



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:12 PM UTC

PDB ID : 1HR9 / pdb_00001hr9
Title : Yeast Mitochondrial Processing Peptidase beta-E73Q Mutant Complexed with Malate Dehydrogenase Signal Peptide
Authors : Taylor, A.B.; Smith, B.S.; Kitada, S.; Kojima, K.; Miyaura, H.; Otwinowski, Z.; Ito, A.; Deisenhofer, J.
Deposited on : 2000-12-21
Resolution : 3.01 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

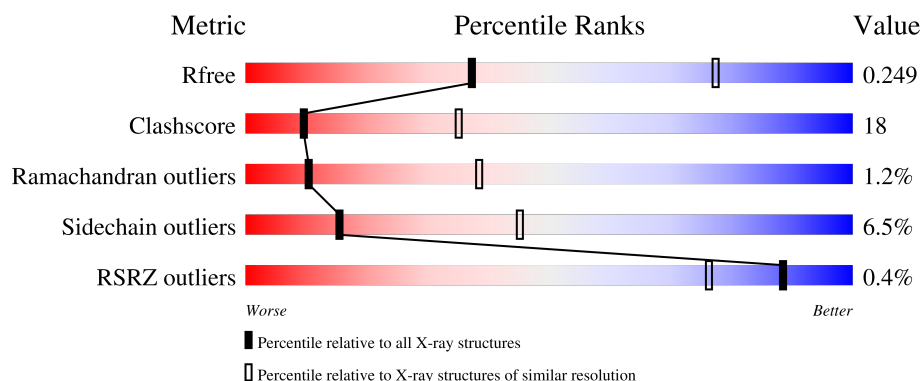
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	475	59% 32% 5% 5%
1	C	475	60% 30% • 6%
1	E	475	58% 32% • 6%
1	G	475	% 60% 32% • 5%
2	B	443	62% 31% 6% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	443	61%32%5% •
2	F	443	62%32%5%
2	H	443	% 63%30%6% •
3	O	8	62%38%
3	P	8	50%50%
3	Q	8	50%50%
3	R	8	12% 25%75%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27925 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3499	2213	594	673	19			
1	C	448	Total	C	N	O	S	0	0	0
			3473	2199	587	668	19			
1	E	446	Total	C	N	O	S	0	0	0
			3465	2193	587	666	19			
1	G	451	Total	C	N	O	S	0	0	0
			3493	2210	593	671	19			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	GLY	GLU	SEE REMARK 999	UNP P11914
A	217	GLY	GLU	SEE REMARK 999	UNP P11914
A	483	HIS	-	expression tag	UNP P11914
A	484	HIS	-	expression tag	UNP P11914
A	485	HIS	-	expression tag	UNP P11914
A	486	HIS	-	expression tag	UNP P11914
A	487	HIS	-	expression tag	UNP P11914
A	488	HIS	-	expression tag	UNP P11914
C	177	GLY	GLU	SEE REMARK 999	UNP P11914
C	217	GLY	GLU	SEE REMARK 999	UNP P11914
C	483	HIS	-	expression tag	UNP P11914
C	484	HIS	-	expression tag	UNP P11914
C	485	HIS	-	expression tag	UNP P11914
C	486	HIS	-	expression tag	UNP P11914
C	487	HIS	-	expression tag	UNP P11914
C	488	HIS	-	expression tag	UNP P11914
E	177	GLY	GLU	SEE REMARK 999	UNP P11914
E	217	GLY	GLU	SEE REMARK 999	UNP P11914
E	483	HIS	-	expression tag	UNP P11914
E	484	HIS	-	expression tag	UNP P11914

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	485	HIS	-	expression tag	UNP P11914
E	486	HIS	-	expression tag	UNP P11914
E	487	HIS	-	expression tag	UNP P11914
E	488	HIS	-	expression tag	UNP P11914
G	177	GLY	GLU	SEE REMARK 999	UNP P11914
G	217	GLY	GLU	SEE REMARK 999	UNP P11914
G	483	HIS	-	expression tag	UNP P11914
G	484	HIS	-	expression tag	UNP P11914
G	485	HIS	-	expression tag	UNP P11914
G	486	HIS	-	expression tag	UNP P11914
G	487	HIS	-	expression tag	UNP P11914
G	488	HIS	-	expression tag	UNP P11914

- Molecule 2 is a protein called MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	439	Total	C	N	O	S	0	0	0
			3414	2148	591	668	7			
2	D	441	Total	C	N	O	S	0	0	0
			3431	2159	594	671	7			
2	F	443	Total	C	N	O	S	0	0	0
			3442	2165	596	674	7			
2	H	440	Total	C	N	O	S	0	0	0
			3422	2154	592	669	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	20	ALA	-	cloning artifact	UNP P10507
B	73	GLN	GLU	engineered mutation	UNP P10507
B	84	PRO	SER	SEE REMARK 999	UNP P10507
B	350	ARG	GLN	SEE REMARK 999	UNP P10507
D	20	ALA	-	cloning artifact	UNP P10507
D	73	GLN	GLU	engineered mutation	UNP P10507
D	84	PRO	SER	SEE REMARK 999	UNP P10507
D	350	ARG	GLN	SEE REMARK 999	UNP P10507
F	20	ALA	-	cloning artifact	UNP P10507
F	73	GLN	GLU	engineered mutation	UNP P10507
F	84	PRO	SER	SEE REMARK 999	UNP P10507
F	350	ARG	GLN	SEE REMARK 999	UNP P10507
H	20	ALA	-	cloning artifact	UNP P10507

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	73	GLN	GLU	engineered mutation	UNP P10507
H	84	PRO	SER	SEE REMARK 999	UNP P10507
H	350	ARG	GLN	SEE REMARK 999	UNP P10507

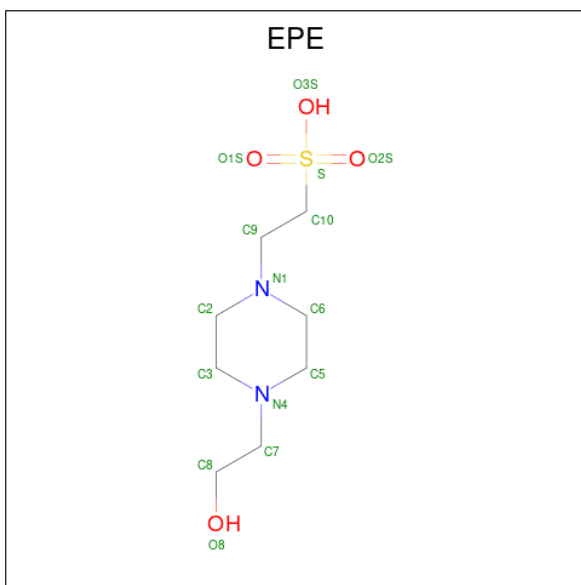
- Molecule 3 is a protein called MALATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	O	8	Total	C	N	O	0	0	0
			63	38	15	10			
3	P	8	Total	C	N	O	0	0	0
			63	38	15	10			
3	Q	8	Total	C	N	O	0	0	0
			63	38	15	10			
3	R	8	Total	C	N	O	0	0	0
			63	38	15	10			

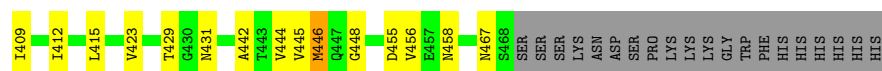
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).

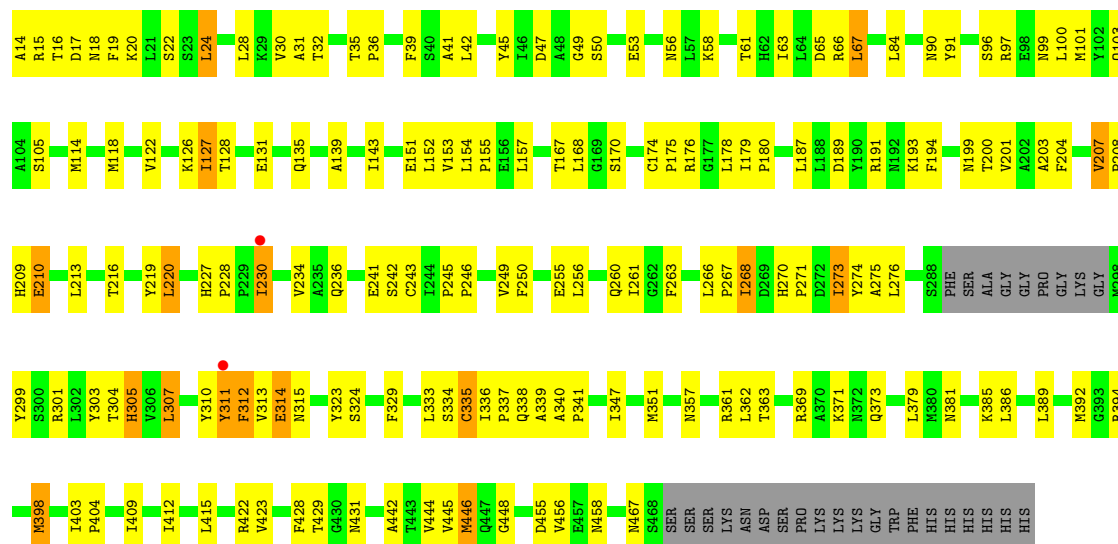


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total 15	C 8	N 2	O 4	S 1	0	0
5	G	1	Total 15	C 8	N 2	O 4	S 1	0	0



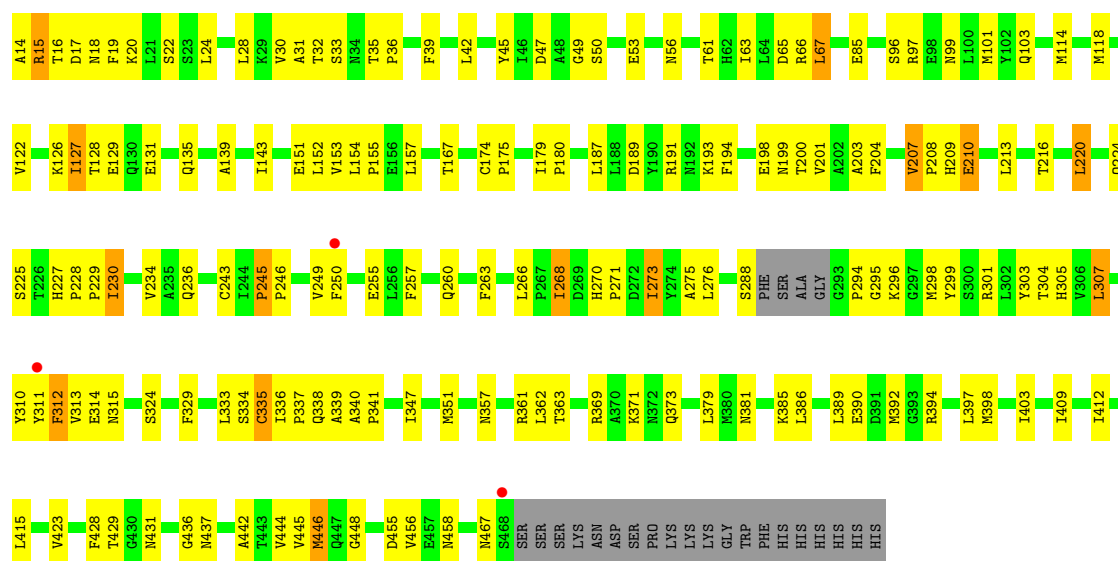
• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

Chain E: 58% 32% 6%



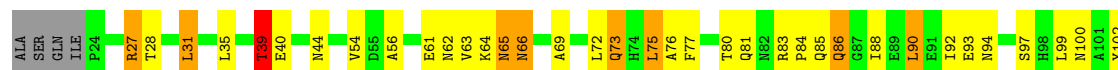
• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

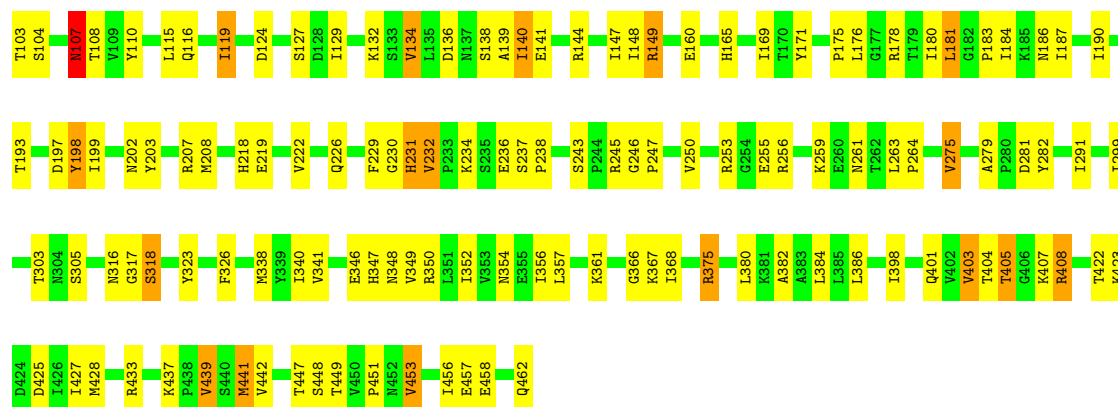
Chain G: 60% 32% 5%



• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

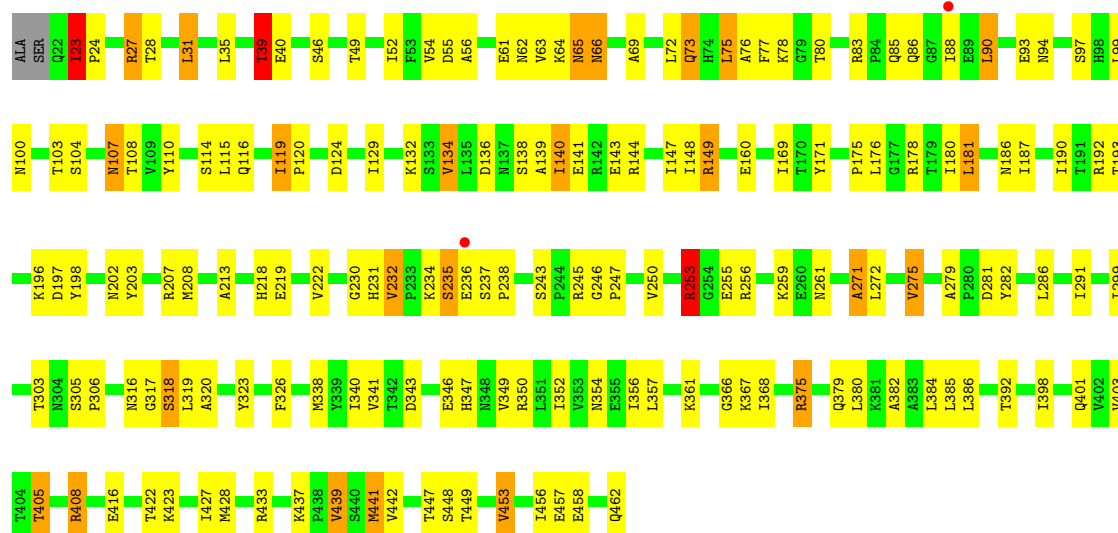
Chain B: 62% 31% 6%





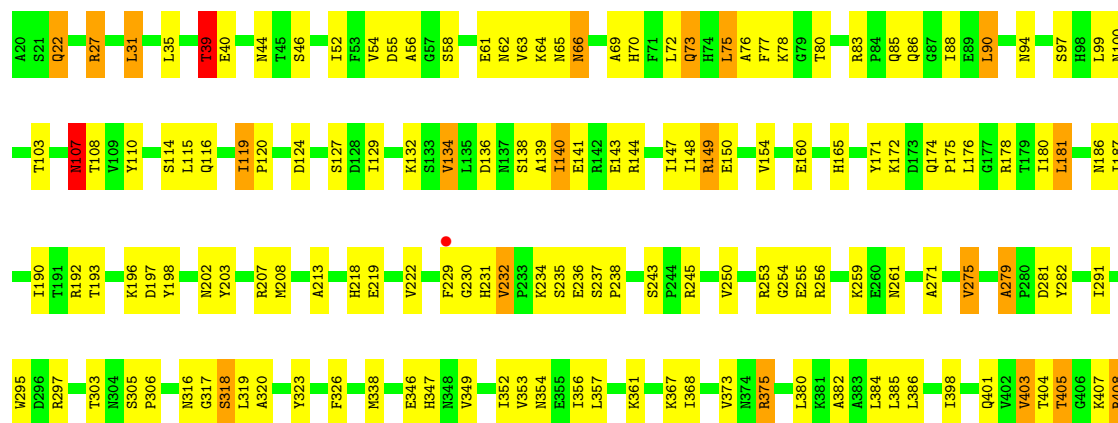
• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

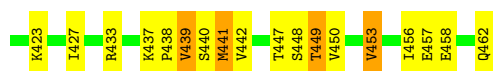
Chain D: 61% 32% 5%



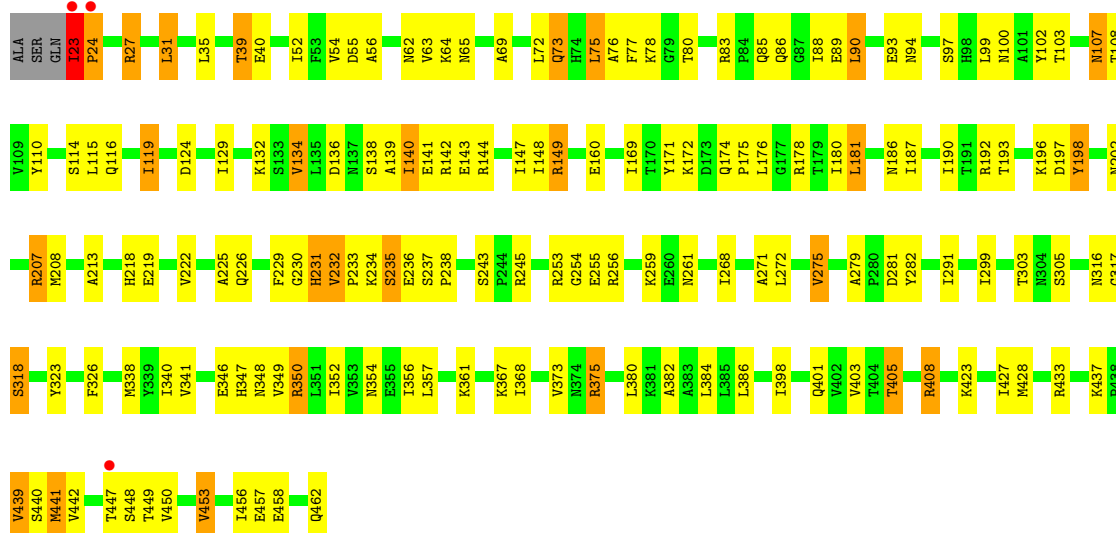
• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

Chain F: 62% 32% 5%

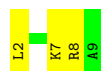




• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT



• Molecule 3: MALATE DEHYDROGENASE



• Molecule 3: MALATE DEHYDROGENASE



• Molecule 3: MALATE DEHYDROGENASE



• Molecule 3: MALATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.37Å 178.52Å 201.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.55 – 3.01 47.55 – 3.01	Depositor EDS
% Data completeness (in resolution range)	93.3 (47.55-3.01) 93.5 (47.55-3.01)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.256 0.213 , 0.249	Depositor DCC
R_{free} test set	2035 reflections (2.25%)	wwPDB-VP
Wilson B-factor (Å ²)	69.5	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27925	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.88	3/3570 (0.1%)	1.15	19/4830 (0.4%)
1	C	0.82	2/3544 (0.1%)	1.12	20/4795 (0.4%)
1	E	0.77	0/3535	1.15	22/4784 (0.5%)
1	G	0.82	2/3564 (0.1%)	1.12	13/4822 (0.3%)
2	B	0.93	5/3478 (0.1%)	1.20	27/4720 (0.6%)
2	D	0.79	3/3495 (0.1%)	1.19	29/4744 (0.6%)
2	F	0.73	4/3506 (0.1%)	1.15	25/4759 (0.5%)
2	H	0.74	5/3486 (0.1%)	1.21	35/4732 (0.7%)
3	O	0.96	0/62	1.03	0/79
3	P	0.87	0/62	1.08	0/79
3	Q	0.79	0/62	0.94	0/79
3	R	0.79	0/62	0.93	0/79
All	All	0.81	24/28426 (0.1%)	1.16	190/38502 (0.5%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	81	GLN	CD-NE2	-11.58	1.08	1.33
2	B	81	GLN	CD-OE1	-11.44	1.01	1.23
2	D	354	ASN	CG-OD1	-9.27	1.05	1.23
2	H	354	ASN	CG-OD1	-8.76	1.06	1.23
2	B	354	ASN	CG-ND2	-8.52	1.15	1.33
2	F	354	ASN	CG-ND2	-8.46	1.15	1.33
2	F	354	ASN	CG-OD1	-8.41	1.07	1.23
2	H	354	ASN	CG-ND2	-7.94	1.16	1.33
2	B	354	ASN	CG-OD1	-7.66	1.08	1.23
1	G	56	ASN	CG-ND2	-7.51	1.17	1.33
2	H	73	GLN	CD-OE1	6.93	1.36	1.23
2	D	354	ASN	CG-ND2	-6.78	1.19	1.33
1	G	56	ASN	CG-OD1	-6.56	1.11	1.23
1	A	114	MET	SD-CE	-6.04	1.64	1.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	73	GLN	CD-OE1	5.88	1.34	1.23
2	F	73	GLN	CD-OE1	5.82	1.34	1.23
1	C	392	MET	SD-CE	-5.71	1.65	1.79
1	A	408	MET	SD-CE	5.67	1.93	1.79
2	H	73	GLN	CA-C	5.50	1.60	1.52
2	D	73	GLN	CD-NE2	5.41	1.44	1.33
2	H	73	GLN	CD-NE2	5.31	1.44	1.33
2	F	73	GLN	N-CA	5.29	1.52	1.46
1	C	114	MET	SD-CE	-5.18	1.66	1.79
1	A	249	VAL	CA-CB	5.01	1.58	1.53

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	253	ARG	NE-CZ-NH2	13.55	131.40	119.20
2	H	207	ARG	NE-CZ-NH2	12.96	130.86	119.20
2	D	253	ARG	NE-CZ-NH1	-12.21	109.30	121.50
2	H	207	ARG	NE-CZ-NH1	-12.17	109.33	121.50
1	E	422	ARG	NE-CZ-NH2	11.75	129.77	119.20
1	E	422	ARG	NE-CZ-NH1	-11.42	110.08	121.50
2	D	253	ARG	CD-NE-CZ	11.30	140.23	124.40
2	H	149	ARG	NE-CZ-NH2	-10.96	109.33	119.20
2	H	149	ARG	CD-NE-CZ	10.47	139.06	124.40
2	H	207	ARG	CD-NE-CZ	9.79	138.10	124.40
1	E	422	ARG	CD-NE-CZ	9.60	137.83	124.40
2	H	149	ARG	NE-CZ-NH1	9.46	130.97	121.50
1	E	312	PHE	N-CA-C	-9.21	101.74	113.16
1	A	312	PHE	N-CA-C	-9.15	101.81	113.16
1	C	312	PHE	N-CA-C	-9.13	101.83	113.16
1	G	312	PHE	N-CA-C	-9.05	101.93	113.16
1	E	15	ARG	N-CA-C	8.80	120.79	111.03
2	B	243	SER	CA-C-N	8.37	128.89	119.93
2	B	243	SER	C-N-CA	8.37	128.89	119.93
2	H	350	ARG	NE-CZ-NH2	-8.31	111.72	119.20
2	H	350	ARG	CG-CD-NE	-8.13	94.12	112.00
2	B	134	VAL	N-CA-C	7.91	118.01	110.42
1	E	153	VAL	N-CA-C	7.87	118.65	110.62
2	F	232	VAL	CA-C-N	7.80	127.86	119.90
2	F	232	VAL	C-N-CA	7.80	127.86	119.90
2	F	347	HIS	N-CA-C	7.61	122.24	109.76
1	A	153	VAL	N-CA-C	7.55	118.32	110.62
2	B	119	ILE	CB-CA-C	-7.37	106.70	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	453	VAL	N-CA-C	7.25	118.02	110.62
2	D	119	ILE	CB-CA-C	-7.22	106.84	113.70
1	G	207	VAL	CA-C-N	7.20	127.61	119.83
1	G	207	VAL	C-N-CA	7.20	127.61	119.83
2	H	119	ILE	CB-CA-C	-7.13	106.93	113.70
2	H	350	ARG	CD-NE-CZ	7.10	134.34	124.40
2	H	347	HIS	N-CA-C	7.05	121.33	109.76
1	E	245	PRO	N-CA-C	7.03	119.28	110.70
2	F	134	VAL	N-CA-C	7.02	117.73	110.36
2	D	134	VAL	N-CA-C	7.00	117.14	110.42
2	H	453	VAL	N-CA-C	6.95	117.09	110.42
1	A	17	ASP	N-CA-C	-6.92	103.82	111.36
1	C	207	VAL	CA-C-N	6.88	127.26	119.83
1	C	207	VAL	C-N-CA	6.88	127.26	119.83
1	G	16	THR	N-CA-C	-6.88	105.82	114.56
2	F	453	VAL	N-CA-C	6.86	117.00	110.42
2	B	63	VAL	N-CA-C	6.84	116.99	110.42
2	H	134	VAL	N-CA-C	6.82	117.52	110.36
2	D	243	SER	CA-C-N	6.79	127.20	119.93
2	D	243	SER	C-N-CA	6.79	127.20	119.93
2	D	347	HIS	N-CA-C	6.76	120.84	109.76
2	F	243	SER	CA-C-N	6.74	128.27	119.84
2	F	243	SER	C-N-CA	6.74	128.27	119.84
2	F	119	ILE	CB-CA-C	-6.74	107.30	113.70
2	B	347	HIS	N-CA-C	6.71	120.76	109.76
2	F	202	ASN	N-CA-C	6.70	121.69	112.04
2	H	450	VAL	N-CA-C	6.70	114.53	107.76
2	H	202	ASN	N-CA-C	6.65	121.69	112.45
2	D	202	ASN	N-CA-C	6.63	121.59	112.04
1	G	153	VAL	N-CA-C	6.59	117.34	110.62
1	G	266	LEU	CA-C-N	6.57	126.33	119.76
1	G	266	LEU	C-N-CA	6.57	126.33	119.76
2	F	63	VAL	N-CA-C	6.54	116.70	110.42
2	B	81	GLN	OE1-CD-NE2	-6.51	116.09	122.60
2	H	63	VAL	N-CA-C	6.45	116.62	110.42
2	F	448	SER	N-CA-C	6.40	120.66	112.34
2	D	448	SER	N-CA-C	6.36	120.61	112.34
2	B	448	SER	N-CA-C	6.36	120.61	112.34
1	A	245	PRO	N-CA-C	6.34	118.44	110.70
2	B	232	VAL	CA-C-N	6.34	126.37	119.90
2	B	232	VAL	C-N-CA	6.34	126.37	119.90
1	G	245	PRO	N-CA-C	6.31	118.40	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	350	ARG	NE-CZ-NH1	6.27	127.77	121.50
2	H	232	VAL	CA-C-N	6.25	126.61	119.93
2	H	232	VAL	C-N-CA	6.25	126.61	119.93
2	H	448	SER	N-CA-C	6.24	120.46	112.34
2	D	63	VAL	N-CA-C	6.22	116.97	110.62
2	B	231	HIS	CA-C-N	-6.16	117.38	123.04
2	B	231	HIS	C-N-CA	-6.16	117.38	123.04
2	F	450	VAL	N-CA-C	6.16	113.98	107.76
1	A	266	LEU	CA-C-N	6.14	125.90	119.76
1	A	266	LEU	C-N-CA	6.14	125.90	119.76
2	D	437	LYS	CA-C-N	6.14	126.05	119.85
2	D	437	LYS	C-N-CA	6.14	126.05	119.85
2	D	108	THR	N-CA-C	-6.14	98.89	108.90
2	B	202	ASN	N-CA-C	6.12	120.85	112.04
2	D	232	VAL	CA-C-N	6.10	126.13	119.90
2	D	232	VAL	C-N-CA	6.10	126.13	119.90
2	D	453	VAL	N-CA-C	6.08	116.26	110.42
1	A	207	VAL	CA-C-N	6.05	126.36	119.83
1	A	207	VAL	C-N-CA	6.05	126.36	119.83
1	G	194	PHE	N-CA-C	6.03	121.69	113.97
2	H	243	SER	CA-C-N	6.00	127.34	119.84
2	H	243	SER	C-N-CA	6.00	127.34	119.84
1	A	295	GLY	N-CA-C	-5.98	107.43	115.21
2	H	231	HIS	CA-C-N	-5.98	117.54	123.04
2	H	231	HIS	C-N-CA	-5.98	117.54	123.04
1	A	16	THR	CA-C-N	5.89	128.66	120.29
1	A	16	THR	C-N-CA	5.89	128.66	120.29
2	B	437	LYS	CA-C-N	5.86	125.77	119.85
2	B	437	LYS	C-N-CA	5.86	125.77	119.85
2	F	22	GLN	N-CA-C	5.86	118.75	109.50
1	E	194	PHE	N-CA-C	5.83	121.44	113.97
2	D	23	ILE	CA-C-N	5.80	127.09	119.84
2	D	23	ILE	C-N-CA	5.80	127.09	119.84
2	H	373	VAL	N-CA-C	-5.79	105.08	110.53
1	C	330	GLY	N-CA-C	5.79	118.96	110.80
1	G	446	MET	N-CA-C	5.77	118.05	108.99
2	B	108	THR	N-CA-C	-5.70	99.61	108.90
1	C	194	PHE	N-CA-C	5.70	121.26	113.97
2	B	107	ASN	N-CA-C	5.67	117.40	108.96
2	B	232	VAL	CA-C-O	5.67	122.87	119.19
2	F	433	ARG	N-CA-C	5.66	119.91	112.89
1	E	207	VAL	CA-C-N	5.64	125.93	119.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	207	VAL	C-N-CA	5.64	125.93	119.83
1	E	266	LEU	CA-C-N	5.64	125.40	119.76
1	E	266	LEU	C-N-CA	5.64	125.40	119.76
1	C	170	SER	CA-C-N	5.63	126.88	119.84
1	C	170	SER	C-N-CA	5.63	126.88	119.84
2	B	433	ARG	N-CA-C	5.62	120.20	113.23
2	H	437	LYS	CA-C-N	5.60	125.51	119.85
2	H	437	LYS	C-N-CA	5.60	125.51	119.85
1	E	335	CYS	N-CA-C	5.60	115.93	108.38
1	C	446	MET	N-CA-C	5.59	117.76	108.99
2	H	23	ILE	CA-C-N	5.54	126.76	119.84
2	H	23	ILE	C-N-CA	5.54	126.76	119.84
2	F	149	ARG	NE-CZ-NH2	5.53	124.17	119.20
2	F	107	ASN	N-CA-C	5.52	117.18	108.96
1	A	56	ASN	N-CA-C	5.50	117.36	111.36
2	F	108	THR	N-CA-C	-5.48	99.96	108.90
2	D	299	ILE	N-CA-C	5.46	118.76	111.44
2	B	39	THR	N-CA-C	5.45	118.44	109.72
1	C	60	CYS	N-CA-C	5.44	116.89	111.07
1	A	66	ARG	N-CA-C	-5.42	106.62	113.18
2	B	149	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	G	257	PHE	N-CA-C	-5.40	101.31	109.85
2	B	198	TYR	N-CA-C	-5.38	105.41	111.28
2	F	437	LYS	CA-C-N	5.38	125.29	119.85
2	F	437	LYS	C-N-CA	5.38	125.29	119.85
2	F	373	VAL	N-CA-C	-5.37	105.48	110.53
1	A	194	PHE	N-CA-C	5.36	120.83	113.97
1	C	84	LEU	N-CA-C	-5.35	105.53	111.36
1	E	170	SER	CA-C-N	5.35	126.53	119.84
1	E	170	SER	C-N-CA	5.35	126.53	119.84
1	E	446	MET	N-CA-C	5.35	117.20	109.07
2	F	271	ALA	N-CA-C	5.34	117.80	109.52
1	C	266	LEU	CA-C-N	5.33	125.09	119.76
1	C	266	LEU	C-N-CA	5.33	125.09	119.76
1	E	219	TYR	N-CA-C	5.33	119.84	113.23
1	G	56	ASN	N-CA-C	5.31	117.14	111.36
2	F	385	LEU	N-CA-C	5.30	120.23	113.55
2	D	379	GLN	N-CA-C	-5.28	105.42	111.07
1	E	56	ASN	N-CA-C	5.27	117.11	111.36
2	D	39	THR	N-CA-C	5.27	118.15	109.72
2	H	108	THR	N-CA-C	-5.27	100.32	108.90
1	C	287	GLY	N-CA-C	-5.26	101.41	112.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	39	THR	N-CA-C	5.26	118.14	109.72
2	H	198	TYR	N-CA-C	-5.26	105.55	111.28
2	B	149	ARG	N-CA-C	-5.25	105.45	111.07
1	C	245	PRO	CA-C-N	5.25	125.01	119.76
1	C	245	PRO	C-N-CA	5.25	125.01	119.76
1	A	330	GLY	N-CA-C	5.25	118.20	110.80
1	E	24	LEU	N-CA-C	-5.24	102.76	110.52
2	H	235	SER	N-CA-C	-5.24	102.73	110.48
1	G	335	CYS	N-CA-C	5.23	116.75	108.96
2	D	433	ARG	N-CA-C	5.20	119.68	113.23
2	D	343	ASP	N-CA-C	-5.17	101.34	109.25
1	C	24	LEU	N-CA-C	-5.16	102.88	110.52
2	H	433	ARG	N-CA-C	5.16	119.63	113.23
1	A	100	LEU	N-CA-C	-5.16	99.69	108.26
1	A	24	LEU	N-CA-C	-5.16	102.89	110.52
2	D	271	ALA	N-CA-C	5.16	117.51	109.52
1	E	174	CYS	N-CA-C	5.15	116.18	109.64
2	B	299	ILE	N-CA-C	5.12	118.31	111.44
2	D	149	ARG	NE-CZ-NH2	5.12	123.81	119.20
2	H	232	VAL	N-CA-C	5.12	114.09	108.05
1	C	257	PHE	N-CA-C	-5.11	101.54	109.72
2	D	235	SER	N-CA-C	-5.11	102.19	110.32
2	B	203	TYR	N-CA-C	5.08	117.82	108.58
1	C	153	VAL	N-CA-C	5.08	115.80	110.62
1	E	100	LEU	N-CA-C	-5.08	99.83	108.26
1	C	335	CYS	N-CA-C	5.08	115.75	108.74
1	C	97	ARG	N-CA-C	-5.06	105.95	111.82
2	F	279	ALA	CA-C-N	5.05	124.54	119.19
2	F	279	ALA	C-N-CA	5.05	124.54	119.19
1	A	71	SER	N-CA-C	5.04	117.21	110.35
2	D	350	ARG	NE-CZ-NH1	-5.04	116.46	121.50
2	H	299	ILE	N-CA-C	5.03	118.18	111.44
2	B	199	ILE	CB-CA-C	-5.02	105.54	111.97
1	A	446	MET	N-CA-C	5.02	116.87	108.99
2	D	385	LEU	N-CA-C	5.02	119.87	113.55
1	E	398	MET	N-CA-C	5.01	119.25	112.04

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3499	0	3460	143	0
1	C	3473	0	3435	128	0
1	E	3465	0	3426	128	0
1	G	3493	0	3455	135	0
2	B	3414	0	3414	125	0
2	D	3431	0	3432	131	0
2	F	3442	0	3442	123	0
2	H	3422	0	3424	118	0
3	O	63	0	73	3	0
3	P	63	0	73	4	0
3	Q	63	0	73	5	0
3	R	63	0	73	6	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
5	E	15	0	17	0	0
5	G	15	0	17	0	0
All	All	27925	0	27814	991	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (991) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:GLY:HA2	2:D:93:GLU:HG2	1.40	1.03
1:C:230:ILE:HD12	1:C:230:ILE:H	1.15	1.02
1:G:230:ILE:H	1:G:230:ILE:HD12	1.21	1.01
1:E:230:ILE:HD12	1:E:230:ILE:H	1.25	1.01
1:A:230:ILE:HD12	1:A:230:ILE:H	1.20	1.00
1:E:14:ALA:HB3	1:E:404:PRO:HB3	1.47	0.97
1:A:14:ALA:N	1:A:19:PHE:HB3	1.82	0.95
1:G:157:LEU:HB3	1:G:445:VAL:HG21	1.45	0.95
1:A:304:THR:HG22	1:A:305:HIS:HD2	1.31	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:14:ALA:N	1:G:19:PHE:HB3	1.83	0.91
1:C:157:LEU:HB3	1:C:445:VAL:HG21	1.53	0.91
1:G:304:THR:HG22	1:G:305:HIS:HD2	1.34	0.90
1:C:246:PRO:HG3	1:C:448:GLY:HA2	1.52	0.90
2:H:186:ASN:O	2:H:190:ILE:HG12	1.73	0.88
2:D:186:ASN:O	2:D:190:ILE:HG12	1.73	0.88
1:A:379:LEU:HD11	1:A:409:ILE:HD11	1.56	0.86
2:D:303:THR:HG22	2:D:305:SER:H	1.41	0.86
2:B:186:ASN:O	2:B:190:ILE:HG12	1.76	0.86
1:A:128:THR:OG1	1:A:131:GLU:HG3	1.76	0.85
2:H:303:THR:HG22	2:H:305:SER:H	1.41	0.84
1:C:299:TYR:CE1	2:D:90:LEU:HD23	2.12	0.84
2:D:181:LEU:HD13	3:P:8:ARG:HG2	1.60	0.84
1:C:379:LEU:HD11	1:C:409:ILE:HD11	1.59	0.84
2:F:136:ASP:OD2	2:F:138:SER:HB3	1.78	0.84
1:E:154:LEU:HB3	1:E:260:GLN:NE2	1.93	0.84
1:E:379:LEU:HD11	1:E:409:ILE:HD11	1.60	0.84
2:H:136:ASP:OD2	2:H:138:SER:HB3	1.77	0.84
2:D:136:ASP:OD2	2:D:138:SER:HB3	1.77	0.83
2:F:303:THR:HG22	2:F:305:SER:H	1.43	0.83
3:R:7:LYS:O	3:R:8:ARG:HD2	1.79	0.82
2:F:256:ARG:HG3	2:F:256:ARG:HH11	1.43	0.82
1:G:154:LEU:HB3	1:G:260:GLN:NE2	1.94	0.82
1:C:230:ILE:H	1:C:230:ILE:CD1	1.92	0.82
1:E:157:LEU:HB3	1:E:445:VAL:HG21	1.59	0.82
2:B:303:THR:HG22	2:B:305:SER:H	1.43	0.81
2:F:181:LEU:HD13	3:Q:8:ARG:HG2	1.62	0.81
1:G:246:PRO:HG3	1:G:448:GLY:HA2	1.63	0.81
1:A:34:ASN:HD21	2:B:44:ASN:HB2	1.45	0.81
1:C:230:ILE:HD12	1:C:230:ILE:N	1.96	0.81
2:D:256:ARG:HG3	2:D:256:ARG:HH11	1.44	0.81
2:H:181:LEU:HD13	3:R:8:ARG:HG2	1.63	0.80
2:F:186:ASN:O	2:F:190:ILE:HG12	1.80	0.80
2:B:375:ARG:HB3	2:B:375:ARG:NH1	1.96	0.80
1:G:379:LEU:HD11	1:G:409:ILE:HD11	1.63	0.80
1:G:24:LEU:HD11	1:G:216:THR:HG22	1.65	0.79
1:C:128:THR:OG1	1:C:131:GLU:HG3	1.83	0.79
2:H:338:MET:HG2	2:H:356:ILE:HD13	1.65	0.79
1:G:15:ARG:O	1:G:15:ARG:HD3	1.83	0.79
2:B:181:LEU:HD13	3:O:8:ARG:HG2	1.65	0.79
2:B:136:ASP:OD2	2:B:138:SER:HB3	1.82	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:PRO:HA	1:A:298:MET:CE	2.13	0.78
1:E:39:PHE:CE1	1:E:385:LYS:HD2	2.18	0.78
1:C:32:THR:C	1:C:392:MET:HE1	2.09	0.78
2:D:375:ARG:HB3	2:D:375:ARG:NH1	1.99	0.78
2:H:375:ARG:NH1	2:H:375:ARG:HB3	2.00	0.77
2:F:116:GLN:O	2:F:119:ILE:HG12	1.84	0.77
2:B:144:ARG:O	2:B:148:ILE:HG12	1.84	0.77
1:E:347:ILE:HG22	1:E:351:MET:HE3	1.67	0.77
1:G:295:GLY:HA2	2:H:93:GLU:HG2	1.67	0.77
1:C:295:GLY:CA	2:D:93:GLU:HG2	2.13	0.76
1:E:299:TYR:CZ	2:F:90:LEU:HD23	2.20	0.76
1:G:230:ILE:H	1:G:230:ILE:CD1	1.99	0.76
2:H:116:GLN:O	2:H:119:ILE:HG12	1.86	0.76
2:H:76:ALA:O	2:H:129:ILE:HG23	1.85	0.76
2:D:338:MET:HG2	2:D:356:ILE:HD13	1.67	0.76
2:F:76:ALA:O	2:F:129:ILE:HG23	1.86	0.76
2:D:375:ARG:HB3	2:D:375:ARG:CZ	2.16	0.76
2:F:375:ARG:CZ	2:F:375:ARG:HB3	2.16	0.76
2:H:375:ARG:HB3	2:H:375:ARG:CZ	2.16	0.76
1:E:236:GLN:HE22	1:G:230:ILE:HD11	1.50	0.75
1:G:128:THR:OG1	1:G:131:GLU:HG3	1.85	0.75
2:H:144:ARG:O	2:H:148:ILE:HG12	1.87	0.75
1:C:101:MET:HE1	1:C:394:ARG:HD2	1.68	0.75
1:G:230:ILE:HD12	1:G:230:ILE:N	2.01	0.75
1:A:230:ILE:HD12	1:A:230:ILE:N	2.00	0.75
1:A:157:LEU:HB3	1:A:445:VAL:HG21	1.69	0.74
2:B:375:ARG:HB3	2:B:375:ARG:CZ	2.14	0.74
2:H:357:LEU:O	2:H:361:LYS:HG3	1.87	0.74
1:C:24:LEU:HD11	1:C:216:THR:HG22	1.69	0.73
1:E:243:CYS:HA	1:E:446:MET:O	1.87	0.73
1:A:347:ILE:HG22	1:A:351:MET:HE3	1.69	0.73
2:B:350:ARG:NE	2:D:416:GLU:OE2	2.18	0.73
1:C:299:TYR:CZ	2:D:90:LEU:HD23	2.23	0.73
1:E:99:ASN:ND2	1:E:101:MET:HE3	2.02	0.73
2:H:256:ARG:HH11	2:H:256:ARG:HG3	1.53	0.73
1:A:24:LEU:HD11	1:A:216:THR:HG22	1.71	0.73
2:D:144:ARG:O	2:D:148:ILE:HG12	1.89	0.72
1:G:14:ALA:N	1:G:17:ASP:OD2	2.23	0.72
2:D:90:LEU:CD1	2:D:94:ASN:HD21	2.03	0.72
2:F:375:ARG:HB3	2:F:375:ARG:NH1	2.03	0.72
1:A:14:ALA:N	1:A:17:ASP:OD2	2.23	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:90:LEU:CD1	2:F:94:ASN:HD21	2.03	0.72
1:E:128:THR:OG1	1:E:131:GLU:HG3	1.90	0.72
2:F:73:GLN:HA	2:F:110:TYR:OH	1.91	0.71
2:D:73:GLN:HA	2:D:110:TYR:OH	1.91	0.71
2:H:90:LEU:CD1	2:H:94:ASN:HD21	2.03	0.71
2:H:73:GLN:HA	2:H:110:TYR:OH	1.89	0.71
2:F:144:ARG:O	2:F:148:ILE:HG12	1.90	0.71
1:A:19:PHE:HD1	1:A:392:MET:HE3	1.55	0.71
1:A:230:ILE:H	1:A:230:ILE:CD1	1.96	0.71
2:D:116:GLN:O	2:D:119:ILE:HG12	1.90	0.71
1:C:347:ILE:HG22	1:C:351:MET:HE3	1.72	0.71
1:G:101:MET:HE1	1:G:394:ARG:HD2	1.72	0.71
2:H:62:ASN:H	2:H:65:ASN:HB3	1.56	0.70
1:A:101:MET:HE1	1:A:394:ARG:HD2	1.73	0.70
2:B:338:MET:HG2	2:B:356:ILE:HD13	1.73	0.70
2:B:357:LEU:O	2:B:361:LYS:HG3	1.91	0.70
2:B:256:ARG:HG3	2:B:256:ARG:HH11	1.57	0.70
1:E:101:MET:HE1	1:E:394:ARG:HD2	1.72	0.70
2:B:368:ILE:O	2:B:423:LYS:HE3	1.92	0.70
2:F:338:MET:HG2	2:F:356:ILE:HD13	1.74	0.70
1:C:246:PRO:HG3	1:C:448:GLY:CA	2.20	0.70
1:E:230:ILE:H	1:E:230:ILE:CD1	2.02	0.69
2:B:62:ASN:H	2:B:65:ASN:HB3	1.57	0.69
1:C:154:LEU:HB3	1:C:260:GLN:NE2	2.08	0.69
2:F:357:LEU:O	2:F:361:LYS:HG3	1.93	0.69
1:C:157:LEU:CB	1:C:445:VAL:HG21	2.21	0.69
1:G:15:ARG:HD3	1:G:15:ARG:C	2.18	0.69
1:A:294:PRO:HA	1:A:298:MET:HE1	1.74	0.69
2:B:76:ALA:O	2:B:129:ILE:HG23	1.92	0.69
2:H:259:LYS:HG3	2:H:447:THR:HG22	1.75	0.69
2:F:62:ASN:H	2:F:65:ASN:HB3	1.58	0.68
1:C:429:THR:O	1:C:429:THR:HG22	1.94	0.68
1:E:230:ILE:HD12	1:E:230:ILE:N	2.04	0.68
1:G:157:LEU:HB3	1:G:445:VAL:CG2	2.23	0.68
2:H:236:GLU:C	2:H:238:PRO:HD3	2.18	0.68
2:D:357:LEU:O	2:D:361:LYS:HG3	1.93	0.68
1:G:19:PHE:HD1	1:G:392:MET:HE3	1.59	0.68
1:A:32:THR:C	1:A:392:MET:HE1	2.19	0.68
1:G:157:LEU:CB	1:G:445:VAL:HG21	2.22	0.68
1:G:347:ILE:HG22	1:G:351:MET:HE3	1.74	0.68
1:C:157:LEU:HB3	1:C:445:VAL:CG2	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:368:ILE:O	2:F:423:LYS:HE3	1.94	0.67
2:H:90:LEU:HD13	2:H:94:ASN:ND2	2.09	0.67
1:A:268:ILE:HD11	1:A:398:MET:SD	2.33	0.67
2:B:116:GLN:O	2:B:119:ILE:HG12	1.94	0.67
1:E:246:PRO:HG3	1:E:448:GLY:HA2	1.76	0.67
2:H:115:LEU:HD12	2:H:115:LEU:H	1.58	0.67
1:C:19:PHE:HD1	1:C:392:MET:HE3	1.59	0.67
1:G:50:SER:HA	1:G:53:GLU:HG3	1.76	0.67
2:D:90:LEU:HD13	2:D:94:ASN:ND2	2.08	0.67
1:E:268:ILE:HD11	1:E:398:MET:SD	2.34	0.67
1:G:268:ILE:HD11	1:G:398:MET:SD	2.35	0.67
1:C:263:PHE:CE2	1:C:442:ALA:HB2	2.30	0.67
1:E:14:ALA:N	1:E:19:PHE:HB3	2.10	0.67
3:P:5:VAL:O	3:P:7:LYS:HG3	1.96	0.66
1:C:340:ALA:HB3	1:C:341:PRO:HD3	1.78	0.66
2:D:368:ILE:O	2:D:423:LYS:HE3	1.95	0.66
1:C:122:VAL:O	1:C:191:ARG:NH2	2.29	0.66
2:D:62:ASN:H	2:D:65:ASN:HB3	1.60	0.66
1:E:14:ALA:CB	1:E:404:PRO:HB3	2.23	0.66
2:F:154:VAL:HG11	3:Q:8:ARG:HH11	1.61	0.66
1:A:429:THR:O	1:A:429:THR:HG22	1.96	0.66
1:A:96:SER:OG	1:A:97:ARG:N	2.24	0.65
2:H:54:VAL:O	2:H:107:ASN:HB3	1.96	0.65
1:G:32:THR:C	1:G:392:MET:HE1	2.20	0.65
1:A:19:PHE:CD1	1:A:392:MET:HE3	2.31	0.65
2:D:76:ALA:O	2:D:129:ILE:HG23	1.96	0.65
1:E:96:SER:OG	1:E:97:ARG:N	2.30	0.65
2:D:253:ARG:HH21	2:D:457:GLU:CD	2.04	0.65
2:H:458:GLU:O	2:H:462:GLN:HB2	1.96	0.65
2:B:115:LEU:HD12	2:B:115:LEU:H	1.61	0.65
1:C:50:SER:HA	1:C:53:GLU:HG3	1.79	0.65
2:F:259:LYS:HG3	2:F:447:THR:HG22	1.79	0.65
2:F:90:LEU:HD13	2:F:94:ASN:ND2	2.11	0.64
3:Q:2:LEU:HD12	3:Q:3:SER:N	2.13	0.64
2:B:458:GLU:CD	2:D:422:THR:HB	2.21	0.64
2:D:259:LYS:HG3	2:D:447:THR:HG22	1.79	0.64
2:H:54:VAL:HG22	2:H:208:MET:HE2	1.79	0.64
2:H:136:ASP:O	2:H:140:ILE:HG13	1.97	0.64
2:B:54:VAL:O	2:B:107:ASN:HB3	1.98	0.64
1:C:347:ILE:CG2	1:C:351:MET:HE3	2.27	0.64
2:H:253:ARG:NH2	2:H:453:VAL:HG12	2.13	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ILE:N	1:A:268:ILE:HD13	2.12	0.64
2:D:90:LEU:HD13	2:D:94:ASN:HD21	1.63	0.64
2:H:368:ILE:O	2:H:423:LYS:HE3	1.97	0.64
2:B:90:LEU:CD1	2:B:94:ASN:HD21	2.10	0.64
1:E:299:TYR:CE1	2:F:90:LEU:HD23	2.32	0.64
1:E:268:ILE:HD13	1:E:268:ILE:N	2.13	0.64
2:H:90:LEU:HD13	2:H:94:ASN:HD21	1.63	0.64
2:B:40:GLU:OE1	2:B:408:ARG:NH2	2.31	0.63
1:G:17:ASP:O	1:G:18:ASN:HB3	1.98	0.63
1:E:263:PHE:CE2	1:E:442:ALA:HB2	2.33	0.63
1:G:268:ILE:HD13	1:G:268:ILE:N	2.14	0.63
2:B:73:GLN:HA	2:B:110:TYR:OH	1.98	0.63
1:C:268:ILE:N	1:C:268:ILE:HD13	2.14	0.63
1:E:429:THR:HG22	1:E:429:THR:O	1.98	0.63
1:A:340:ALA:HB3	1:A:341:PRO:HD3	1.80	0.63
2:B:259:LYS:HG3	2:B:447:THR:HG22	1.80	0.63
1:E:347:ILE:CG2	1:E:351:MET:HE3	2.29	0.63
2:H:207:ARG:HH11	2:H:245:ARG:NH1	1.97	0.63
1:G:96:SER:OG	1:G:97:ARG:N	2.29	0.62
1:G:340:ALA:HB3	1:G:341:PRO:HD3	1.81	0.62
1:G:455:ASP:OD1	1:G:458:ASN:HB2	1.99	0.62
3:R:5:VAL:O	3:R:7:LYS:HG3	1.99	0.62
2:B:458:GLU:O	2:B:462:GLN:HB2	1.99	0.62
2:D:115:LEU:HD12	2:D:115:LEU:H	1.64	0.62
1:G:246:PRO:HG3	1:G:448:GLY:CA	2.30	0.62
1:C:17:ASP:O	1:C:18:ASN:HB3	1.99	0.62
2:F:236:GLU:C	2:F:238:PRO:HD3	2.24	0.62
2:D:64:LYS:O	2:D:186:ASN:ND2	2.33	0.62
1:E:24:LEU:HD11	1:E:216:THR:HG22	1.80	0.62
1:A:263:PHE:CE2	1:A:442:ALA:HB2	2.34	0.62
1:E:16:THR:HG22	2:F:44:ASN:ND2	2.14	0.62
1:E:99:ASN:HD22	1:E:101:MET:HE3	1.62	0.62
1:E:122:VAL:O	1:E:191:ARG:NH2	2.33	0.61
1:G:154:LEU:HB3	1:G:260:GLN:HE21	1.65	0.61
2:B:90:LEU:HD13	2:B:94:ASN:ND2	2.16	0.61
1:E:32:THR:C	1:E:392:MET:HE1	2.24	0.61
1:C:455:ASP:OD1	1:C:458:ASN:HB2	1.99	0.61
2:B:140:ILE:HG22	2:B:140:ILE:O	2.00	0.61
1:G:99:ASN:ND2	1:G:101:MET:HE3	2.15	0.61
2:D:458:GLU:O	2:D:462:GLN:HB2	1.99	0.61
1:E:340:ALA:HB3	1:E:341:PRO:HD3	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:455:ASP:OD1	1:E:458:ASN:HB2	2.01	0.61
1:A:246:PRO:HG3	1:A:448:GLY:HA2	1.83	0.60
2:B:281:ASP:OD1	2:B:281:ASP:N	2.35	0.60
1:A:304:THR:HG22	1:A:305:HIS:CD2	2.23	0.60
2:B:64:LYS:O	2:B:186:ASN:ND2	2.35	0.60
1:C:96:SER:OG	1:C:97:ARG:N	2.31	0.60
2:D:236:GLU:C	2:D:238:PRO:HD3	2.27	0.60
1:A:455:ASP:OD1	1:A:458:ASN:HB2	2.01	0.60
2:B:144:ARG:NH2	2:B:190:ILE:N	2.48	0.60
1:E:50:SER:HA	1:E:53:GLU:HG3	1.82	0.60
1:G:19:PHE:CD1	1:G:392:MET:HE3	2.37	0.60
2:D:286:LEU:HD13	3:P:2:LEU:HD13	1.83	0.60
1:A:455:ASP:CG	1:A:458:ASN:HB2	2.27	0.59
2:D:256:ARG:HG3	2:D:256:ARG:NH1	2.16	0.59
2:D:441:MET:HG2	2:D:442:VAL:N	2.16	0.59
1:E:157:LEU:CB	1:E:445:VAL:HG21	2.32	0.59
2:F:56:ALA:HB1	2:F:198:TYR:OH	2.01	0.59
1:C:99:ASN:ND2	1:C:101:MET:HE3	2.17	0.59
1:G:304:THR:HG22	1:G:305:HIS:CD2	2.25	0.59
2:H:64:LYS:O	2:H:186:ASN:ND2	2.34	0.59
1:A:304:THR:CG2	1:A:305:HIS:HD2	2.11	0.59
1:A:178:LEU:HD11	1:E:178:LEU:HD11	1.85	0.59
2:D:54:VAL:HG22	2:D:208:MET:HE2	1.83	0.59
2:D:56:ALA:HB1	2:D:198:TYR:OH	2.03	0.59
1:A:347:ILE:CG2	1:A:351:MET:HE3	2.32	0.59
1:G:122:VAL:O	1:G:191:ARG:NH2	2.36	0.59
1:A:175:PRO:HB3	1:E:175:PRO:HB3	1.84	0.59
2:B:136:ASP:O	2:B:140:ILE:HG13	2.03	0.59
1:C:268:ILE:HD11	1:C:398:MET:SD	2.43	0.59
1:E:157:LEU:HB3	1:E:445:VAL:CG2	2.31	0.59
1:C:19:PHE:CD1	1:C:392:MET:HE3	2.38	0.59
1:G:310:TYR:CD1	1:G:312:PHE:CZ	2.91	0.58
1:C:455:ASP:CG	1:C:458:ASN:HB2	2.28	0.58
1:A:99:ASN:ND2	1:A:101:MET:HE3	2.17	0.58
2:F:54:VAL:O	2:F:107:ASN:HB3	2.03	0.58
2:F:253:ARG:NH2	2:F:453:VAL:HG12	2.19	0.58
2:H:303:THR:HG22	2:H:305:SER:N	2.15	0.58
1:E:101:MET:HE1	1:E:394:ARG:CD	2.32	0.58
2:F:303:THR:HG22	2:F:305:SER:N	2.16	0.58
1:A:14:ALA:HB2	1:A:402:LYS:O	2.03	0.58
2:H:62:ASN:CG	2:H:65:ASN:HB2	2.28	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:207:ARG:HH11	2:H:245:ARG:HH12	1.51	0.58
1:A:19:PHE:HD1	1:A:392:MET:CE	2.14	0.58
1:E:154:LEU:HB3	1:E:260:GLN:HE21	1.68	0.58
2:F:115:LEU:HD12	2:F:115:LEU:H	1.68	0.58
1:G:299:TYR:CZ	2:H:90:LEU:HD23	2.37	0.58
2:B:441:MET:HG2	2:B:442:VAL:N	2.19	0.58
2:D:140:ILE:HG22	2:D:140:ILE:O	2.03	0.58
1:G:371:LYS:HE3	1:G:412:ILE:O	2.04	0.58
1:G:455:ASP:CG	1:G:458:ASN:HB2	2.29	0.58
2:D:75:LEU:HD21	2:D:140:ILE:HG12	1.86	0.57
2:F:255:GLU:HB3	2:F:453:VAL:HG23	1.86	0.57
1:C:101:MET:HE1	1:C:394:ARG:CD	2.34	0.57
1:C:295:GLY:H	2:D:93:GLU:HG3	1.69	0.57
2:D:207:ARG:NH1	2:D:245:ARG:NH1	2.52	0.57
1:E:63:ILE:O	1:E:67:LEU:HB2	2.03	0.57
1:A:371:LYS:HE3	1:A:412:ILE:O	2.05	0.57
1:A:242:SER:OG	1:E:176:ARG:NH2	2.37	0.57
2:F:218:HIS:O	2:F:222:VAL:HG23	2.04	0.57
2:F:458:GLU:O	2:F:462:GLN:HB2	2.04	0.57
1:A:34:ASN:HD21	2:B:44:ASN:CB	2.15	0.57
1:A:154:LEU:HB3	1:A:260:GLN:NE2	2.18	0.57
2:B:236:GLU:C	2:B:238:PRO:HD3	2.30	0.57
1:C:310:TYR:CD1	1:C:312:PHE:CZ	2.93	0.57
2:D:441:MET:HE2	2:D:456:ILE:HD12	1.87	0.57
1:A:50:SER:HA	1:A:53:GLU:HG3	1.86	0.57
2:F:193:THR:HG22	2:F:197:ASP:OD2	2.05	0.57
2:F:256:ARG:HG3	2:F:256:ARG:NH1	2.15	0.57
2:F:136:ASP:O	2:F:140:ILE:HG13	2.04	0.57
1:C:20:LYS:HD2	1:C:209:HIS:HB2	1.87	0.57
1:E:17:ASP:O	1:E:18:ASN:HB3	2.02	0.57
1:G:139:ALA:O	1:G:143:ILE:HD13	2.05	0.57
1:G:304:THR:CG2	1:G:305:HIS:HD2	2.11	0.57
2:H:76:ALA:HB1	2:H:129:ILE:CG2	2.35	0.57
2:H:441:MET:HG2	2:H:442:VAL:N	2.20	0.57
1:A:17:ASP:O	1:A:18:ASN:HB3	2.05	0.56
1:G:39:PHE:CE1	1:G:385:LYS:HD2	2.40	0.56
2:B:439:VAL:HG22	2:B:453:VAL:HG13	1.87	0.56
2:F:62:ASN:CG	2:F:65:ASN:HB2	2.30	0.56
2:F:76:ALA:HB1	2:F:129:ILE:HG22	1.87	0.56
2:F:140:ILE:HG22	2:F:140:ILE:O	2.05	0.56
1:C:249:VAL:HG23	1:C:249:VAL:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:429:THR:HG22	1:G:429:THR:O	2.04	0.56
1:A:20:LYS:HD2	1:A:209:HIS:HB2	1.86	0.56
1:E:455:ASP:CG	1:E:458:ASN:HB2	2.30	0.56
1:C:96:SER:HB3	1:C:99:ASN:OD1	2.06	0.56
1:E:371:LYS:HE3	1:E:412:ILE:O	2.05	0.56
2:H:207:ARG:NH1	2:H:245:ARG:NH1	2.53	0.56
2:H:255:GLU:HB3	2:H:453:VAL:HG23	1.86	0.56
2:B:423:LYS:O	2:B:427:ILE:HG13	2.06	0.56
2:D:136:ASP:O	2:D:140:ILE:HG13	2.05	0.56
2:D:207:ARG:NH1	2:D:245:ARG:HH12	2.04	0.56
2:D:303:THR:HG22	2:D:305:SER:N	2.16	0.56
1:G:20:LYS:HD2	1:G:209:HIS:HB2	1.87	0.56
1:E:20:LYS:HD2	1:E:209:HIS:HB2	1.87	0.56
1:G:296:LYS:HE2	1:G:298:MET:HE2	1.87	0.56
2:H:56:ALA:HB1	2:H:198:TYR:OH	2.05	0.56
2:B:218:HIS:O	2:B:222:VAL:HG23	2.06	0.55
2:H:75:LEU:HD21	2:H:140:ILE:HG12	1.87	0.55
1:A:122:VAL:O	1:A:191:ARG:NH2	2.40	0.55
1:G:210:GLU:OE1	1:G:210:GLU:HA	2.06	0.55
3:R:2:LEU:HD12	3:R:3:SER:N	2.20	0.55
1:G:19:PHE:HD1	1:G:392:MET:CE	2.19	0.55
2:H:76:ALA:HB1	2:H:129:ILE:HG22	1.88	0.55
2:H:275:VAL:HG22	2:H:279:ALA:CB	2.37	0.55
1:A:45:TYR:OH	1:A:389:LEU:HG	2.07	0.55
2:D:144:ARG:NH2	2:D:190:ILE:N	2.55	0.55
1:E:210:GLU:HA	1:E:210:GLU:OE1	2.06	0.55
2:F:54:VAL:HG22	2:F:208:MET:HE2	1.88	0.55
2:F:75:LEU:HD21	2:F:140:ILE:HG12	1.89	0.55
2:F:165:HIS:HD2	2:F:256:ARG:HE	1.55	0.55
2:F:76:ALA:HB1	2:F:129:ILE:CG2	2.37	0.55
2:H:193:THR:HG22	2:H:197:ASP:OD2	2.07	0.55
1:C:298:MET:HG2	2:D:93:GLU:OE2	2.07	0.54
1:A:19:PHE:CD1	1:A:392:MET:CE	2.90	0.54
2:B:56:ALA:HB1	2:B:198:TYR:OH	2.06	0.54
2:D:54:VAL:O	2:D:107:ASN:HB3	2.07	0.54
3:Q:2:LEU:HD12	3:Q:3:SER:H	1.71	0.54
2:B:75:LEU:HD21	2:B:140:ILE:HG12	1.88	0.54
1:C:210:GLU:HA	1:C:210:GLU:OE1	2.07	0.54
2:D:62:ASN:CG	2:D:65:ASN:HB2	2.33	0.54
2:F:207:ARG:NH1	2:F:245:ARG:NH1	2.55	0.54
1:A:299:TYR:OH	2:B:86:GLN:HG2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:317:GLY:O	2:D:318:SER:CB	2.56	0.54
2:F:97:SER:OG	2:F:114:SER:HB3	2.08	0.54
2:F:382:ALA:HB1	2:F:386:LEU:HD12	1.89	0.54
1:G:296:LYS:HG2	1:G:298:MET:HE2	1.89	0.54
1:A:63:ILE:O	1:A:67:LEU:HB2	2.08	0.54
2:B:62:ASN:CG	2:B:65:ASN:HB2	2.32	0.54
2:D:382:ALA:HB1	2:D:386:LEU:HD12	1.89	0.54
1:G:14:ALA:N	1:G:17:ASP:HB2	2.22	0.54
2:D:175:PRO:HA	2:D:178:ARG:NH1	2.23	0.54
2:D:255:GLU:HB3	2:D:453:VAL:HG23	1.90	0.54
2:H:275:VAL:HG11	2:H:282:TYR:HA	1.90	0.54
1:A:139:ALA:O	1:A:143:ILE:HD13	2.07	0.54
2:B:253:ARG:HH21	2:B:457:GLU:CD	2.16	0.54
2:B:303:THR:HG22	2:B:305:SER:N	2.16	0.54
2:B:382:ALA:HB1	2:B:386:LEU:HD12	1.90	0.54
2:D:76:ALA:HB1	2:D:129:ILE:CG2	2.37	0.54
1:G:96:SER:HB3	1:G:99:ASN:OD1	2.08	0.54
2:D:441:MET:HE2	2:D:456:ILE:CD1	2.38	0.54
2:F:275:VAL:HG11	2:F:282:TYR:HA	1.89	0.54
1:A:310:TYR:CD1	1:A:312:PHE:CZ	2.96	0.53
2:B:147:ILE:HG22	2:B:187:ILE:HD13	1.90	0.53
1:G:347:ILE:CG2	1:G:351:MET:HE3	2.37	0.53
2:H:253:ARG:HH21	2:H:457:GLU:CD	2.16	0.53
1:E:28:LEU:HD21	1:E:220:LEU:HD23	1.90	0.53
1:E:310:TYR:CD1	1:E:312:PHE:CZ	2.97	0.53
2:F:64:LYS:O	2:F:186:ASN:ND2	2.40	0.53
1:G:63:ILE:O	1:G:67:LEU:HB2	2.08	0.53
1:G:101:MET:HE1	1:G:394:ARG:CD	2.36	0.53
2:F:62:ASN:OD1	2:F:65:ASN:HB2	2.09	0.53
2:H:218:HIS:O	2:H:222:VAL:HG23	2.09	0.53
2:H:317:GLY:O	2:H:318:SER:CB	2.57	0.53
2:B:349:VAL:O	2:B:352:ILE:HG22	2.08	0.53
1:G:263:PHE:CE2	1:G:442:ALA:HB2	2.42	0.53
2:H:140:ILE:O	2:H:140:ILE:HG22	2.08	0.53
1:G:298:MET:HG2	2:H:93:GLU:OE2	2.08	0.53
1:A:210:GLU:OE1	1:A:210:GLU:HA	2.09	0.53
2:F:165:HIS:HD2	2:F:256:ARG:NE	2.06	0.53
1:A:403:ILE:HG23	1:A:403:ILE:O	2.07	0.53
1:A:312:PHE:O	1:A:335:CYS:HB2	2.09	0.52
1:E:241:GLU:HA	1:E:444:VAL:O	2.09	0.52
2:F:441:MET:HG2	2:F:442:VAL:N	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:VAL:HG11	2:B:282:TYR:HA	1.92	0.52
1:G:403:ILE:HG23	1:G:403:ILE:O	2.08	0.52
2:B:83:ARG:NH2	2:B:124:ASP:OD2	2.42	0.52
2:B:366:GLY:HA2	2:B:427:ILE:HD13	1.90	0.52
1:E:379:LEU:HD11	1:E:409:ILE:CD1	2.37	0.52
2:H:453:VAL:O	2:H:457:GLU:HG3	2.09	0.52
1:A:224:GLN:CD	1:G:129:GLU:HG3	2.34	0.52
1:C:268:ILE:CD1	1:C:324:SER:HA	2.40	0.52
2:F:83:ARG:NH2	2:F:124:ASP:OD2	2.41	0.52
1:A:85:GLU:OE2	2:B:303:THR:HG23	2.10	0.52
1:A:129:GLU:HG3	1:G:224:GLN:OE1	2.08	0.52
2:B:90:LEU:HD13	2:B:94:ASN:HD21	1.74	0.52
1:C:114:MET:HE2	1:C:118:MET:HE3	1.90	0.52
2:F:160:GLU:OE1	2:F:160:GLU:HA	2.10	0.52
1:A:429:THR:CG2	1:A:431:ASN:HD22	2.23	0.52
2:B:76:ALA:HB1	2:B:129:ILE:CG2	2.40	0.52
1:A:14:ALA:HB3	1:A:404:PRO:HB3	1.92	0.52
1:A:379:LEU:HD11	1:A:409:ILE:CD1	2.35	0.52
1:G:200:THR:HG22	1:G:201:VAL:N	2.25	0.52
2:D:192:ARG:NH1	2:D:196:LYS:HD2	2.25	0.52
1:C:28:LEU:HD21	1:C:220:LEU:HD23	1.92	0.51
2:D:147:ILE:HG22	2:D:187:ILE:HD13	1.92	0.51
2:D:192:ARG:HH12	2:D:196:LYS:HD2	1.75	0.51
2:B:453:VAL:O	2:B:457:GLU:HG3	2.10	0.51
1:C:246:PRO:HG3	1:C:448:GLY:C	2.34	0.51
2:F:349:VAL:O	2:F:352:ILE:HG22	2.10	0.51
2:B:165:HIS:HD2	2:B:256:ARG:NE	2.08	0.51
1:C:33:SER:HB3	1:C:392:MET:CE	2.40	0.51
1:G:369:ARG:O	1:G:373:GLN:HG3	2.11	0.51
1:G:412:ILE:O	1:G:415:LEU:HB2	2.11	0.51
2:B:76:ALA:HB1	2:B:129:ILE:HG22	1.92	0.51
2:B:207:ARG:NH1	2:B:245:ARG:NH1	2.58	0.51
2:F:207:ARG:NH1	2:F:245:ARG:HH12	2.08	0.51
2:F:253:ARG:HH21	2:F:457:GLU:CD	2.18	0.51
1:G:243:CYS:HA	1:G:446:MET:O	2.09	0.51
2:B:134:VAL:HG12	2:B:136:ASP:N	2.25	0.51
2:D:181:LEU:HD13	3:P:8:ARG:CG	2.36	0.51
2:D:218:HIS:O	2:D:222:VAL:HG23	2.11	0.51
1:A:157:LEU:CB	1:A:445:VAL:HG21	2.41	0.51
1:C:371:LYS:HE3	1:C:412:ILE:O	2.11	0.51
2:H:281:ASP:OD1	2:H:281:ASP:N	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:MET:HE1	1:A:394:ARG:CD	2.41	0.51
1:C:429:THR:O	1:C:467:ASN:HB2	2.10	0.51
2:D:76:ALA:HB1	2:D:129:ILE:HG22	1.92	0.51
1:E:268:ILE:HD13	1:E:268:ILE:H	1.75	0.51
1:E:45:TYR:OH	1:E:389:LEU:HG	2.11	0.51
2:F:423:LYS:O	2:F:427:ILE:HG13	2.10	0.51
2:B:193:THR:HG22	2:B:197:ASP:OD2	2.11	0.51
1:C:19:PHE:HD1	1:C:392:MET:CE	2.24	0.51
1:C:301:ARG:NH2	1:C:362:LEU:HD23	2.25	0.51
1:C:336:ILE:HG22	1:C:338:GLN:H	1.75	0.51
1:A:261:ILE:HG12	1:A:444:VAL:HG22	1.92	0.51
1:C:99:ASN:HD22	1:C:101:MET:HE3	1.75	0.51
1:C:275:ALA:HB3	1:C:423:VAL:HG21	1.93	0.51
1:E:139:ALA:O	1:E:143:ILE:HD13	2.10	0.51
2:F:134:VAL:HG12	2:F:136:ASP:N	2.25	0.51
1:G:379:LEU:HD11	1:G:409:ILE:CD1	2.40	0.51
1:E:19:PHE:HD1	1:E:392:MET:HE3	1.75	0.50
2:F:22:GLN:HA	2:F:22:GLN:NE2	2.26	0.50
2:F:326:PHE:CD1	2:F:326:PHE:C	2.89	0.50
1:G:249:VAL:O	1:G:249:VAL:HG23	2.12	0.50
2:H:256:ARG:HG3	2:H:256:ARG:NH1	2.24	0.50
1:G:152:LEU:O	1:G:155:PRO:HD2	2.11	0.50
2:H:83:ARG:NH2	2:H:124:ASP:OD2	2.44	0.50
1:C:45:TYR:OH	1:C:389:LEU:HG	2.12	0.50
1:E:312:PHE:O	1:E:335:CYS:HB2	2.12	0.50
2:B:237:SER:N	2:B:238:PRO:HD3	2.27	0.50
2:F:144:ARG:NH2	2:F:190:ILE:N	2.60	0.50
2:H:40:GLU:OE1	2:H:408:ARG:NH2	2.44	0.50
2:B:54:VAL:HG22	2:B:208:MET:HE2	1.93	0.50
2:D:193:THR:HG22	2:D:197:ASP:OD2	2.11	0.50
1:E:403:ILE:HG23	1:E:403:ILE:O	2.10	0.50
1:A:157:LEU:HB3	1:A:445:VAL:CG2	2.39	0.50
2:D:83:ARG:NH2	2:D:124:ASP:OD2	2.45	0.50
2:F:103:THR:O	2:F:180:ILE:HD13	2.12	0.50
1:G:179:ILE:N	1:G:180:PRO:CD	2.74	0.50
2:H:144:ARG:NH2	2:H:190:ILE:N	2.59	0.50
2:H:147:ILE:HG22	2:H:187:ILE:HD13	1.92	0.50
2:H:175:PRO:HA	2:H:178:ARG:NH1	2.27	0.50
2:D:139:ALA:C	2:D:141:GLU:H	2.20	0.49
2:F:192:ARG:HH12	2:F:196:LYS:HD2	1.77	0.49
2:F:192:ARG:NH1	2:F:196:LYS:HD2	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:281:ASP:OD1	2:F:281:ASP:N	2.41	0.49
2:D:97:SER:OG	2:D:114:SER:HB3	2.12	0.49
2:D:275:VAL:HG11	2:D:282:TYR:HA	1.94	0.49
2:F:317:GLY:O	2:F:318:SER:CB	2.59	0.49
2:H:69:ALA:HB2	2:H:198:TYR:CZ	2.47	0.49
2:F:181:LEU:HD13	3:Q:8:ARG:CG	2.39	0.49
2:H:382:ALA:HB1	2:H:386:LEU:HD12	1.95	0.49
1:E:200:THR:HG22	1:E:201:VAL:N	2.27	0.49
2:F:147:ILE:HG22	2:F:187:ILE:HD13	1.93	0.49
2:B:69:ALA:HB2	2:B:198:TYR:CZ	2.48	0.49
2:B:458:GLU:OE2	2:D:422:THR:HB	2.13	0.49
1:C:154:LEU:HB3	1:C:260:GLN:HE21	1.76	0.49
2:D:380:LEU:HD11	2:D:384:LEU:HD11	1.94	0.49
1:C:42:LEU:HD23	1:C:42:LEU:N	2.27	0.49
1:C:312:PHE:O	1:C:335:CYS:HB2	2.12	0.49
1:E:32:THR:HG22	1:E:204:PHE:HB2	1.95	0.49
1:E:249:VAL:HG23	1:E:249:VAL:O	2.13	0.49
2:F:401:GLN:O	2:F:405:THR:HB	2.12	0.49
1:G:429:THR:O	1:G:467:ASN:HB2	2.13	0.49
1:A:189:ASP:OD2	1:A:193:LYS:HE3	2.13	0.49
1:A:268:ILE:HD13	1:A:268:ILE:H	1.75	0.49
2:B:375:ARG:NH1	2:B:375:ARG:CB	2.73	0.49
2:D:234:LYS:HG2	2:D:235:SER:N	2.27	0.49
2:D:253:ARG:NH2	2:D:453:VAL:HG12	2.27	0.49
1:G:45:TYR:OH	1:G:389:LEU:HG	2.12	0.49
3:R:2:LEU:HD12	3:R:3:SER:H	1.78	0.49
1:A:28:LEU:HD21	1:A:220:LEU:HD23	1.93	0.49
1:A:336:ILE:HG22	1:A:338:GLN:H	1.78	0.49
2:H:62:ASN:OD1	2:H:65:ASN:HB2	2.13	0.49
1:A:429:THR:O	1:A:467:ASN:HB2	2.13	0.49
2:B:253:ARG:NH2	2:B:453:VAL:HG12	2.28	0.49
1:G:303:TYR:HA	1:G:307:LEU:HB2	1.93	0.49
2:H:62:ASN:ND2	2:H:65:ASN:HB2	2.28	0.49
2:H:348:ASN:OD1	2:H:350:ARG:HB3	2.12	0.49
2:H:398:ILE:HA	2:H:408:ARG:HG3	1.94	0.49
1:C:32:THR:HG22	1:C:204:PHE:HB2	1.95	0.48
2:D:281:ASP:OD1	2:D:281:ASP:N	2.43	0.48
1:E:179:ILE:N	1:E:180:PRO:CD	2.76	0.48
1:E:261:ILE:HG12	1:E:444:VAL:HG22	1.94	0.48
1:E:311:TYR:CD2	1:E:311:TYR:N	2.80	0.48
2:H:441:MET:HE2	2:H:456:ILE:CD1	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:MET:HE2	1:A:118:MET:HE3	1.95	0.48
1:C:31:ALA:HB1	1:C:392:MET:HE2	1.94	0.48
1:A:224:GLN:OE1	1:G:129:GLU:HG3	2.13	0.48
1:A:339:ALA:O	1:A:340:ALA:C	2.57	0.48
1:C:139:ALA:O	1:C:143:ILE:HD13	2.13	0.48
1:A:403:ILE:O	1:A:403:ILE:CG2	2.62	0.48
1:C:179:ILE:N	1:C:180:PRO:CD	2.77	0.48
1:C:429:THR:O	1:C:429:THR:CG2	2.61	0.48
1:E:230:ILE:HD11	1:G:236:GLN:HE22	1.79	0.48
1:E:301:ARG:NH2	1:E:362:LEU:HD23	2.29	0.48
2:F:69:ALA:HB2	2:F:198:TYR:CZ	2.47	0.48
2:F:171:TYR:CE2	2:F:176:LEU:HD23	2.49	0.48
1:G:19:PHE:CD1	1:G:392:MET:CE	2.96	0.48
1:G:32:THR:HG22	1:G:204:PHE:HB2	1.94	0.48
1:G:246:PRO:HG3	1:G:448:GLY:C	2.39	0.48
1:A:35:THR:HB	1:A:36:PRO:CD	2.44	0.48
1:E:14:ALA:N	1:E:17:ASP:OD2	2.47	0.48
1:G:268:ILE:CD1	1:G:324:SER:HA	2.44	0.48
2:H:160:GLU:OE1	2:H:160:GLU:HA	2.13	0.48
1:A:152:LEU:O	1:A:155:PRO:HD2	2.13	0.48
1:A:249:VAL:HG23	1:A:249:VAL:O	2.13	0.48
2:F:27:ARG:HB3	2:F:27:ARG:NH1	2.28	0.48
2:H:27:ARG:HB3	2:H:27:ARG:NH1	2.28	0.48
2:H:441:MET:HE2	2:H:456:ILE:HD12	1.95	0.48
1:A:39:PHE:CE1	1:A:385:LYS:HD2	2.49	0.48
1:C:412:ILE:O	1:C:415:LEU:HB2	2.13	0.48
1:E:429:THR:O	1:E:467:ASN:HB2	2.13	0.48
2:H:207:ARG:NH1	2:H:245:ARG:HH12	2.11	0.48
2:H:326:PHE:CD1	2:H:326:PHE:C	2.91	0.48
1:A:256:LEU:HD11	1:A:314:GLU:HG2	1.96	0.48
2:F:175:PRO:HA	2:F:178:ARG:NH1	2.29	0.48
1:A:49:GLY:HA2	1:A:61:THR:HG21	1.95	0.48
2:D:27:ARG:NH1	2:D:27:ARG:HB3	2.29	0.48
2:D:62:ASN:OD1	2:D:65:ASN:HB2	2.13	0.48
1:A:268:ILE:N	1:A:268:ILE:CD1	2.77	0.47
1:C:403:ILE:O	1:C:403:ILE:HG23	2.13	0.47
1:E:270:HIS:O	1:E:273:ILE:HB	2.14	0.47
1:E:303:TYR:HA	1:E:307:LEU:HB2	1.96	0.47
1:A:429:THR:HG22	1:A:431:ASN:HD22	1.77	0.47
2:B:27:ARG:NH1	2:B:27:ARG:HB3	2.29	0.47
1:G:276:LEU:HD11	1:G:329:PHE:CD2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:THR:CG2	1:C:431:ASN:HD22	2.27	0.47
2:F:27:ARG:HB3	2:F:27:ARG:HH11	1.79	0.47
1:G:301:ARG:NH2	1:G:362:LEU:HD23	2.29	0.47
1:G:429:THR:CG2	1:G:431:ASN:HD22	2.26	0.47
2:F:90:LEU:CD1	2:F:94:ASN:ND2	2.70	0.47
2:H:88:ILE:HG21	2:H:129:ILE:HD11	1.96	0.47
2:H:234:LYS:HG2	2:H:235:SER:N	2.29	0.47
1:A:412:ILE:O	1:A:415:LEU:HB2	2.14	0.47
2:H:349:VAL:O	2:H:352:ILE:HG22	2.14	0.47
1:A:369:ARG:HG3	2:B:94:ASN:HA	1.96	0.47
1:C:63:ILE:O	1:C:67:LEU:HB2	2.15	0.47
1:C:256:LEU:HD11	1:C:314:GLU:HG2	1.96	0.47
1:E:96:SER:HB3	1:E:99:ASN:OD1	2.14	0.47
1:G:85:GLU:OE2	2:H:303:THR:HG23	2.14	0.47
2:H:40:GLU:O	2:H:213:ALA:HA	2.14	0.47
1:A:47:ASP:HB3	1:A:199:ASN:OD1	2.14	0.47
2:B:62:ASN:OD1	2:B:65:ASN:HB2	2.14	0.47
1:C:379:LEU:HD11	1:C:409:ILE:CD1	2.39	0.47
1:G:30:VAL:HG22	1:G:216:THR:HG21	1.96	0.47
2:B:171:TYR:CE2	2:B:176:LEU:HD23	2.49	0.47
2:B:401:GLN:O	2:B:405:THR:HB	2.14	0.47
1:C:288:SER:OG	1:C:307:LEU:HD12	2.15	0.47
1:C:295:GLY:H	2:D:93:GLU:CG	2.27	0.47
2:H:192:ARG:HH12	2:H:196:LYS:HD2	1.80	0.47
2:H:439:VAL:HG22	2:H:453:VAL:HG13	1.96	0.47
1:G:270:HIS:O	1:G:273:ILE:HB	2.15	0.47
1:G:403:ILE:O	1:G:403:ILE:CG2	2.63	0.47
1:A:317:VAL:HG22	1:A:318:ALA:N	2.29	0.47
1:C:256:LEU:CD1	1:C:314:GLU:HG2	2.45	0.47
1:G:444:VAL:HG11	1:G:456:VAL:HG11	1.97	0.47
2:B:256:ARG:HG3	2:B:256:ARG:NH1	2.28	0.46
1:C:152:LEU:O	1:C:155:PRO:HD2	2.14	0.46
1:C:311:TYR:CD2	1:C:311:TYR:N	2.83	0.46
2:D:134:VAL:HG12	2:D:136:ASP:N	2.30	0.46
2:D:349:VAL:O	2:D:352:ILE:HG22	2.15	0.46
1:G:67:LEU:HD13	1:G:135:GLN:HG3	1.97	0.46
1:G:339:ALA:O	1:G:340:ALA:C	2.57	0.46
1:G:390:GLU:O	1:G:394:ARG:HG3	2.15	0.46
2:H:27:ARG:HB3	2:H:27:ARG:HH11	1.80	0.46
1:A:204:PHE:CD1	1:A:204:PHE:N	2.83	0.46
2:B:27:ARG:HB3	2:B:27:ARG:HH11	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:TYR:CZ	3:O:7:LYS:HE2	2.51	0.46
1:C:49:GLY:HA2	1:C:61:THR:HG21	1.97	0.46
1:C:204:PHE:CD1	1:C:204:PHE:N	2.83	0.46
2:D:69:ALA:HB2	2:D:198:TYR:CZ	2.50	0.46
1:E:312:PHE:CE1	1:E:313:VAL:HG23	2.50	0.46
2:B:39:THR:HB	2:B:218:HIS:ND1	2.30	0.46
1:C:200:THR:HG22	1:C:201:VAL:N	2.30	0.46
1:E:187:LEU:O	1:E:191:ARG:HG3	2.15	0.46
1:E:204:PHE:N	1:E:204:PHE:CD1	2.82	0.46
2:F:139:ALA:C	2:F:141:GLU:H	2.22	0.46
1:G:99:ASN:HD22	1:G:101:MET:HE3	1.78	0.46
1:G:275:ALA:HB3	1:G:423:VAL:HG21	1.97	0.46
2:H:230:GLY:C	2:H:232:VAL:H	2.24	0.46
1:A:200:THR:HG22	1:A:201:VAL:N	2.31	0.46
1:C:126:LYS:O	1:C:127:ILE:C	2.58	0.46
1:E:90:ASN:ND2	1:E:105:SER:OG	2.46	0.46
1:E:268:ILE:H	1:E:268:ILE:CD1	2.27	0.46
2:F:230:GLY:C	2:F:232:VAL:H	2.24	0.46
1:C:17:ASP:O	1:C:18:ASN:CB	2.63	0.46
2:F:398:ILE:HA	2:F:408:ARG:HG3	1.97	0.46
2:F:439:VAL:HG22	2:F:453:VAL:HG13	1.97	0.46
2:B:102:TYR:CE1	3:O:7:LYS:HE2	2.51	0.46
2:B:139:ALA:C	2:B:141:GLU:H	2.24	0.46
1:G:227:HIS:N	1:G:228:PRO:CD	2.79	0.46
1:G:312:PHE:CE1	1:G:313:VAL:HG23	2.51	0.46
1:A:268:ILE:H	1:A:268:ILE:CD1	2.29	0.46
2:B:88:ILE:HG21	2:B:129:ILE:HD11	1.97	0.46
1:E:114:MET:HE2	1:E:118:MET:HE3	1.97	0.46
1:E:242:SER:HB3	1:E:445:VAL:HG23	1.97	0.46
1:A:256:LEU:CD1	1:A:314:GLU:HG2	2.46	0.46
2:B:160:GLU:HA	2:B:160:GLU:OE1	2.15	0.46
2:D:139:ALA:C	2:D:141:GLU:N	2.73	0.46
1:E:256:LEU:CD1	1:E:314:GLU:HG2	2.46	0.46
2:F:77:PHE:O	2:F:85:GLN:HG3	2.15	0.46
2:F:237:SER:N	2:F:238:PRO:HD3	2.30	0.46
2:H:232:VAL:HG13	2:H:233:PRO:HD2	1.98	0.46
1:A:126:LYS:O	1:A:127:ILE:C	2.57	0.46
2:B:380:LEU:HD11	2:B:384:LEU:HD11	1.98	0.46
1:C:299:TYR:CD1	2:D:90:LEU:HD23	2.51	0.46
1:C:303:TYR:HA	1:C:307:LEU:HB2	1.98	0.46
2:D:90:LEU:CD1	2:D:94:ASN:ND2	2.72	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:336:ILE:HG22	1:E:338:GLN:H	1.81	0.46
1:E:444:VAL:HG11	1:E:456:VAL:HG11	1.98	0.46
1:G:268:ILE:N	1:G:268:ILE:CD1	2.78	0.46
1:A:315:ASN:HB3	1:A:334:SER:HB2	1.98	0.46
2:B:207:ARG:NH1	2:B:245:ARG:HH12	2.14	0.46
1:A:96:SER:HB3	1:A:99:ASN:OD1	2.16	0.45
2:B:230:GLY:C	2:B:232:VAL:H	2.24	0.45
1:E:256:LEU:HD11	1:E:314:GLU:HG2	1.97	0.45
1:G:17:ASP:O	1:G:18:ASN:CB	2.61	0.45
2:H:134:VAL:HG12	2:H:136:ASP:N	2.31	0.45
1:A:275:ALA:HB3	1:A:423:VAL:HG21	1.97	0.45
1:A:312:PHE:CE1	1:A:313:VAL:HG23	2.51	0.45
2:B:422:THR:HG23	2:B:425:ASP:OD2	2.15	0.45
1:C:270:HIS:O	1:C:273:ILE:HB	2.16	0.45
1:G:28:LEU:HD21	1:G:220:LEU:HD23	1.98	0.45
1:G:33:SER:HB3	1:G:392:MET:CE	2.46	0.45
2:H:77:PHE:O	2:H:85:GLN:HG3	2.17	0.45
2:H:139:ALA:C	2:H:141:GLU:H	2.24	0.45
1:A:301:ARG:NH2	1:A:362:LEU:HD23	2.31	0.45
2:D:326:PHE:CD1	2:D:326:PHE:C	2.93	0.45
2:D:423:LYS:O	2:D:427:ILE:HG13	2.16	0.45
1:E:47:ASP:HB3	1:E:199:ASN:OD1	2.16	0.45
1:G:270:HIS:ND1	1:G:271:PRO:HD2	2.31	0.45
2:H:192:ARG:NH1	2:H:196:LYS:HD2	2.31	0.45
1:C:19:PHE:CD1	1:C:392:MET:CE	2.99	0.45
1:C:213:LEU:HD23	1:C:213:LEU:HA	1.75	0.45
1:C:268:ILE:N	1:C:268:ILE:CD1	2.79	0.45
1:E:275:ALA:HB3	1:E:423:VAL:HG21	1.98	0.45
1:E:429:THR:O	1:E:429:THR:CG2	2.65	0.45
2:F:323:TYR:CD1	2:F:323:TYR:C	2.95	0.45
1:A:35:THR:HB	1:A:36:PRO:HD2	1.99	0.45
1:A:429:THR:O	1:A:429:THR:CG2	2.63	0.45
2:B:263:LEU:HA	2:B:264:PRO:HD3	1.83	0.45
1:C:357:ASN:C	1:C:357:ASN:OD1	2.60	0.45
2:D:366:GLY:HA2	2:D:427:ILE:HD13	1.99	0.45
1:E:268:ILE:N	1:E:268:ILE:CD1	2.77	0.45
1:A:273:ILE:CG2	1:A:274:TYR:N	2.80	0.45
2:B:35:LEU:CD1	2:B:208:MET:HG3	2.46	0.45
1:C:275:ALA:CB	1:C:423:VAL:HG21	2.47	0.45
1:C:369:ARG:O	1:C:373:GLN:HG3	2.17	0.45
2:D:52:ILE:O	2:D:52:ILE:HG23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:GLU:OE1	2:D:66:ASN:HA	2.17	0.45
2:D:88:ILE:HG21	2:D:129:ILE:HD11	1.99	0.45
2:D:207:ARG:HH11	2:D:245:ARG:HH12	1.64	0.45
1:E:236:GLN:NE2	1:G:230:ILE:HD11	2.25	0.45
2:F:380:LEU:HD11	2:F:384:LEU:HD11	1.98	0.45
1:A:179:ILE:N	1:A:180:PRO:CD	2.79	0.45
1:A:303:TYR:HA	1:A:307:LEU:HB2	1.97	0.45
2:B:127:SER:HB3	2:B:229:PHE:CE2	2.51	0.45
2:D:319:LEU:O	2:D:320:ALA:HB2	2.16	0.45
1:E:31:ALA:O	1:E:203:ALA:HA	2.17	0.45
1:G:126:LYS:O	1:G:127:ILE:C	2.59	0.45
2:B:80:THR:HB	2:B:132:LYS:O	2.17	0.45
1:C:429:THR:HG22	1:C:431:ASN:HD22	1.82	0.45
2:F:139:ALA:C	2:F:141:GLU:N	2.74	0.45
2:F:275:VAL:HG22	2:F:279:ALA:CB	2.47	0.45
1:G:35:THR:HB	1:G:36:PRO:HD2	1.99	0.45
1:A:243:CYS:HA	1:A:446:MET:O	2.17	0.45
1:G:315:ASN:HB3	1:G:334:SER:HB2	1.99	0.45
1:A:255:GLU:O	1:A:337:PRO:HD3	2.17	0.45
2:B:326:PHE:CD1	2:B:326:PHE:C	2.94	0.45
1:C:268:ILE:HD13	1:C:268:ILE:H	1.79	0.45
1:C:317:VAL:HG22	1:C:318:ALA:N	2.32	0.45
1:G:42:LEU:N	1:G:42:LEU:HD23	2.31	0.45
1:G:351:MET:HG2	1:G:428:PHE:CE1	2.51	0.45
1:A:207:VAL:HA	1:A:208:PRO:HD3	1.81	0.44
2:F:31:LEU:HD22	2:F:35:LEU:HD23	1.99	0.44
2:F:375:ARG:NH1	2:F:375:ARG:CB	2.79	0.44
2:D:275:VAL:HG22	2:D:279:ALA:CB	2.47	0.44
1:E:35:THR:HB	1:E:36:PRO:HD2	1.99	0.44
1:E:403:ILE:O	1:E:403:ILE:CG2	2.64	0.44
1:G:187:LEU:O	1:G:191:ARG:HG3	2.17	0.44
1:A:268:ILE:CD1	1:A:324:SER:HA	2.48	0.44
2:B:340:ILE:HG22	2:B:341:VAL:N	2.32	0.44
1:E:35:THR:HB	1:E:36:PRO:CD	2.48	0.44
2:F:52:ILE:HG23	2:F:52:ILE:O	2.17	0.44
2:F:55:ASP:CG	2:F:55:ASP:O	2.58	0.44
1:G:50:SER:OG	1:G:97:ARG:HA	2.16	0.44
1:G:296:LYS:HE2	1:G:298:MET:CE	2.47	0.44
1:G:299:TYR:CE1	2:H:90:LEU:HD23	2.52	0.44
1:G:429:THR:HG22	1:G:431:ASN:HD22	1.83	0.44
1:C:47:ASP:HB3	1:C:199:ASN:OD1	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:441:MET:HG2	2:D:442:VAL:H	1.82	0.44
1:A:312:PHE:CD1	1:A:313:VAL:HG23	2.53	0.44
1:A:168:LEU:HD13	1:A:323:TYR:CD2	2.53	0.44
1:A:295:GLY:HA2	2:B:93:GLU:HG2	1.99	0.44
1:C:403:ILE:O	1:C:403:ILE:CG2	2.65	0.44
1:E:16:THR:HG22	2:F:44:ASN:HD21	1.83	0.44
1:E:30:VAL:HG22	1:E:216:THR:HG21	1.99	0.44
1:E:42:LEU:N	1:E:42:LEU:HD23	2.32	0.44
1:G:336:ILE:HG22	1:G:338:GLN:H	1.82	0.44
2:H:97:SER:OG	2:H:114:SER:HB3	2.18	0.44
2:H:237:SER:N	2:H:238:PRO:HD3	2.31	0.44
2:H:268:ILE:HD12	2:H:268:ILE:N	2.33	0.44
1:A:42:LEU:HD23	1:A:42:LEU:N	2.32	0.44
1:A:176:ARG:NH2	1:E:242:SER:OG	2.50	0.44
2:B:165:HIS:HD2	2:B:256:ARG:HE	1.63	0.44
2:B:398:ILE:HA	2:B:408:ARG:HG3	2.00	0.44
2:D:23:ILE:HA	2:D:24:PRO:HD3	1.86	0.44
2:D:398:ILE:HA	2:D:408:ARG:HG3	1.99	0.44
2:D:453:VAL:O	2:D:457:GLU:HG3	2.18	0.44
1:E:67:LEU:HD13	1:E:135:GLN:HG3	1.99	0.44
2:F:40:GLU:O	2:F:213:ALA:HA	2.18	0.44
2:F:349:VAL:N	2:F:449:THR:OG1	2.51	0.44
2:H:259:LYS:HG3	2:H:447:THR:CG2	2.46	0.44
2:F:88:ILE:HG21	2:F:129:ILE:HD11	1.99	0.44
1:G:204:PHE:N	1:G:204:PHE:CD1	2.85	0.44
2:B:103:THR:O	2:B:180:ILE:HD13	2.18	0.44
2:B:255:GLU:HB3	2:B:453:VAL:HG23	2.00	0.44
1:C:444:VAL:HG11	1:C:456:VAL:HG11	2.00	0.44
1:G:227:HIS:N	1:G:228:PRO:HD3	2.33	0.44
1:G:268:ILE:CD1	1:G:268:ILE:H	2.31	0.44
2:H:171:TYR:CE2	2:H:176:LEU:HD23	2.52	0.44
2:B:77:PHE:O	2:B:85:GLN:HG3	2.18	0.43
2:B:183:PRO:O	2:B:184:ILE:C	2.60	0.43
1:G:35:THR:HB	1:G:36:PRO:CD	2.48	0.43
1:G:49:GLY:HA2	1:G:61:THR:HG21	2.00	0.43
1:A:299:TYR:CD1	2:B:90:LEU:HD23	2.53	0.43
1:C:32:THR:O	1:C:392:MET:HE1	2.18	0.43
1:C:100:LEU:HD21	1:C:195:TYR:OH	2.18	0.43
2:D:40:GLU:O	2:D:213:ALA:HA	2.18	0.43
2:D:375:ARG:NH1	2:D:375:ARG:CB	2.77	0.43
1:E:369:ARG:O	1:E:373:GLN:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:ILE:O	1:E:415:LEU:HB2	2.19	0.43
2:B:348:ASN:OD1	2:B:350:ARG:HB3	2.18	0.43
2:B:441:MET:HG2	2:B:442:VAL:H	1.82	0.43
2:D:139:ALA:O	2:D:141:GLU:N	2.51	0.43
2:D:382:ALA:CB	2:D:386:LEU:HD12	2.48	0.43
1:E:207:VAL:HA	1:E:208:PRO:HD3	1.84	0.43
1:G:30:VAL:CG2	1:G:216:THR:HG21	2.48	0.43
2:H:31:LEU:HD22	2:H:35:LEU:HD23	1.99	0.43
2:H:340:ILE:HG22	2:H:341:VAL:N	2.34	0.43
2:B:275:VAL:HG22	2:B:279:ALA:CB	2.48	0.43
1:C:314:GLU:OE2	1:C:315:ASN:HB2	2.19	0.43
1:C:379:LEU:HD13	2:D:46:SER:HB2	2.01	0.43
1:E:152:LEU:O	1:E:155:PRO:HD2	2.18	0.43
2:F:382:ALA:CB	2:F:386:LEU:HD12	2.48	0.43
2:F:405:THR:HG22	2:F:407:LYS:H	1.82	0.43
1:A:227:HIS:N	1:A:228:PRO:HD3	2.33	0.43
2:B:139:ALA:C	2:B:141:GLU:N	2.76	0.43
2:B:317:GLY:O	2:B:318:SER:CB	2.66	0.43
2:D:27:ARG:HB2	2:D:218:HIS:ND1	2.33	0.43
2:D:78:LYS:HE3	2:D:143:GLU:OE1	2.18	0.43
2:F:203:TYR:N	2:F:203:TYR:CD1	2.87	0.43
1:A:67:LEU:HD13	1:A:135:GLN:HG3	2.00	0.43
2:B:441:MET:HE2	2:B:456:ILE:CD1	2.49	0.43
2:D:62:ASN:ND2	2:D:65:ASN:HB2	2.34	0.43
2:D:439:VAL:HG22	2:D:453:VAL:HG13	2.00	0.43
1:E:312:PHE:CD1	1:E:313:VAL:HG23	2.54	0.43
1:E:351:MET:HG2	1:E:428:PHE:CE1	2.54	0.43
1:E:379:LEU:HD13	2:F:46:SER:HB2	2.00	0.43
2:H:139:ALA:O	2:H:141:GLU:N	2.52	0.43
2:D:78:LYS:O	2:D:85:GLN:HB2	2.19	0.43
2:F:139:ALA:O	2:F:141:GLU:N	2.51	0.43
2:F:305:SER:HA	2:F:306:PRO:HD3	1.79	0.43
1:G:228:PRO:HA	1:G:229:PRO:HD3	1.84	0.43
2:H:27:ARG:HB2	2:H:218:HIS:ND1	2.34	0.43
1:A:333:LEU:C	1:A:333:LEU:HD13	2.44	0.43
2:D:77:PHE:O	2:D:85:GLN:HG3	2.19	0.43
2:D:171:TYR:CE2	2:D:176:LEU:HD23	2.54	0.43
1:E:50:SER:OG	1:E:97:ARG:HA	2.19	0.43
1:E:273:ILE:CG2	1:E:274:TYR:N	2.80	0.43
2:H:103:THR:O	2:H:180:ILE:HD13	2.18	0.43
2:D:119:ILE:N	2:D:120:PRO:HD2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:245:ARG:HA	2:D:245:ARG:HE	1.84	0.43
1:E:189:ASP:OD2	1:E:193:LYS:HE3	2.18	0.43
2:F:61:GLU:OE1	2:F:66:ASN:HA	2.19	0.43
1:A:246:PRO:HG3	1:A:448:GLY:CA	2.49	0.42
2:B:403:VAL:HG13	2:B:404:THR:HG23	1.99	0.42
1:C:31:ALA:O	1:C:203:ALA:HA	2.18	0.42
2:D:39:THR:HB	2:D:218:HIS:ND1	2.33	0.42
2:D:246:GLY:HA3	2:D:247:PRO:HD3	1.85	0.42
2:D:271:ALA:C	2:D:272:LEU:HD12	2.44	0.42
2:H:375:ARG:NH1	2:H:375:ARG:CB	2.77	0.42
2:B:35:LEU:HD13	2:B:208:MET:HG3	2.01	0.42
2:B:403:VAL:CG1	2:B:404:THR:HG23	2.50	0.42
1:C:381:ASN:HD22	1:C:381:ASN:HA	1.56	0.42
2:D:27:ARG:HB3	2:D:27:ARG:HH11	1.82	0.42
1:E:213:LEU:HD23	1:E:213:LEU:HA	1.72	0.42
1:G:245:PRO:HA	1:G:246:PRO:HD3	1.90	0.42
2:H:423:LYS:O	2:H:427:ILE:HG13	2.18	0.42
1:A:14:ALA:N	1:A:19:PHE:CB	2.68	0.42
1:A:99:ASN:HD22	1:A:101:MET:HE3	1.81	0.42
2:B:441:MET:HE1	2:B:451:PRO:O	2.18	0.42
2:D:103:THR:O	2:D:180:ILE:HD13	2.20	0.42
2:D:203:TYR:CD1	2:D:203:TYR:N	2.87	0.42
2:D:237:SER:N	2:D:238:PRO:HD3	2.35	0.42
2:D:340:ILE:HG22	2:D:341:VAL:N	2.33	0.42
1:E:19:PHE:CD1	1:E:392:MET:HE3	2.53	0.42
1:E:267:PRO:HA	1:E:323:TYR:O	2.20	0.42
1:G:213:LEU:HA	1:G:213:LEU:HD23	1.79	0.42
1:G:312:PHE:O	1:G:335:CYS:HB2	2.19	0.42
2:H:52:ILE:HG23	2:H:52:ILE:O	2.19	0.42
1:A:45:TYR:CD1	1:A:45:TYR:N	2.87	0.42
2:B:84:PRO:O	2:B:85:GLN:C	2.62	0.42
2:B:245:ARG:HA	2:B:245:ARG:NE	2.34	0.42
1:C:187:LEU:O	1:C:191:ARG:HG3	2.18	0.42
1:E:58:LYS:HA	1:E:58:LYS:HD3	1.80	0.42
1:G:304:THR:CG2	1:G:305:HIS:CD2	2.97	0.42
2:H:139:ALA:C	2:H:141:GLU:N	2.76	0.42
2:H:401:GLN:O	2:H:405:THR:HB	2.19	0.42
1:A:32:THR:HG22	1:A:204:PHE:HB2	2.00	0.42
1:A:266:LEU:HA	1:A:267:PRO:HD3	1.84	0.42
2:D:80:THR:HB	2:D:132:LYS:O	2.20	0.42
2:F:78:LYS:HE3	2:F:143:GLU:OE1	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:268:ILE:HD13	1:G:268:ILE:H	1.79	0.42
2:H:88:ILE:HD13	2:H:129:ILE:HD11	2.01	0.42
2:H:90:LEU:CD1	2:H:94:ASN:ND2	2.73	0.42
1:A:34:ASN:ND2	2:B:44:ASN:CB	2.81	0.42
1:A:369:ARG:HG3	2:B:93:GLU:O	2.19	0.42
2:B:61:GLU:OE1	2:B:66:ASN:HA	2.20	0.42
2:B:140:ILE:O	2:B:140:ILE:CG2	2.67	0.42
2:B:441:MET:HE2	2:B:456:ILE:HD12	2.02	0.42
1:C:168:LEU:HD13	1:C:323:TYR:CD2	2.54	0.42
1:C:304:THR:HG22	1:C:305:HIS:ND1	2.34	0.42
2:D:380:LEU:HD12	2:D:380:LEU:O	2.20	0.42
2:F:62:ASN:ND2	2:F:65:ASN:HB2	2.34	0.42
2:F:259:LYS:HG3	2:F:447:THR:CG2	2.48	0.42
1:G:310:TYR:HD1	1:G:312:PHE:CE2	2.37	0.42
1:G:357:ASN:C	1:G:357:ASN:OD1	2.61	0.42
2:H:31:LEU:HD21	2:H:226:GLN:HA	2.01	0.42
1:A:31:ALA:HB1	1:A:392:MET:HE2	2.01	0.42
1:A:198:GLU:OE1	1:A:225:SER:HB2	2.19	0.42
1:C:116:GLN:HB2	1:C:219:TYR:CZ	2.55	0.42
1:C:174:CYS:HA	1:C:175:PRO:HD3	1.89	0.42
2:D:401:GLN:O	2:D:405:THR:HB	2.20	0.42
1:E:255:GLU:O	1:E:337:PRO:HD3	2.19	0.42
2:F:441:MET:HE2	2:F:456:ILE:CD1	2.50	0.42
1:G:114:MET:HE2	1:G:118:MET:HE3	2.01	0.42
1:C:261:ILE:HG12	1:C:444:VAL:HG22	2.01	0.42
2:D:49:THR:HG21	2:D:392:THR:HA	2.02	0.42
2:F:127:SER:HB3	2:F:229:PHE:CE2	2.55	0.42
1:G:31:ALA:O	1:G:203:ALA:HA	2.20	0.42
1:G:189:ASP:OD2	1:G:193:LYS:HE3	2.20	0.42
1:G:198:GLU:OE1	1:G:225:SER:HB2	2.19	0.42
2:H:102:TYR:CD1	3:R:7:LYS:HD3	2.55	0.42
2:H:441:MET:HG2	2:H:442:VAL:H	1.85	0.42
2:B:27:ARG:HB2	2:B:218:HIS:ND1	2.35	0.42
2:B:92:ILE:HG23	2:B:97:SER:HB2	2.00	0.42
2:B:175:PRO:HA	2:B:178:ARG:NH1	2.35	0.42
2:B:405:THR:HG22	2:B:407:LYS:H	1.84	0.42
1:E:429:THR:HG22	1:E:431:ASN:HD22	1.85	0.42
2:H:78:LYS:HE3	2:H:143:GLU:OE1	2.19	0.42
1:A:270:HIS:O	1:A:273:ILE:HB	2.20	0.42
1:C:28:LEU:CD1	1:C:200:THR:HB	2.50	0.42
1:C:369:ARG:HG3	2:D:94:ASN:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:88:ILE:HD13	2:D:129:ILE:HD11	2.02	0.42
1:E:315:ASN:HB3	1:E:334:SER:HB2	2.01	0.42
1:E:429:THR:CG2	1:E:431:ASN:HD22	2.32	0.42
2:F:207:ARG:HH11	2:F:245:ARG:HH12	1.65	0.42
2:F:245:ARG:HE	2:F:245:ARG:HA	1.85	0.42
2:F:245:ARG:HA	2:F:245:ARG:NE	2.34	0.42
2:F:295:TRP:CZ2	2:F:297:ARG:HA	2.55	0.42
1:G:369:ARG:HG3	2:H:94:ASN:HA	2.01	0.42
2:H:225:ALA:O	2:H:229:PHE:HB2	2.19	0.42
1:A:228:PRO:HA	1:A:229:PRO:HD3	1.82	0.41
1:A:276:LEU:HD11	1:A:329:PHE:CD2	2.54	0.41
1:C:39:PHE:CE1	1:C:385:LYS:HD2	2.55	0.41
1:C:228:PRO:HA	1:C:229:PRO:HD3	1.80	0.41
1:C:267:PRO:HD2	1:C:270:HIS:HB2	2.02	0.41
2:F:40:GLU:OE1	2:F:408:ARG:NH2	2.52	0.41
2:H:172:LYS:O	2:H:174:GLN:HG3	2.20	0.41
2:H:323:TYR:CD1	2:H:323:TYR:C	2.98	0.41
1:A:227:HIS:N	1:A:228:PRO:CD	2.83	0.41
1:C:310:TYR:HD1	1:C:312:PHE:CE2	2.38	0.41
1:C:312:PHE:CD1	1:C:313:VAL:HG23	2.55	0.41
2:D:305:SER:HA	2:D:306:PRO:HD3	1.78	0.41
1:E:304:THR:HG22	1:E:305:HIS:ND1	2.35	0.41
1:C:268:ILE:CD1	1:C:268:ILE:H	2.32	0.41
1:C:307:LEU:HD13	1:C:307:LEU:HA	1.86	0.41
1:E:84:LEU:HD13	1:E:91:TYR:CZ	2.54	0.41
1:G:201:VAL:HG23	1:G:397:LEU:HD13	2.01	0.41
1:G:294:PRO:HB3	2:H:89:GLU:HA	2.02	0.41
1:A:304:THR:CG2	1:A:305:HIS:CD2	2.96	0.41
1:E:268:ILE:CD1	1:E:324:SER:HA	2.51	0.41
1:E:276:LEU:HD11	1:E:329:PHE:CD2	2.55	0.41
1:C:50:SER:OG	1:C:97:ARG:HA	2.20	0.41
1:C:80:MET:SD	1:C:117:LEU:HD22	2.61	0.41
2:D:230:GLY:C	2:D:232:VAL:H	2.28	0.41
2:D:234:LYS:HB2	2:D:234:LYS:HE3	1.89	0.41
2:D:253:ARG:NH2	2:D:457:GLU:OE1	2.52	0.41
2:D:323:TYR:CD1	2:D:323:TYR:C	2.98	0.41
1:E:246:PRO:HG3	1:E:448:GLY:CA	2.49	0.41
1:E:270:HIS:ND1	1:E:271:PRO:HD2	2.36	0.41
2:F:70:HIS:HE1	2:F:150:GLU:OE2	1.98	0.41
2:F:441:MET:HE2	2:F:456:ILE:HD12	2.02	0.41
2:H:23:ILE:N	2:H:24:PRO:HD3	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:SER:OG	1:A:97:ARG:HA	2.20	0.41
1:A:118:MET:O	1:A:121:THR:HG22	2.19	0.41
2:B:88:ILE:HD13	2:B:129:ILE:HD11	2.02	0.41
1:C:227:HIS:N	1:C:228:PRO:HD3	2.35	0.41
2:D:160:GLU:OE1	2:D:160:GLU:HA	2.20	0.41
1:E:126:LYS:O	1:E:127:ILE:C	2.64	0.41
2:F:234:LYS:HG2	2:F:235:SER:N	2.36	0.41
1:A:369:ARG:O	1:A:373:GLN:HG3	2.21	0.41
2:D:55:ASP:O	2:D:55:ASP:CG	2.64	0.41
2:D:140:ILE:O	2:D:140:ILE:CG2	2.69	0.41
1:E:241:GLU:HG2	1:E:444:VAL:HB	2.03	0.41
1:E:369:ARG:HG3	2:F:94:ASN:HA	2.03	0.41
1:G:312:PHE:CD1	1:G:313:VAL:HG23	2.56	0.41
2:H:39:THR:HB	2:H:218:HIS:ND1	2.35	0.41
2:H:55:ASP:O	2:H:55:ASP:CG	2.64	0.41
1:A:31:ALA:O	1:A:203:ALA:HA	2.20	0.41
1:A:90:ASN:ND2	1:A:105:SER:OG	2.51	0.41
1:A:267:PRO:HA	1:A:323:TYR:O	2.20	0.41
1:E:41:ALA:HB1	1:E:389:LEU:HD22	2.02	0.41
1:G:255:GLU:O	1:G:337:PRO:HD3	2.21	0.41
1:G:305:HIS:CD2	1:G:305:HIS:N	2.87	0.41
1:G:436:GLY:O	1:G:437:ASN:C	2.62	0.41
2:H:254:GLY:O	2:H:440:SER:HA	2.21	0.41
1:A:467:ASN:ND2	1:A:469:SER:O	2.54	0.41
2:B:104:SER:HA	2:B:180:ILE:CD1	2.51	0.41
1:C:99:ASN:HD22	1:C:101:MET:HG2	1.86	0.41
1:C:312:PHE:CE1	1:C:313:VAL:HG23	2.56	0.41
1:C:339:ALA:O	1:C:340:ALA:C	2.63	0.41
1:E:30:VAL:CG2	1:E:216:THR:HG21	2.51	0.41
2:F:172:LYS:O	2:F:174:GLN:HG3	2.20	0.41
2:F:319:LEU:O	2:F:320:ALA:HB2	2.20	0.41
2:F:438:PRO:HA	2:F:457:GLU:OE2	2.20	0.41
2:H:139:ALA:CA	2:H:142:ARG:HH21	2.34	0.41
2:H:380:LEU:HD11	2:H:384:LEU:HD11	2.01	0.41
1:C:35:THR:HB	1:C:36:PRO:CD	2.51	0.41
2:D:104:SER:HA	2:D:180:ILE:CD1	2.51	0.41
1:E:227:HIS:N	1:E:228:PRO:HD3	2.36	0.41
2:F:80:THR:HB	2:F:132:LYS:O	2.21	0.41
2:F:119:ILE:N	2:F:120:PRO:HD2	2.35	0.41
1:A:17:ASP:O	1:A:18:ASN:CB	2.69	0.40
1:A:100:LEU:HD21	1:A:195:TYR:OH	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:39:THR:HB	2:F:218:HIS:ND1	2.36	0.40
2:F:254:GLY:O	2:F:440:SER:HA	2.21	0.40
2:F:439:VAL:O	2:F:439:VAL:CG2	2.68	0.40
1:G:47:ASP:HB3	1:G:199:ASN:OD1	2.21	0.40
2:H:139:ALA:N	2:H:142:ARG:HH21	2.19	0.40
1:A:233:LYS:HB3	1:A:233:LYS:HE2	1.89	0.40
1:A:297:GLY:HA2	2:B:93:GLU:OE1	2.21	0.40
1:A:317:VAL:CG2	1:A:318:ALA:N	2.85	0.40
1:A:357:ASN:OD1	1:A:357:ASN:C	2.64	0.40
2:B:234:LYS:HB2	2:B:234:LYS:HE3	1.91	0.40
1:C:135:GLN:OE1	1:C:135:GLN:HA	2.20	0.40
1:C:233:LYS:HB3	1:C:233:LYS:HE2	1.88	0.40
2:D:31:LEU:HD22	2:D:35:LEU:HD23	2.02	0.40
2:D:35:LEU:HD13	2:D:208:MET:HG3	2.03	0.40
1:E:357:ASN:C	1:E:357:ASN:OD1	2.63	0.40
2:F:58:SER:HA	2:F:61:GLU:HG3	2.04	0.40
2:F:403:VAL:HG13	2:F:404:THR:HG23	2.04	0.40
1:G:207:VAL:HA	1:G:208:PRO:HD3	1.82	0.40
1:A:270:HIS:ND1	1:A:271:PRO:HD2	2.36	0.40
1:A:299:TYR:CE1	2:B:90:LEU:HD23	2.56	0.40
2:B:245:ARG:HA	2:B:245:ARG:HE	1.87	0.40
1:C:243:CYS:HA	1:C:446:MET:O	2.21	0.40
1:C:315:ASN:HB3	1:C:334:SER:HB2	2.04	0.40
1:E:339:ALA:O	1:E:340:ALA:C	2.64	0.40
2:H:271:ALA:C	2:H:272:LEU:HD12	2.46	0.40
1:A:298:MET:H	1:A:298:MET:HG2	1.70	0.40
1:A:378:LEU:O	1:A:379:LEU:C	2.64	0.40
2:B:31:LEU:HD21	2:B:226:GLN:HA	2.02	0.40
2:B:246:GLY:HA3	2:B:247:PRO:HD3	1.93	0.40
1:C:266:LEU:HA	1:C:267:PRO:HD3	1.85	0.40
2:D:245:ARG:HA	2:D:245:ARG:NE	2.36	0.40
1:E:168:LEU:HD13	1:E:323:TYR:CD2	2.57	0.40
2:F:352:ILE:HG23	2:F:353:VAL:N	2.37	0.40
2:B:39:THR:HG23	2:B:40:GLU:N	2.36	0.40
2:B:323:TYR:C	2:B:323:TYR:CD1	3.00	0.40
1:C:90:ASN:ND2	1:C:105:SER:OG	2.52	0.40
1:E:49:GLY:HA2	1:E:61:THR:HG21	2.03	0.40
1:G:174:CYS:HA	1:G:175:PRO:HD3	1.96	0.40
2:H:80:THR:HB	2:H:132:LYS:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	448/475 (94%)	417 (93%)	27 (6%)	4 (1%)	14	46
1	C	444/475 (94%)	413 (93%)	27 (6%)	4 (1%)	14	46
1	E	442/475 (93%)	412 (93%)	27 (6%)	3 (1%)	18	51
1	G	447/475 (94%)	412 (92%)	32 (7%)	3 (1%)	18	51
2	B	437/443 (99%)	403 (92%)	27 (6%)	7 (2%)	7	32
2	D	439/443 (99%)	401 (91%)	31 (7%)	7 (2%)	7	32
2	F	441/443 (100%)	408 (92%)	26 (6%)	7 (2%)	7	32
2	H	438/443 (99%)	397 (91%)	34 (8%)	7 (2%)	7	32
3	O	6/8 (75%)	6 (100%)	0	0	100	100
3	P	6/8 (75%)	6 (100%)	0	0	100	100
3	Q	6/8 (75%)	6 (100%)	0	0	100	100
3	R	6/8 (75%)	6 (100%)	0	0	100	100
All	All	3560/3704 (96%)	3287 (92%)	231 (6%)	42 (1%)	10	38

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	PHE
1	C	250	PHE
1	E	250	PHE
1	G	250	PHE
2	B	367	LYS
1	A	34	ASN
2	B	231	HIS
2	B	261	ASN
2	D	231	HIS
2	D	318	SER
2	D	367	LYS
2	F	231	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	261	ASN
2	F	318	SER
2	F	367	LYS
2	H	24	PRO
2	H	231	HIS
2	H	261	ASN
2	H	318	SER
2	B	66	ASN
2	B	316	ASN
2	B	318	SER
1	C	296	LYS
2	D	140	ILE
2	D	261	ASN
2	D	316	ASN
2	F	140	ILE
2	F	316	ASN
2	H	140	ILE
2	H	316	ASN
2	H	367	LYS
1	A	167	THR
1	C	167	THR
2	D	66	ASN
1	E	167	THR
2	F	66	ASN
1	G	167	THR
2	B	140	ILE
1	A	127	ILE
1	C	127	ILE
1	E	127	ILE
1	G	127	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	381/401 (95%)	362 (95%)	19 (5%)	22 54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	379/401 (94%)	355 (94%)	24 (6%)	16	46
1	E	378/401 (94%)	357 (94%)	21 (6%)	19	51
1	G	380/401 (95%)	358 (94%)	22 (6%)	18	49
2	B	376/379 (99%)	348 (93%)	28 (7%)	13	40
2	D	378/379 (100%)	348 (92%)	30 (8%)	11	37
2	F	379/379 (100%)	355 (94%)	24 (6%)	16	46
2	H	377/379 (100%)	351 (93%)	26 (7%)	14	43
3	O	6/6 (100%)	5 (83%)	1 (17%)	2	11
3	P	6/6 (100%)	6 (100%)	0	100	100
3	Q	6/6 (100%)	5 (83%)	1 (17%)	2	11
3	R	6/6 (100%)	5 (83%)	1 (17%)	2	11
All	All	3052/3144 (97%)	2855 (94%)	197 (6%)	15	45

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ASP
1	A	66	ARG
1	A	67	LEU
1	A	103	GLN
1	A	151	GLU
1	A	210	GLU
1	A	220	LEU
1	A	230	ILE
1	A	234	VAL
1	A	268	ILE
1	A	273	ILE
1	A	307	LEU
1	A	311	TYR
1	A	314	GLU
1	A	333	LEU
1	A	361	ARG
1	A	363	THR
1	A	381	ASN
1	A	386	LEU
2	B	27	ARG
2	B	28	THR
2	B	31	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	39	THR
2	B	65	ASN
2	B	72	LEU
2	B	75	LEU
2	B	86	GLN
2	B	90	LEU
2	B	99	LEU
2	B	100	ASN
2	B	107	ASN
2	B	149	ARG
2	B	169	ILE
2	B	181	LEU
2	B	219	GLU
2	B	250	VAL
2	B	275	VAL
2	B	291	ILE
2	B	346	GLU
2	B	375	ARG
2	B	403	VAL
2	B	405	THR
2	B	408	ARG
2	B	428	MET
2	B	439	VAL
2	B	441	MET
2	B	449	THR
1	C	16	THR
1	C	22	SER
1	C	65	ASP
1	C	66	ARG
1	C	67	LEU
1	C	103	GLN
1	C	151	GLU
1	C	210	GLU
1	C	220	LEU
1	C	230	ILE
1	C	234	VAL
1	C	268	ILE
1	C	273	ILE
1	C	288	SER
1	C	305	HIS
1	C	307	LEU
1	C	311	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	314	GLU
1	C	333	LEU
1	C	361	ARG
1	C	363	THR
1	C	381	ASN
1	C	382	LEU
1	C	386	LEU
2	D	23	ILE
2	D	27	ARG
2	D	28	THR
2	D	31	LEU
2	D	39	THR
2	D	65	ASN
2	D	72	LEU
2	D	75	LEU
2	D	86	GLN
2	D	90	LEU
2	D	99	LEU
2	D	100	ASN
2	D	107	ASN
2	D	149	ARG
2	D	169	ILE
2	D	181	LEU
2	D	219	GLU
2	D	250	VAL
2	D	253	ARG
2	D	275	VAL
2	D	291	ILE
2	D	346	GLU
2	D	375	ARG
2	D	403	VAL
2	D	405	THR
2	D	408	ARG
2	D	428	MET
2	D	439	VAL
2	D	441	MET
2	D	449	THR
1	E	22	SER
1	E	65	ASP
1	E	66	ARG
1	E	67	LEU
1	E	103	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	151	GLU
1	E	210	GLU
1	E	220	LEU
1	E	230	ILE
1	E	234	VAL
1	E	268	ILE
1	E	273	ILE
1	E	305	HIS
1	E	307	LEU
1	E	311	TYR
1	E	314	GLU
1	E	333	LEU
1	E	361	ARG
1	E	363	THR
1	E	381	ASN
1	E	386	LEU
2	F	27	ARG
2	F	31	LEU
2	F	39	THR
2	F	72	LEU
2	F	75	LEU
2	F	86	GLN
2	F	90	LEU
2	F	99	LEU
2	F	100	ASN
2	F	107	ASN
2	F	149	ARG
2	F	181	LEU
2	F	219	GLU
2	F	250	VAL
2	F	275	VAL
2	F	291	ILE
2	F	346	GLU
2	F	375	ARG
2	F	403	VAL
2	F	405	THR
2	F	408	ARG
2	F	439	VAL
2	F	441	MET
2	F	449	THR
1	G	15	ARG
1	G	22	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	65	ASP
1	G	66	ARG
1	G	67	LEU
1	G	103	GLN
1	G	151	GLU
1	G	210	GLU
1	G	220	LEU
1	G	230	ILE
1	G	234	VAL
1	G	268	ILE
1	G	273	ILE
1	G	288	SER
1	G	307	LEU
1	G	311	TYR
1	G	314	GLU
1	G	333	LEU
1	G	361	ARG
1	G	363	THR
1	G	381	ASN
1	G	386	LEU
2	H	23	ILE
2	H	27	ARG
2	H	31	LEU
2	H	39	THR
2	H	72	LEU
2	H	75	LEU
2	H	86	GLN
2	H	90	LEU
2	H	99	LEU
2	H	100	ASN
2	H	107	ASN
2	H	149	ARG
2	H	169	ILE
2	H	181	LEU
2	H	219	GLU
2	H	275	VAL
2	H	291	ILE
2	H	346	GLU
2	H	375	ARG
2	H	403	VAL
2	H	405	THR
2	H	408	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	428	MET
2	H	439	VAL
2	H	441	MET
2	H	449	THR
3	O	2	LEU
3	Q	4	ARG
3	R	4	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	90	ASN
1	A	99	ASN
1	A	260	GLN
1	A	305	HIS
1	A	320	ASN
1	A	342	GLN
1	A	350	GLN
1	A	381	ASN
1	A	399	HIS
1	A	406	ASN
1	A	431	ASN
2	B	44	ASN
2	B	65	ASN
2	B	81	GLN
2	B	94	ASN
2	B	98	HIS
2	B	100	ASN
2	B	137	ASN
2	B	165	HIS
2	B	223	GLN
2	B	304	ASN
2	B	316	ASN
2	B	374	ASN
2	B	417	GLN
2	B	436	ASN
2	B	452	ASN
1	C	90	ASN
1	C	99	ASN
1	C	260	GLN
1	C	315	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	320	ASN
1	C	350	GLN
1	C	381	ASN
1	C	399	HIS
1	C	406	ASN
1	C	431	ASN
2	D	65	ASN
2	D	73	GLN
2	D	85	GLN
2	D	100	ASN
2	D	107	ASN
2	D	137	ASN
2	D	223	GLN
2	D	316	ASN
2	D	354	ASN
2	D	374	ASN
2	D	452	ASN
1	E	90	ASN
1	E	99	ASN
1	E	236	GLN
1	E	252	ASN
1	E	260	GLN
1	E	315	ASN
1	E	320	ASN
1	E	342	GLN
1	E	381	ASN
1	E	399	HIS
1	E	406	ASN
1	E	431	ASN
1	E	447	GLN
2	F	44	ASN
2	F	65	ASN
2	F	73	GLN
2	F	85	GLN
2	F	94	ASN
2	F	100	ASN
2	F	107	ASN
2	F	137	ASN
2	F	165	HIS
2	F	223	GLN
2	F	316	ASN
2	F	374	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	417	GLN
2	F	452	ASN
1	G	90	ASN
1	G	236	GLN
1	G	260	GLN
1	G	305	HIS
1	G	315	ASN
1	G	320	ASN
1	G	381	ASN
1	G	399	HIS
1	G	406	ASN
1	G	431	ASN
2	H	44	ASN
2	H	65	ASN
2	H	66	ASN
2	H	73	GLN
2	H	85	GLN
2	H	94	ASN
2	H	100	ASN
2	H	137	ASN
2	H	223	GLN
2	H	316	ASN
2	H	374	ASN
2	H	436	ASN
2	H	452	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EPE	G	489	-	15,15,15	1.81	5 (33%)	19,20,20	0.83	1 (5%)
5	EPE	E	489	-	15,15,15	1.72	5 (33%)	19,20,20	0.86	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EPE	G	489	-	-	0/9/19/19	0/1/1/1
5	EPE	E	489	-	-	2/9/19/19	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	489	EPE	C10-S	4.05	1.83	1.77
5	E	489	EPE	C10-S	3.05	1.81	1.77
5	E	489	EPE	C6-N1	2.86	1.54	1.46
5	E	489	EPE	C9-N1	2.57	1.53	1.47
5	G	489	EPE	C7-N4	2.49	1.53	1.47
5	G	489	EPE	C6-N1	2.46	1.53	1.46
5	E	489	EPE	C2-N1	2.42	1.53	1.46
5	E	489	EPE	C9-C10	2.14	1.58	1.52
5	G	489	EPE	C9-N1	2.14	1.52	1.47
5	G	489	EPE	C2-N1	2.12	1.52	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	489	EPE	C7-N4-C5	-2.05	105.79	111.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	489	EPE	C10-C9-N1-C2
5	E	489	EPE	C10-C9-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	452/475 (95%)	-0.45	2 (0%) 88 76	24, 52, 92, 101	0
1	C	448/475 (94%)	-0.40	1 (0%) 91 83	30, 54, 90, 101	0
1	E	446/475 (93%)	-0.32	2 (0%) 88 76	36, 63, 98, 101	0
1	G	451/475 (94%)	-0.41	3 (0%) 84 66	28, 57, 94, 101	0
2	B	439/443 (99%)	-0.44	0 100 100	26, 51, 83, 101	0
2	D	441/443 (99%)	-0.07	2 (0%) 87 72	23, 75, 101, 101	0
2	F	443/443 (100%)	-0.04	1 (0%) 91 83	47, 84, 101, 101	0
2	H	440/443 (99%)	0.06	3 (0%) 84 66	50, 95, 101, 101	0
3	O	8/8 (100%)	-0.12	0 100 100	36, 50, 81, 88	0
3	P	8/8 (100%)	0.21	0 100 100	79, 94, 101, 101	0
3	Q	8/8 (100%)	-0.01	0 100 100	65, 96, 101, 101	0
3	R	8/8 (100%)	0.50	1 (12%) 8 5	84, 97, 101, 101	0
All	All	3592/3704 (96%)	-0.26	15 (0%) 88 76	23, 66, 101, 101	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	23	ILE	3.2
1	A	287	GLY	3.0
1	E	311	TYR	3.0
1	G	250	PHE	2.9
3	R	2	LEU	2.7
1	G	311	TYR	2.6
1	E	230	ILE	2.5
2	F	229	PHE	2.4
2	H	24	PRO	2.2
1	C	249	VAL	2.1
1	A	34	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	447	THR	2.1
2	D	88	ILE	2.1
2	D	236	GLU	2.1
1	G	468	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EPE	G	489	15/15	0.91	0.15	91,91,91,91	0
5	EPE	E	489	15/15	0.92	0.13	84,84,84,84	0
4	ZN	F	503	1/1	0.98	0.04	91,91,91,91	0
4	ZN	D	502	1/1	0.99	0.03	99,99,99,99	0
4	ZN	H	504	1/1	0.99	0.04	101,101,101,101	0
4	ZN	B	501	1/1	1.00	0.01	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.