



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:28 PM UTC

PDB ID : 1DE5 / pdb_00001de5
Title : L-RHAMNOSE ISOMERASE
Authors : Korndorfer, I.P.; Fessner, W.D.; Matthews, B.W.
Deposited on : 1999-11-12
Resolution : 2.20 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

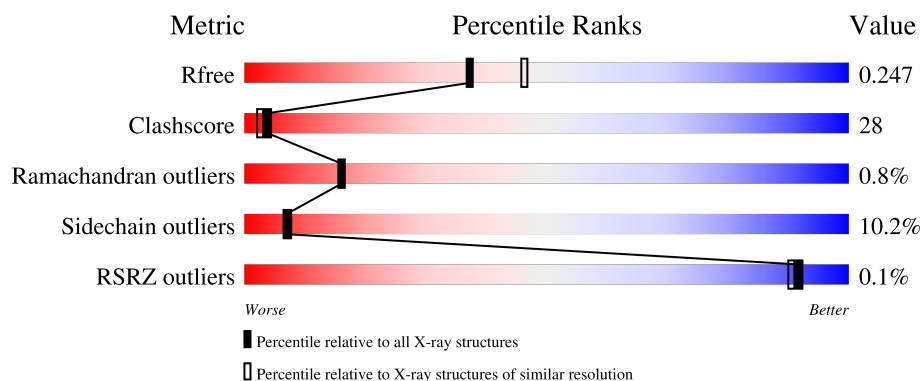
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	426	 48% 36% 11% ..
1	B	426	 49% 36% 12% ..
1	C	426	 48% 37% 11% ..
1	D	426	 47% 37% 13% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14315 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 L-RHAMNOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3316	2094	588	621	13			
1	B	416	Total	C	N	O	S	0	0	0
			3309	2090	587	619	13			
1	C	416	Total	C	N	O	S	0	0	0
			3309	2090	587	619	13			
1	D	416	Total	C	N	O	S	0	0	0
			3309	2090	587	619	13			

There are 28 discrepancies between the modelled and reference sequences:

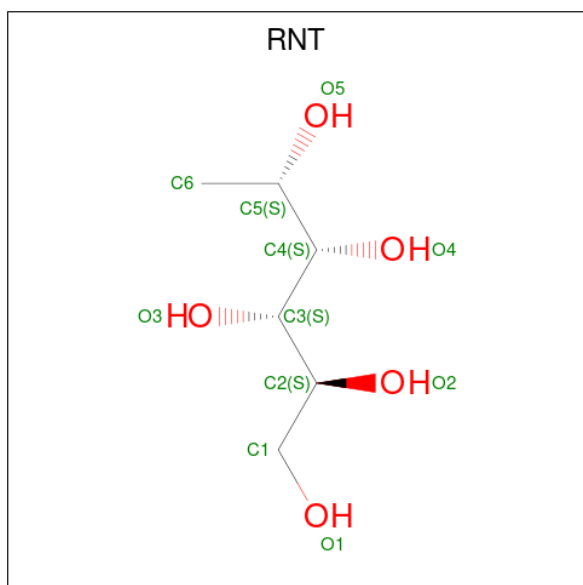
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	expression tag	UNP P32170
A	3	HIS	-	expression tag	UNP P32170
A	4	HIS	-	expression tag	UNP P32170
A	5	HIS	-	expression tag	UNP P32170
A	6	HIS	-	expression tag	UNP P32170
A	7	HIS	-	expression tag	UNP P32170
A	8	HIS	-	expression tag	UNP P32170
B	2	GLY	-	expression tag	UNP P32170
B	3	HIS	-	expression tag	UNP P32170
B	4	HIS	-	expression tag	UNP P32170
B	5	HIS	-	expression tag	UNP P32170
B	6	HIS	-	expression tag	UNP P32170
B	7	HIS	-	expression tag	UNP P32170
B	8	HIS	-	expression tag	UNP P32170
C	2	GLY	-	expression tag	UNP P32170
C	3	HIS	-	expression tag	UNP P32170
C	4	HIS	-	expression tag	UNP P32170
C	5	HIS	-	expression tag	UNP P32170
C	6	HIS	-	expression tag	UNP P32170
C	7	HIS	-	expression tag	UNP P32170
C	8	HIS	-	expression tag	UNP P32170

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	2	GLY	-	expression tag	UNP P32170
D	3	HIS	-	expression tag	UNP P32170
D	4	HIS	-	expression tag	UNP P32170
D	5	HIS	-	expression tag	UNP P32170
D	6	HIS	-	expression tag	UNP P32170
D	7	HIS	-	expression tag	UNP P32170
D	8	HIS	-	expression tag	UNP P32170

- Molecule 2 is L-RHAMNITOL (CCD ID: RNT) (formula: C₆H₁₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	C	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0

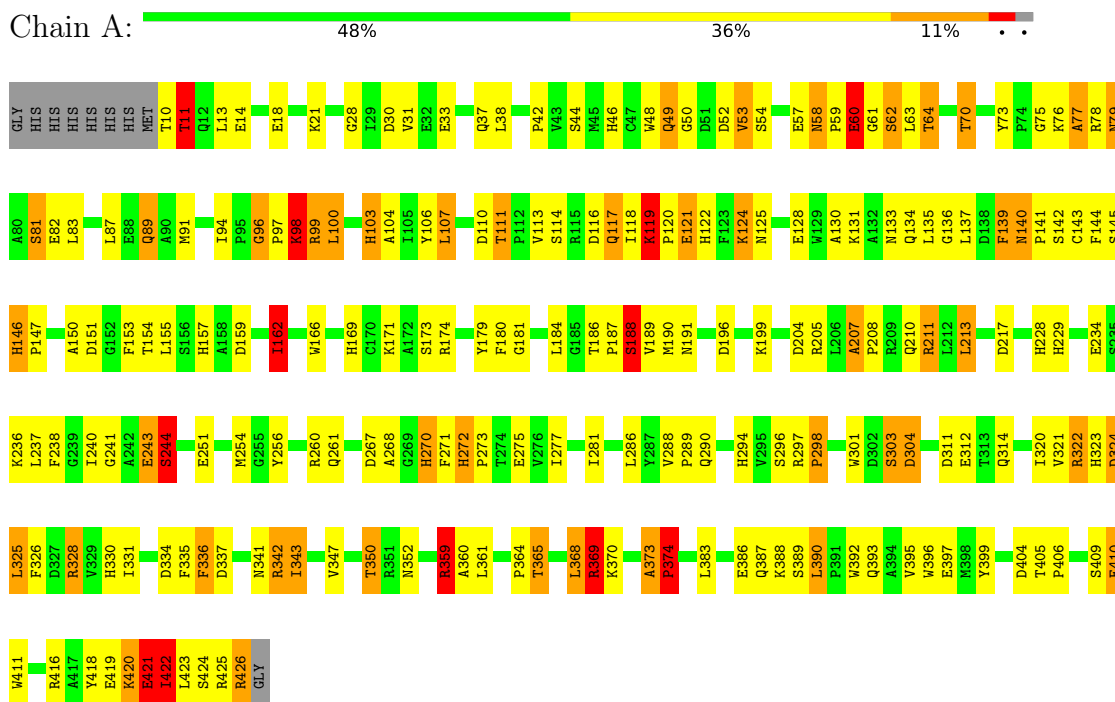
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	247	Total 247	O 247	0	0
4	B	286	Total 286	O 286	0	0
4	C	254	Total 254	O 254	0	0
4	D	237	Total 237	O 237	0	0

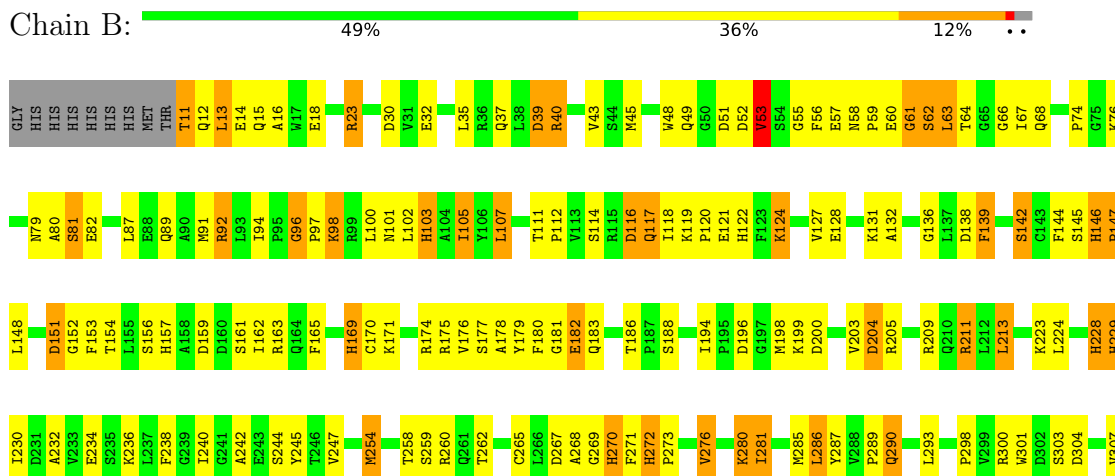
3 Residue-property plots

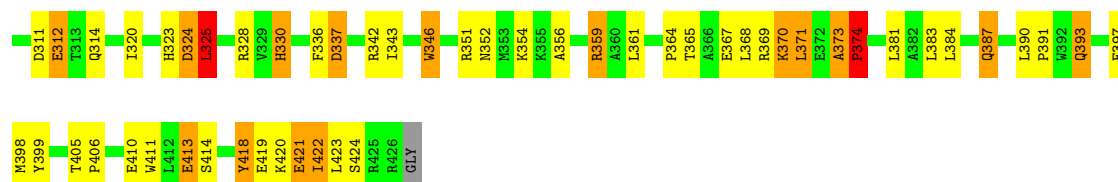
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: L-RHAMNOSE ISOMERASE



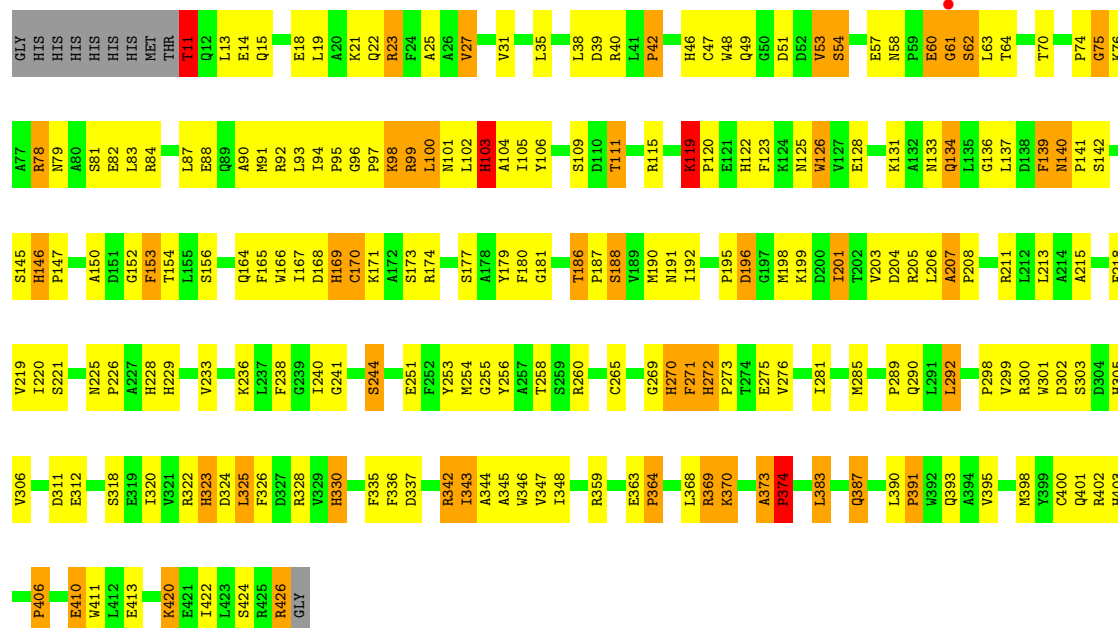
• Molecule 1: L-RHAMNOSE ISOMERASE





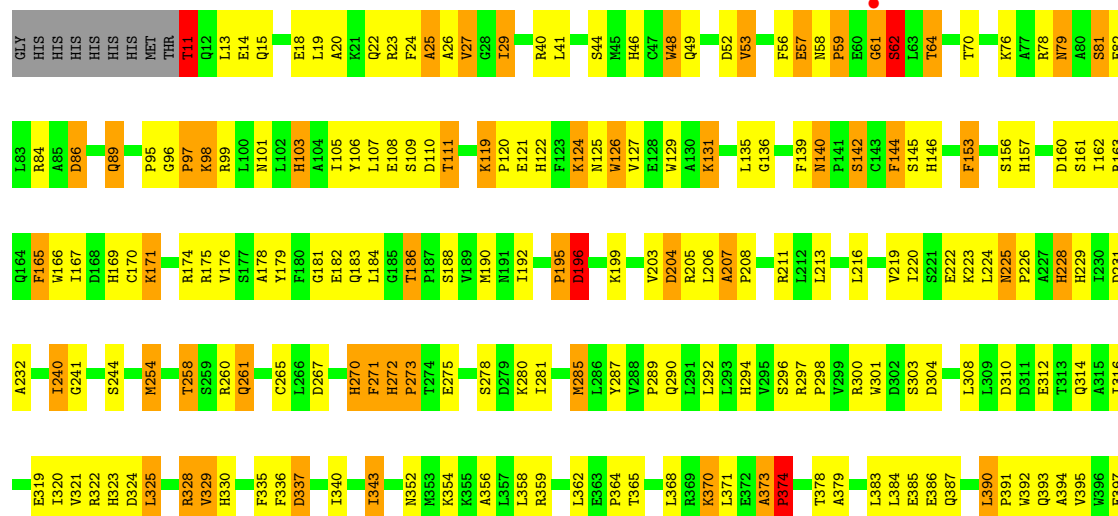
• Molecule 1: L-RHAMNOSE ISOMERASE

Chain C: 48% 37% 11% ..



• Molecule 1: L-RHAMNOSE ISOMERASE

Chain D: 47% 37% 13% ..



M398	Y399	Q400	Q401	R402	R403	D404	T405	P406	A407	G408	S409	E410	W411	L412	E413	R416	A417	Y418	E419	K420	E421	I422	L423	S424	R425	R426	GLY
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.44Å 162.69Å 77.02Å 90.00° 110.68° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20 15.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	81.0 (15.00-2.20) 86.1 (15.00-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 2.20Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.156 , 0.275 (Not available) , 0.247	Depositor DCC
R_{free} test set	4333 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 111.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14315	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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: ZN, RNT

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	1.39	12/3396 (0.4%)	1.97	88/4612 (1.9%)
1	B	1.37	5/3389 (0.1%)	1.90	70/4602 (1.5%)
1	C	1.34	10/3389 (0.3%)	1.88	81/4602 (1.8%)
1	D	1.33	8/3389 (0.2%)	1.87	73/4602 (1.6%)
All	All	1.36	35/13563 (0.3%)	1.91	312/18418 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	C	1	0
1	D	1	0
All	All	3	0

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	HIS	ND1-CE1	8.64	1.41	1.32
1	C	146	HIS	ND1-CE1	8.29	1.40	1.32
1	A	146	HIS	ND1-CE1	7.72	1.40	1.32
1	B	142	SER	CA-C	-7.21	1.43	1.53
1	C	272	HIS	ND1-CE1	7.07	1.39	1.32
1	C	374	PRO	CA-C	-6.88	1.46	1.52
1	B	229	HIS	ND1-CE1	6.72	1.39	1.32
1	B	228	HIS	ND1-CE1	6.61	1.39	1.32
1	D	272	HIS	ND1-CE1	6.58	1.39	1.32
1	A	272	HIS	CG-CD2	6.54	1.43	1.35
1	B	272	HIS	ND1-CE1	6.45	1.39	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374	PRO	CA-C	-6.43	1.46	1.52
1	A	374	PRO	N-CA	-6.34	1.42	1.47
1	A	146	HIS	CG-CD2	6.28	1.42	1.35
1	D	103	HIS	ND1-CE1	6.20	1.38	1.32
1	D	140	ASN	CG-OD1	6.13	1.35	1.23
1	A	422	ILE	CA-C	-5.75	1.45	1.52
1	D	229	HIS	ND1-CE1	5.73	1.38	1.32
1	C	103	HIS	CG-CD2	5.71	1.42	1.35
1	D	146	HIS	ND1-CE1	5.62	1.38	1.32
1	A	228	HIS	CG-CD2	5.57	1.42	1.35
1	B	103	HIS	CD2-NE2	-5.56	1.31	1.37
1	C	251	GLU	CD-OE2	5.45	1.35	1.25
1	C	146	HIS	CG-CD2	5.43	1.41	1.35
1	D	260	ARG	CA-C	-5.41	1.45	1.52
1	D	422	ILE	CA-CB	-5.40	1.50	1.55
1	C	229	HIS	ND1-CE1	5.37	1.38	1.32
1	C	140	ASN	CG-OD1	5.35	1.33	1.23
1	C	228	HIS	ND1-CE1	5.35	1.37	1.32
1	A	229	HIS	CD2-NE2	-5.34	1.31	1.37
1	D	228	HIS	CD2-NE2	-5.24	1.32	1.37
1	C	103	HIS	ND1-CE1	5.21	1.37	1.32
1	A	229	HIS	ND1-CE1	5.13	1.37	1.32
1	A	103	HIS	CD2-NE2	-5.11	1.32	1.37
1	A	421	GLU	N-CA	-5.08	1.40	1.46

All (312) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	422	ILE	N-CA-C	12.53	122.14	110.74
1	A	217	ASP	CA-CB-CG	-11.28	101.32	112.60
1	B	373	ALA	C-N-CD	-10.90	80.31	125.00
1	A	373	ALA	C-N-CD	-10.69	81.16	125.00
1	B	254	MET	N-CA-C	-10.03	100.31	111.14
1	C	150	ALA	N-CA-C	10.00	124.58	112.38
1	A	60	GLU	N-CA-CB	9.98	127.36	111.20
1	A	11	THR	N-CA-C	-9.72	97.70	110.53
1	A	153	PHE	CA-CB-CG	-9.47	104.33	113.80
1	D	228	HIS	CB-CG-CD2	-9.34	119.06	131.20
1	A	374	PRO	CA-N-CD	-8.89	99.56	112.00
1	C	373	ALA	C-N-CD	-8.64	89.57	125.00
1	B	228	HIS	CB-CG-CD2	-8.59	120.04	131.20
1	A	390	LEU	N-CA-C	-8.55	99.33	109.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	228	HIS	CB-CG-CD2	-8.53	120.11	131.20
1	C	272	HIS	CB-CG-CD2	-8.45	120.21	131.20
1	C	229	HIS	CB-CG-CD2	-8.40	120.28	131.20
1	D	136	GLY	N-CA-C	-8.39	99.62	112.89
1	D	207	ALA	CA-C-N	-8.29	110.16	119.28
1	D	207	ALA	C-N-CA	-8.29	110.16	119.28
1	C	146	HIS	CB-CG-CD2	-8.22	120.52	131.20
1	A	62	SER	N-CA-C	8.20	128.26	110.80
1	D	25	ALA	N-CA-C	-8.20	102.35	111.28
1	A	136	GLY	N-CA-C	-8.18	100.01	113.02
1	A	229	HIS	CB-CG-CD2	-8.12	120.64	131.20
1	B	57	GLU	CB-CA-C	-8.11	98.09	110.90
1	A	365	THR	N-CA-C	8.07	120.80	111.11
1	D	229	HIS	CB-CG-CD2	-8.05	120.73	131.20
1	A	58	ASN	CA-C-N	8.05	128.50	119.32
1	A	58	ASN	C-N-CA	8.05	128.50	119.32
1	B	272	HIS	CB-CG-CD2	-7.93	120.89	131.20
1	C	254	MET	N-CA-C	-7.88	102.62	111.14
1	B	374	PRO	CA-N-CD	-7.86	101.00	112.00
1	D	103	HIS	CB-CG-CD2	-7.80	121.05	131.20
1	D	365	THR	N-CA-C	7.79	120.46	111.11
1	C	186	THR	CB-CA-C	7.74	120.68	109.45
1	D	373	ALA	C-N-CD	-7.74	93.27	125.00
1	C	422	ILE	CB-CA-C	-7.70	104.12	111.44
1	B	62	SER	N-CA-C	7.66	127.11	110.80
1	D	422	ILE	N-CA-C	7.62	118.64	111.48
1	A	244	SER	N-CA-C	7.59	122.84	113.50
1	B	103	HIS	CB-CG-CD2	-7.58	121.35	131.20
1	C	60	GLU	N-CA-C	-7.56	96.54	108.63
1	D	272	HIS	CB-CG-CD2	-7.55	121.38	131.20
1	C	374	PRO	CA-N-CD	-7.53	101.46	112.00
1	A	272	HIS	CB-CG-CD2	-7.49	121.47	131.20
1	D	146	HIS	CB-CG-CD2	-7.47	121.49	131.20
1	A	187	PRO	N-CA-CB	7.40	110.22	103.34
1	A	119	LYS	O-C-N	7.40	127.05	121.65
1	B	311	ASP	CA-CB-CG	7.38	119.98	112.60
1	D	48	TRP	N-CA-C	7.38	121.72	112.87
1	A	150	ALA	N-CA-C	7.34	120.33	111.82
1	C	330	HIS	CA-CB-CG	-7.26	106.54	113.80
1	A	146	HIS	CB-CG-CD2	-7.25	121.77	131.20
1	B	281	ILE	N-CA-C	7.25	117.38	110.42
1	B	48	TRP	N-CA-C	7.23	121.55	112.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	THR	N-CA-CB	7.15	123.66	111.50
1	A	189	VAL	CA-C-N	-7.13	112.98	123.11
1	A	189	VAL	C-N-CA	-7.13	112.98	123.11
1	B	271	PHE	CA-CB-CG	-7.06	106.74	113.80
1	A	96	GLY	CA-C-N	7.04	127.44	119.83
1	A	96	GLY	C-N-CA	7.04	127.44	119.83
1	B	312	GLU	N-CA-C	7.04	118.96	111.28
1	B	138	ASP	CA-CB-CG	-7.01	105.58	112.60
1	A	330	HIS	CA-CB-CG	-6.95	106.85	113.80
1	A	254	MET	N-CA-C	-6.84	103.75	111.07
1	B	146	HIS	CB-CG-CD2	-6.80	122.36	131.20
1	C	133	ASN	CA-CB-CG	-6.79	105.81	112.60
1	A	350	THR	N-CA-C	6.78	118.33	111.07
1	C	238	PHE	CA-CB-CG	-6.78	107.02	113.80
1	D	343	ILE	N-CA-C	-6.78	103.87	110.72
1	B	276	VAL	N-CA-C	6.77	117.86	108.12
1	C	187	PRO	N-CA-CB	6.75	109.23	103.35
1	D	254	MET	N-CA-C	-6.74	103.85	111.07
1	D	270	HIS	N-CA-C	6.73	121.20	112.92
1	D	153	PHE	CA-CB-CG	-6.71	107.09	113.80
1	C	206	LEU	N-CA-C	6.70	118.47	111.03
1	D	329	VAL	CB-CA-C	-6.66	100.90	110.83
1	D	374	PRO	CA-N-CD	-6.66	102.67	112.00
1	A	103	HIS	CB-CG-CD2	-6.66	122.55	131.20
1	D	196	ASP	N-CA-C	6.65	120.02	110.24
1	A	322	ARG	N-CA-CB	6.64	119.88	110.12
1	B	169	HIS	CA-CB-CG	-6.64	107.16	113.80
1	A	100	LEU	N-CA-CB	6.63	122.36	110.83
1	C	270	HIS	N-CA-C	6.61	120.25	112.72
1	C	153	PHE	CA-CB-CG	-6.58	107.22	113.80
1	D	219	VAL	CA-C-N	-6.54	112.34	122.09
1	D	219	VAL	C-N-CA	-6.54	112.34	122.09
1	D	272	HIS	CA-C-N	-6.53	113.04	119.76
1	D	272	HIS	C-N-CA	-6.53	113.04	119.76
1	C	330	HIS	CA-C-N	-6.49	114.59	122.90
1	C	330	HIS	C-N-CA	-6.49	114.59	122.90
1	A	228	HIS	CB-CG-CD2	-6.48	122.78	131.20
1	C	391	PRO	CB-CA-C	-6.45	104.44	112.89
1	A	334	ASP	CA-CB-CG	6.40	119.00	112.60
1	D	228	HIS	CB-CA-C	-6.40	97.68	110.42
1	B	229	HIS	CB-CG-CD2	-6.39	122.89	131.20
1	B	370	LYS	O-C-N	-6.35	115.53	122.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	281	ILE	N-CA-C	6.31	116.79	110.23
1	B	175	ARG	NE-CZ-NH2	-6.30	113.53	119.20
1	D	352	ASN	CA-CB-CG	-6.29	106.31	112.60
1	A	298	PRO	CB-CA-C	-6.28	101.65	110.63
1	D	271	PHE	CA-CB-CG	-6.27	107.53	113.80
1	A	188	SER	CA-C-N	-6.25	114.55	122.37
1	A	188	SER	C-N-CA	-6.25	114.55	122.37
1	A	369	ARG	N-CA-CB	-6.25	100.93	110.12
1	D	328	ARG	NE-CZ-NH2	-6.25	113.58	119.20
1	D	421	GLU	CA-C-N	-6.24	116.85	122.97
1	D	421	GLU	C-N-CA	-6.24	116.85	122.97
1	D	285	MET	N-CA-C	6.23	120.35	112.87
1	D	140	ASN	CB-CA-C	-6.22	101.56	109.65
1	D	328	ARG	CA-C-N	-6.22	115.48	123.19
1	D	328	ARG	C-N-CA	-6.22	115.48	123.19
1	C	140	ASN	CB-CA-C	-6.19	101.60	109.65
1	C	11	THR	CB-CA-C	6.18	122.70	109.10
1	B	370	LYS	CA-C-N	-6.15	112.04	120.28
1	B	370	LYS	C-N-CA	-6.15	112.04	120.28
1	C	125	ASN	CA-CB-CG	-6.14	106.46	112.60
1	A	270	HIS	N-CA-C	6.13	119.50	112.57
1	B	91	MET	CA-CB-CG	-6.13	101.84	114.10
1	D	195	PRO	CA-C-N	-6.12	112.30	121.05
1	D	195	PRO	C-N-CA	-6.12	112.30	121.05
1	C	422	ILE	N-CA-C	6.11	116.82	111.56
1	D	301	TRP	O-C-N	-6.09	117.53	123.26
1	D	204	ASP	N-CA-C	6.05	119.55	107.62
1	A	270	HIS	N-CA-CB	-6.04	101.37	110.91
1	C	364	PRO	CB-CA-C	-6.04	104.34	112.97
1	A	331	ILE	CA-C-N	-6.01	117.12	122.47
1	A	331	ILE	C-N-CA	-6.01	117.12	122.47
1	B	270	HIS	N-CA-C	5.97	120.19	113.02
1	B	124	LYS	N-CA-C	5.95	117.77	111.28
1	D	273	PRO	N-CA-CB	5.95	108.60	103.31
1	C	48	TRP	N-CA-C	5.94	119.62	112.38
1	D	320	ILE	CB-CA-C	-5.92	104.26	112.02
1	D	144	PHE	CA-CB-CG	-5.92	107.88	113.80
1	A	139	PHE	N-CA-CB	-5.91	102.05	111.62
1	B	39	ASP	CA-CB-CG	-5.90	106.70	112.60
1	D	103	HIS	CB-CG-ND1	5.90	131.54	122.70
1	A	312	GLU	N-CA-C	5.88	117.77	111.36
1	A	60	GLU	CB-CA-C	5.87	121.05	109.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	VAL	N-CA-C	5.87	115.99	110.30
1	C	136	GLY	N-CA-C	-5.85	103.64	112.89
1	C	40	ARG	CB-CA-C	-5.85	100.67	110.56
1	D	231	ASP	CB-CA-C	-5.85	99.65	109.48
1	B	337	ASP	CA-CB-CG	-5.85	106.75	112.60
1	C	58	ASN	CA-C-N	5.84	127.13	119.84
1	C	58	ASN	C-N-CA	5.84	127.13	119.84
1	C	126	TRP	CA-C-O	5.83	126.94	120.82
1	D	401	GLN	N-CA-CB	5.82	118.68	110.12
1	A	303	SER	CA-C-N	-5.82	114.26	122.34
1	A	303	SER	C-N-CA	-5.82	114.26	122.34
1	D	330	HIS	CA-CB-CG	-5.82	107.98	113.80
1	B	330	HIS	CA-CB-CG	-5.81	107.99	113.80
1	A	60	GLU	CA-C-N	-5.79	110.06	121.41
1	A	60	GLU	C-N-CA	-5.79	110.06	121.41
1	C	103	HIS	CB-CG-CD2	-5.78	123.68	131.20
1	C	244	SER	N-CA-C	5.77	120.46	112.90
1	D	160	ASP	N-CA-C	5.77	118.34	111.71
1	B	112	PRO	N-CA-CB	5.76	108.36	103.35
1	B	124	LYS	CB-CA-C	-5.74	101.27	110.79
1	D	298	PRO	CB-CA-C	-5.74	102.43	110.63
1	B	242	ALA	N-CA-C	-5.72	103.66	110.41
1	C	306	VAL	N-CA-C	5.72	116.45	109.30
1	B	204	ASP	N-CA-C	5.72	119.19	107.69
1	D	244	SER	N-CA-C	5.71	120.32	113.23
1	B	286	LEU	N-CA-C	-5.71	105.81	112.89
1	C	348	ILE	CA-C-N	5.71	126.27	119.94
1	C	348	ILE	C-N-CA	5.71	126.27	119.94
1	B	139	PHE	N-CA-CB	-5.70	102.38	111.62
1	A	103	HIS	CA-CB-CG	-5.70	108.10	113.80
1	D	403	HIS	CA-CB-CG	5.70	119.50	113.80
1	A	211	ARG	NE-CZ-NH2	-5.67	114.10	119.20
1	C	342	ARG	N-CA-C	5.65	118.21	111.71
1	B	304	ASP	CA-CB-CG	-5.64	106.95	112.60
1	C	170	CYS	CA-C-N	-5.64	113.11	120.44
1	C	170	CYS	C-N-CA	-5.64	113.11	120.44
1	A	328	ARG	CA-C-N	-5.63	116.20	123.19
1	A	328	ARG	C-N-CA	-5.63	116.20	123.19
1	B	287	TYR	N-CA-C	5.63	120.81	113.88
1	A	162	ILE	N-CA-C	-5.62	105.02	110.42
1	A	49	GLN	N-CA-C	-5.62	105.68	112.54
1	C	311	ASP	N-CA-CB	5.62	118.36	109.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	16	ALA	CA-C-N	5.61	128.06	120.65
1	B	16	ALA	C-N-CA	5.61	128.06	120.65
1	D	81	SER	N-CA-C	5.61	117.07	111.07
1	A	331	ILE	N-CA-C	5.60	115.33	107.37
1	A	281	ILE	N-CA-C	5.59	116.04	110.23
1	A	368	LEU	CA-C-N	5.57	127.74	120.28
1	A	368	LEU	C-N-CA	5.57	127.74	120.28
1	B	136	GLY	N-CA-C	-5.55	104.20	113.02
1	A	241	GLY	CA-C-O	5.54	125.14	119.10
1	D	272	HIS	CB-CG-ND1	5.53	130.99	122.70
1	D	225	ASN	CA-C-N	5.52	125.88	119.47
1	D	225	ASN	C-N-CA	5.52	125.88	119.47
1	D	304	ASP	N-CA-C	5.52	119.25	111.52
1	C	139	PHE	N-CA-C	5.52	117.18	108.96
1	A	304	ASP	N-CA-C	5.51	119.23	111.52
1	A	388	LYS	CA-C-N	-5.50	113.85	122.49
1	A	388	LYS	C-N-CA	-5.50	113.85	122.49
1	C	281	ILE	N-CA-C	5.50	115.95	110.23
1	A	98	LYS	CA-CB-CG	-5.50	103.11	114.10
1	A	244	SER	CB-CA-C	5.49	119.28	109.29
1	D	29	ILE	N-CA-C	5.48	115.75	107.80
1	A	60	GLU	N-CA-C	-5.48	101.19	109.85
1	B	271	PHE	N-CA-C	5.47	118.18	109.65
1	B	116	ASP	CA-CB-CG	-5.46	107.14	112.60
1	C	11	THR	N-CA-CB	5.46	120.79	111.50
1	C	229	HIS	CB-CG-ND1	5.45	130.88	122.70
1	D	126	TRP	N-CA-C	-5.44	105.25	111.07
1	B	103	HIS	CA-CB-CG	-5.43	108.36	113.80
1	C	58	ASN	N-CA-CB	-5.43	100.71	110.37
1	C	271	PHE	N-CA-C	5.43	118.12	109.65
1	A	404	ASP	CA-CB-CG	-5.41	107.19	112.60
1	D	296	SER	N-CA-CB	-5.41	102.86	111.62
1	D	271	PHE	N-CA-C	5.40	118.49	109.96
1	A	322	ARG	CA-C-N	-5.40	114.52	122.83
1	A	322	ARG	C-N-CA	-5.40	114.52	122.83
1	D	86	ASP	CA-CB-CG	-5.40	107.20	112.60
1	B	307	VAL	N-CA-C	5.40	115.96	108.84
1	B	387	GLN	OE1-CD-NE2	5.39	127.99	122.60
1	C	23	ARG	CD-NE-CZ	-5.38	116.86	124.40
1	C	93	LEU	CA-C-O	5.38	125.72	119.32
1	C	326	PHE	CA-CB-CG	-5.37	108.43	113.80
1	B	107	LEU	CA-C-N	-5.37	115.53	123.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	LEU	C-N-CA	-5.37	115.53	123.05
1	C	146	HIS	CB-CG-ND1	5.37	130.76	122.70
1	D	119	LYS	CA-C-O	5.36	125.38	119.91
1	C	343	ILE	N-CA-C	-5.35	105.31	110.72
1	A	99	ARG	CA-C-N	-5.34	114.92	122.94
1	A	99	ARG	C-N-CA	-5.34	114.92	122.94
1	D	11	THR	N-CA-CB	5.34	120.58	111.50
1	C	198	MET	N-CA-C	5.34	118.26	109.72
1	C	187	PRO	CA-C-N	-5.33	115.36	122.72
1	C	187	PRO	C-N-CA	-5.33	115.36	122.72
1	A	191	ASN	CA-C-N	-5.33	115.86	123.11
1	A	191	ASN	C-N-CA	-5.33	115.86	123.11
1	A	368	LEU	N-CA-C	5.33	117.51	111.11
1	C	195	PRO	CB-CA-C	-5.33	102.77	111.56
1	A	139	PHE	N-CA-C	5.32	117.07	109.14
1	C	373	ALA	CA-C-N	5.32	127.18	121.00
1	C	373	ALA	C-N-CA	5.32	127.18	121.00
1	C	207	ALA	CA-C-O	5.32	123.23	118.33
1	B	418	TYR	CA-C-O	5.31	126.11	120.10
1	A	28	GLY	CA-C-N	-5.31	116.61	123.19
1	A	28	GLY	C-N-CA	-5.31	116.61	123.19
1	A	11	THR	CA-CB-OG1	5.31	117.56	109.60
1	D	196	ASP	CA-CB-CG	5.31	117.91	112.60
1	C	204	ASP	N-CA-C	5.30	118.76	107.67
1	D	81	SER	CB-CA-C	5.29	119.18	110.88
1	C	292	LEU	CA-C-N	-5.28	115.66	123.05
1	C	292	LEU	C-N-CA	-5.28	115.66	123.05
1	A	140	ASN	CB-CA-C	-5.28	101.80	109.45
1	B	359	ARG	NE-CZ-NH2	-5.27	114.45	119.20
1	C	27	VAL	CB-CA-C	5.26	119.92	111.29
1	D	229	HIS	CB-CG-ND1	5.26	130.59	122.70
1	A	364	PRO	N-CA-CB	5.26	106.08	102.35
1	B	60	GLU	N-CA-C	-5.24	101.23	109.25
1	D	390	LEU	N-CA-C	-5.24	102.42	110.07
1	C	169	HIS	CA-C-O	5.24	126.10	120.55
1	D	261	GLN	CB-CA-C	-5.24	104.84	111.86
1	B	96	GLY	CA-C-N	5.23	125.47	119.83
1	B	96	GLY	C-N-CA	5.23	125.47	119.83
1	C	91	MET	N-CA-C	5.22	118.43	111.75
1	C	226	PRO	N-CA-CB	5.21	108.72	103.25
1	A	146	HIS	CB-CG-ND1	5.21	130.51	122.70
1	B	352	ASN	CA-CB-CG	-5.21	107.39	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	387	GLN	CA-C-O	5.21	126.07	120.55
1	C	42	PRO	CA-C-N	-5.19	116.38	123.12
1	C	42	PRO	C-N-CA	-5.19	116.38	123.12
1	D	303	SER	CA-C-N	-5.18	115.14	122.34
1	D	303	SER	C-N-CA	-5.18	115.14	122.34
1	C	119	LYS	CA-C-O	5.17	125.26	120.50
1	A	359	ARG	NE-CZ-NH2	-5.17	114.55	119.20
1	B	371	LEU	CA-C-O	5.17	126.03	120.55
1	B	228	HIS	CB-CG-ND1	5.16	130.44	122.70
1	B	342	ARG	N-CA-CB	5.15	117.79	110.06
1	C	323	HIS	CA-CB-CG	-5.15	108.65	113.80
1	B	359	ARG	CB-CG-CD	-5.15	99.46	111.30
1	A	420	LYS	CA-C-O	5.14	126.00	120.70
1	C	402	ARG	CA-C-O	5.13	125.72	119.05
1	B	147	PRO	CB-CA-C	-5.13	104.53	113.20
1	C	203	VAL	N-CA-C	-5.13	107.40	111.81
1	D	97	PRO	N-CA-C	5.13	119.26	111.15
1	A	180	PHE	CB-CA-C	-5.13	102.83	110.88
1	B	74	PRO	CB-CA-C	-5.13	104.23	110.95
1	B	211	ARG	NE-CZ-NH2	-5.13	114.59	119.20
1	D	165	PHE	CA-CB-CG	-5.13	108.67	113.80
1	B	151	ASP	N-CA-C	-5.12	106.98	113.18
1	D	337	ASP	CA-C-N	-5.11	114.10	122.54
1	D	337	ASP	C-N-CA	-5.11	114.10	122.54
1	B	232	ALA	CA-C-N	-5.11	115.84	122.94
1	B	232	ALA	C-N-CA	-5.11	115.84	122.94
1	A	243	GLU	N-CA-C	5.10	117.58	111.71
1	C	320	ILE	O-C-N	5.10	127.40	121.94
1	A	320	ILE	CB-CA-C	-5.10	105.30	111.87
1	A	77	ALA	N-CA-C	-5.09	103.32	110.50
1	C	75	GLY	CA-C-N	-5.08	113.35	120.82
1	C	75	GLY	C-N-CA	-5.08	113.35	120.82
1	C	406	PRO	N-CA-CB	5.08	107.83	103.31
1	B	40	ARG	N-CA-C	-5.05	105.84	112.41
1	C	225	ASN	CA-C-N	5.04	126.14	119.84
1	C	225	ASN	C-N-CA	5.04	126.14	119.84
1	A	261	GLN	CB-CG-CD	-5.04	104.03	112.60
1	A	113	VAL	N-CA-C	5.03	115.21	108.17
1	B	175	ARG	CD-NE-CZ	5.03	131.44	124.40
1	B	280	LYS	CA-C-N	-5.02	114.23	120.56
1	B	280	LYS	C-N-CA	-5.02	114.23	120.56
1	A	207	ALA	CA-C-O	5.02	123.25	118.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	99	ARG	CA-C-N	-5.02	115.02	122.74
1	C	99	ARG	C-N-CA	-5.02	115.02	122.74
1	B	57	GLU	O-C-N	5.00	127.49	122.09
1	B	381	LEU	CA-C-O	5.00	125.85	120.55

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	10	THR	CA
1	C	150	ALA	CA
1	D	70	THR	CB

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3316	0	3238	228	0
1	B	3309	0	3231	188	0
1	C	3309	0	3231	175	0
1	D	3309	0	3231	194	0
2	A	11	0	12	4	0
2	B	11	0	13	1	0
2	C	11	0	12	1	0
2	D	11	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	247	0	0	16	0
4	B	286	0	0	22	0
4	C	254	0	0	11	2
4	D	237	0	0	10	0
All	All	14315	0	12980	743	2

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 28.

All (743) 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:B:269:GLY:HA2	1:B:298:PRO:HG3	1.38	1.04
1:A:369:ARG:HH11	1:A:369:ARG:HG3	1.25	1.00
1:D:64:THR:HG22	1:D:145:SER:H	1.27	1.00
1:D:422:ILE:HG22	1:D:423:LEU:HD23	1.41	0.99
1:C:272:HIS:HE1	4:D:4640:HOH:O	1.44	0.98
1:A:70:THR:HG22	1:C:199:LYS:HZ2	1.26	0.97
1:A:119:LYS:H	1:A:122:HIS:HD2	1.13	0.93
1:D:49:GLN:HE22	1:D:337:ASP:H	1.17	0.92
1:A:207:ALA:HB3	1:A:208:PRO:HD3	1.52	0.92
1:A:70:THR:HG22	1:C:199:LYS:NZ	1.85	0.91
1:C:368:LEU:HD21	1:C:383:LEU:HB3	1.53	0.91
1:C:142:SER:H	1:C:169:HIS:HE1	1.12	0.91
1:D:142:SER:H	1:D:169:HIS:HE1	1.14	0.91
1:D:119:LYS:H	1:D:122:HIS:HD2	1.20	0.89
1:D:182:GLU:OE1	1:D:228:HIS:CE1	2.26	0.87
1:B:64:THR:HG22	1:B:145:SER:HA	1.57	0.87
1:D:119:LYS:H	1:D:122:HIS:CD2	1.93	0.87
1:A:142:SER:H	1:A:169:HIS:HE1	1.19	0.86
1:B:146:HIS:CG	1:B:147:PRO:HD2	2.10	0.86
1:B:12:GLN:HE22	1:C:22:GLN:NE2	1.73	0.85
1:D:64:THR:HG22	1:D:145:SER:N	1.93	0.83
1:A:91:MET:HE1	1:A:135:LEU:HD11	1.59	0.83
1:D:371:LEU:HD13	1:D:379:ALA:CB	2.08	0.83
1:C:207:ALA:HB3	1:C:208:PRO:HD3	1.61	0.83
1:B:153:PHE:CZ	1:B:198:MET:HE2	2.12	0.83
1:B:92:ARG:HD3	4:B:2489:HOH:O	1.79	0.83
1:B:314:GLN:HE21	1:B:359:ARG:HH11	1.24	0.82
1:C:393:GLN:HB2	4:C:3548:HOH:O	1.79	0.81
1:D:371:LEU:HD13	1:D:379:ALA:HB1	1.64	0.80
1:C:79:ASN:ND2	1:C:82:GLU:H	1.78	0.80
1:B:153:PHE:HZ	1:B:198:MET:HE2	1.44	0.80
1:C:119:LYS:H	1:C:122:HIS:HD2	1.27	0.80
1:A:91:MET:HE1	1:A:135:LEU:CD1	2.12	0.79
1:A:421:GLU:CD	1:A:422:ILE:HD12	2.06	0.79
1:B:205:ARG:HD2	4:B:2539:HOH:O	1.81	0.79
1:C:272:HIS:HB3	1:C:273:PRO:HD2	1.63	0.79
1:D:364:PRO:HD3	1:D:387:GLN:NE2	1.97	0.79
1:C:119:LYS:H	1:C:122:HIS:CD2	2.01	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:MET:O	1:D:258:THR:HG23	1.83	0.78
1:D:127:VAL:HG11	1:D:183:GLN:HG2	1.63	0.78
1:A:64:THR:HG22	1:A:145:SER:HA	1.65	0.78
2:A:1460:RNT:H12	4:A:1462:HOH:O	1.84	0.77
1:A:64:THR:HG23	4:A:1619:HOH:O	1.83	0.77
1:D:205:ARG:HD2	4:D:4584:HOH:O	1.84	0.77
1:C:167:ILE:HG21	1:C:218:GLU:OE2	1.86	0.76
1:C:92:ARG:HD3	4:C:3496:HOH:O	1.86	0.76
1:A:64:THR:HG22	1:A:145:SER:CA	2.15	0.76
1:D:79:ASN:HD22	1:D:81:SER:N	1.84	0.75
1:A:119:LYS:H	1:A:122:HIS:CD2	2.02	0.75
1:C:84:ARG:O	1:C:88:GLU:HG3	1.86	0.74
1:A:64:THR:HG22	1:A:145:SER:H	1.51	0.74
1:A:110:ASP:HB2	4:A:1648:HOH:O	1.86	0.74
1:B:79:ASN:ND2	1:B:81:SER:HB2	2.02	0.74
1:B:49:GLN:HE22	1:B:337:ASP:H	1.34	0.74
1:B:142:SER:H	1:B:169:HIS:HE1	1.37	0.73
1:A:205:ARG:HD2	4:B:2470:HOH:O	1.87	0.73
1:B:64:THR:HG22	1:B:145:SER:CA	2.18	0.73
1:B:64:THR:HG23	4:B:2590:HOH:O	1.89	0.73
1:C:323:HIS:HB2	1:C:325:LEU:HD22	1.68	0.73
1:A:323:HIS:O	1:A:325:LEU:HD13	1.89	0.73
1:A:79:ASN:HD22	1:A:81:SER:H	1.36	0.73
1:B:119:LYS:H	1:B:122:HIS:CD2	2.06	0.73
1:C:205:ARG:HD2	4:D:4476:HOH:O	1.88	0.73
1:A:213:LEU:HD12	1:A:213:LEU:O	1.88	0.72
1:A:137:LEU:O	1:A:188:SER:HB2	1.87	0.72
1:D:406:PRO:HG2	1:D:411:TRP:HB3	1.70	0.72
1:C:156:SER:O	1:C:211:ARG:HD2	1.89	0.72
1:B:406:PRO:HG2	1:B:411:TRP:HB3	1.71	0.72
1:A:79:ASN:ND2	1:A:82:GLU:H	1.87	0.72
1:D:312:GLU:O	1:D:316:ILE:HG13	1.89	0.72
1:D:289:PRO:O	1:D:328:ARG:HD2	1.90	0.71
1:B:314:GLN:NE2	1:B:359:ARG:HH11	1.89	0.71
1:D:86:ASP:HB3	1:D:343:ILE:HD11	1.72	0.71
1:D:142:SER:H	1:D:169:HIS:CE1	2.05	0.71
1:C:137:LEU:O	1:C:188:SER:HB2	1.91	0.71
1:B:64:THR:HG21	4:B:2499:HOH:O	1.91	0.71
1:D:157:HIS:O	1:D:163:ARG:HD3	1.91	0.70
1:D:142:SER:N	1:D:169:HIS:HE1	1.88	0.70
1:A:64:THR:HG22	1:A:145:SER:N	2.06	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:GLU:HG2	1:B:422:ILE:HG13	1.72	0.70
1:D:11:THR:O	1:D:15:GLN:HG3	1.92	0.69
1:A:70:THR:CG2	1:C:199:LYS:HD2	2.23	0.69
1:B:119:LYS:HB3	1:B:120:PRO:HD2	1.75	0.69
1:B:205:ARG:O	1:B:209:ARG:HG3	1.93	0.69
1:A:50:GLY:HA3	1:A:83:LEU:HD11	1.75	0.68
1:D:79:ASN:HD22	1:D:81:SER:H	1.40	0.68
1:D:416:ARG:O	1:D:419:GLU:HB3	1.92	0.68
1:D:387:GLN:NE2	4:D:4669:HOH:O	2.27	0.68
1:A:142:SER:N	1:A:169:HIS:HE1	1.89	0.68
1:D:418:TYR:HE2	1:D:423:LEU:HD21	1.59	0.68
1:A:369:ARG:HG3	1:A:369:ARG:NH1	1.99	0.68
1:B:58:ASN:ND2	1:B:61:GLY:HA3	2.09	0.68
1:A:142:SER:H	1:A:169:HIS:CE1	2.09	0.67
1:B:421:GLU:HG3	4:B:2669:HOH:O	1.94	0.67
1:C:78:ARG:CZ	1:C:426:ARG:HB3	2.25	0.67
1:C:94:ILE:O	1:C:98:LYS:NZ	2.26	0.67
1:D:314:GLN:NE2	1:D:356:ALA:HA	2.10	0.67
1:B:66:GLY:HA2	1:B:240:ILE:O	1.94	0.67
1:C:134:GLN:HA	1:C:134:GLN:NE2	2.10	0.67
1:D:64:THR:CG2	1:D:145:SER:H	2.06	0.67
1:D:78:ARG:N	1:D:82:GLU:OE1	2.27	0.67
1:A:243:GLU:HB3	1:C:299:VAL:HG12	1.76	0.67
1:B:323:HIS:O	1:B:325:LEU:HD13	1.95	0.67
1:B:170:CYS:O	1:B:174:ARG:HG3	1.95	0.66
1:D:358:LEU:O	1:D:362:LEU:HG	1.95	0.66
1:A:114:SER:HB3	1:A:117:GLN:HG3	1.77	0.66
1:B:234:GLU:HB2	1:B:265:CYS:HB3	1.76	0.66
1:C:142:SER:N	1:C:169:HIS:HE1	1.90	0.66
1:D:373:ALA:HB3	1:D:374:PRO:HD2	1.77	0.66
1:A:244:SER:HB2	4:A:1610:HOH:O	1.95	0.65
1:A:94:ILE:O	1:A:98:LYS:NZ	2.28	0.65
1:B:367:GLU:HG3	4:B:2533:HOH:O	1.96	0.65
1:D:258:THR:O	1:D:261:GLN:NE2	2.28	0.65
1:C:79:ASN:HD21	1:C:82:GLU:H	1.44	0.65
1:A:204:ASP:OD2	1:B:369:ARG:NH1	2.30	0.65
1:A:387:GLN:O	1:A:390:LEU:HB2	1.97	0.65
1:D:412:LEU:HG	1:D:416:ARG:HD2	1.77	0.65
1:A:277:ILE:HG12	4:A:1616:HOH:O	1.97	0.65
1:B:79:ASN:HD22	1:B:81:SER:H	1.45	0.65
1:D:176:VAL:O	1:D:179:TYR:HB3	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ASN:HD22	1:A:81:SER:N	1.94	0.64
1:A:94:ILE:HD13	1:A:350:THR:HB	1.79	0.64
1:A:119:LYS:N	1:A:122:HIS:HD2	1.91	0.64
1:B:58:ASN:HD21	1:B:61:GLY:HA3	1.62	0.64
1:C:35:LEU:HD21	1:C:395:VAL:HG12	1.79	0.64
1:C:369:ARG:NE	4:C:3699:HOH:O	2.29	0.64
1:A:87:LEU:HD22	1:A:100:LEU:HD13	1.78	0.64
1:A:421:GLU:OE1	1:A:422:ILE:N	2.30	0.64
1:D:84:ARG:HD2	1:D:129:TRP:CD1	2.32	0.64
1:A:405:THR:HG22	1:A:406:PRO:HD2	1.80	0.64
1:A:134:GLN:HA	1:A:134:GLN:NE2	2.12	0.64
1:A:154:THR:OG1	1:A:155:LEU:N	2.31	0.64
1:A:365:THR:O	1:A:369:ARG:HB2	1.98	0.64
1:B:142:SER:N	1:B:169:HIS:HE1	1.95	0.64
1:D:418:TYR:CE2	1:D:423:LEU:HD21	2.33	0.63
1:A:270:HIS:NE2	2:A:1460:RNT:O2	2.31	0.63
1:C:146:HIS:CG	1:C:147:PRO:HD2	2.33	0.63
1:A:91:MET:HG2	1:A:98:LYS:HD2	1.80	0.63
1:D:139:PHE:O	1:D:190:MET:HA	1.98	0.63
1:B:151:ASP:HB2	4:B:2485:HOH:O	1.97	0.63
1:A:422:ILE:HG22	1:A:423:LEU:N	2.13	0.63
1:B:64:THR:CG2	1:B:145:SER:H	2.12	0.63
1:B:127:VAL:O	1:B:131:LYS:HG3	1.99	0.63
1:B:154:THR:O	1:B:157:HIS:HB2	1.97	0.63
1:D:418:TYR:HA	1:D:421:GLU:OE1	1.98	0.63
1:C:285:MET:CE	1:C:325:LEU:HD11	2.30	0.62
1:A:146:HIS:CG	1:A:147:PRO:HD2	2.34	0.62
1:A:272:HIS:HB3	1:A:273:PRO:HD2	1.82	0.62
1:A:373:ALA:HB3	1:A:374:PRO:HD2	1.79	0.62
1:D:371:LEU:HD13	1:D:379:ALA:HB3	1.80	0.62
1:A:107:LEU:HD23	1:A:107:LEU:O	1.99	0.62
1:A:54:SER:HB3	1:A:59:PRO:O	1.99	0.62
1:A:387:GLN:NE2	1:A:390:LEU:HD12	2.15	0.62
1:A:49:GLN:HE21	1:A:335:PHE:HD1	1.47	0.62
1:B:205:ARG:HB3	1:B:245:TYR:CE1	2.35	0.62
1:A:314:GLN:HE21	1:A:359:ARG:HH11	1.46	0.62
1:D:289:PRO:O	1:D:290:GLN:HG3	2.00	0.62
1:B:118:ILE:HD12	1:B:176:VAL:HG21	1.81	0.61
1:D:120:PRO:HB3	1:D:179:TYR:CD2	2.34	0.61
1:C:79:ASN:HD22	1:C:81:SER:N	1.97	0.61
1:C:120:PRO:HB3	1:C:179:TYR:CD2	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:GLN:HE22	1:D:356:ALA:HA	1.65	0.61
1:A:121:GLU:HB3	4:A:1692:HOH:O	2.00	0.61
1:B:63:LEU:HD13	1:B:67:ILE:O	2.00	0.61
1:C:373:ALA:HB3	1:C:374:PRO:HD2	1.83	0.61
1:D:64:THR:HG23	4:D:4613:HOH:O	2.00	0.61
1:B:240:ILE:HD12	1:B:301:TRP:CZ3	2.35	0.61
1:B:89:GLN:HG3	1:B:418:TYR:CE1	2.36	0.60
1:B:240:ILE:HD13	1:D:240:ILE:CD1	2.30	0.60
1:C:152:GLY:O	1:C:196:ASP:HA	2.00	0.60
1:C:258:THR:HG23	4:C:3512:HOH:O	2.01	0.60
1:A:75:GLY:O	1:A:76:LYS:C	2.43	0.60
1:D:131:LYS:HE3	1:D:183:GLN:HG3	1.83	0.60
1:A:393:GLN:HB2	4:A:1530:HOH:O	2.00	0.60
1:D:61:GLY:O	1:D:62:SER:HB2	2.01	0.60
1:A:64:THR:HG21	4:A:1483:HOH:O	2.01	0.60
1:B:391:PRO:C	1:B:393:GLN:HE21	2.09	0.60
1:B:64:THR:HG22	1:B:145:SER:N	2.17	0.60
1:B:370:LYS:O	1:B:374:PRO:HD2	2.02	0.60
1:C:49:GLN:HE22	1:C:337:ASP:H	1.50	0.60
1:C:359:ARG:NH1	4:C:3701:HOH:O	2.35	0.60
1:B:64:THR:CG2	1:B:145:SER:HA	2.31	0.60
1:B:359:ARG:NH2	4:B:2700:HOH:O	2.34	0.60
1:B:116:ASP:C	1:B:117:GLN:HG2	2.25	0.59
1:B:176:VAL:O	1:B:179:TYR:HB3	2.02	0.59
1:C:134:GLN:HA	1:C:134:GLN:HE21	1.66	0.59
1:A:44:SER:HA	1:A:99:ARG:HB2	1.83	0.59
1:C:318:SER:O	1:C:322:ARG:HG3	2.01	0.59
1:D:64:THR:HG22	1:D:145:SER:CA	2.33	0.59
1:D:275:GLU:OE1	1:D:280:LYS:NZ	2.34	0.59
1:B:236:LYS:HE2	1:B:238:PHE:O	2.02	0.59
1:C:413:GLU:HA	1:C:413:GLU:OE1	2.00	0.59
1:B:64:THR:HG22	1:B:145:SER:H	1.68	0.59
1:A:91:MET:CE	1:A:135:LEU:HD11	2.31	0.59
1:D:290:GLN:HG2	1:D:328:ARG:HA	1.83	0.59
1:D:370:LYS:HG2	4:D:4529:HOH:O	2.01	0.59
1:A:405:THR:CG2	1:A:406:PRO:HD2	2.33	0.59
1:B:49:GLN:HE22	1:B:337:ASP:N	2.01	0.59
1:B:142:SER:H	1:B:169:HIS:CE1	2.20	0.58
1:C:220:ILE:O	1:C:221:SER:C	2.46	0.58
1:C:343:ILE:O	1:C:347:VAL:HG23	2.03	0.58
1:B:413:GLU:N	1:B:413:GLU:OE2	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ARG:HH12	1:C:186:THR:CG2	2.15	0.58
1:B:365:THR:O	1:B:369:ARG:HB2	2.03	0.58
1:D:397:GLU:HG2	1:D:407:ALA:HB1	1.85	0.58
1:D:175:ARG:HD3	1:D:222:GLU:OE1	2.04	0.58
1:D:79:ASN:ND2	1:D:82:GLU:H	2.01	0.58
1:C:142:SER:H	1:C:169:HIS:CE1	2.05	0.58
1:B:45:MET:O	1:B:100:LEU:HD12	2.04	0.58
1:B:55:GLY:HA3	1:B:105:ILE:HG13	1.86	0.58
1:B:89:GLN:HG3	1:B:418:TYR:CD1	2.39	0.58
1:D:321:VAL:O	1:D:322:ARG:C	2.46	0.58
1:D:57:GLU:HG3	4:D:4619:HOH:O	2.04	0.58
1:C:174:ARG:HG2	1:C:190:MET:HE1	1.86	0.57
1:D:119:LYS:N	1:D:122:HIS:CD2	2.68	0.57
1:D:86:ASP:CB	1:D:343:ILE:HD11	2.32	0.57
1:C:272:HIS:CE1	1:D:275:GLU:HA	2.40	0.57
1:D:49:GLN:NE2	1:D:337:ASP:H	1.95	0.57
1:A:213:LEU:HD12	1:A:213:LEU:C	2.28	0.57
1:C:35:LEU:HD21	1:C:395:VAL:CG1	2.34	0.57
1:C:369:ARG:NH1	1:D:204:ASP:OD2	2.36	0.57
1:B:373:ALA:HB3	1:B:374:PRO:HD2	1.85	0.57
1:C:13:LEU:HD23	1:C:398:MET:HE2	1.87	0.57
1:C:96:GLY:HA2	1:C:403:HIS:CE1	2.39	0.57
1:D:13:LEU:CD2	1:D:398:MET:HE2	2.34	0.57
1:A:64:THR:CG2	1:A:145:SER:H	2.17	0.57
1:C:233:VAL:HB	1:C:253:TYR:CD2	2.40	0.57
1:C:120:PRO:HB3	1:C:179:TYR:CG	2.40	0.57
1:D:422:ILE:HG22	1:D:423:LEU:N	2.20	0.57
1:A:70:THR:HG22	1:C:199:LYS:CE	2.35	0.56
1:A:70:THR:HG22	1:C:199:LYS:HD2	1.87	0.56
1:A:424:SER:C	1:A:425:ARG:HG2	2.29	0.56
1:C:177:SER:O	1:C:180:PHE:HB2	2.05	0.56
1:B:79:ASN:ND2	1:B:82:GLU:H	2.03	0.56
1:D:162:ILE:O	1:D:165:PHE:HB3	2.05	0.56
1:A:70:THR:HG23	4:C:3491:HOH:O	2.04	0.56
1:A:392:TRP:H	1:A:392:TRP:CD1	2.23	0.56
1:B:61:GLY:C	4:B:2715:HOH:O	2.48	0.56
1:C:141:PRO:HD2	1:C:191:ASN:O	2.06	0.56
1:D:97:PRO:C	1:D:98:LYS:HG2	2.29	0.56
1:A:13:LEU:HD23	1:A:13:LEU:O	2.04	0.56
1:A:60:GLU:OE1	1:A:61:GLY:N	2.37	0.56
1:B:213:LEU:C	1:B:213:LEU:HD12	2.29	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:GLN:HG2	1:B:330:HIS:NE2	2.20	0.56
1:A:119:LYS:HB3	1:A:120:PRO:HD2	1.87	0.56
1:B:79:ASN:HD22	1:B:81:SER:HB2	1.71	0.56
1:A:79:ASN:ND2	1:A:82:GLU:HG3	2.21	0.55
1:A:238:PHE:CD2	1:C:300:ARG:HD3	2.41	0.55
1:C:181:GLY:HA2	1:C:186:THR:O	2.06	0.55
1:C:285:MET:HE1	1:C:325:LEU:HD11	1.88	0.55
1:D:44:SER:HA	1:D:99:ARG:HB2	1.86	0.55
1:C:164:GLN:NE2	1:C:168:ASP:OD1	2.35	0.55
1:B:79:ASN:HD22	1:B:81:SER:N	2.03	0.55
1:B:267:ASP:HB3	1:B:270:HIS:CG	2.42	0.55
1:D:370:LYS:O	1:D:374:PRO:HD2	2.05	0.55
1:A:79:ASN:HD21	1:A:82:GLU:H	1.55	0.55
1:C:11:THR:HG23	1:C:15:GLN:HE21	1.72	0.55
1:B:213:LEU:HD12	1:B:213:LEU:O	2.07	0.55
1:B:370:LYS:O	1:B:371:LEU:C	2.46	0.55
1:B:405:THR:HG23	1:B:406:PRO:HD2	1.88	0.55
1:A:143:CYS:HA	1:A:166:TRP:CZ3	2.42	0.55
1:B:37:GLN:O	1:B:40:ARG:HB2	2.06	0.55
1:B:157:HIS:O	1:B:163:ARG:HD3	2.06	0.55
1:C:406:PRO:HG2	1:C:411:TRP:HB3	1.88	0.55
1:B:116:ASP:OD1	1:B:117:GLN:HG2	2.06	0.55
1:B:422:ILE:HD13	4:B:2724:HOH:O	2.05	0.55
1:A:424:SER:O	1:A:425:ARG:HG2	2.06	0.54
1:A:77:ALA:HB3	1:A:83:LEU:HD13	1.89	0.54
1:C:64:THR:OG1	1:C:145:SER:HA	2.07	0.54
1:D:216:LEU:O	1:D:220:ILE:HG12	2.08	0.54
1:A:288:VAL:HB	1:A:289:PRO:HD2	1.90	0.54
1:C:236:LYS:HG3	1:C:270:HIS:ND1	2.22	0.54
1:A:119:LYS:N	1:A:122:HIS:CD2	2.71	0.54
1:A:159:ASP:OD2	1:A:162:ILE:HG13	2.08	0.54
1:B:369:ARG:NH1	1:B:369:ARG:HG3	2.22	0.54
1:D:27:VAL:HG23	1:D:27:VAL:O	2.08	0.54
1:A:49:GLN:NE2	1:A:335:PHE:HD1	2.06	0.54
1:A:304:ASP:HB3	1:A:336:PHE:H	1.73	0.54
1:A:370:LYS:O	1:A:374:PRO:HD2	2.08	0.54
1:A:389:SER:HA	1:D:393:GLN:HG2	1.90	0.54
1:B:369:ARG:NH1	4:B:2738:HOH:O	2.39	0.54
1:D:79:ASN:ND2	1:D:81:SER:N	2.55	0.54
1:D:119:LYS:HE2	1:D:121:GLU:OE2	2.08	0.54
1:D:199:LYS:HB2	1:D:241:GLY:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ALA:HB3	1:A:296:SER:H	1.73	0.53
1:A:271:PHE:HB3	1:A:275:GLU:OE2	2.07	0.53
1:A:386:GLU:HB3	4:A:1542:HOH:O	2.07	0.53
1:B:49:GLN:NE2	1:B:336:PHE:HA	2.22	0.53
1:C:13:LEU:CD2	1:C:398:MET:HE2	2.38	0.53
1:C:215:ALA:O	1:C:219:VAL:HG23	2.07	0.53
1:D:127:VAL:CG1	1:D:183:GLN:HG2	2.37	0.53
1:D:156:SER:O	1:D:211:ARG:HD2	2.07	0.53
1:C:75:GLY:O	1:C:76:LYS:C	2.45	0.53
1:C:256:TYR:CZ	1:C:260:ARG:HG2	2.43	0.53
1:C:342:ARG:HG3	1:C:342:ARG:HH11	1.72	0.53
1:A:52:ASP:C	1:A:53:VAL:HG23	2.31	0.53
1:C:289:PRO:O	1:C:328:ARG:HD2	2.09	0.53
1:D:207:ALA:O	1:D:208:PRO:C	2.46	0.53
1:A:13:LEU:HD23	1:A:13:LEU:C	2.34	0.53
1:C:87:LEU:O	1:C:90:ALA:HB3	2.09	0.53
1:C:342:ARG:HG3	4:C:3625:HOH:O	2.09	0.53
1:A:87:LEU:CD2	1:A:100:LEU:HD13	2.38	0.53
1:D:358:LEU:HD21	1:D:395:VAL:HG12	1.91	0.53
1:A:421:GLU:OE1	1:A:422:ILE:HD12	2.08	0.53
1:B:405:THR:CG2	1:B:406:PRO:HD2	2.39	0.53
1:B:199:LYS:HZ2	1:D:70:THR:HG23	1.73	0.53
1:D:225:ASN:O	1:D:228:HIS:N	2.39	0.53
1:B:146:HIS:ND1	1:B:147:PRO:HD2	2.24	0.52
1:C:236:LYS:HG3	1:C:270:HIS:CE1	2.44	0.52
1:C:51:ASP:OD2	1:C:51:ASP:N	2.41	0.52
1:D:406:PRO:HG2	1:D:411:TRP:CB	2.39	0.52
1:A:78:ARG:N	1:A:82:GLU:OE1	2.41	0.52
1:A:342:ARG:HG3	1:A:342:ARG:HH11	1.74	0.52
1:C:272:HIS:HB3	1:C:273:PRO:CD	2.36	0.52
1:C:368:LEU:HD21	1:C:383:LEU:CB	2.33	0.52
1:D:422:ILE:CG2	1:D:423:LEU:HD23	2.28	0.52
1:C:61:GLY:O	1:C:62:SER:HB2	2.08	0.52
1:A:50:GLY:HA3	1:A:83:LEU:CD1	2.40	0.52
1:A:314:GLN:HE21	1:A:359:ARG:NH1	2.08	0.52
1:D:265:CYS:HB2	1:D:292:LEU:HD23	1.92	0.52
1:A:243:GLU:HB3	1:C:299:VAL:CG1	2.39	0.51
1:A:423:LEU:C	1:A:425:ARG:H	2.18	0.51
1:B:178:ALA:HB2	1:B:224:LEU:HD13	1.92	0.51
1:D:79:ASN:HD21	1:D:82:GLU:H	1.58	0.51
1:A:341:ASN:HB3	1:D:378:THR:HG21	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ILE:HG22	1:A:423:LEU:HD23	1.92	0.51
1:B:64:THR:CG2	1:B:145:SER:N	2.73	0.51
1:C:46:HIS:NE2	1:C:335:PHE:O	2.43	0.51
1:C:119:LYS:N	1:C:122:HIS:CD2	2.75	0.51
1:A:301:TRP:CE2	1:A:303:SER:HB3	2.45	0.51
1:B:393:GLN:OE1	1:C:391:PRO:HA	2.10	0.51
1:C:359:ARG:NH2	4:C:3687:HOH:O	2.42	0.51
1:D:23:ARG:O	1:D:26:ALA:HB3	2.10	0.51
1:D:391:PRO:HA	4:D:4671:HOH:O	2.09	0.51
1:D:418:TYR:CE1	1:D:422:ILE:HD12	2.46	0.51
1:B:300:ARG:O	1:B:301:TRP:HB3	2.11	0.51
1:A:204:ASP:HB2	1:B:369:ARG:NH1	2.26	0.51
1:B:89:GLN:O	1:B:92:ARG:HG2	2.11	0.51
1:A:343:ILE:N	1:A:343:ILE:HD13	2.26	0.50
1:A:421:GLU:HA	1:A:425:ARG:NH2	2.26	0.50
1:B:12:GLN:HE22	1:C:22:GLN:HE22	1.55	0.50
1:B:61:GLY:N	4:B:2715:HOH:O	2.44	0.50
1:A:267:ASP:HA	1:A:294:HIS:HB2	1.92	0.50
1:C:387:GLN:NE2	1:C:390:LEU:HD12	2.26	0.50
1:D:167:ILE:O	1:D:171:LYS:HG3	2.11	0.50
1:B:211:ARG:NH2	4:B:2721:HOH:O	2.44	0.50
1:D:368:LEU:HD21	1:D:383:LEU:HB3	1.93	0.50
1:A:240:ILE:HD11	1:C:240:ILE:HD12	1.94	0.50
1:A:421:GLU:O	1:A:425:ARG:HG3	2.10	0.50
1:C:46:HIS:HA	1:C:101:ASN:HB3	1.94	0.50
1:A:70:THR:HG21	1:C:241:GLY:HA2	1.92	0.50
1:B:289:PRO:O	1:B:328:ARG:HD2	2.11	0.50
1:C:323:HIS:HB2	1:C:325:LEU:CD2	2.38	0.50
1:A:373:ALA:CB	1:A:374:PRO:HD2	2.36	0.50
1:D:20:ALA:HB2	1:D:394:ALA:HB3	1.93	0.50
1:C:22:GLN:O	1:C:23:ARG:C	2.52	0.50
1:A:421:GLU:CG	1:A:422:ILE:HD12	2.42	0.49
1:C:123:PHE:O	1:C:126:TRP:HB2	2.12	0.49
1:C:344:ALA:O	1:C:345:ALA:C	2.51	0.49
1:B:182:GLU:HG3	1:B:228:HIS:ND1	2.27	0.49
1:C:79:ASN:ND2	1:C:81:SER:HB2	2.27	0.49
1:D:297:ARG:HD2	4:D:4581:HOH:O	2.11	0.49
1:A:89:GLN:C	1:A:89:GLN:HE21	2.18	0.49
1:A:124:LYS:NZ	1:A:125:ASN:ND2	2.60	0.49
1:C:370:LYS:O	1:C:374:PRO:HD2	2.12	0.49
1:D:323:HIS:HB2	1:D:325:LEU:HD22	1.92	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:THR:HB	1:A:14:GLU:H	1.78	0.49
1:A:18:GLU:OE1	1:A:18:GLU:HA	2.11	0.49
1:A:196:ASP:OD1	1:A:196:ASP:N	2.45	0.49
1:B:14:GLU:O	1:B:18:GLU:HG2	2.12	0.49
1:B:107:LEU:HG	1:B:107:LEU:O	2.12	0.49
1:D:119:LYS:N	1:D:122:HIS:HD2	2.01	0.49
1:B:124:LYS:O	1:B:128:GLU:HG3	2.13	0.49
1:B:229:HIS:O	1:B:230:ILE:HG13	2.13	0.49
1:B:152:GLY:O	1:B:196:ASP:HA	2.13	0.49
1:C:373:ALA:CB	1:C:374:PRO:HD2	2.42	0.49
1:D:285:MET:HE1	1:D:325:LEU:HD11	1.94	0.49
1:A:64:THR:CG2	1:A:145:SER:HA	2.37	0.49
1:A:89:GLN:NE2	1:A:89:GLN:CA	2.75	0.49
1:B:293:LEU:CD1	1:B:320:ILE:HD11	2.43	0.49
1:B:351:ARG:HH22	1:B:405:THR:HG22	1.77	0.49
1:D:107:LEU:N	1:D:107:LEU:HD23	2.27	0.49
1:D:195:PRO:O	1:D:196:ASP:C	2.54	0.49
1:A:419:GLU:O	1:A:424:SER:HB3	2.12	0.49
1:B:14:GLU:OE2	1:B:18:GLU:OE2	2.30	0.49
1:B:151:ASP:OD2	1:B:157:HIS:NE2	2.46	0.49
1:B:269:GLY:HA2	1:B:298:PRO:CG	2.27	0.49
1:C:134:GLN:HE21	1:C:134:GLN:CA	2.24	0.49
1:C:269:GLY:HA2	1:C:298:PRO:HG3	1.94	0.49
1:A:46:HIS:HB2	1:A:48:TRP:CE2	2.48	0.48
1:A:91:MET:HE2	1:A:98:LYS:HB2	1.94	0.48
1:C:15:GLN:HA	4:C:3685:HOH:O	2.12	0.48
1:A:79:ASN:ND2	1:A:81:SER:H	2.10	0.48
1:B:181:GLY:HA3	1:B:228:HIS:O	2.14	0.48
1:C:39:ASP:O	1:C:97:PRO:HG3	2.13	0.48
1:C:79:ASN:ND2	1:C:82:GLU:N	2.57	0.48
1:C:153:PHE:CD1	1:C:153:PHE:N	2.79	0.48
1:C:213:LEU:HD11	1:C:260:ARG:NH2	2.29	0.48
1:D:192:ILE:N	1:D:232:ALA:O	2.43	0.48
1:A:272:HIS:HB3	1:A:273:PRO:CD	2.44	0.48
1:B:119:LYS:H	1:B:122:HIS:HD2	1.59	0.48
1:A:78:ARG:NH2	1:A:426:ARG:HB3	2.28	0.48
1:B:228:HIS:CD2	1:B:228:HIS:N	2.77	0.48
1:A:78:ARG:HD3	4:A:1515:HOH:O	2.12	0.48
1:A:79:ASN:HD21	1:A:82:GLU:HG3	1.79	0.48
1:C:330:HIS:HB3	4:C:3522:HOH:O	2.13	0.48
1:A:286:LEU:HD22	4:B:2740:HOH:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:TYR:CE1	1:B:183:GLN:HG3	2.49	0.48
1:B:337:ASP:OD1	1:D:199:LYS:NZ	2.41	0.48
1:A:157:HIS:CD2	1:A:162:ILE:HG21	2.49	0.48
1:B:268:ALA:HB1	4:B:2576:HOH:O	2.14	0.48
1:C:79:ASN:HD21	1:C:82:GLU:N	2.09	0.48
1:A:134:GLN:NE2	1:A:134:GLN:CA	2.75	0.48
1:B:384:LEU:O	1:B:387:GLN:HB2	2.14	0.48
1:A:159:ASP:CG	1:A:162:ILE:HG13	2.39	0.47
1:A:419:GLU:O	1:A:424:SER:N	2.46	0.47
1:B:270:HIS:NE2	2:B:2460:RNT:O2	2.47	0.47
1:B:124:LYS:O	1:B:124:LYS:HG2	2.13	0.47
1:B:128:GLU:HG2	4:B:2713:HOH:O	2.13	0.47
1:B:262:THR:O	1:B:289:PRO:HD2	2.13	0.47
1:B:162:ILE:O	1:B:165:PHE:HB3	2.14	0.47
1:C:103:HIS:O	1:C:104:ALA:C	2.52	0.47
1:A:133:ASN:O	1:A:134:GLN:HB2	2.13	0.47
1:C:103:HIS:CD2	2:C:3460:RNT:H61	2.49	0.47
1:D:56:PHE:O	1:D:59:PRO:HD3	2.15	0.47
1:A:114:SER:HB3	1:A:117:GLN:CG	2.43	0.47
1:A:314:GLN:NE2	1:A:359:ARG:HD3	2.29	0.47
1:B:23:ARG:HA	1:B:23:ARG:HD2	1.64	0.47
1:C:13:LEU:HD13	1:C:401:GLN:NE2	2.29	0.47
1:C:84:ARG:HG2	1:C:126:TRP:CZ3	2.50	0.47
1:C:99:ARG:HH12	1:C:186:THR:HG21	1.78	0.47
1:A:240:ILE:HD11	1:C:240:ILE:CD1	2.44	0.47
1:A:386:GLU:O	1:A:387:GLN:C	2.55	0.47
1:D:265:CYS:HA	1:D:292:LEU:O	2.14	0.47
1:A:352:ASN:ND2	1:D:385:GLU:OE1	2.48	0.47
1:A:370:LYS:O	1:A:374:PRO:HG2	2.15	0.47
1:B:301:TRP:HA	4:B:2519:HOH:O	2.14	0.46
1:B:364:PRO:O	1:B:368:LEU:HG	2.15	0.46
1:B:390:LEU:HD23	1:B:390:LEU:HA	1.81	0.46
1:C:174:ARG:HG2	1:C:190:MET:CE	2.45	0.46
1:D:46:HIS:ND1	1:D:46:HIS:N	2.61	0.46
1:A:204:ASP:CG	1:B:369:ARG:HH12	2.23	0.46
1:B:94:ILE:O	1:B:98:LYS:NZ	2.34	0.46
1:B:114:SER:HB3	1:B:116:ASP:OD1	2.15	0.46
1:B:178:ALA:HA	1:B:229:HIS:HB2	1.97	0.46
1:C:14:GLU:OE2	1:C:18:GLU:HG3	2.16	0.46
1:C:21:LYS:HG3	1:C:31:VAL:HG22	1.97	0.46
1:C:363:GLU:HG3	1:C:364:PRO:HD2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:ASP:CB	1:D:294:HIS:HB2	2.45	0.46
1:A:238:PHE:HB2	1:A:243:GLU:HA	1.98	0.46
1:B:146:HIS:CE1	1:B:148:LEU:HB2	2.50	0.46
1:C:115:ARG:HB2	1:C:165:PHE:CZ	2.51	0.46
1:D:109:SER:HB3	1:D:111:THR:O	2.15	0.46
1:D:297:ARG:NE	1:D:308:LEU:HG	2.31	0.46
1:A:324:ASP:OD1	1:A:326:PHE:HE2	1.99	0.46
1:A:337:ASP:OD1	1:C:199:LYS:NZ	2.41	0.46
1:A:21:LYS:HG3	1:A:31:VAL:CG2	2.46	0.46
1:D:181:GLY:HA2	1:D:186:THR:O	2.16	0.46
1:D:213:LEU:HD12	1:D:213:LEU:O	2.15	0.46
1:A:91:MET:HE1	1:A:135:LEU:HD13	1.92	0.46
1:A:236:LYS:HG3	1:A:270:HIS:ND1	2.31	0.46
1:A:289:PRO:O	1:A:328:ARG:HD2	2.15	0.46
1:A:342:ARG:HG3	4:A:1608:HOH:O	2.15	0.46
1:C:51:ASP:O	1:C:54:SER:OG	2.29	0.46
1:C:271:PHE:HB3	1:C:275:GLU:OE2	2.16	0.46
1:D:58:ASN:O	1:D:59:PRO:C	2.58	0.46
1:D:108:GLU:OE2	1:D:125:ASN:HB2	2.16	0.46
1:D:170:CYS:O	1:D:174:ARG:HG3	2.15	0.46
1:A:393:GLN:NE2	1:D:393:GLN:NE2	2.64	0.46
1:C:174:ARG:CG	1:C:190:MET:HE1	2.45	0.46
1:B:39:ASP:OD1	1:B:399:TYR:OH	2.32	0.46
1:B:51:ASP:OD1	1:B:55:GLY:N	2.42	0.46
1:B:418:TYR:HE2	1:B:423:LEU:HD21	1.81	0.46
1:D:162:ILE:O	1:D:163:ARG:C	2.59	0.46
1:D:373:ALA:CB	1:D:374:PRO:HD2	2.40	0.46
1:B:131:LYS:O	1:B:132:ALA:C	2.56	0.46
1:C:109:SER:OG	1:C:111:THR:O	2.29	0.46
1:D:56:PHE:C	1:D:59:PRO:HD3	2.41	0.46
1:B:199:LYS:NZ	1:D:70:THR:CG2	2.79	0.46
1:B:419:GLU:O	1:B:424:SER:N	2.44	0.46
1:C:47:CYS:HB3	1:C:100:LEU:HD11	1.98	0.46
1:C:104:ALA:C	1:C:106:TYR:H	2.24	0.46
1:D:272:HIS:O	1:D:273:PRO:C	2.56	0.46
1:D:370:LYS:O	1:D:371:LEU:C	2.58	0.45
1:D:418:TYR:HA	1:D:421:GLU:CD	2.41	0.45
1:B:56:PHE:CZ	1:B:80:ALA:HA	2.51	0.45
1:B:87:LEU:HD21	1:B:346:TRP:CZ2	2.51	0.45
1:B:177:SER:O	1:B:180:PHE:HB2	2.17	0.45
1:C:368:LEU:HB3	1:D:203:VAL:HG21	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:HD23	1:A:107:LEU:C	2.40	0.45
1:B:285:MET:HE1	1:B:325:LEU:HD11	1.99	0.45
1:B:325:LEU:HD12	1:B:325:LEU:HA	1.49	0.45
1:B:383:LEU:HD23	1:B:383:LEU:HA	1.73	0.45
1:C:207:ALA:N	1:C:208:PRO:CD	2.79	0.45
1:D:22:GLN:O	1:D:23:ARG:C	2.59	0.45
1:B:240:ILE:CD1	1:B:301:TRP:CZ3	3.00	0.45
1:B:421:GLU:HG2	1:B:421:GLU:O	2.15	0.45
1:D:20:ALA:CB	1:D:394:ALA:HB3	2.47	0.45
1:D:89:GLN:CG	1:D:418:TYR:CD1	3.00	0.45
1:A:368:LEU:HD21	1:A:383:LEU:CB	2.47	0.45
1:B:144:PHE:O	1:B:145:SER:C	2.58	0.45
1:D:224:LEU:O	1:D:226:PRO:HD3	2.16	0.45
1:C:128:GLU:O	1:C:131:LYS:HB2	2.17	0.45
1:C:236:LYS:HG3	1:C:270:HIS:CG	2.52	0.45
1:D:86:ASP:CA	1:D:343:ILE:HD11	2.46	0.45
1:D:300:ARG:HB3	4:D:4564:HOH:O	2.17	0.45
1:D:392:TRP:O	1:D:395:VAL:HB	2.17	0.45
1:A:73:TYR:O	1:A:342:ARG:NH2	2.35	0.45
1:A:181:GLY:HA2	1:A:186:THR:O	2.17	0.45
1:B:165:PHE:HA	4:B:2552:HOH:O	2.16	0.45
1:B:391:PRO:HA	1:B:393:GLN:NE2	2.32	0.45
1:C:370:LYS:O	1:C:374:PRO:HG2	2.17	0.45
1:D:52:ASP:C	1:D:53:VAL:HG23	2.42	0.45
1:D:95:PRO:O	1:D:354:LYS:NZ	2.31	0.45
1:D:285:MET:CE	1:D:325:LEU:HD11	2.47	0.45
1:D:410:GLU:H	1:D:410:GLU:HG3	1.30	0.45
1:D:19:LEU:HD23	1:D:19:LEU:HA	1.72	0.45
1:A:130:ALA:O	1:A:131:LYS:C	2.55	0.44
1:B:391:PRO:CA	1:B:393:GLN:NE2	2.80	0.44
1:B:418:TYR:CE2	1:B:423:LEU:HD21	2.52	0.44
1:D:278:SER:O	1:D:319:GLU:HG3	2.17	0.44
1:D:413:GLU:OE1	1:D:416:ARG:HD3	2.18	0.44
1:D:373:ALA:CB	1:D:374:PRO:CD	2.95	0.44
1:A:70:THR:HG22	1:C:199:LYS:CD	2.47	0.44
1:A:418:TYR:HE2	1:A:423:LEU:HD21	1.82	0.44
1:B:102:LEU:O	1:B:139:PHE:HA	2.18	0.44
1:B:240:ILE:HD13	1:D:240:ILE:HD13	1.98	0.44
1:C:95:PRO:HG3	1:C:400:CYS:SG	2.57	0.44
1:C:105:ILE:HG23	1:C:142:SER:CB	2.48	0.44
1:C:269:GLY:O	1:C:302:ASP:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:PHE:O	1:D:25:ALA:C	2.57	0.44
1:D:46:HIS:HB2	1:D:48:TRP:CE2	2.53	0.44
1:A:237:LEU:HB3	4:A:1607:HOH:O	2.16	0.44
1:A:405:THR:HG22	1:A:406:PRO:CD	2.47	0.44
1:B:13:LEU:HD11	1:B:397:GLU:HB3	1.99	0.44
1:B:79:ASN:ND2	1:B:81:SER:CB	2.78	0.44
1:D:46:HIS:NE2	1:D:335:PHE:O	2.51	0.44
1:A:321:VAL:HB	1:A:360:ALA:HB1	1.99	0.44
1:B:64:THR:O	1:B:144:PHE:HB2	2.17	0.44
1:C:410:GLU:H	1:C:410:GLU:HG3	1.42	0.44
1:D:79:ASN:ND2	1:D:81:SER:H	2.13	0.44
1:D:423:LEU:HD23	1:D:423:LEU:N	2.31	0.44
1:A:322:ARG:HD3	1:B:203:VAL:O	2.17	0.44
1:A:383:LEU:HD23	1:A:383:LEU:HA	1.82	0.44
1:B:119:LYS:CB	1:B:120:PRO:HD2	2.41	0.44
1:C:42:PRO:HA	1:C:97:PRO:HB2	2.00	0.44
1:A:89:GLN:HE21	1:A:89:GLN:CA	2.30	0.44
1:D:84:ARG:HD2	1:D:129:TRP:CG	2.53	0.44
1:D:96:GLY:H	1:D:403:HIS:CD2	2.35	0.44
1:A:79:ASN:HD22	1:A:79:ASN:C	2.25	0.44
1:A:421:GLU:OE1	1:A:422:ILE:HB	2.16	0.44
1:C:276:VAL:HB	1:C:312:GLU:OE2	2.17	0.44
1:A:174:ARG:HG3	1:A:190:MET:HE1	2.00	0.44
1:C:154:THR:HB	1:C:166:TRP:CG	2.53	0.44
1:D:129:TRP:CZ3	1:D:135:LEU:HD12	2.52	0.44
1:C:119:LYS:N	1:C:122:HIS:HD2	2.06	0.43
1:A:251:GLU:CD	1:A:251:GLU:H	2.26	0.43
1:A:392:TRP:O	1:A:395:VAL:HB	2.18	0.43
4:B:2652:HOH:O	1:D:199:LYS:HE3	2.18	0.43
1:B:398:MET:HE2	1:B:398:MET:HB2	1.85	0.43
1:D:13:LEU:HD23	1:D:398:MET:HE2	2.00	0.43
1:A:159:ASP:HB3	1:A:162:ILE:HG13	2.00	0.43
1:A:341:ASN:OD1	1:A:343:ILE:N	2.51	0.43
1:B:159:ASP:OD2	1:B:162:ILE:HG13	2.17	0.43
1:B:314:GLN:HE21	1:B:359:ARG:NH1	2.05	0.43
1:A:410:GLU:O	1:A:411:TRP:C	2.61	0.43
1:A:416:ARG:HB3	4:A:1498:HOH:O	2.18	0.43
1:B:254:MET:HE3	1:B:258:THR:OG1	2.19	0.43
1:C:83:LEU:HD12	1:C:83:LEU:HA	1.81	0.43
1:C:119:LYS:O	1:C:120:PRO:C	2.62	0.43
1:C:134:GLN:NE2	1:C:134:GLN:CA	2.78	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:ALA:O	1:D:179:TYR:C	2.59	0.43
1:D:371:LEU:CD1	1:D:379:ALA:HB1	2.43	0.43
1:A:42:PRO:HA	1:A:97:PRO:HB2	2.00	0.43
1:A:373:ALA:CB	1:A:374:PRO:CD	2.96	0.43
1:A:393:GLN:OE1	1:D:393:GLN:OE1	2.37	0.43
1:B:100:LEU:HD12	1:B:100:LEU:HA	1.73	0.43
1:D:135:LEU:HA	1:D:135:LEU:HD23	1.77	0.43
1:A:151:ASP:HB2	4:A:1471:HOH:O	2.17	0.43
1:B:146:HIS:CD2	1:B:147:PRO:HD2	2.52	0.43
1:D:314:GLN:NE2	1:D:359:ARG:HD3	2.33	0.43
1:D:390:LEU:HB3	1:D:391:PRO:HD2	1.99	0.43
1:A:79:ASN:CG	1:A:82:GLU:HG3	2.44	0.43
1:C:13:LEU:HD21	1:C:398:MET:HA	2.00	0.43
1:C:300:ARG:HG2	1:C:300:ARG:HH11	1.84	0.43
1:D:89:GLN:HG3	1:D:418:TYR:CG	2.54	0.43
1:D:325:LEU:HB3	1:D:329:VAL:CG2	2.49	0.43
1:D:386:GLU:O	1:D:387:GLN:C	2.61	0.43
1:D:399:TYR:CE1	1:D:403:HIS:CE1	3.07	0.43
1:D:403:HIS:O	1:D:405:THR:HG23	2.19	0.43
1:A:121:GLU:N	4:A:1692:HOH:O	2.40	0.43
1:B:30:ASP:OD1	1:B:32:GLU:HB2	2.18	0.43
1:B:127:VAL:CG1	1:B:131:LYS:HE3	2.49	0.43
1:C:342:ARG:HG3	1:C:342:ARG:NH1	2.34	0.43
1:D:371:LEU:HD11	1:D:383:LEU:HD12	1.99	0.43
1:A:49:GLN:HE22	1:A:337:ASP:H	1.67	0.42
1:B:314:GLN:HE22	1:B:356:ALA:HA	1.83	0.42
1:D:418:TYR:O	1:D:419:GLU:C	2.61	0.42
1:A:135:LEU:HA	1:A:135:LEU:HD23	1.66	0.42
1:A:139:PHE:O	1:A:190:MET:HA	2.19	0.42
1:A:144:PHE:CD1	1:A:144:PHE:N	2.87	0.42
1:B:314:GLN:NE2	1:B:359:ARG:HD3	2.33	0.42
1:B:393:GLN:CG	1:C:393:GLN:HE22	2.32	0.42
1:D:84:ARG:HG2	1:D:126:TRP:CZ3	2.54	0.42
1:D:86:ASP:O	1:D:343:ILE:HD12	2.19	0.42
1:D:120:PRO:HB3	1:D:179:TYR:CG	2.54	0.42
1:A:207:ALA:HB1	1:A:211:ARG:NH2	2.35	0.42
1:A:418:TYR:CE2	1:A:423:LEU:HD21	2.55	0.42
1:B:43:VAL:HG23	1:B:354:LYS:HE2	2.02	0.42
1:D:131:LYS:CE	1:D:183:GLN:HG3	2.47	0.42
1:D:325:LEU:HD12	1:D:325:LEU:HA	1.68	0.42
1:A:311:ASP:OD1	1:D:310:ASP:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:LYS:O	1:D:124:LYS:HG2	2.18	0.42
1:A:30:ASP:HB3	1:A:33:GLU:HB3	2.01	0.42
1:A:207:ALA:HB3	1:A:208:PRO:CD	2.35	0.42
1:B:63:LEU:CD1	1:B:68:GLN:HA	2.49	0.42
1:C:420:LYS:O	1:C:424:SER:OG	2.28	0.42
1:D:254:MET:HE3	1:D:258:THR:CG2	2.49	0.42
1:A:89:GLN:NE2	1:A:89:GLN:HA	2.35	0.42
1:A:314:GLN:HE22	1:A:359:ARG:HD3	1.85	0.42
1:B:240:ILE:CD1	1:D:240:ILE:HD13	2.50	0.42
1:B:272:HIS:HB3	1:B:273:PRO:HD2	2.02	0.42
1:C:49:GLN:NE2	1:C:336:PHE:HA	2.35	0.42
1:D:86:ASP:HB3	1:D:343:ILE:CD1	2.45	0.42
1:A:79:ASN:ND2	1:A:79:ASN:C	2.78	0.42
1:A:213:LEU:HD11	1:A:260:ARG:NH2	2.35	0.42
1:A:213:LEU:CD1	1:A:256:TYR:HE1	2.32	0.42
1:B:105:ILE:HG23	1:B:142:SER:CB	2.49	0.42
1:C:170:CYS:O	1:C:174:ARG:HG3	2.19	0.42
1:D:383:LEU:O	1:D:384:LEU:C	2.60	0.42
1:A:94:ILE:HD11	1:A:347:VAL:HA	2.02	0.42
1:A:96:GLY:O	1:A:98:LYS:HE2	2.20	0.42
1:A:97:PRO:C	1:A:98:LYS:HG2	2.45	0.42
1:A:124:LYS:HE3	1:A:128:GLU:OE2	2.20	0.42
1:C:265:CYS:HA	1:C:292:LEU:O	2.20	0.42
1:D:18:GLU:O	1:D:19:LEU:C	2.62	0.42
1:A:46:HIS:NE2	1:A:49:GLN:HB2	2.34	0.42
1:A:49:GLN:NE2	1:A:335:PHE:CD1	2.81	0.42
1:A:111:THR:HG23	4:A:1648:HOH:O	2.19	0.42
1:A:204:ASP:CG	1:B:369:ARG:NH1	2.77	0.42
1:A:234:GLU:OE2	1:A:267:ASP:HB2	2.20	0.42
1:A:405:THR:CG2	1:A:406:PRO:CD	2.98	0.42
1:A:418:TYR:O	1:A:421:GLU:OE1	2.37	0.42
1:B:100:LEU:HD12	1:B:101:ASN:H	1.85	0.42
1:B:280:LYS:O	1:B:281:ILE:C	2.61	0.42
1:D:79:ASN:ND2	1:D:79:ASN:C	2.78	0.42
1:D:153:PHE:CD2	1:D:196:ASP:HB3	2.54	0.42
1:D:408:GLY:O	1:D:411:TRP:HD1	2.02	0.42
1:A:325:LEU:HA	1:A:325:LEU:HD12	1.59	0.42
1:B:96:GLY:HA3	1:B:97:PRO:HD2	1.82	0.42
1:B:369:ARG:CG	1:B:369:ARG:HH11	2.32	0.42
1:C:22:GLN:O	1:C:25:ALA:N	2.52	0.42
1:C:169:HIS:O	1:C:173:SER:OG	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:SER:OG	1:C:305:HIS:ND1	2.45	0.42
1:D:184:LEU:HD23	1:D:184:LEU:HA	1.66	0.42
1:D:297:ARG:HE	1:D:308:LEU:HG	1.84	0.42
1:A:119:LYS:HB3	1:A:120:PRO:CD	2.49	0.41
1:B:148:LEU:HD23	1:B:148:LEU:HA	1.91	0.41
1:C:102:LEU:O	1:C:139:PHE:HA	2.20	0.41
1:C:301:TRP:O	1:C:303:SER:N	2.52	0.41
2:A:1460:RNT:H4	2:A:1460:RNT:H11	1.92	0.41
1:B:52:ASP:C	1:B:53:VAL:HG23	2.46	0.41
1:B:301:TRP:CE2	1:B:303:SER:HB3	2.55	0.41
1:C:38:LEU:HD12	1:C:38:LEU:HA	1.88	0.41
1:C:100:LEU:HD21	1:C:102:LEU:HD21	2.02	0.41
1:D:166:TRP:O	1:D:167:ILE:C	2.63	0.41
1:A:38:LEU:HG	1:A:399:TYR:CZ	2.55	0.41
1:A:120:PRO:HB3	1:A:179:TYR:CG	2.55	0.41
1:B:37:GLN:CB	1:B:361:LEU:HD22	2.50	0.41
1:B:156:SER:O	1:B:211:ARG:HD2	2.19	0.41
1:B:323:HIS:O	1:B:324:ASP:C	2.63	0.41
1:C:146:HIS:CG	1:C:147:PRO:CD	3.03	0.41
1:B:15:GLN:OE1	1:C:19:LEU:HD21	2.21	0.41
1:C:115:ARG:HB2	1:C:165:PHE:HZ	1.86	0.41
1:C:131:LYS:O	1:C:134:GLN:NE2	2.53	0.41
1:D:79:ASN:HD22	1:D:79:ASN:C	2.28	0.41
1:A:297:ARG:HA	1:A:298:PRO:HD2	1.94	0.41
1:B:285:MET:HE3	1:B:328:ARG:NH2	2.35	0.41
1:C:46:HIS:ND1	1:C:46:HIS:N	2.63	0.41
1:C:119:LYS:HB3	1:C:120:PRO:HD2	2.03	0.41
1:D:23:ARG:O	1:D:27:VAL:HG13	2.21	0.41
1:D:46:HIS:HA	1:D:101:ASN:HB3	2.02	0.41
1:A:119:LYS:HA	1:A:120:PRO:HD3	1.73	0.41
1:C:79:ASN:ND2	1:C:79:ASN:C	2.78	0.41
1:D:29:ILE:HD13	1:D:29:ILE:HA	1.88	0.41
1:A:210:GLN:HG3	1:B:286:LEU:HD21	2.01	0.41
1:B:12:GLN:NE2	1:C:22:GLN:NE2	2.55	0.41
1:B:240:ILE:CD1	1:D:240:ILE:CD1	2.98	0.41
1:D:53:VAL:HA	1:D:106:TYR:OH	2.20	0.41
1:D:267:ASP:HB2	1:D:294:HIS:HB2	2.02	0.41
1:A:75:GLY:O	1:A:426:ARG:HD2	2.21	0.41
1:A:111:THR:HG23	1:A:111:THR:H	1.46	0.41
1:A:114:SER:OG	1:A:116:ASP:OD1	2.28	0.41
1:A:125:ASN:O	1:A:128:GLU:HG2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LYS:HG3	1:A:270:HIS:CE1	2.54	0.41
1:A:396:TRP:O	1:A:397:GLU:C	2.63	0.41
1:B:35:LEU:HD22	1:B:399:TYR:HD1	1.86	0.41
1:C:99:ARG:HH12	1:C:186:THR:HG23	1.83	0.41
1:C:137:LEU:HB3	1:C:180:PHE:CD2	2.56	0.41
1:C:170:CYS:O	1:C:171:LYS:C	2.62	0.41
1:D:105:ILE:HG13	1:D:106:TYR:CD1	2.56	0.41
1:D:124:LYS:NZ	1:D:125:ASN:ND2	2.69	0.41
1:D:325:LEU:HB3	1:D:329:VAL:HG23	2.03	0.41
1:A:78:ARG:CZ	1:A:426:ARG:HB2	2.51	0.41
1:A:104:ALA:C	1:A:106:TYR:N	2.78	0.41
1:A:118:ILE:O	1:A:119:LYS:HG3	2.20	0.41
1:A:199:LYS:HE3	1:C:70:THR:OG1	2.21	0.41
1:B:213:LEU:HD11	1:B:260:ARG:NH2	2.35	0.41
1:C:201:ILE:H	1:C:201:ILE:HG12	1.60	0.41
1:D:270:HIS:CE1	2:D:4460:RNT:O2	2.74	0.41
1:A:146:HIS:HA	1:A:147:PRO:HD3	1.92	0.40
1:B:367:GLU:HG2	4:B:2706:HOH:O	2.21	0.40
1:A:37:GLN:CB	1:A:361:LEU:HD22	2.51	0.40
1:A:137:LEU:HB2	1:A:184:LEU:CD1	2.51	0.40
1:B:204:ASP:HA	4:B:2618:HOH:O	2.21	0.40
1:B:276:VAL:HB	1:B:312:GLU:OE2	2.21	0.40
1:C:177:SER:OG	1:C:188:SER:OG	2.30	0.40
1:C:373:ALA:CB	1:C:374:PRO:CD	2.98	0.40
1:D:40:ARG:C	1:D:41:LEU:HG	2.46	0.40
1:A:141:PRO:HB3	1:A:173:SER:OG	2.22	0.40
1:B:200:ASP:HA	1:B:244:SER:OG	2.21	0.40
1:C:255:GLY:HA3	1:D:287:TYR:CD1	2.57	0.40
1:C:323:HIS:CE1	1:D:206:LEU:HB3	2.56	0.40
1:C:406:PRO:HB3	1:C:410:GLU:OE1	2.22	0.40
1:D:144:PHE:CD1	1:D:144:PHE:N	2.89	0.40
1:A:58:ASN:N	1:A:59:PRO:HD3	2.36	0.40
1:A:104:ALA:C	1:A:106:TYR:H	2.28	0.40
1:A:270:HIS:CE1	2:A:1460:RNT:O2	2.74	0.40
1:A:368:LEU:HD21	1:A:383:LEU:HB3	2.03	0.40
1:B:127:VAL:HG12	1:B:131:LYS:HE3	2.04	0.40
1:B:182:GLU:HG3	1:B:228:HIS:CE1	2.56	0.40
1:C:119:LYS:O	1:C:122:HIS:N	2.49	0.40
1:D:107:LEU:N	1:D:107:LEU:CD2	2.83	0.40
1:D:271:PHE:HB3	1:D:275:GLU:CG	2.52	0.40
1:A:79:ASN:ND2	1:A:81:SER:N	2.65	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:HD12	1:A:83:LEU:HA	1.90	0.40
1:A:87:LEU:HD21	1:A:100:LEU:CD1	2.52	0.40
1:A:267:ASP:CB	1:A:294:HIS:HB2	2.51	0.40
1:B:373:ALA:CB	1:B:374:PRO:HD2	2.44	0.40
1:C:23:ARG:HH11	1:C:23:ARG:HD3	1.63	0.40
1:C:74:PRO:HA	4:C:3630:HOH:O	2.21	0.40
1:C:236:LYS:HE3	1:C:302:ASP:OD2	2.22	0.40
1:D:225:ASN:OD1	1:D:226:PRO:HD2	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:3475:HOH:O	4:C:3475:HOH:O[2_556]	1.99	0.21
4:C:3481:HOH:O	4:C:3481:HOH:O[2_556]	2.15	0.05

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	415/426 (97%)	383 (92%)	32 (8%)	0	100	100
1	B	414/426 (97%)	386 (93%)	23 (6%)	5 (1%)	10	8
1	C	414/426 (97%)	387 (94%)	23 (6%)	4 (1%)	12	11
1	D	414/426 (97%)	384 (93%)	26 (6%)	4 (1%)	12	11
All	All	1657/1704 (97%)	1540 (93%)	104 (6%)	13 (1%)	16	16

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	62	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	62	SER
1	B	61	GLY
1	B	59	PRO
1	C	61	GLY
1	C	62	SER
1	D	59	PRO
1	D	61	GLY
1	B	325	LEU
1	D	420	LYS
1	C	201	ILE
1	B	53	VAL
1	C	53	VAL

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	352/359 (98%)	311 (88%)	41 (12%)	5	5
1	B	351/359 (98%)	315 (90%)	36 (10%)	7	7
1	C	351/359 (98%)	321 (92%)	30 (8%)	10	11
1	D	351/359 (98%)	314 (90%)	37 (10%)	6	6
All	All	1405/1436 (98%)	1261 (90%)	144 (10%)	7	7

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	11	THR
1	A	53	VAL
1	A	57	GLU
1	A	60	GLU
1	A	62	SER
1	A	63	LEU
1	A	64	THR
1	A	70	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	79	ASN
1	A	81	SER
1	A	89	GLN
1	A	98	LYS
1	A	103	HIS
1	A	107	LEU
1	A	111	THR
1	A	117	GLN
1	A	119	LYS
1	A	121	GLU
1	A	124	LYS
1	A	140	ASN
1	A	162	ILE
1	A	171	LYS
1	A	188	SER
1	A	213	LEU
1	A	244	SER
1	A	290	GLN
1	A	324	ASP
1	A	325	LEU
1	A	336	PHE
1	A	342	ARG
1	A	343	ILE
1	A	359	ARG
1	A	369	ARG
1	A	374	PRO
1	A	409	SER
1	A	410	GLU
1	A	420	LYS
1	A	421	GLU
1	A	422	ILE
1	A	426	ARG
1	B	11	THR
1	B	13	LEU
1	B	23	ARG
1	B	53	VAL
1	B	63	LEU
1	B	76	LYS
1	B	81	SER
1	B	92	ARG
1	B	98	LYS
1	B	103	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	105	ILE
1	B	111	THR
1	B	117	GLN
1	B	121	GLU
1	B	161	SER
1	B	171	LYS
1	B	182	GLU
1	B	186	THR
1	B	188	SER
1	B	194	ILE
1	B	213	LEU
1	B	223	LYS
1	B	259	SER
1	B	290	GLN
1	B	324	ASP
1	B	325	LEU
1	B	343	ILE
1	B	346	TRP
1	B	374	PRO
1	B	393	GLN
1	B	410	GLU
1	B	413	GLU
1	B	414	SER
1	B	420	LYS
1	B	421	GLU
1	B	422	ILE
1	C	11	THR
1	C	27	VAL
1	C	53	VAL
1	C	54	SER
1	C	57	GLU
1	C	60	GLU
1	C	63	LEU
1	C	78	ARG
1	C	98	LYS
1	C	100	LEU
1	C	103	HIS
1	C	111	THR
1	C	119	LYS
1	C	134	GLN
1	C	140	ASN
1	C	188	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	192	ILE
1	C	196	ASP
1	C	244	SER
1	C	290	GLN
1	C	324	ASP
1	C	325	LEU
1	C	346	TRP
1	C	369	ARG
1	C	370	LYS
1	C	374	PRO
1	C	383	LEU
1	C	410	GLU
1	C	420	LYS
1	C	426	ARG
1	D	11	THR
1	D	14	GLU
1	D	27	VAL
1	D	53	VAL
1	D	57	GLU
1	D	62	SER
1	D	64	THR
1	D	76	LYS
1	D	79	ASN
1	D	89	GLN
1	D	98	LYS
1	D	103	HIS
1	D	110	ASP
1	D	111	THR
1	D	124	LYS
1	D	131	LYS
1	D	140	ASN
1	D	142	SER
1	D	161	SER
1	D	171	LYS
1	D	186	THR
1	D	188	SER
1	D	196	ASP
1	D	223	LYS
1	D	240	ILE
1	D	258	THR
1	D	324	ASP
1	D	325	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	336	PHE
1	D	340	ILE
1	D	370	LYS
1	D	374	PRO
1	D	409	SER
1	D	410	GLU
1	D	420	LYS
1	D	421	GLU
1	D	425	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	37	GLN
1	A	49	GLN
1	A	68	GLN
1	A	79	ASN
1	A	89	GLN
1	A	122	HIS
1	A	125	ASN
1	A	134	GLN
1	A	169	HIS
1	A	314	GLN
1	A	387	GLN
1	B	49	GLN
1	B	58	ASN
1	B	79	ASN
1	B	117	GLN
1	B	122	HIS
1	B	140	ASN
1	B	169	HIS
1	B	228	HIS
1	B	314	GLN
1	B	387	GLN
1	C	15	GLN
1	C	22	GLN
1	C	49	GLN
1	C	58	ASN
1	C	68	GLN
1	C	79	ASN
1	C	122	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	125	ASN
1	C	134	GLN
1	C	140	ASN
1	C	169	HIS
1	C	272	HIS
1	C	314	GLN
1	C	387	GLN
1	C	401	GLN
1	D	49	GLN
1	D	79	ASN
1	D	89	GLN
1	D	122	HIS
1	D	125	ASN
1	D	134	GLN
1	D	169	HIS
1	D	314	GLN
1	D	387	GLN
1	D	403	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
2	RNT	B	2460	3	10,10,10	0.93	0	13,13,13	1.31	2 (15%)
2	RNT	D	4460	3	10,10,10	1.07	1 (10%)	13,13,13	0.94	0
2	RNT	A	1460	3	10,10,10	0.83	0	13,13,13	1.20	1 (7%)
2	RNT	C	3460	3	10,10,10	1.10	1 (10%)	13,13,13	1.32	2 (15%)

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
2	RNT	B	2460	3	-	6/14/14/14	-
2	RNT	D	4460	3	-	6/14/14/14	-
2	RNT	A	1460	3	-	6/14/14/14	-
2	RNT	C	3460	3	-	6/14/14/14	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3460	RNT	C2-C3	2.45	1.57	1.53
2	D	4460	RNT	C4-C3	2.12	1.57	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2460	RNT	O3-C3-C2	2.83	115.37	108.93
2	C	3460	RNT	C6-C5-C4	2.71	115.43	112.11
2	B	2460	RNT	C1-C2-C3	2.52	117.31	112.17
2	C	3460	RNT	C1-C2-C3	2.41	117.08	112.17
2	A	1460	RNT	C1-C2-C3	2.32	116.89	112.17

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1460	RNT	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1460	RNT	C1-C2-C3-C4
2	A	1460	RNT	O2-C2-C3-C4
2	A	1460	RNT	O2-C2-C3-O3
2	B	2460	RNT	C1-C2-C3-C4
2	B	2460	RNT	O2-C2-C3-C4
2	B	2460	RNT	O2-C2-C3-O3
2	C	3460	RNT	C1-C2-C3-C4
2	C	3460	RNT	C1-C2-C3-O3
2	C	3460	RNT	O2-C2-C3-C4
2	C	3460	RNT	O2-C2-C3-O3
2	D	4460	RNT	C1-C2-C3-C4
2	D	4460	RNT	O2-C2-C3-C4
2	D	4460	RNT	O2-C2-C3-O3
2	A	1460	RNT	O1-C1-C2-O2
2	A	1460	RNT	C1-C2-C3-O3
2	B	2460	RNT	C1-C2-C3-O3
2	D	4460	RNT	C1-C2-C3-O3
2	B	2460	RNT	O1-C1-C2-C3
2	C	3460	RNT	O1-C1-C2-C3
2	D	4460	RNT	O1-C1-C2-C3
2	B	2460	RNT	O1-C1-C2-O2
2	D	4460	RNT	O1-C1-C2-O2
2	C	3460	RNT	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2460	RNT	1	0
2	D	4460	RNT	1	0
2	A	1460	RNT	4	0
2	C	3460	RNT	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	417/426 (97%)	-0.59	0	100 100	11, 25, 55, 94	0
1	B	416/426 (97%)	-0.64	0	100 100	13, 24, 48, 84	0
1	C	416/426 (97%)	-0.62	1 (0%)	91 90	12, 24, 49, 97	0
1	D	416/426 (97%)	-0.51	1 (0%)	91 90	12, 27, 57, 93	0
All	All	1665/1704 (97%)	-0.59	2 (0%)	92 90	11, 25, 52, 97	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	61	GLY	4.4
1	C	61	GLY	2.6

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
2	RNT	C	3460	11/11	0.93	0.09	22,25,37,42	0
2	RNT	D	4460	11/11	0.93	0.08	21,22,34,40	0
2	RNT	A	1460	11/11	0.94	0.08	25,26,40,44	0
2	RNT	B	2460	11/11	0.95	0.09	19,23,35,39	0
3	ZN	B	450	1/1	0.99	0.03	35,35,35,35	0
3	ZN	D	450	1/1	0.99	0.03	34,34,34,34	0
3	ZN	C	450	1/1	1.00	0.02	33,33,33,33	0
3	ZN	A	450	1/1	1.00	0.03	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.