



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:51 PM UTC

PDB ID : 8IGU / pdb_00008igu
Title : Hexameric Ring Complex of Engineered V1-ATPase: A3(De)3_empty
Authors : Kosugi, T.; Tanabe, M.; Koga, N.
Deposited on : 2023-02-21
Resolution : 2.77 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
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

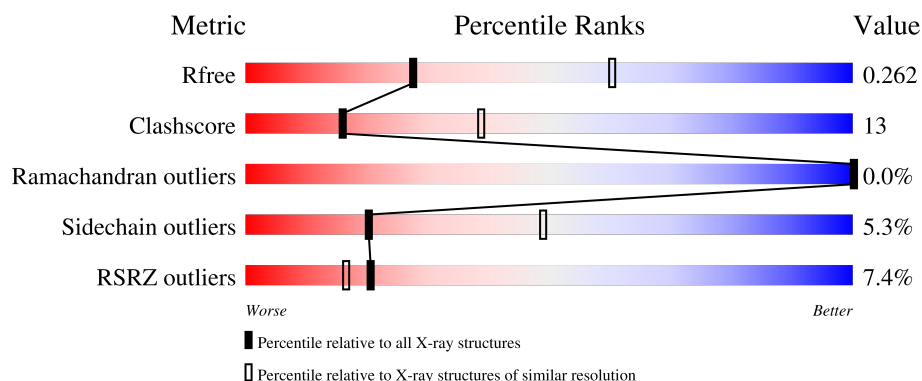
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	596	0% 80% 18% .
1	B	596	3% 66% 31% ..
1	C	596	5% 62% 31% 5% .
2	D	458	10% 65% 26% . 6%
2	E	458	19% 68% 25% 5% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	458	10% 67% 27% ••

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24292 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 V-type sodium ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	0	0
			4562	2866	766	904	26			
1	B	586	Total	C	N	O	S	0	0	0
			4562	2866	766	904	26			
1	C	584	Total	C	N	O	S	0	1	0
			4560	2864	768	902	26			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q08636
A	-1	SER	-	expression tag	UNP Q08636
A	0	GLY	-	expression tag	UNP Q08636
B	-2	SER	-	expression tag	UNP Q08636
B	-1	SER	-	expression tag	UNP Q08636
B	0	GLY	-	expression tag	UNP Q08636
C	-2	SER	-	expression tag	UNP Q08636
C	-1	SER	-	expression tag	UNP Q08636
C	0	GLY	-	expression tag	UNP Q08636

- Molecule 2 is a protein called V-type sodium ATPase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	432	Total	C	N	O	S	0	0	0
			3369	2134	576	646	13			
2	E	449	Total	C	N	O	S	0	0	0
			3509	2224	601	670	14			
2	F	445	Total	C	N	O	S	0	0	0
			3477	2204	597	662	14			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	151	GLY	SER	engineered mutation	UNP Q08637
D	152	PRO	GLY	engineered mutation	UNP Q08637
D	153	PRO	SER	engineered mutation	UNP Q08637
D	155	ALA	LEU	engineered mutation	UNP Q08637
D	156	GLY	PRO	engineered mutation	UNP Q08637
D	157	LYS	HIS	engineered mutation	UNP Q08637
D	158	SER	LYS	engineered mutation	UNP Q08637
D	159	ALA	GLU	engineered mutation	UNP Q08637
D	248	GLU	THR	engineered mutation	UNP Q08637
D	339	SER	GLN	engineered mutation	UNP Q08637
E	151	GLY	SER	engineered mutation	UNP Q08637
E	152	PRO	GLY	engineered mutation	UNP Q08637
E	153	PRO	SER	engineered mutation	UNP Q08637
E	155	ALA	LEU	engineered mutation	UNP Q08637
E	156	GLY	PRO	engineered mutation	UNP Q08637
E	157	LYS	HIS	engineered mutation	UNP Q08637
E	158	SER	LYS	engineered mutation	UNP Q08637
E	159	ALA	GLU	engineered mutation	UNP Q08637
E	248	GLU	THR	engineered mutation	UNP Q08637
E	339	SER	GLN	engineered mutation	UNP Q08637
F	151	GLY	SER	engineered mutation	UNP Q08637
F	152	PRO	GLY	engineered mutation	UNP Q08637
F	153	PRO	SER	engineered mutation	UNP Q08637
F	155	ALA	LEU	engineered mutation	UNP Q08637
F	156	GLY	PRO	engineered mutation	UNP Q08637
F	157	LYS	HIS	engineered mutation	UNP Q08637
F	158	SER	LYS	engineered mutation	UNP Q08637
F	159	ALA	GLU	engineered mutation	UNP Q08637
F	248	GLU	THR	engineered mutation	UNP Q08637
F	339	SER	GLN	engineered mutation	UNP Q08637

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	99	Total O 99 99	0	0
3	B	35	Total O 35 35	0	0
3	C	47	Total O 47 47	0	0
3	D	22	Total O 22 22	0	0
3	E	30	Total O 30 30	0	0

Continued on next page...

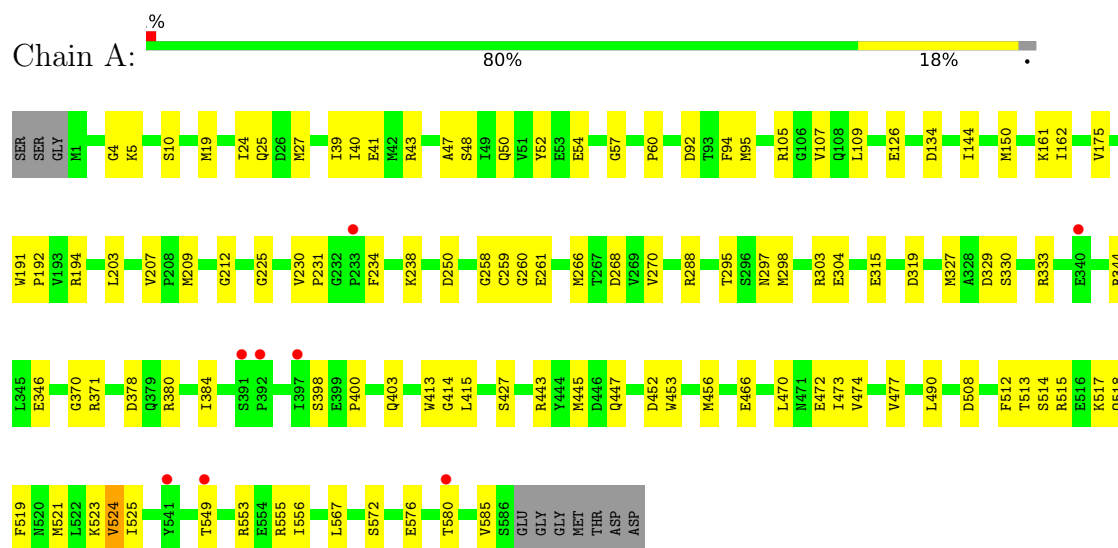
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	20	Total	O	0	0
			20	20		

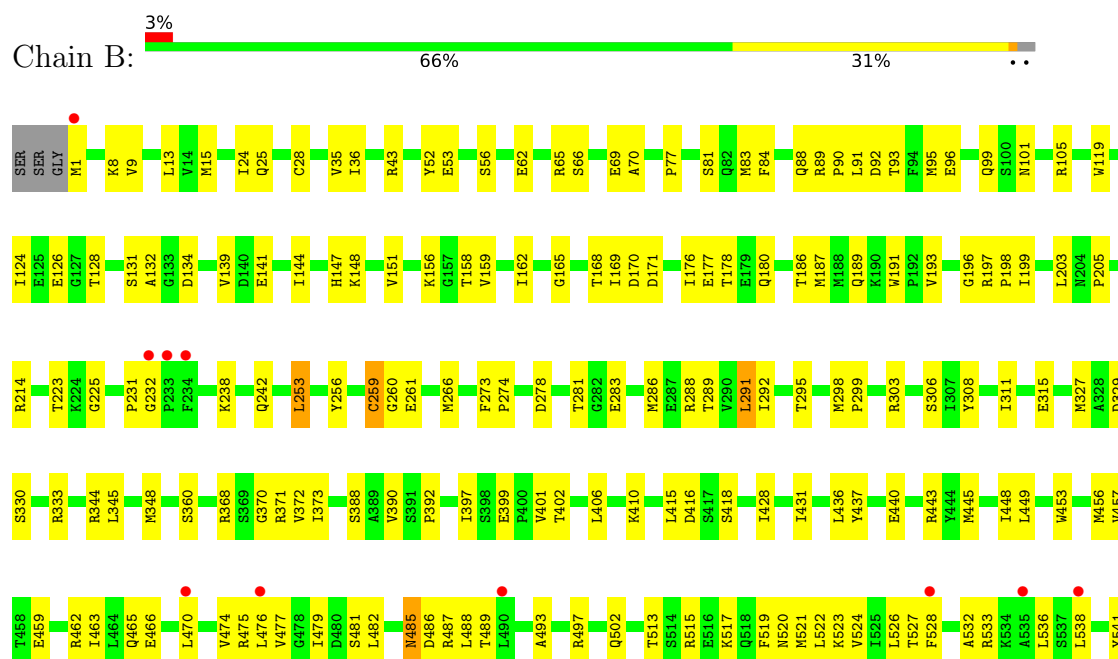
3 Residue-property plots

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: V-type sodium ATPase catalytic subunit A

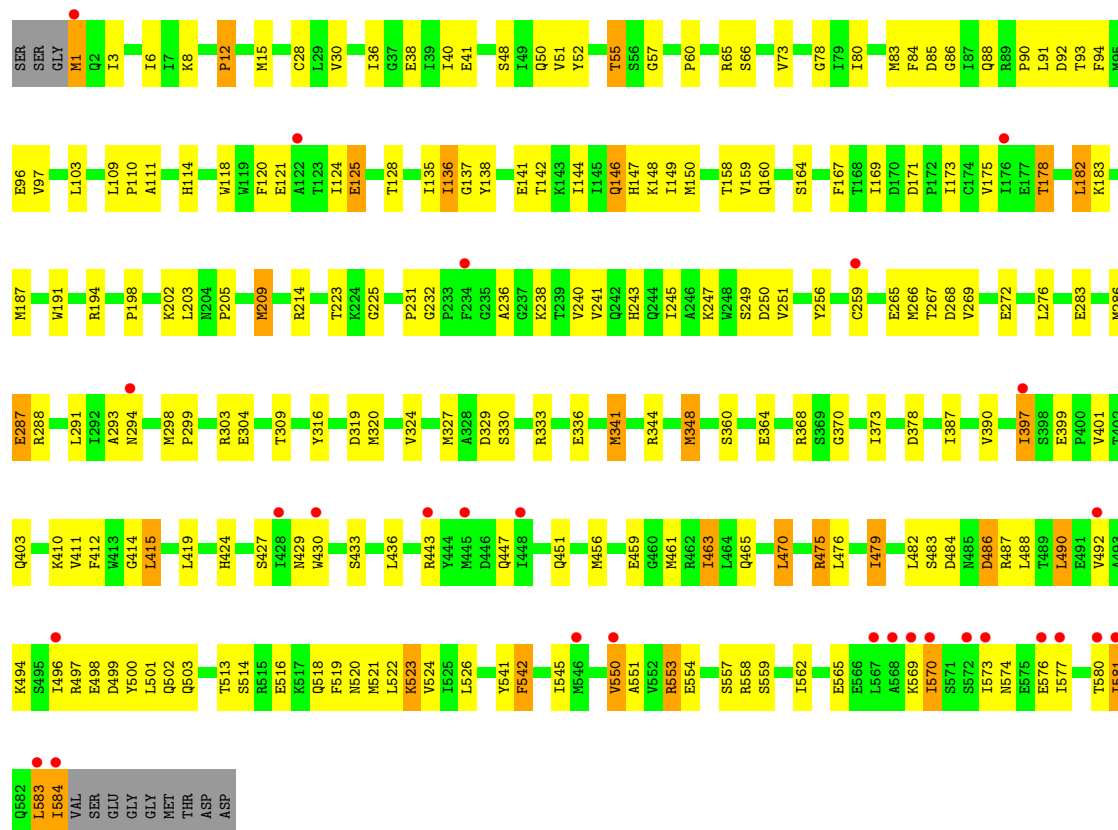


- Molecule 1: V-type sodium ATPase catalytic subunit A

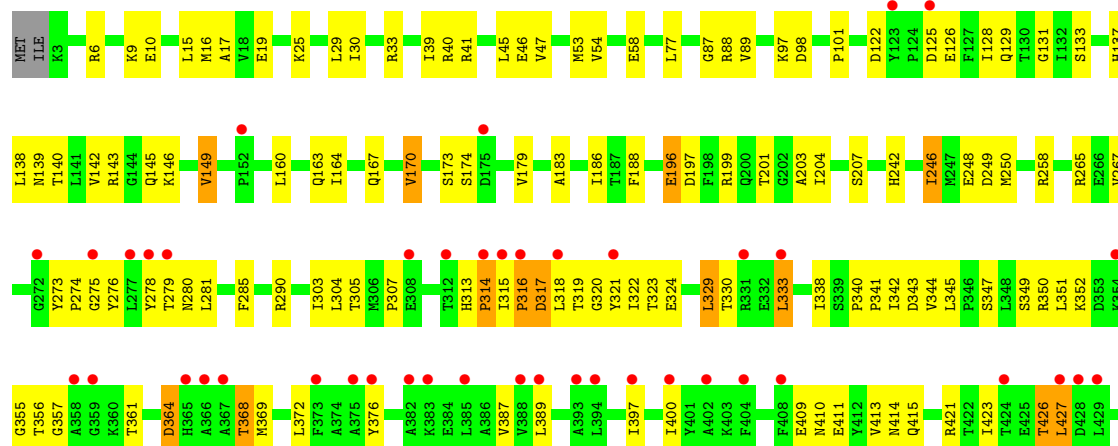


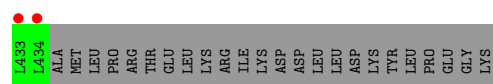


• Molecule 1: V-type sodium ATPase catalytic subunit A

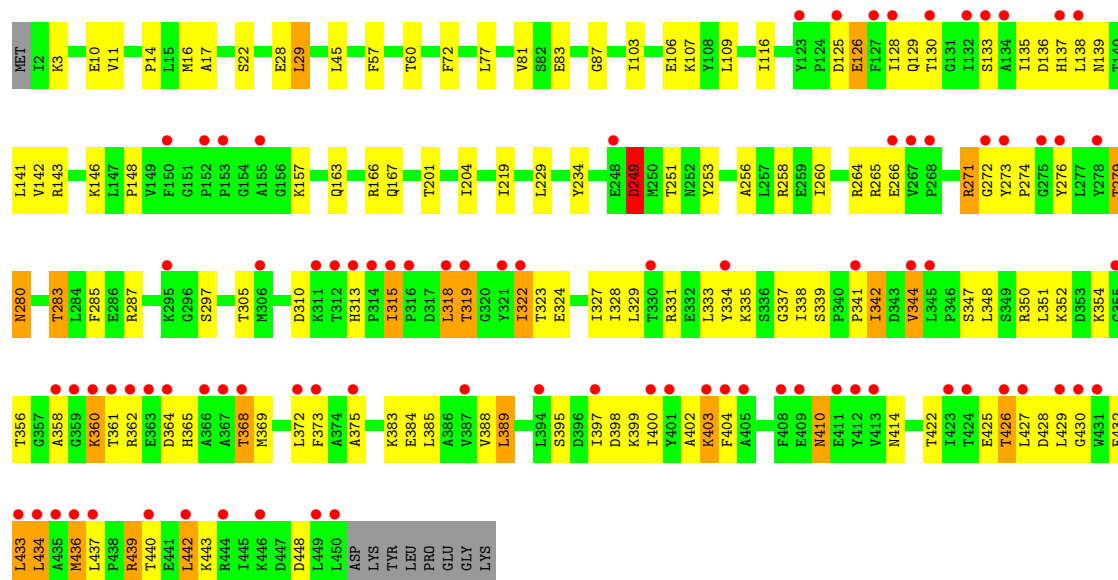


• Molecule 2: V-type sodium ATPase subunit B

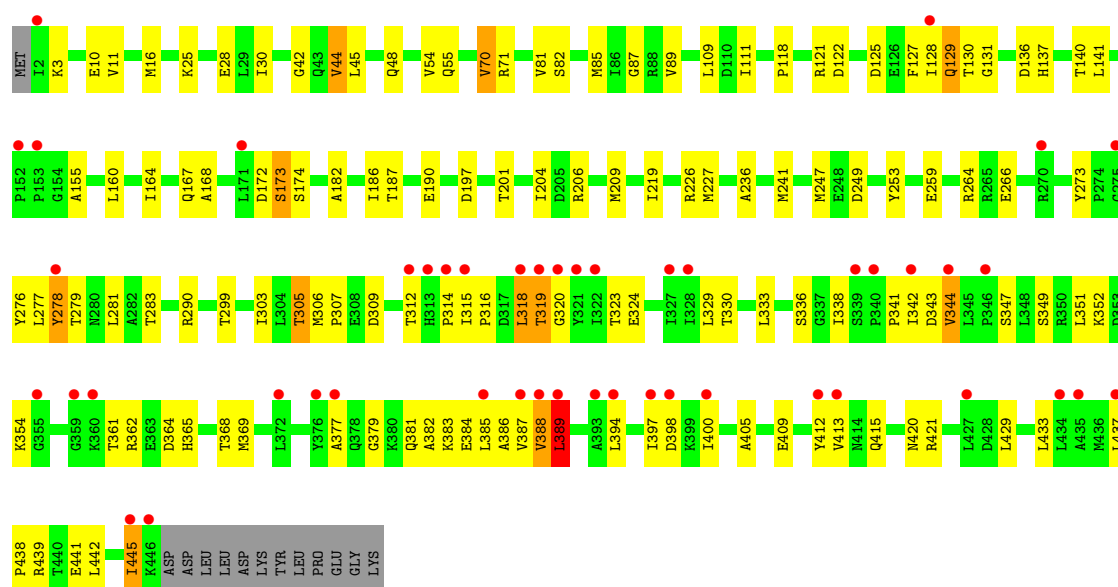




• Molecule 2: V-type sodium ATPase subunit B



• Molecule 2: V-type sodium ATPase subunit B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.45Å 122.65Å 128.70Å 90.00° 90.74° 90.00°	Depositor
Resolution (Å)	44.64 – 2.77 44.64 – 2.77	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.64-2.77) 99.9 (44.64-2.77)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.216 , 0.262 0.219 , 0.262	Depositor DCC
R_{free} test set	4712 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.007 for -h,-l,-k 0.000 for -l,k,h 0.000 for -k,-h,-l 0.000 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k 0.000 for l,-h,-k 0.000 for -k,-l,h 0.015 for h,-k,-l 0.011 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24292	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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

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	0.30	1/4638 (0.0%)	0.53	0/6275
1	B	0.22	0/4638	0.50	1/6275 (0.0%)
1	C	0.30	0/4636	0.60	6/6271 (0.1%)
2	D	0.26	0/3429	0.60	4/4637 (0.1%)
2	E	0.29	0/3570	0.64	5/4826 (0.1%)
2	F	0.32	0/3538	0.70	4/4782 (0.1%)
All	All	0.28	1/24449 (0.0%)	0.59	20/33066 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	PHE	C-O	-5.12	1.18	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	388	VAL	CB-CA-C	-15.76	85.45	111.29
2	F	389	LEU	N-CA-CB	11.41	129.77	110.49
2	D	314	PRO	N-CA-C	-9.65	94.72	110.74
2	E	439	ARG	CB-CA-C	8.29	127.81	110.32
2	D	174	SER	N-CA-C	-8.00	101.34	112.45
1	C	287	GLU	CB-CA-C	7.75	123.60	110.74
1	C	288	ARG	N-CA-C	7.41	121.73	113.21
2	F	389	LEU	N-CA-C	-7.03	95.83	110.80
1	B	437	TYR	N-CA-C	6.73	121.09	113.01
1	C	288	ARG	N-CA-CB	-6.71	100.84	110.57
2	E	440	THR	N-CA-C	6.60	124.86	110.80
1	C	523	LYS	CA-CB-CG	6.49	127.08	114.10
2	E	249	ASP	N-CA-C	6.13	118.08	110.91
2	F	264	ARG	N-CA-C	5.73	120.04	112.25
1	C	553	ARG	CB-CG-CD	-5.59	98.45	111.30
1	C	550	VAL	CA-CB-CG1	-5.55	100.97	110.40
2	E	266	GLU	N-CA-C	5.42	118.23	111.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	272	GLY	N-CA-C	-5.28	108.72	115.42
2	D	173	SER	CB-CA-C	-5.15	104.28	111.80
2	D	316	PRO	CB-CA-C	-5.04	104.31	112.62

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	4562	0	4528	67	1
1	B	4562	0	4528	124	0
1	C	4560	0	4526	148	0
2	D	3369	0	3377	103	0
2	E	3509	0	3535	103	0
2	F	3477	0	3507	107	0
3	A	99	0	0	1	0
3	B	35	0	0	3	0
3	C	47	0	0	3	0
3	D	22	0	0	1	0
3	E	30	0	0	1	0
3	F	20	0	0	2	0
All	All	24292	0	24001	634	1

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 13.

All (634) 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)
2:E:333:LEU:HB3	2:E:338:ILE:HG21	1.43	0.99
2:F:388:VAL:HG12	2:F:388:VAL:O	1.63	0.94
2:E:434:LEU:HA	2:E:437:LEU:HD23	1.47	0.94
2:F:128:ILE:HD12	2:F:141:LEU:HG	1.52	0.91
1:C:570:ILE:O	1:C:573:ILE:HG12	1.71	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:GLY:HA3	1:C:238:LYS:HE2	1.54	0.89
2:F:388:VAL:O	2:F:389:LEU:HD23	1.75	0.86
1:C:203:LEU:HD11	1:C:373:ILE:HG13	1.55	0.86
1:B:555:ARG:NH2	1:B:576:GLU:OE1	2.11	0.83
2:E:333:LEU:CB	2:E:338:ILE:HG21	2.01	0.83
1:C:173:ILE:HD13	1:C:187:MET:HG3	1.61	0.83
1:B:56:SER:O	1:B:105:ARG:NH2	2.11	0.82
2:D:313:HIS:HB3	2:D:314:PRO:HD2	1.61	0.80
2:E:166:ARG:HD3	2:E:201:THR:HG21	1.63	0.80
1:C:461:MET:HG3	1:C:465:GLN:HE21	1.46	0.80
2:F:130:THR:OG1	2:F:136:ASP:OD1	1.99	0.79
1:B:62:GLU:OE2	3:B:601:HOH:O	2.01	0.78
1:B:573:ILE:O	1:B:577:ILE:HG13	1.84	0.78
1:B:77:PRO:HG2	1:B:187:MET:HE2	1.66	0.77
1:C:503:GLN:NE2	3:C:601:HOH:O	2.11	0.76
1:B:281:THR:HG23	1:B:283:GLU:H	1.51	0.76
1:B:242:GLN:HB3	1:B:327:MET:HE1	1.67	0.76
2:E:338:ILE:HG23	2:E:341:PRO:HB3	1.66	0.76
2:E:422:THR:HG22	2:E:425:GLU:HG3	1.69	0.75
2:F:323:THR:OG1	3:F:501:HOH:O	2.05	0.74
2:E:337:GLY:O	2:E:414:ASN:ND2	2.20	0.74
1:C:124:ILE:HD11	1:C:159:VAL:HG11	1.68	0.74
1:B:485:ASN:HD21	1:B:533:ARG:HG3	1.53	0.73
2:D:25:LYS:NZ	3:D:501:HOH:O	2.21	0.73
2:E:404:PHE:CE1	2:E:433:LEU:HD21	2.23	0.73
1:B:83:MET:HE2	1:B:291:LEU:HD22	1.70	0.73
1:B:43:ARG:HG2	2:F:10:GLU:HG3	1.70	0.73
1:C:429:ASN:O	1:C:433:SER:OG	2.07	0.73
1:C:52:TYR:O	1:C:299:PRO:HB3	1.88	0.72
1:A:107:VAL:HG12	1:A:109:LEU:CD1	2.20	0.72
1:A:10:SER:HB2	2:D:46:GLU:HG3	1.70	0.72
2:F:314:PRO:O	2:F:318:LEU:HB2	1.90	0.72
2:F:277:LEU:O	2:F:277:LEU:HD12	1.88	0.72
2:E:361:THR:HG21	2:E:365:HIS:ND1	2.05	0.71
2:E:258:ARG:HG2	2:E:274:PRO:HD3	1.71	0.71
1:C:298:MET:O	1:C:303:ARG:NH1	2.24	0.71
1:B:486:ASP:O	1:B:489:THR:OG1	2.09	0.70
2:E:106:GLU:OE1	2:E:234:TYR:OH	2.09	0.70
1:A:261:GLU:OE2	1:A:330:SER:N	2.24	0.70
1:C:520:ASN:O	1:C:523:LYS:HB3	1.92	0.70
1:C:573:ILE:HG13	1:C:574:ASN:N	2.06	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:107:LYS:HE2	2:E:109:LEU:HD21	1.75	0.69
1:A:298:MET:O	1:A:303:ARG:NH1	2.26	0.68
2:D:276:TYR:HB2	2:D:279:THR:OG1	1.92	0.68
2:F:312:THR:OG1	2:F:316:PRO:HG2	1.94	0.68
2:E:3:LYS:NZ	2:E:22:SER:O	2.26	0.68
1:A:555:ARG:NH2	1:A:572:SER:OG	2.26	0.68
1:C:461:MET:O	1:C:465:GLN:HG3	1.92	0.68
2:E:11:VAL:HG22	2:E:16:MET:HG2	1.76	0.67
1:B:482:LEU:O	1:B:487:ARG:NH1	2.26	0.67
1:C:86:GLY:N	1:C:294:ASN:HD21	1.92	0.67
1:B:169:ILE:O	1:B:186:THR:OG1	2.13	0.67
1:B:482:LEU:HD23	1:B:487:ARG:HH11	1.60	0.67
2:E:130:THR:OG1	2:E:136:ASP:OD1	2.10	0.67
1:C:51:VAL:HG11	1:C:55:THR:HG23	1.76	0.66
1:B:231:PRO:HA	1:B:390:VAL:HG23	1.77	0.66
2:D:278:TYR:HA	2:D:318:LEU:HD21	1.77	0.66
1:C:80:ILE:HG22	1:C:287:GLU:O	1.96	0.66
1:B:453:TRP:HA	1:B:456:MET:HE3	1.78	0.66
2:D:307:PRO:HA	2:D:313:HIS:CE1	2.31	0.66
1:A:24:ILE:HG22	1:A:25:GLN:HG2	1.77	0.65
1:C:148:LYS:NZ	3:C:602:HOH:O	2.30	0.65
2:E:385:LEU:O	2:E:389:LEU:HB2	1.96	0.65
2:E:138:LEU:HD11	2:E:373:PHE:HD2	1.61	0.65
1:A:346:GLU:HG2	2:D:267:VAL:HG21	1.80	0.64
1:A:517:LYS:O	1:A:521:MET:HG3	1.97	0.64
2:F:439:ARG:HA	2:F:442:LEU:HD21	1.79	0.64
2:D:357:GLY:H	2:D:361:THR:HG22	1.61	0.64
2:F:329:LEU:HD22	2:F:341:PRO:HD2	1.78	0.64
1:B:462:ARG:NH1	1:B:466:GLU:OE1	2.30	0.64
1:C:514:SER:O	1:C:518:GLN:HG3	1.96	0.64
2:F:388:VAL:O	2:F:388:VAL:CG1	2.20	0.64
1:A:194:ARG:NH1	1:A:304:GLU:OE2	2.31	0.64
1:C:3:ILE:CD1	1:C:65:ARG:HD3	2.28	0.64
1:C:80:ILE:CG2	1:C:287:GLU:O	2.46	0.63
2:E:138:LEU:HG	2:E:369:MET:HG3	1.80	0.63
2:F:141:LEU:HD11	2:F:299:THR:HG21	1.79	0.63
1:B:144:ILE:HG21	1:B:288:ARG:HD3	1.81	0.63
2:F:129:GLN:O	2:F:168:ALA:HA	1.97	0.63
2:F:128:ILE:HG22	2:F:129:GLN:N	2.13	0.63
2:D:250:MET:HB2	2:D:304:LEU:HD13	1.79	0.63
1:C:256:TYR:HB3	1:C:291:LEU:HD12	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:VAL:HG13	1:C:551:ALA:N	2.14	0.63
1:B:523:LYS:O	1:B:527:THR:HG23	1.99	0.63
1:C:231:PRO:HA	1:C:390:VAL:O	1.99	0.62
1:B:580:THR:O	1:B:584:ILE:HG13	1.99	0.62
2:D:364:ASP:O	2:D:368:THR:HG22	2.00	0.62
2:F:131:GLY:O	2:F:415:GLN:NE2	2.32	0.62
1:C:333:ARG:NH2	1:C:336:GLU:OE2	2.33	0.62
2:E:265:ARG:NH2	3:E:503:HOH:O	2.33	0.61
2:D:249:ASP:OD2	2:D:305:THR:OG1	2.18	0.61
2:F:172:ASP:O	2:F:174:SER:N	2.32	0.61
1:B:119:TRP:O	3:B:602:HOH:O	2.16	0.61
1:B:397:ILE:HB	1:B:402:THR:HG21	1.83	0.61
2:E:258:ARG:HG2	2:E:273:TYR:HA	1.81	0.61
2:D:356:THR:OG1	2:D:361:THR:HG21	2.00	0.61
2:E:397:ILE:HD12	2:E:400:ILE:HD11	1.82	0.61
2:D:368:THR:O	2:D:372:LEU:HB2	2.01	0.61
2:D:146:LYS:HD2	2:D:285:PHE:O	2.02	0.60
1:A:231:PRO:HG2	1:A:414:GLY:HA2	1.84	0.60
1:C:486:ASP:OD2	1:C:486:ASP:N	2.34	0.60
2:D:143:ARG:HH21	2:D:170:VAL:HG11	1.65	0.60
1:C:497:ARG:O	1:C:502:GLN:HG3	2.00	0.60
2:D:315:ILE:HG22	2:D:317:ASP:OD1	2.01	0.60
1:C:142:THR:HG22	1:C:144:ILE:H	1.67	0.60
1:C:430:TRP:HE3	1:C:430:TRP:H	1.47	0.60
1:C:399:GLU:OE1	1:C:401:VAL:HB	2.00	0.60
2:F:306:MET:HE3	2:F:307:PRO:HD2	1.83	0.60
1:B:273:PHE:HE2	1:B:289:THR:HG21	1.67	0.60
1:C:135:ILE:HD13	1:C:148:LYS:HD3	1.84	0.60
2:F:127:PHE:HE1	2:F:140:THR:HG23	1.66	0.60
2:E:428:ASP:O	2:E:432:GLU:HG2	2.01	0.59
1:A:43:ARG:HG3	2:E:10:GLU:HG3	1.84	0.59
1:C:341:MET:SD	3:C:644:HOH:O	2.57	0.59
2:F:249:ASP:OD1	2:F:305:THR:OG1	2.19	0.59
1:B:541:TYR:H	1:B:544:GLU:HG3	1.67	0.59
1:C:573:ILE:HG13	1:C:574:ASN:H	1.66	0.59
2:D:133:SER:OG	2:D:426:THR:OG1	2.20	0.59
1:C:558:ARG:HH21	1:C:558:ARG:HG3	1.68	0.59
1:C:36:ILE:HG23	1:C:52:TYR:HB2	1.84	0.59
1:B:298:MET:O	1:B:303:ARG:NH1	2.34	0.58
1:B:203:LEU:HB2	1:B:371:ARG:HD3	1.85	0.58
2:D:258:ARG:HA	2:D:274:PRO:HD3	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:368:THR:HG22	2:E:372:LEU:HD11	1.84	0.58
1:B:477:VAL:HG13	1:B:481:SER:HB3	1.85	0.58
1:B:456:MET:HE1	1:B:519:PHE:CE1	2.38	0.58
1:C:124:ILE:CD1	1:C:159:VAL:HG11	2.33	0.58
2:F:320:GLY:O	3:F:501:HOH:O	2.17	0.58
1:C:167:PHE:HB3	1:C:171:ASP:HB2	1.86	0.58
1:A:443:ARG:O	1:A:447:GLN:HG3	2.04	0.58
2:F:387:VAL:HG22	2:F:388:VAL:HG23	1.86	0.58
1:B:532:ALA:O	1:B:536:LEU:HB2	2.03	0.58
1:C:482:LEU:HD12	1:C:483:SER:H	1.69	0.57
1:C:550:VAL:HA	1:C:553:ARG:HH22	1.68	0.57
2:F:122:ASP:HB3	2:F:290:ARG:HB2	1.87	0.57
1:B:126:GLU:HG2	1:B:162:ILE:HG22	1.85	0.57
1:C:348:MET:SD	2:D:265:ARG:HA	2.45	0.57
1:C:475:ARG:HG2	1:C:476:LEU:HD22	1.85	0.57
2:D:364:ASP:OD1	2:D:364:ASP:N	2.31	0.57
1:B:440:GLU:OE1	1:B:443:ARG:NH1	2.37	0.57
1:B:274:PRO:HA	1:B:286:MET:HG2	1.87	0.57
2:E:146:LYS:HE3	2:E:285:PHE:HB3	1.87	0.57
2:F:45:LEU:HD11	2:F:55:GLN:HB2	1.87	0.57
2:F:182:ALA:HB3	2:F:247:MET:HG2	1.86	0.57
2:D:146:LYS:CD	2:D:285:PHE:O	2.52	0.56
1:B:168:THR:HG23	1:B:170:ASP:H	1.69	0.56
1:A:107:VAL:HG12	1:A:109:LEU:HD13	1.85	0.56
2:D:197:ASP:O	2:D:201:THR:HG22	2.05	0.56
1:A:231:PRO:HD2	1:A:413:TRP:O	2.05	0.56
2:D:196:GLU:HG2	2:D:199:ARG:NH2	2.20	0.56
2:F:127:PHE:CE1	2:F:140:THR:HG23	2.39	0.56
1:A:50:GLN:NE2	1:A:344:ARG:HH21	2.03	0.56
1:A:576:GLU:O	1:A:580:THR:HG23	2.06	0.56
1:C:225:GLY:O	1:C:370:GLY:HA2	2.05	0.56
1:A:266:MET:O	1:A:270:VAL:HG13	2.06	0.56
1:C:470:LEU:HB3	1:C:490:LEU:HD11	1.87	0.56
2:D:276:TYR:HD2	2:D:280:ASN:ND2	2.03	0.56
1:B:416:ASP:OD1	1:B:418:SER:OG	2.24	0.56
2:D:343:ASP:O	2:D:347:SER:OG	2.22	0.56
2:E:249:ASP:OD1	2:E:251:THR:OG1	2.23	0.56
1:A:445:MET:HE1	1:A:515:ARG:HG3	1.88	0.55
2:E:364:ASP:OD1	2:E:364:ASP:N	2.36	0.55
1:A:456:MET:HE3	1:A:523:LYS:HE2	1.87	0.55
1:C:83:MET:HG2	1:C:291:LEU:HD23	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:LEU:HG	1:C:424:HIS:HB3	1.87	0.55
1:C:125:GLU:O	1:C:128:THR:HG22	2.05	0.55
2:D:122:ASP:HB3	2:D:290:ARG:HB2	1.87	0.55
2:D:352:LYS:O	2:D:356:THR:HG22	2.07	0.55
1:B:189:GLN:NE2	1:B:197:ARG:HH12	2.04	0.55
2:E:310:ASP:OD2	2:E:310:ASP:N	2.38	0.55
2:F:319:THR:O	2:F:323:THR:HG23	2.06	0.55
1:C:378:ASP:OD1	1:C:378:ASP:N	2.36	0.55
2:D:10:GLU:HB2	2:D:17:ALA:HB3	1.89	0.55
2:E:129:GLN:NE2	2:E:136:ASP:OD2	2.39	0.55
1:A:60:PRO:HD3	2:D:47:VAL:HG13	1.88	0.55
1:C:327:MET:HA	1:C:387:ILE:O	2.07	0.55
2:D:40:ARG:HD3	2:D:58:GLU:HB2	1.89	0.55
2:D:183:ALA:HB1	2:D:186:ILE:HG12	1.89	0.55
2:F:140:THR:O	2:F:349:SER:OG	2.21	0.55
1:C:93:THR:HA	1:C:96:GLU:HG2	1.89	0.54
2:D:368:THR:O	2:D:372:LEU:CB	2.56	0.54
2:F:342:ILE:O	2:F:342:ILE:HG23	2.07	0.54
1:C:550:VAL:HA	1:C:553:ARG:NH2	2.22	0.54
2:D:88:ARG:NH2	2:D:101:PRO:O	2.41	0.54
2:D:307:PRO:HA	2:D:313:HIS:ND1	2.23	0.54
1:A:40:ILE:HD13	1:A:50:GLN:HG2	1.89	0.54
1:B:517:LYS:O	1:B:521:MET:HG3	2.07	0.54
2:E:383:LYS:HD3	2:E:402:ALA:HB1	1.88	0.54
2:D:315:ILE:CG2	2:D:317:ASP:OD1	2.55	0.54
2:E:271:ARG:C	2:E:273:TYR:H	2.15	0.54
1:A:50:GLN:HE21	1:A:344:ARG:HH21	1.55	0.54
2:F:11:VAL:HG22	2:F:16:MET:HG2	1.90	0.54
2:F:342:ILE:CG2	2:F:413:VAL:HG13	2.38	0.53
1:B:214:ARG:HH11	1:B:513:THR:HG21	1.74	0.53
1:C:245:ILE:O	1:C:249:SER:OG	2.18	0.53
1:C:519:PHE:O	1:C:523:LYS:HB2	2.08	0.53
2:D:281:LEU:HD12	2:D:318:LEU:HD22	1.91	0.53
2:D:317:ASP:O	2:D:321:TYR:HB2	2.07	0.53
1:B:119:TRP:O	1:B:139:VAL:HG22	2.08	0.53
2:F:324:GLU:OE1	2:F:351:LEU:HD11	2.08	0.53
1:B:52:TYR:O	1:B:299:PRO:HB3	2.09	0.53
2:E:375:ALA:HB3	2:E:404:PHE:CE2	2.44	0.53
1:C:266:MET:HE2	1:C:293:ALA:HA	1.90	0.53
2:E:137:HIS:O	2:E:365:HIS:NE2	2.40	0.53
2:F:442:LEU:HD23	2:F:442:LEU:H	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:437:LEU:HD13	2:F:441:GLU:HB2	1.89	0.53
1:C:41:GLU:HB2	1:C:48:SER:HB2	1.91	0.52
2:D:160:LEU:O	2:D:164:ILE:HD12	2.08	0.52
2:D:276:TYR:O	2:D:279:THR:OG1	2.23	0.52
2:E:334:TYR:HA	2:E:338:ILE:CG2	2.39	0.52
1:A:473:ILE:O	1:A:477:VAL:HG22	2.09	0.52
1:C:236:ALA:HB1	1:C:415:LEU:HD22	1.89	0.52
2:F:362:ARG:HG2	2:F:364:ASP:CG	2.34	0.52
1:B:141:GLU:OE2	1:B:147:HIS:ND1	2.41	0.52
1:B:273:PHE:CE2	1:B:289:THR:HG21	2.44	0.52
1:B:459:GLU:O	1:B:463:ILE:HG13	2.10	0.52
2:E:10:GLU:HB3	2:E:17:ALA:HB3	1.90	0.52
2:D:316:PRO:HA	2:D:319:THR:OG1	2.08	0.52
2:F:278:TYR:CD2	2:F:278:TYR:N	2.71	0.52
1:A:513:THR:HG23	1:A:517:LYS:HD3	1.90	0.52
1:B:203:LEU:HD11	1:B:373:ILE:HG13	1.91	0.52
1:C:78:GLY:N	1:C:141:GLU:OE2	2.36	0.52
1:C:209:MET:HE3	1:C:249:SER:HB3	1.90	0.52
2:E:264:ARG:O	2:E:265:ARG:HD3	2.10	0.52
2:E:356:THR:HG22	2:E:365:HIS:CE1	2.45	0.52
2:E:133:SER:OG	2:E:426:THR:HB	2.10	0.52
1:C:265:GLU:O	1:C:269:VAL:HG23	2.09	0.52
1:B:440:GLU:CD	1:B:443:ARG:HH12	2.18	0.51
1:C:28:CYS:HB3	1:C:66:SER:HA	1.91	0.51
1:C:3:ILE:HD13	1:C:65:ARG:HD3	1.92	0.51
2:F:307:PRO:HG3	2:F:316:PRO:HG3	1.91	0.51
1:B:92:ASP:OD1	1:B:93:THR:N	2.44	0.51
2:D:423:ILE:O	2:D:427:LEU:HD22	2.10	0.51
2:F:412:TYR:O	2:F:421:ARG:NH2	2.43	0.51
1:A:453:TRP:HZ3	1:A:519:PHE:HA	1.75	0.51
1:B:256:TYR:HB3	1:B:291:LEU:HD12	1.92	0.51
2:F:128:ILE:CG2	2:F:129:GLN:N	2.72	0.51
1:B:456:MET:HE1	1:B:519:PHE:HE1	1.74	0.51
2:F:137:HIS:O	2:F:369:MET:HE2	2.10	0.51
2:F:437:LEU:HD12	2:F:438:PRO:O	2.11	0.51
1:A:549:THR:HG23	1:A:553:ARG:HH11	1.75	0.51
1:B:131:SER:OG	1:B:132:ALA:N	2.44	0.51
2:E:125:ASP:HA	2:E:354:LYS:HB3	1.93	0.51
2:F:3:LYS:O	2:F:71:ARG:HA	2.11	0.51
1:B:445:MET:HE1	1:B:515:ARG:HE	1.76	0.51
2:D:313:HIS:HB3	2:D:314:PRO:CD	2.37	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:28:GLU:O	2:F:44:VAL:HG13	2.11	0.51
1:B:475:ARG:HG3	1:B:476:LEU:HD23	1.92	0.50
2:E:29:LEU:HD21	2:E:77:LEU:HG	1.93	0.50
2:E:375:ALA:HB3	2:E:404:PHE:HE2	1.76	0.50
2:F:364:ASP:O	2:F:368:THR:HG22	2.12	0.50
2:D:276:TYR:HD2	2:D:280:ASN:HD22	1.59	0.50
2:D:137:HIS:NE2	2:D:368:THR:HG23	2.27	0.50
2:E:400:ILE:HB	2:E:436:MET:HE1	1.93	0.50
1:C:92:ASP:OD1	1:C:93:THR:N	2.42	0.50
2:E:429:LEU:HA	2:E:432:GLU:CG	2.42	0.50
1:B:36:ILE:HG23	1:B:52:TYR:HB2	1.94	0.50
1:B:479:ILE:HD12	1:B:482:LEU:HD21	1.93	0.50
2:D:340:PRO:HD2	2:D:413:VAL:O	2.12	0.50
2:E:384:GLU:O	2:E:388:VAL:HG12	2.11	0.50
2:F:277:LEU:HD12	2:F:277:LEU:C	2.35	0.50
1:B:84:PHE:HB2	1:B:292:ILE:HD13	1.94	0.50
2:E:148:PRO:HG3	2:E:323:THR:HG21	1.94	0.50
2:D:29:LEU:HD21	2:D:77:LEU:HG	1.93	0.49
2:E:315:ILE:HG22	2:E:318:LEU:H	1.77	0.49
2:E:404:PHE:HE1	2:E:433:LEU:HD21	1.72	0.49
1:C:118:TRP:CH2	1:C:141:GLU:HG3	2.47	0.49
2:E:81:VAL:HB	2:E:234:TYR:CD2	2.48	0.49
1:B:238:LYS:O	1:B:242:GLN:HG3	2.11	0.49
1:C:500:TYR:OH	1:C:518:GLN:HB3	2.12	0.49
1:A:4:GLY:HA3	1:A:19:MET:HE3	1.95	0.49
2:E:385:LEU:HA	2:E:388:VAL:CG1	2.43	0.49
1:C:93:THR:O	1:C:97:VAL:HG23	2.12	0.49
1:C:522:LEU:HG	1:C:526:LEU:HD12	1.94	0.49
2:D:143:ARG:NH2	2:D:170:VAL:HG11	2.27	0.49
1:A:161:LYS:HE2	1:A:175:VAL:HG23	1.95	0.49
1:B:168:THR:HG22	1:B:171:ASP:CG	2.37	0.49
2:E:327:ILE:HG23	2:E:342:ILE:HG21	1.93	0.49
1:A:400:PRO:HA	1:A:403:GLN:HE21	1.78	0.49
1:B:199:ILE:HD12	1:B:372:VAL:HG23	1.94	0.49
1:C:73:VAL:HG11	1:C:309:THR:HG23	1.94	0.49
1:C:412:PHE:HD2	1:C:433:SER:HA	1.78	0.49
2:E:329:LEU:HD12	2:E:342:ILE:HG23	1.95	0.49
2:F:226:ARG:NH2	2:F:253:TYR:OH	2.45	0.49
1:C:150:MET:HE1	1:C:319:ASP:O	2.12	0.49
2:F:197:ASP:O	2:F:201:THR:HG22	2.12	0.48
2:F:338:ILE:HD11	2:F:409:GLU:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:400:ILE:HG22	2:D:400:ILE:O	2.12	0.48
2:E:157:LYS:NZ	2:E:305:THR:HG22	2.28	0.48
1:C:8:LYS:HD2	2:F:48:GLN:HG3	1.94	0.48
2:F:130:THR:HG22	2:F:164:ILE:HG23	1.96	0.48
1:B:205:PRO:HB2	1:B:223:THR:OG1	2.13	0.48
1:C:1:MET:HE3	1:C:1:MET:HB3	1.61	0.48
2:D:89:VAL:HB	2:D:98:ASP:HB3	1.95	0.48
1:A:126:GLU:HG2	1:A:162:ILE:HG22	1.96	0.48
2:D:16:MET:HB3	2:D:54:VAL:HG22	1.95	0.48
2:E:142:VAL:HG21	2:E:351:LEU:O	2.13	0.48
1:A:319:ASP:O	1:A:380:ARG:NH1	2.47	0.48
1:C:286:MET:O	1:C:287:GLU:C	2.55	0.48
2:F:82:SER:O	2:F:85:MET:HG3	2.13	0.48
1:A:41:GLU:HB2	1:A:48:SER:HB2	1.95	0.48
1:B:485:ASN:ND2	1:B:533:ARG:HG3	2.25	0.48
2:E:368:THR:C	2:E:372:LEU:HD12	2.39	0.48
2:F:141:LEU:HD11	2:F:299:THR:CG2	2.43	0.48
1:A:203:LEU:HB2	1:A:371:ARG:HG2	1.94	0.48
1:C:38:GLU:OE1	1:C:52:TYR:OH	2.27	0.48
1:C:148:LYS:O	1:C:320:MET:HE2	2.13	0.48
1:C:484:ASP:OD1	1:C:542:PHE:HB3	2.13	0.48
1:B:134:ASP:O	1:B:151:VAL:HG23	2.14	0.48
1:B:259:CYS:HB3	1:B:306:SER:OG	2.13	0.48
1:C:84:PHE:HB3	1:C:88:GLN:HA	1.94	0.48
2:F:379:GLY:O	2:F:383:LYS:HG3	2.14	0.48
1:B:119:TRP:CZ3	1:B:165:GLY:HA2	2.49	0.48
1:B:225:GLY:O	1:B:370:GLY:HA2	2.14	0.48
1:C:191:TRP:CZ2	1:C:198:PRO:HD3	2.49	0.48
1:C:414:GLY:H	1:C:433:SER:HB3	1.79	0.48
1:C:498:GLU:HA	1:C:502:GLN:NE2	2.29	0.48
1:C:581:ILE:O	1:C:584:ILE:HG23	2.13	0.48
1:C:259:CYS:O	1:C:333:ARG:HB2	2.14	0.47
2:D:142:VAL:HG23	2:D:145:GLN:HB2	1.96	0.47
2:E:146:LYS:HE2	2:E:322:ILE:O	2.14	0.47
1:A:212:GLY:HA3	1:A:512:PHE:CD1	2.49	0.47
1:C:521:MET:HE2	1:C:521:MET:HB2	1.79	0.47
1:A:333:ARG:NH1	2:D:321:TYR:O	2.47	0.47
1:B:35:VAL:HG13	1:B:53:GLU:HG3	1.97	0.47
1:C:214:ARG:NH2	1:C:503:GLN:HG2	2.29	0.47
2:E:253:TYR:OH	2:E:280:ASN:OD1	2.31	0.47
1:A:144:ILE:HG21	1:A:288:ARG:HD3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:GLU:O	1:A:470:LEU:HG	2.14	0.47
1:B:189:GLN:HE22	1:B:197:ARG:HH22	1.62	0.47
2:E:265:ARG:O	2:E:265:ARG:HG2	2.14	0.47
2:E:403:LYS:HB3	2:E:403:LYS:HE3	1.62	0.47
1:B:156:LYS:O	1:B:178:THR:HG22	2.15	0.47
1:B:197:ARG:HD3	1:B:315:GLU:HB3	1.97	0.47
1:C:268:ASP:O	1:C:272:GLU:HG3	2.14	0.47
1:C:479:ILE:HG12	1:C:487:ARG:HD2	1.97	0.47
2:D:196:GLU:HG2	2:D:199:ARG:HH21	1.80	0.47
2:E:385:LEU:HA	2:E:388:VAL:HG12	1.96	0.47
2:F:386:ALA:HA	2:F:389:LEU:O	2.14	0.47
1:A:521:MET:O	1:A:525:ILE:HG12	2.15	0.47
1:B:176:ILE:HG22	1:B:178:THR:HG23	1.97	0.47
2:D:33:ARG:HG2	2:D:39:ILE:HG12	1.95	0.47
2:D:415:GLN:HG2	2:D:421:ARG:NH1	2.29	0.47
2:E:57:PHE:CD1	2:E:219:ILE:HD12	2.49	0.47
2:E:157:LYS:HZ1	2:E:305:THR:HG22	1.79	0.47
2:E:334:TYR:HA	2:E:338:ILE:HG22	1.94	0.47
2:E:395:SER:O	2:E:399:LYS:N	2.46	0.47
2:F:155:ALA:O	2:F:341:PRO:HG2	2.14	0.47
1:A:258:GLY:HA2	1:A:329:ASP:O	2.15	0.47
1:C:461:MET:CG	1:C:465:GLN:HE21	2.24	0.47
2:D:87:GLY:HA2	2:D:204:ILE:O	2.15	0.47
2:E:135:ILE:HG12	2:E:327:ILE:HD13	1.97	0.47
2:F:385:LEU:HD21	2:F:394:LEU:HD23	1.97	0.47
1:A:315:GLU:HA	1:A:384:ILE:HD11	1.97	0.47
1:C:144:ILE:HD11	1:C:283:GLU:HB2	1.97	0.47
2:D:344:VAL:HG23	2:D:345:LEU:HD23	1.96	0.47
2:F:30:ILE:HG22	2:F:42:GLY:C	2.40	0.47
2:F:437:LEU:HD12	2:F:437:LEU:C	2.40	0.47
1:A:54:GLU:HB2	1:A:105:ARG:HD3	1.97	0.46
2:E:28:GLU:OE1	2:E:72:PHE:HB3	2.14	0.46
2:E:148:PRO:HD3	2:E:323:THR:HB	1.97	0.46
1:B:308:TYR:HA	1:B:311:ILE:HG22	1.97	0.46
2:E:319:THR:O	2:E:323:THR:HG23	2.15	0.46
2:F:186:ILE:HB	2:F:190:GLU:HG3	1.96	0.46
2:D:329:LEU:HD22	2:D:342:ILE:HG13	1.97	0.46
2:E:338:ILE:HG23	2:E:338:ILE:O	2.15	0.46
1:A:107:VAL:CG1	1:A:109:LEU:CD1	2.91	0.46
1:B:333:ARG:HA	1:B:333:ARG:HD3	1.61	0.46
2:D:313:HIS:CB	2:D:314:PRO:HD2	2.39	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ARG:HD3	1:C:513:THR:HG21	1.98	0.46
2:D:131:GLY:HA3	2:D:167:GLN:HE21	1.79	0.46
2:E:360:LYS:HB2	2:E:360:LYS:HE3	1.56	0.46
2:F:397:ILE:HA	2:F:400:ILE:HG12	1.98	0.46
1:B:24:ILE:HG22	1:B:25:GLN:NE2	2.31	0.46
2:E:229:LEU:HD13	2:E:287:ARG:HD3	1.97	0.46
1:B:8:LYS:HB3	1:B:15:MET:HB2	1.98	0.46
1:B:96:GLU:O	1:B:99:GLN:NE2	2.48	0.46
2:E:334:TYR:HD1	2:E:341:PRO:HG3	1.81	0.46
1:B:84:PHE:HB3	1:B:88:GLN:HA	1.98	0.46
2:E:362:ARG:HB2	2:E:427:LEU:HD13	1.98	0.46
2:F:361:THR:OG1	2:F:362:ARG:N	2.49	0.46
1:C:399:GLU:O	1:C:403:GLN:HG3	2.16	0.46
1:C:412:PHE:CD2	1:C:433:SER:HA	2.51	0.46
1:C:93:THR:HG22	1:C:109:LEU:HD21	1.98	0.46
1:C:456:MET:HE1	1:C:523:LYS:HD3	1.96	0.46
1:C:499:ASP:CG	1:C:557:SER:HA	2.41	0.45
2:F:87:GLY:HA2	2:F:204:ILE:O	2.15	0.45
2:F:362:ARG:HG2	2:F:364:ASP:OD1	2.17	0.45
1:B:410:LYS:HB3	1:B:436:LEU:HB2	1.98	0.45
2:E:126:GLU:O	2:E:143:ARG:HG3	2.16	0.45
2:F:160:LEU:O	2:F:164:ILE:HG13	2.16	0.45
1:C:147:HIS:CE1	1:C:316:TYR:HE2	2.35	0.45
1:C:521:MET:O	1:C:524:VAL:HG22	2.17	0.45
2:D:129:GLN:NE2	2:D:423:ILE:H	2.15	0.45
2:D:142:VAL:CG1	2:D:355:GLY:HA3	2.46	0.45
2:E:348:LEU:HD21	2:E:350:ARG:HE	1.80	0.45
2:F:125:ASP:HA	2:F:354:LYS:HB3	1.98	0.45
2:F:137:HIS:CD2	2:F:369:MET:HB2	2.51	0.45
2:F:273:TYR:OH	2:F:315:ILE:HD11	2.17	0.45
1:B:415:LEU:HD23	1:B:428:ILE:HD13	1.98	0.45
1:C:520:ASN:O	1:C:524:VAL:HG13	2.16	0.45
2:D:320:GLY:HA2	2:D:323:THR:OG1	2.16	0.45
2:D:338:ILE:HD12	2:D:414:ASN:HB2	1.99	0.45
2:F:168:ALA:O	2:F:206:ARG:NH2	2.48	0.45
1:B:329:ASP:HA	1:B:330:SER:HA	1.60	0.45
1:B:488:LEU:HD11	1:B:532:ALA:HB1	1.97	0.45
1:C:91:LEU:HD13	2:F:118:PRO:HD2	1.98	0.45
1:C:488:LEU:O	1:C:492:VAL:HG13	2.17	0.45
2:F:44:VAL:HA	2:F:54:VAL:HG12	1.98	0.45
1:B:128:THR:O	1:B:159:VAL:HG23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:TRP:O	1:B:457:VAL:HG23	2.17	0.45
2:E:138:LEU:HD13	2:E:344:VAL:CG1	2.47	0.45
1:B:191:TRP:CZ2	1:B:198:PRO:HD3	2.51	0.45
1:B:528:PHE:C	1:B:528:PHE:CD2	2.94	0.45
1:C:85:ASP:HB3	1:C:91:LEU:HD21	1.99	0.45
2:D:9:LYS:HG3	2:D:19:GLU:CD	2.41	0.45
1:A:207:VAL:HG23	1:A:207:VAL:O	2.16	0.45
1:A:327:MET:HE3	1:A:327:MET:HB3	1.88	0.45
2:E:334:TYR:CA	2:E:338:ILE:HG22	2.46	0.45
1:C:175:VAL:HG12	1:C:182:LEU:HD11	1.99	0.45
2:D:128:ILE:HD11	2:D:143:ARG:HG2	1.98	0.45
2:D:163:GLN:O	2:D:167:GLN:HG2	2.17	0.45
1:A:191:TRP:CD2	1:A:192:PRO:HD2	2.52	0.45
1:B:360:SER:OG	2:F:259:GLU:OE1	2.32	0.45
1:B:528:PHE:HA	1:B:577:ILE:HG21	1.99	0.44
2:D:179:VAL:O	2:D:207:SER:HA	2.17	0.44
2:D:201:THR:HG23	2:D:203:ALA:H	1.82	0.44
1:A:453:TRP:CZ3	1:A:519:PHE:HA	2.51	0.44
1:B:95:MET:HE2	1:B:95:MET:HB3	1.67	0.44
1:B:344:ARG:HG2	3:B:634:HOH:O	2.17	0.44
2:E:16:MET:HB3	2:E:16:MET:HE3	1.75	0.44
1:B:69:GLU:HG3	1:B:70:ALA:O	2.18	0.44
1:B:445:MET:HA	1:B:448:ILE:HG22	1.99	0.44
2:E:139:ASN:OD1	2:E:347:SER:OG	2.27	0.44
1:A:234:PHE:CE1	2:D:350:ARG:HG3	2.53	0.44
2:F:333:LEU:HA	2:F:336:SER:HB3	1.99	0.44
1:A:524:VAL:CG1	1:A:556:ILE:HG12	2.48	0.44
2:E:87:GLY:HA2	2:E:204:ILE:O	2.18	0.44
1:B:399:GLU:OE2	1:B:401:VAL:HB	2.18	0.44
1:B:522:LEU:HG	1:B:526:LEU:HD11	1.99	0.44
1:C:28:CYS:CB	1:C:66:SER:HA	2.48	0.44
1:C:545:ILE:HG13	1:C:583:LEU:HD22	1.99	0.44
2:D:376:TYR:OH	2:D:409:GLU:OE2	2.29	0.44
2:D:409:GLU:HA	2:D:413:VAL:HG22	2.00	0.44
2:F:279:THR:O	2:F:283:THR:HG23	2.18	0.44
2:F:379:GLY:HA3	2:F:405:ALA:HB2	2.00	0.44
1:A:415:LEU:HA	1:A:427:SER:O	2.17	0.44
1:B:520:ASN:O	1:B:524:VAL:HG13	2.18	0.44
2:E:358:ALA:HA	2:E:361:THR:O	2.18	0.44
2:E:430:GLY:O	2:E:434:LEU:HD12	2.18	0.44
2:F:168:ALA:O	2:F:206:ARG:NH1	2.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:MET:HE1	1:A:52:TYR:CZ	2.53	0.43
1:A:378:ASP:OD1	1:A:378:ASP:N	2.51	0.43
1:B:101:ASN:O	2:E:116:ILE:HD12	2.18	0.43
1:A:514:SER:O	1:A:518:GLN:HG3	2.18	0.43
1:B:169:ILE:HD13	1:B:169:ILE:HA	1.80	0.43
1:C:8:LYS:HB3	1:C:15:MET:HB2	1.99	0.43
1:C:463:ILE:CD1	1:C:492:VAL:HG23	2.48	0.43
2:D:410:ASN:O	2:D:414:ASN:HB3	2.19	0.43
2:E:138:LEU:HD13	2:E:344:VAL:HG12	1.99	0.43
1:C:6:ILE:HG22	1:C:60:PRO:HA	2.00	0.43
1:B:348:MET:HE3	2:F:266:GLU:O	2.19	0.43
2:D:126:GLU:HG2	2:D:143:ARG:NH2	2.34	0.43
2:D:149:VAL:HG13	2:D:303:ILE:HG13	1.99	0.43
2:D:316:PRO:O	2:D:320:GLY:N	2.38	0.43
1:A:329:ASP:HA	1:A:330:SER:HA	1.65	0.43
1:C:90:PRO:HD3	1:C:111:ALA:HA	2.00	0.43
2:F:343:ASP:O	2:F:347:SER:OG	2.37	0.43
2:F:383:LYS:HB2	2:F:383:LYS:HE2	1.87	0.43
1:A:57:GLY:O	2:D:25:LYS:HD2	2.19	0.43
1:B:448:ILE:HG23	1:B:449:LEU:HD23	2.00	0.43
1:C:121:GLU:HA	1:C:164:SER:OG	2.18	0.43
1:C:456:MET:HE1	1:C:523:LYS:CD	2.49	0.43
1:C:484:ASP:CG	1:C:542:PHE:HB3	2.44	0.43
2:E:443:LYS:HA	2:E:443:LYS:HD3	1.63	0.43
1:B:28:CYS:HB3	1:B:66:SER:HA	2.00	0.43
1:B:91:LEU:HD23	1:B:91:LEU:HA	1.78	0.43
1:B:278:ASP:HB3	1:B:281:THR:HG22	2.01	0.43
1:B:327:MET:HE3	1:B:327:MET:HB3	1.69	0.43
1:B:392:PRO:HG2	1:B:397:ILE:HG22	2.01	0.43
2:D:143:ARG:NH1	2:D:242:HIS:CE1	2.87	0.43
2:E:429:LEU:HA	2:E:432:GLU:HG2	2.00	0.43
1:A:39:ILE:HG12	1:A:47:ALA:HB1	2.00	0.43
1:C:136:ILE:HG22	1:C:149:ILE:O	2.19	0.43
1:C:205:PRO:HB2	1:C:223:THR:OG1	2.18	0.43
1:A:260:GLY:CA	1:A:303:ARG:HD2	2.49	0.43
1:B:565:GLU:N	1:B:565:GLU:OE1	2.52	0.43
1:C:120:PHE:CE1	1:C:137:GLY:HA3	2.53	0.43
1:C:178:THR:HG21	1:C:183:LYS:HE3	2.01	0.43
2:D:146:LYS:HD3	2:D:285:PHE:O	2.19	0.43
1:A:238:LYS:HE2	1:A:238:LYS:HB3	1.90	0.43
1:A:472:GLU:OE2	1:A:472:GLU:HA	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:LEU:HD23	1:B:415:LEU:HA	1.80	0.43
1:C:187:MET:HE3	1:C:187:MET:HB2	1.90	0.43
2:D:137:HIS:CD2	2:D:369:MET:HB2	2.54	0.43
2:E:324:GLU:HB3	2:E:351:LEU:HD13	1.99	0.43
2:F:111:ILE:HG21	2:F:227:MET:HG3	2.00	0.43
1:B:232:GLY:HA3	1:B:238:LYS:HD3	2.01	0.42
1:B:238:LYS:HE3	1:B:238:LYS:HB3	1.79	0.42
1:B:260:GLY:HA2	1:B:303:ARG:HD2	2.00	0.42
1:B:497:ARG:O	1:B:502:GLN:HG3	2.19	0.42
1:B:585:VAL:O	1:B:585:VAL:HG12	2.19	0.42
1:C:329:ASP:HA	1:C:330:SER:HA	1.64	0.42
2:D:333:LEU:HD13	2:D:341:PRO:O	2.18	0.42
1:C:142:THR:HG23	1:C:287:GLU:OE1	2.19	0.42
2:D:324:GLU:HG2	2:D:351:LEU:HD13	2.01	0.42
2:E:442:LEU:HD23	2:E:448:ASP:CG	2.44	0.42
2:F:281:LEU:HD12	2:F:318:LEU:HB3	2.01	0.42
1:B:90:PRO:HB2	1:B:93:THR:HB	2.00	0.42
1:C:57:GLY:C	2:F:25:LYS:HB3	2.44	0.42
1:C:94:PHE:CE1	1:C:103:LEU:HA	2.53	0.42
1:C:483:SER:HB2	1:C:486:ASP:OD2	2.19	0.42
2:D:149:VAL:CG1	2:D:303:ILE:HG13	2.50	0.42
2:D:248:GLU:HA	2:D:249:ASP:HA	1.76	0.42
2:F:249:ASP:N	2:F:303:ILE:O	2.53	0.42
1:C:554:GLU:O	1:C:558:ARG:HG2	2.19	0.42
2:E:14:PRO:HA	2:E:60:THR:HG23	2.01	0.42
1:C:12:PRO:HD3	1:C:344:ARG:NH1	2.34	0.42
1:C:459:GLU:O	1:C:463:ILE:HG23	2.19	0.42
1:C:576:GLU:O	1:C:580:THR:HG23	2.19	0.42
2:D:329:LEU:CD2	2:D:342:ILE:HG13	2.49	0.42
1:C:451:GLN:HG2	1:C:519:PHE:CE1	2.55	0.42
2:D:400:ILE:O	2:D:400:ILE:CG2	2.66	0.42
2:E:361:THR:HG22	2:E:362:ARG:O	2.20	0.42
2:E:410:ASN:O	2:E:414:ASN:HB3	2.19	0.42
1:A:126:GLU:HG3	3:A:608:HOH:O	2.20	0.42
1:A:567:LEU:HD23	1:A:567:LEU:HA	1.87	0.42
1:C:109:LEU:HD12	1:C:110:PRO:HD2	2.02	0.42
1:C:214:ARG:HG3	1:C:503:GLN:OE1	2.20	0.42
1:C:410:LYS:HB3	1:C:436:LEU:HB2	2.01	0.42
1:C:497:ARG:HA	1:C:501:LEU:HB2	2.02	0.42
1:C:565:GLU:OE2	1:C:565:GLU:N	2.44	0.42
2:D:30:ILE:HD13	2:D:54:VAL:HG21	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ARG:NH1	1:B:513:THR:HG21	2.35	0.42
2:D:15:LEU:HD22	2:D:45:LEU:HD21	2.01	0.42
2:D:246:ILE:HG23	2:D:303:ILE:CD1	2.50	0.42
2:F:236:ALA:HA	2:F:241:MET:O	2.20	0.42
2:F:382:ALA:HB2	2:F:398:ASP:OD1	2.20	0.42
1:B:158:THR:HG22	1:B:177:GLU:HB3	2.01	0.42
1:B:581:ILE:HA	1:B:584:ILE:HD12	2.01	0.42
1:C:541:TYR:O	1:C:545:ILE:HD12	2.20	0.42
2:E:276:TYR:HA	2:E:279:THR:HG23	2.00	0.42
2:F:30:ILE:HD11	2:F:70:VAL:HG13	2.01	0.42
2:F:344:VAL:HA	2:F:347:SER:OG	2.20	0.42
2:F:381:GLN:HA	2:F:384:GLU:HG3	2.01	0.42
1:A:209:MET:HG3	1:A:250:ASP:OD1	2.20	0.42
1:B:196:GLY:HA2	1:B:368:ARG:HH21	1.84	0.42
1:B:406:LEU:HD23	1:B:406:LEU:HA	1.85	0.42
1:C:114:HIS:HA	1:C:169:ILE:HG12	2.02	0.42
2:D:139:ASN:HA	2:D:349:SER:HB2	2.01	0.42
2:D:273:TYR:O	2:D:275:GLY:N	2.53	0.42
2:F:140:THR:HB	2:F:352:LYS:CB	2.49	0.42
2:F:333:LEU:HB3	2:F:338:ILE:HB	2.01	0.42
2:E:128:ILE:HG22	2:E:141:LEU:O	2.20	0.41
2:E:163:GLN:HE21	2:E:167:GLN:HE22	1.67	0.41
2:E:256:ALA:O	2:E:260:ILE:HG12	2.20	0.41
2:F:338:ILE:HD11	2:F:409:GLU:C	2.45	0.41
1:C:40:ILE:HG13	1:C:41:GLU:HG3	2.01	0.41
1:C:397:ILE:H	1:C:397:ILE:HG13	1.30	0.41
2:F:89:VAL:HG22	2:F:209:MET:HB2	2.02	0.41
2:F:160:LEU:HD22	2:F:329:LEU:HD21	2.02	0.41
2:F:329:LEU:HA	2:F:341:PRO:O	2.19	0.41
1:C:138:TYR:CZ	1:C:146:GLN:HB3	2.55	0.41
2:F:318:LEU:HA	2:F:318:LEU:HD13	1.29	0.41
1:B:266:MET:HA	1:B:266:MET:HE3	2.02	0.41
1:B:295:THR:OG1	1:B:298:MET:HG3	2.20	0.41
1:B:523:LYS:HD3	1:B:574:ASN:ND2	2.35	0.41
2:D:281:LEU:HD23	2:D:281:LEU:HA	1.90	0.41
2:E:45:LEU:HD21	2:E:264:ARG:CZ	2.50	0.41
1:A:134:ASP:O	1:A:150:MET:HA	2.21	0.41
1:B:573:ILE:H	1:B:573:ILE:HG13	1.69	0.41
1:C:272:GLU:O	1:C:276:LEU:HD13	2.21	0.41
2:D:314:PRO:O	2:D:314:PRO:CG	2.69	0.41
2:E:137:HIS:CD2	2:E:427:LEU:HD23	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:167:GLN:HB3	2:F:420:ASN:ND2	2.34	0.41
1:A:191:TRP:CG	1:A:192:PRO:HD2	2.55	0.41
1:B:89:ARG:HA	1:B:90:PRO:HD3	1.93	0.41
1:C:194:ARG:NH1	1:C:304:GLU:OE1	2.53	0.41
1:C:482:LEU:HG	1:C:486:ASP:HB2	2.01	0.41
2:E:126:GLU:C	2:E:143:ARG:HG3	2.46	0.41
1:C:559:SER:HA	1:C:562:ILE:CD1	2.51	0.41
2:D:397:ILE:HD12	2:D:397:ILE:HA	1.89	0.41
2:E:429:LEU:HA	2:E:432:GLU:HG3	2.01	0.41
1:C:150:MET:HB3	1:C:150:MET:HE3	1.75	0.41
1:C:202:LYS:HG2	2:D:188:PHE:CE2	2.55	0.41
1:C:250:ASP:OD1	1:C:250:ASP:N	2.48	0.41
2:D:316:PRO:O	2:D:319:THR:N	2.54	0.41
2:F:172:ASP:O	2:F:173:SER:C	2.64	0.41
1:B:199:ILE:HG21	1:B:372:VAL:HG21	2.01	0.41
1:B:261:GLU:O	1:B:295:THR:HA	2.21	0.41
1:C:364:GLU:O	1:C:368:ARG:HG3	2.21	0.41
2:D:138:LEU:HD13	2:D:369:MET:HG2	2.03	0.41
2:D:246:ILE:HG23	2:D:303:ILE:HD13	2.01	0.41
2:E:146:LYS:CD	2:E:285:PHE:HB3	2.51	0.41
2:E:280:ASN:O	2:E:283:THR:HB	2.21	0.41
1:B:493:ALA:O	1:B:497:ARG:HG3	2.21	0.41
2:F:44:VAL:HG12	2:F:54:VAL:HG12	2.03	0.41
2:F:81:VAL:HG11	2:F:109:LEU:HD12	2.03	0.41
1:A:225:GLY:O	1:A:370:GLY:HA2	2.22	0.40
1:A:261:GLU:O	1:A:295:THR:HA	2.20	0.40
1:C:360:SER:O	1:C:364:GLU:HG3	2.20	0.40
2:D:248:GLU:HG3	2:D:249:ASP:HB2	2.03	0.40
2:F:167:GLN:HB3	2:F:420:ASN:CG	2.46	0.40
2:F:381:GLN:HA	2:F:384:GLU:CG	2.51	0.40
1:A:297:ASN:OD1	1:A:297:ASN:N	2.51	0.40
1:B:542:PHE:O	1:B:546:MET:HG2	2.21	0.40
1:C:50:GLN:OE1	1:C:341:MET:HE2	2.21	0.40
1:C:202:LYS:HG2	2:D:188:PHE:CZ	2.56	0.40
1:C:243:HIS:HB3	1:C:276:LEU:HD21	2.03	0.40
2:D:30:ILE:O	2:D:41:ARG:HD3	2.22	0.40
2:F:137:HIS:NE2	2:F:368:THR:HG23	2.36	0.40
2:F:140:THR:HB	2:F:352:LYS:HB2	2.03	0.40
1:C:238:LYS:O	1:C:241:VAL:HG22	2.21	0.40
1:C:419:LEU:HD23	1:C:427:SER:HA	2.03	0.40
2:E:331:ARG:O	2:E:335:LYS:HG2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:333:LEU:HB3	2:E:338:ILE:CG2	2.32	0.40
2:F:445:ILE:HD13	2:F:445:ILE:HA	1.68	0.40
1:A:490:LEU:HD23	1:A:490:LEU:HA	1.82	0.40
1:B:13:LEU:HD21	1:B:345:LEU:HD21	2.04	0.40
1:C:267:THR:HG21	2:F:121:ARG:HB3	2.03	0.40
1:C:494:LYS:HA	1:C:497:ARG:NH2	2.37	0.40
2:D:133:SER:N	2:D:415:GLN:HE22	2.19	0.40
2:E:397:ILE:HG23	2:E:398:ASP:OD1	2.20	0.40
1:B:253:LEU:HD23	1:B:288:ARG:O	2.21	0.40
1:B:299:PRO:O	1:B:303:ARG:HG3	2.21	0.40
2:D:53:MET:HE2	2:D:53:MET:HB2	1.84	0.40
2:F:187:THR:OG1	2:F:190:GLU:HG2	2.22	0.40
2:F:361:THR:HG21	2:F:365:HIS:ND1	2.36	0.40
2:F:377:ALA:O	2:F:381:GLN:HG2	2.21	0.40

All (1) 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)
1:A:5:LYS:NZ	1:A:508:ASP:OD2[2_656]	2.10	0.10

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	584/596 (98%)	574 (98%)	10 (2%)	0	100	100
1	B	584/596 (98%)	567 (97%)	17 (3%)	0	100	100
1	C	583/596 (98%)	567 (97%)	16 (3%)	0	100	100
2	D	430/458 (94%)	408 (95%)	22 (5%)	0	100	100
2	E	447/458 (98%)	422 (94%)	25 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	443/458 (97%)	412 (93%)	30 (7%)	1 (0%)	43	70
All	All	3071/3162 (97%)	2950 (96%)	120 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	173	SER

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	502/509 (99%)	492 (98%)	10 (2%)	48	77
1	B	502/509 (99%)	479 (95%)	23 (5%)	24	55
1	C	501/509 (98%)	462 (92%)	39 (8%)	11	32
2	D	356/380 (94%)	336 (94%)	20 (6%)	19	46
2	E	372/380 (98%)	341 (92%)	31 (8%)	10	29
2	F	368/380 (97%)	352 (96%)	16 (4%)	26	57
All	All	2601/2667 (98%)	2462 (95%)	139 (5%)	20	49

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ASP
1	A	95	MET
1	A	230	VAL
1	A	259	CYS
1	A	268	ASP
1	A	398	SER
1	A	452	ASP
1	A	474	VAL
1	A	524	VAL
1	A	585	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1	MET
1	B	9	VAL
1	B	65	ARG
1	B	81	SER
1	B	124	ILE
1	B	148	LYS
1	B	180	GLN
1	B	193	VAL
1	B	253	LEU
1	B	259	CYS
1	B	291	LEU
1	B	388	SER
1	B	431	ILE
1	B	465	GLN
1	B	470	LEU
1	B	474	VAL
1	B	485	ASN
1	B	538	LEU
1	B	544	GLU
1	B	545	ILE
1	B	552	VAL
1	B	567	LEU
1	B	581	ILE
1	C	1	MET
1	C	12	PRO
1	C	30	VAL
1	C	55	THR
1	C	125	GLU
1	C	136	ILE
1	C	146	GLN
1	C	158	THR
1	C	160	GLN
1	C	178	THR
1	C	182	LEU
1	C	209	MET
1	C	240	VAL
1	C	247	LYS
1	C	251	VAL
1	C	324	VAL
1	C	341	MET
1	C	348	MET
1	C	397	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	411	VAL
1	C	415	LEU
1	C	443[A]	ARG
1	C	443[B]	ARG
1	C	447	GLN
1	C	463	ILE
1	C	470	LEU
1	C	475	ARG
1	C	479	ILE
1	C	486	ASP
1	C	490	LEU
1	C	496	ILE
1	C	516	GLU
1	C	542	PHE
1	C	569	LYS
1	C	570	ILE
1	C	577	ILE
1	C	581	ILE
1	C	583	LEU
1	C	584	ILE
2	D	6	ARG
2	D	97	LYS
2	D	125	ASP
2	D	140	THR
2	D	149	VAL
2	D	170	VAL
2	D	196	GLU
2	D	246	ILE
2	D	317	ASP
2	D	322	ILE
2	D	329	LEU
2	D	330	THR
2	D	333	LEU
2	D	364	ASP
2	D	368	THR
2	D	387	VAL
2	D	389	LEU
2	D	411	GLU
2	D	426	THR
2	D	427	LEU
2	E	29	LEU
2	E	83	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	103	ILE
2	E	126	GLU
2	E	249	ASP
2	E	271	ARG
2	E	279	THR
2	E	280	ASN
2	E	283	THR
2	E	297	SER
2	E	313	HIS
2	E	315	ILE
2	E	318	LEU
2	E	319	THR
2	E	322	ILE
2	E	328	ILE
2	E	339	SER
2	E	342	ILE
2	E	344	VAL
2	E	352	LYS
2	E	360	LYS
2	E	368	THR
2	E	389	LEU
2	E	403	LYS
2	E	410	ASN
2	E	426	THR
2	E	433	LEU
2	E	434	LEU
2	E	436	MET
2	E	439	ARG
2	E	442	LEU
2	F	44	VAL
2	F	70	VAL
2	F	129	GLN
2	F	219	ILE
2	F	276	TYR
2	F	278	TYR
2	F	305	THR
2	F	309	ASP
2	F	318	LEU
2	F	319	THR
2	F	330	THR
2	F	344	VAL
2	F	389	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	429	LEU
2	F	433	LEU
2	F	445	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	99	GLN
1	A	244	GLN
1	A	403	GLN
1	A	447	GLN
1	A	502	GLN
1	A	520	ASN
1	B	25	GLN
1	B	99	GLN
1	B	108	GLN
1	B	160	GLN
1	B	180	GLN
1	B	189	GLN
1	B	485	ASN
1	B	520	ASN
1	C	146	GLN
1	C	160	GLN
1	C	180	GLN
1	C	294	ASN
1	C	379	GLN
1	C	421	GLN
1	C	465	GLN
1	C	469	GLN
1	C	582	GLN
2	D	139	ASN
2	D	167	GLN
2	D	280	ASN
2	E	163	GLN
2	E	371	GLN
2	E	415	GLN
2	F	410	ASN

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](#)

There are no ligands in this entry.

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	586/596 (98%)	-0.14	8 (1%) 73 67	32, 49, 82, 119	0
1	B	586/596 (98%)	0.29	15 (2%) 57 49	39, 69, 129, 145	0
1	C	584/596 (97%)	0.50	28 (4%) 35 30	37, 71, 122, 142	1 (0%)
2	D	432/458 (94%)	0.59	45 (10%) 11 9	37, 65, 141, 166	0
2	E	449/458 (98%)	0.83	85 (18%) 3 2	33, 71, 142, 167	0
2	F	445/458 (97%)	0.71	47 (10%) 11 9	41, 79, 157, 179	0
All	All	3082/3162 (97%)	0.43	228 (7%) 20 16	32, 66, 133, 179	1 (0%)

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	319	THR	7.4
2	E	267	VAL	5.9
2	F	318	LEU	4.8
2	E	437	LEU	4.7
2	E	272	GLY	4.5
2	D	315	ILE	4.5
1	A	340	GLU	4.4
2	D	318	LEU	4.4
2	E	361	THR	4.4
2	F	342	ILE	4.3
2	E	278	TYR	4.3
1	C	567	LEU	4.3
2	E	434	LEU	4.3
2	D	428	ASP	4.1
1	C	584	ILE	4.1
2	F	128	ILE	4.0
2	E	318	LEU	4.0
1	B	538	LEU	3.9
2	E	314	PRO	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	404	PHE	3.9
2	D	123	TYR	3.8
2	D	314	PRO	3.8
2	E	431	TRP	3.8
2	E	408	PHE	3.8
1	C	576	GLU	3.7
2	F	394	LEU	3.6
2	E	321	TYR	3.6
2	D	424	THR	3.6
2	E	450	LEU	3.6
2	F	2	ILE	3.6
2	E	358	ALA	3.5
2	E	363	GLU	3.5
2	F	388	VAL	3.5
2	E	444	ARG	3.5
1	C	259	CYS	3.5
1	C	448	ILE	3.5
2	E	268	PRO	3.5
2	F	328	ILE	3.4
2	D	279	THR	3.4
2	E	423	ILE	3.4
2	E	275	GLY	3.4
2	F	385	LEU	3.4
2	E	360	LYS	3.3
2	E	405	ALA	3.3
2	D	278	TYR	3.3
2	F	446	LYS	3.3
2	E	152	PRO	3.3
2	E	359	GLY	3.3
1	B	535	ALA	3.3
1	C	122	ALA	3.3
2	D	375	ALA	3.2
2	F	387	VAL	3.2
1	C	443[A]	ARG	3.2
2	F	322	ILE	3.2
2	D	433	LEU	3.2
1	A	392	PRO	3.2
1	A	541	TYR	3.2
2	E	276	TYR	3.2
2	F	321	TYR	3.2
2	E	128	ILE	3.1
2	D	388	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	355	GLY	3.1
2	E	322	ILE	3.1
1	B	542	PHE	3.1
2	D	272	GLY	3.0
1	C	1	MET	3.0
2	E	429	LEU	3.0
2	F	340	PRO	3.0
1	C	430	TRP	3.0
1	C	550	VAL	3.0
1	C	570	ILE	2.9
2	E	404	PHE	2.9
2	E	312	THR	2.9
2	E	367	ALA	2.9
2	D	434	LEU	2.9
1	C	569	LYS	2.9
1	C	568	ALA	2.9
2	E	366	ALA	2.9
2	E	446	LYS	2.9
2	E	400	ILE	2.9
2	E	273	TYR	2.9
2	E	427	LEU	2.9
1	B	234	PHE	2.9
2	E	411	GLU	2.8
2	D	397	ILE	2.8
2	E	449	LEU	2.8
1	C	397	ILE	2.8
2	D	389	LEU	2.8
2	E	412	TYR	2.8
2	E	125	ASP	2.8
2	E	127	PHE	2.8
2	E	344	VAL	2.8
1	C	234	PHE	2.7
2	F	315	ILE	2.7
2	F	327	ILE	2.7
2	F	397	ILE	2.7
2	D	354	LYS	2.7
2	E	397	ILE	2.7
2	E	138	LEU	2.7
1	C	580	THR	2.7
2	F	359	GLY	2.7
1	C	546	MET	2.6
2	E	313	HIS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	360	LYS	2.6
2	F	152	PRO	2.6
2	F	275	GLY	2.6
2	D	358	ALA	2.6
2	E	155	ALA	2.6
2	D	175	ASP	2.6
2	D	394	LEU	2.6
2	E	150	PHE	2.6
2	E	372	LEU	2.6
2	E	401	TYR	2.6
2	D	152	PRO	2.6
2	E	315	ILE	2.5
2	F	270	ARG	2.5
2	D	308	GLU	2.5
1	C	428	ILE	2.5
1	C	581	ILE	2.5
2	D	321	TYR	2.5
2	F	445	ILE	2.5
2	F	389	LEU	2.5
2	F	278	TYR	2.5
1	B	233	PRO	2.5
2	E	387	VAL	2.5
2	D	366	ALA	2.5
2	D	373	PHE	2.5
2	D	408	PHE	2.5
2	E	394	LEU	2.5
2	F	339	SER	2.5
2	E	364	ASP	2.5
2	D	367	ALA	2.5
2	E	134	ALA	2.5
1	A	549	THR	2.4
2	F	314	PRO	2.4
2	E	375	ALA	2.4
2	F	437	LEU	2.4
2	F	435	ALA	2.4
2	D	400	ILE	2.4
2	E	442	LEU	2.4
2	E	266	GLU	2.4
2	E	413	VAL	2.4
2	E	362	ARG	2.4
2	E	130	THR	2.4
2	F	313	HIS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	295	LYS	2.4
2	F	344	VAL	2.4
2	F	413	VAL	2.4
2	E	373	PHE	2.4
2	E	440	THR	2.3
2	E	430	GLY	2.3
1	B	470	LEU	2.3
1	C	583	LEU	2.3
2	D	277	LEU	2.3
2	D	333	LEU	2.3
1	C	496	ILE	2.3
2	E	426	THR	2.3
1	B	232	GLY	2.3
1	A	397	ILE	2.3
1	C	573	ILE	2.3
2	E	132	ILE	2.3
2	F	400	ILE	2.3
2	E	316	PRO	2.3
1	B	585	VAL	2.3
1	C	577	ILE	2.3
2	D	376	TYR	2.3
1	C	572	SER	2.3
2	D	365	HIS	2.2
1	C	445	MET	2.2
2	D	125	ASP	2.2
2	F	398	ASP	2.2
1	B	548	GLY	2.2
2	D	427	LEU	2.2
2	E	137	HIS	2.2
2	E	334	TYR	2.2
2	D	275	GLY	2.2
1	B	583	LEU	2.2
2	E	436	MET	2.2
2	D	312	THR	2.2
2	D	331	ARG	2.2
2	D	359	GLY	2.2
2	F	320	GLY	2.2
1	A	391	SER	2.2
1	B	581	ILE	2.2
2	E	153	PRO	2.2
2	D	429	LEU	2.2
2	E	433	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	434	LEU	2.2
2	E	424	THR	2.1
2	D	316	PRO	2.1
2	F	153	PRO	2.1
2	F	376	TYR	2.1
2	E	345	LEU	2.1
2	F	427	LEU	2.1
1	C	176	ILE	2.1
2	F	377	ALA	2.1
2	E	248	GLU	2.1
2	E	409	GLU	2.1
2	E	319	THR	2.1
1	B	476	LEU	2.1
2	D	385	LEU	2.1
2	E	123	TYR	2.1
2	E	133	SER	2.1
2	D	382	ALA	2.1
2	D	402	ALA	2.1
2	E	368	THR	2.1
1	A	233	PRO	2.1
2	F	171	LEU	2.1
1	C	294	ASN	2.1
2	F	355	GLY	2.1
2	D	393	ALA	2.1
2	E	435	ALA	2.1
2	D	383	LYS	2.1
2	E	403	LYS	2.1
1	B	490	LEU	2.1
2	F	372	LEU	2.1
1	C	492	VAL	2.1
2	F	393	ALA	2.0
2	E	311	LYS	2.0
1	A	580	THR	2.0
2	E	330	THR	2.0
2	E	306	MET	2.0
2	F	346	PRO	2.0
1	B	528	PHE	2.0
1	B	1	MET	2.0
2	E	341	PRO	2.0
2	F	312	THR	2.0
2	F	412	TYR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.