



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:26 PM UTC

PDB ID : 6ZNJ / pdb_00006znj
Title : MaeB full-length enzyme apoprotein form
Authors : Lovering, A.L.; Harding, C.J.
Deposited on : 2020-07-06
Resolution : 3.70 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

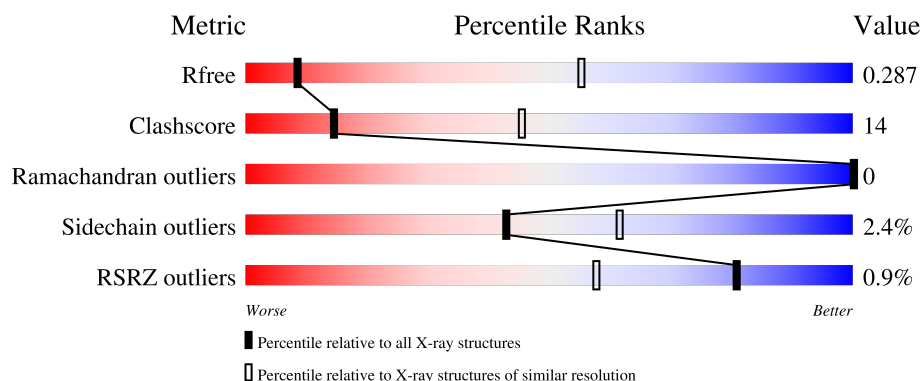
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	791	% 62% 32% . .
1	B	791	% 64% 29% . .
1	C	791	% 65% 29% . .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17400 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 NADP-dependent malate dehydrogenase, Malate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	761	Total	C	N	O	S	0	2	0
			5800	3684	992	1096	28			
1	C	761	Total	C	N	O	S	0	2	0
			5800	3684	992	1096	28			
1	A	761	Total	C	N	O	S	0	2	0
			5800	3684	992	1096	28			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	initiating methionine	UNP Q6MM14
B	-9	GLY	-	expression tag	UNP Q6MM14
B	-8	SER	-	expression tag	UNP Q6MM14
B	-7	SER	-	expression tag	UNP Q6MM14
B	-6	HIS	-	expression tag	UNP Q6MM14
B	-5	HIS	-	expression tag	UNP Q6MM14
B	-4	HIS	-	expression tag	UNP Q6MM14
B	-3	HIS	-	expression tag	UNP Q6MM14
B	-2	HIS	-	expression tag	UNP Q6MM14
B	-1	HIS	-	expression tag	UNP Q6MM14
B	0	SER	-	expression tag	UNP Q6MM14
B	121	ASP	-	linker	UNP Q6MM14
B	122	ILE	-	linker	UNP Q6MM14
B	123	GLU	-	linker	UNP Q6MM14
B	124	VAL	-	linker	UNP Q6MM14
C	-10	MET	-	initiating methionine	UNP Q6MM14
C	-9	GLY	-	expression tag	UNP Q6MM14
C	-8	SER	-	expression tag	UNP Q6MM14
C	-7	SER	-	expression tag	UNP Q6MM14
C	-6	HIS	-	expression tag	UNP Q6MM14
C	-5	HIS	-	expression tag	UNP Q6MM14
C	-4	HIS	-	expression tag	UNP Q6MM14

Continued on next page...

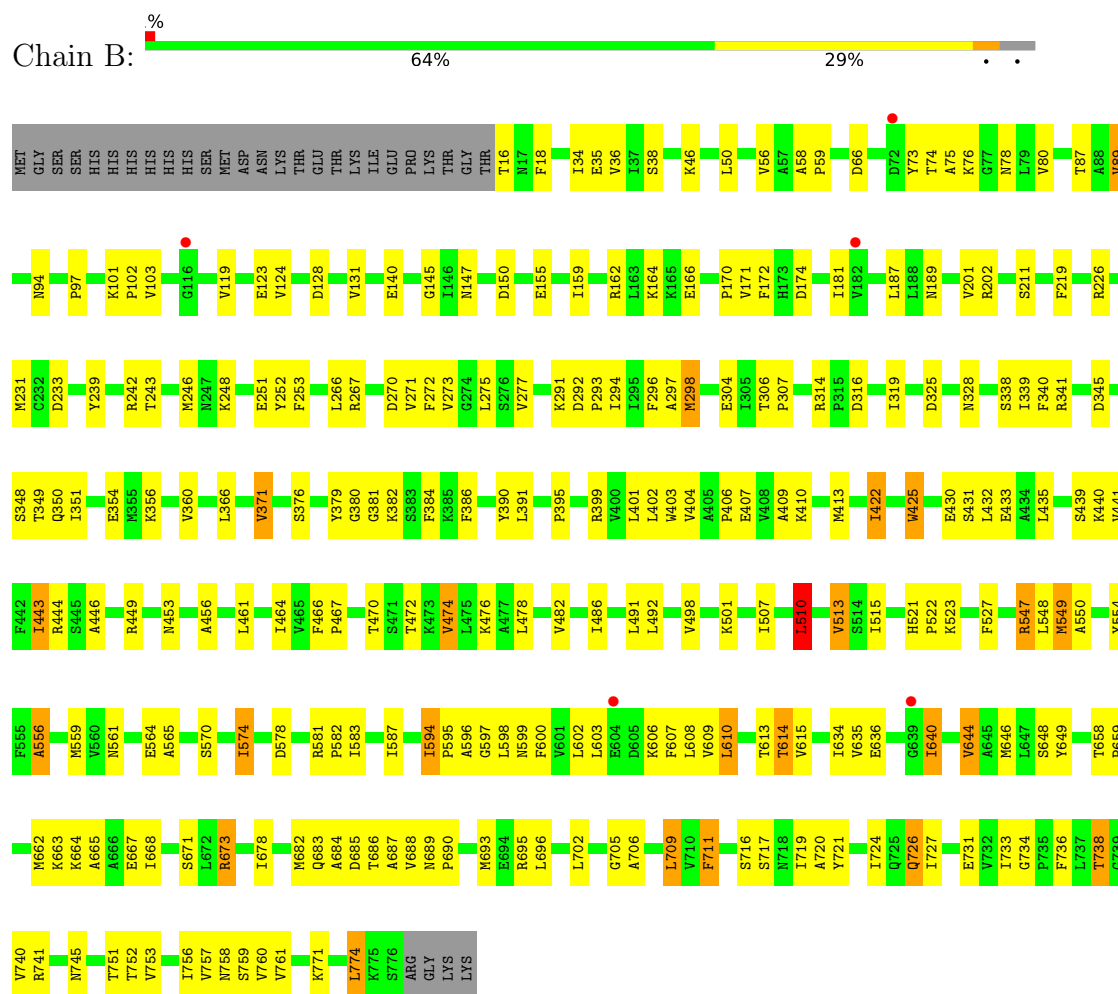
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	HIS	-	expression tag	UNP Q6MM14
C	-2	HIS	-	expression tag	UNP Q6MM14
C	-1	HIS	-	expression tag	UNP Q6MM14
C	0	SER	-	expression tag	UNP Q6MM14
C	121	ASP	-	linker	UNP Q6MM14
C	122	ILE	-	linker	UNP Q6MM14
C	123	GLU	-	linker	UNP Q6MM14
C	124	VAL	-	linker	UNP Q6MM14
A	-10	MET	-	initiating methionine	UNP Q6MM14
A	-9	GLY	-	expression tag	UNP Q6MM14
A	-8	SER	-	expression tag	UNP Q6MM14
A	-7	SER	-	expression tag	UNP Q6MM14
A	-6	HIS	-	expression tag	UNP Q6MM14
A	-5	HIS	-	expression tag	UNP Q6MM14
A	-4	HIS	-	expression tag	UNP Q6MM14
A	-3	HIS	-	expression tag	UNP Q6MM14
A	-2	HIS	-	expression tag	UNP Q6MM14
A	-1	HIS	-	expression tag	UNP Q6MM14
A	0	SER	-	expression tag	UNP Q6MM14
A	121	ASP	-	linker	UNP Q6MM14
A	122	ILE	-	linker	UNP Q6MM14
A	123	GLU	-	linker	UNP Q6MM14
A	124	VAL	-	linker	UNP Q6MM14

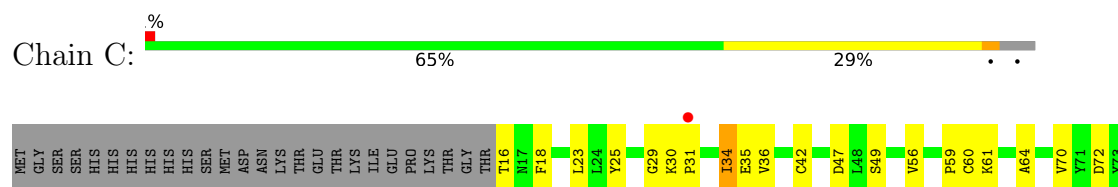
3 Residue-property plots

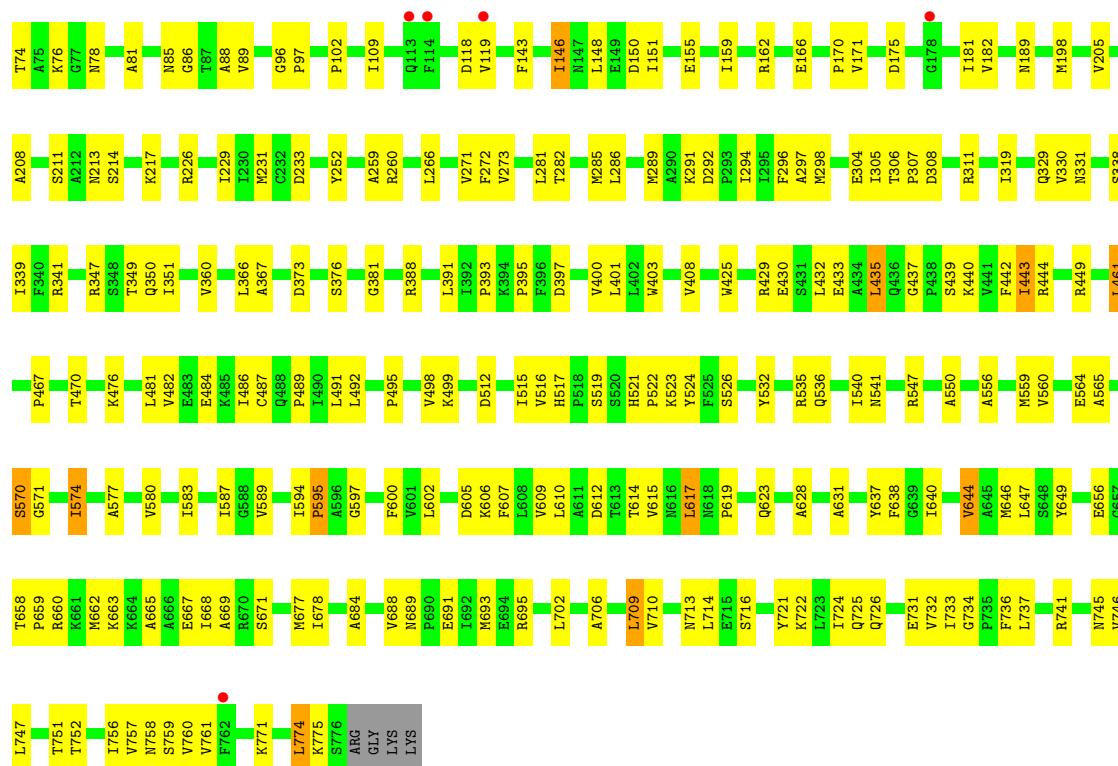
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NADP-dependent malate dehydrogenase, Malate dehydrogenase

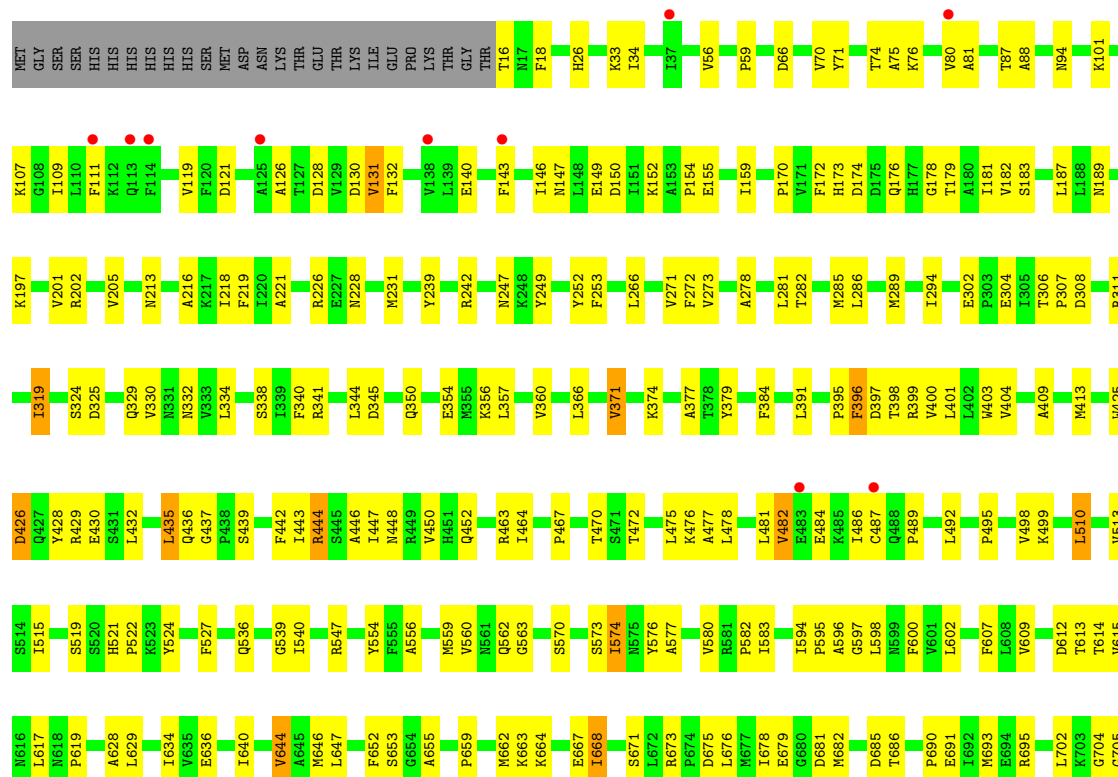


- Molecule 1: NADP-dependent malate dehydrogenase, Malate dehydrogenase





• Molecule 1: NADP-dependent malate dehydrogenase, Malate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	81.70Å 273.58Å 308.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.77 – 3.70 66.77 – 3.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (66.77-3.70) 96.6 (66.77-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 3.68Å)	Xtriage
Refinement program	PHENIX v1.0	Depositor
R, R_{free}	0.210 , 0.270 0.226 , 0.287	Depositor DCC
R_{free} test set	1791 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	101.5	Xtriage
Anisotropy	0.946	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17400	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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	0.85	0/5909	1.22	28/8004 (0.3%)
1	B	0.82	2/5909 (0.0%)	1.19	27/8004 (0.3%)
1	C	0.80	1/5909 (0.0%)	1.15	18/8004 (0.2%)
All	All	0.83	3/17727 (0.0%)	1.19	73/24012 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	456	ALA	CA-CB	-5.47	1.45	1.53
1	C	171	VAL	CA-CB	-5.44	1.47	1.54
1	B	610	LEU	CA-C	5.16	1.58	1.52

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	436	GLN	N-CA-C	-10.77	91.26	109.24
1	A	436	GLN	CB-CA-C	10.43	130.00	109.35
1	B	689	ASN	CA-C-N	9.12	128.85	119.64
1	B	689	ASN	C-N-CA	9.12	128.85	119.64
1	C	146	ILE	N-CA-C	7.91	119.48	107.77
1	B	119	VAL	N-CA-C	7.89	119.70	108.17
1	C	775	LYS	N-CA-C	7.76	119.37	111.07
1	B	727	ILE	CB-CA-C	-7.53	104.07	111.30
1	A	732	VAL	N-CA-C	7.18	118.40	107.77
1	A	644	VAL	N-CA-C	7.04	118.03	108.17
1	B	673	ARG	CA-C-N	7.02	127.17	119.87
1	B	673	ARG	C-N-CA	7.02	127.17	119.87
1	A	131	VAL	CA-C-N	6.83	129.31	120.44
1	A	131	VAL	C-N-CA	6.83	129.31	120.44
1	A	131	VAL	CB-CA-C	-6.80	103.27	111.97
1	B	461	LEU	CA-C-N	6.72	127.09	119.83
1	B	461	LEU	C-N-CA	6.72	127.09	119.83
1	B	644	VAL	N-CA-C	6.70	117.55	108.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	595	PRO	CA-C-O	-6.70	114.23	121.27
1	C	644	VAL	N-CA-C	6.62	117.44	108.17
1	C	119	VAL	N-CA-C	6.59	117.79	108.17
1	B	711	PHE	N-CA-C	6.52	118.94	110.40
1	C	724	ILE	CB-CA-C	-6.35	103.84	111.97
1	A	437	GLY	N-CA-C	6.31	125.20	112.34
1	A	652	PHE	N-CA-C	6.25	120.18	111.74
1	B	464	ILE	N-CA-C	6.18	117.02	108.12
1	C	437	GLY	CA-C-N	6.07	125.75	119.56
1	C	437	GLY	C-N-CA	6.07	125.75	119.56
1	B	58	ALA	CA-C-N	-6.04	112.27	118.85
1	B	58	ALA	C-N-CA	-6.04	112.27	118.85
1	A	146	ILE	CB-CA-C	-6.04	102.20	110.77
1	B	510	LEU	N-CA-C	5.96	118.58	110.06
1	A	218	ILE	N-CA-C	5.95	116.60	110.82
1	B	140	GLU	CA-C-N	-5.92	112.76	119.28
1	B	140	GLU	C-N-CA	-5.92	112.76	119.28
1	C	229	ILE	N-CA-C	5.89	116.34	107.80
1	A	371	VAL	CA-C-N	5.87	125.82	119.78
1	A	371	VAL	C-N-CA	5.87	125.82	119.78
1	A	426	ASP	N-CA-C	-5.86	104.80	111.07
1	A	617	LEU	N-CA-C	5.78	117.38	111.14
1	B	339	ILE	N-CA-C	5.74	115.92	110.53
1	A	704	GLY	N-CA-C	-5.71	107.31	115.64
1	A	547	ARG	N-CA-C	5.65	118.37	111.82
1	B	549	MET	N-CA-C	-5.64	106.24	113.01
1	A	119	VAL	N-CA-C	5.52	116.23	108.17
1	A	140	GLU	CA-C-N	-5.48	113.25	119.28
1	A	140	GLU	C-N-CA	-5.48	113.25	119.28
1	C	614	THR	CB-CA-C	-5.39	102.12	109.28
1	B	243	THR	N-CA-C	-5.38	107.37	114.31
1	B	556	ALA	N-CA-C	-5.37	105.33	111.07
1	A	464	ILE	N-CA-C	5.34	115.81	108.12
1	B	89	VAL	N-CA-C	5.34	115.27	108.12
1	B	614	THR	N-CA-C	5.34	122.17	110.80
1	A	668	ILE	CB-CA-C	-5.33	105.14	111.97
1	C	617	LEU	CA-C-N	-5.30	117.61	122.28
1	C	617	LEU	C-N-CA	-5.30	117.61	122.28
1	B	339	ILE	CB-CA-C	-5.29	105.08	112.02
1	C	97	PRO	N-CA-C	-5.27	106.66	113.57
1	C	570	SER	N-CA-C	5.24	115.05	108.45
1	C	649	TYR	N-CA-C	-5.19	106.72	113.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	461	LEU	CA-C-N	5.19	125.44	119.83
1	C	461	LEU	C-N-CA	5.19	125.44	119.83
1	A	146	ILE	N-CA-C	5.17	115.31	107.75
1	B	371	VAL	CA-C-N	5.13	125.41	119.92
1	B	371	VAL	C-N-CA	5.13	125.41	119.92
1	A	302	GLU	CA-C-N	5.13	125.11	120.03
1	A	302	GLU	C-N-CA	5.13	125.11	120.03
1	A	319	ILE	N-CA-C	5.13	116.10	108.46
1	B	474	VAL	CB-CA-C	-5.07	105.47	111.97
1	B	298	MET	N-CA-C	5.06	118.77	112.59
1	C	49	SER	N-CA-C	-5.05	107.06	113.18
1	A	109	ILE	N-CA-C	-5.01	105.61	110.42
1	A	396	PHE	N-CA-C	5.01	118.54	112.93

There are no chirality outliers.

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	5800	0	5906	172	0
1	B	5800	0	5906	171	0
1	C	5800	0	5906	169	0
All	All	17400	0	17718	493	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (493) 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:607:PHE:HE2	1:B:640:ILE:HD12	1.32	0.94
1:C:443:ILE:HD11	1:C:758:ASN:HB3	1.49	0.94
1:C:607:PHE:HE2	1:C:640:ILE:HD12	1.34	0.91
1:A:226:ARG:HH21	1:A:253:PHE:HD1	1.20	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:PRO:HA	1:A:319:ILE:HD13	1.55	0.87
1:C:307:PRO:HA	1:C:319:ILE:HD13	1.58	0.86
1:A:443:ILE:HD11	1:A:758:ASN:HD22	1.41	0.86
1:B:443:ILE:HD11	1:B:758:ASN:HB3	1.58	0.84
1:B:422:ILE:HB	1:B:425:TRP:HZ3	1.44	0.82
1:A:613:THR:HG22	1:A:717:SER:HB2	1.61	0.82
1:C:498:VAL:HG21	1:C:515:ILE:HG21	1.61	0.81
1:B:613:THR:HG22	1:B:717:SER:HB2	1.62	0.81
1:B:467:PRO:HG2	1:B:570:SER:HB3	1.63	0.80
1:B:226:ARG:NH2	1:B:252:TYR:O	2.15	0.80
1:C:491:LEU:HB2	1:C:515:ILE:HG12	1.66	0.77
1:A:308:ASP:OD1	1:A:311:ARG:NH2	2.16	0.77
1:C:547:ARG:NH2	1:A:573:SER:O	2.17	0.76
1:B:594:ILE:HD12	1:B:595:PRO:HD2	1.68	0.75
1:B:510:LEU:HG	1:B:513:VAL:HG13	1.68	0.75
1:C:646:MET:HB3	1:C:662:MET:HE3	1.68	0.74
1:A:354:GLU:OE1	1:A:354:GLU:N	2.20	0.74
1:C:271:VAL:HG22	1:C:294:ILE:HB	1.70	0.73
1:B:597:GLY:HA3	1:B:614:THR:OG1	1.89	0.73
1:A:189:ASN:ND2	1:A:391:LEU:O	2.23	0.71
1:A:430:GLU:HG2	1:A:444:ARG:HD2	1.72	0.71
1:B:527:PHE:HB3	1:B:549:MET:HE3	1.72	0.70
1:B:226:ARG:HH22	1:B:253:PHE:HA	1.56	0.70
1:B:644:VAL:HB	1:B:678:ILE:HG23	1.71	0.70
1:B:341:ARG:NH2	1:B:345:ASP:OD1	2.25	0.70
1:A:101:LYS:NZ	1:A:121:ASP:OD2	2.24	0.70
1:A:486:ILE:HD13	1:A:761:VAL:HG22	1.72	0.70
1:A:226:ARG:HH22	1:A:253:PHE:HA	1.57	0.69
1:C:439:SER:HA	1:C:602:LEU:HD22	1.74	0.69
1:B:271:VAL:HG22	1:B:294:ILE:HB	1.74	0.69
1:C:433:GLU:OE1	1:C:444:ARG:HD2	1.93	0.68
1:C:76:LYS:NZ	1:C:143:PHE:O	2.22	0.68
1:A:226:ARG:NH2	1:A:252:TYR:O	2.28	0.66
1:A:226:ARG:NH2	1:A:253:PHE:HA	2.10	0.66
1:A:366:LEU:HD13	1:A:403:TRP:CD2	2.30	0.66
1:A:439:SER:HA	1:A:602:LEU:HD22	1.78	0.65
1:B:422:ILE:HB	1:B:425:TRP:CZ3	2.27	0.65
1:B:16:THR:HG22	1:B:18:PHE:H	1.62	0.65
1:C:745:ASN:ND2	1:C:759:SER:OG	2.30	0.65
1:C:583:ILE:HG23	1:C:587:ILE:HD12	1.78	0.64
1:B:189:ASN:ND2	1:B:391:LEU:O	2.29	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LYS:HE3	1:A:398:THR:HG21	1.79	0.64
1:B:702:LEU:HD11	1:B:706:ALA:HB2	1.80	0.64
1:A:594:ILE:HD12	1:A:595:PRO:HD2	1.78	0.64
1:C:442:PHE:HD2	1:C:602:LEU:HD21	1.63	0.64
1:C:170:PRO:HB3	1:C:351:ILE:HG13	1.80	0.64
1:C:594:ILE:HD12	1:C:595:PRO:HD2	1.80	0.64
1:C:349:THR:O	1:C:350:GLN:HG3	1.97	0.63
1:C:617:LEU:HD12	1:C:714:LEU:HD22	1.79	0.63
1:C:281:LEU:HD21	1:C:286:LEU:HD21	1.81	0.63
1:C:481:LEU:HD23	1:C:486:ILE:HD12	1.81	0.63
1:C:467:PRO:HG2	1:C:570:SER:HB3	1.81	0.63
1:A:226:ARG:NH2	1:A:253:PHE:HD1	1.95	0.63
1:A:628:ALA:HB2	1:A:710:VAL:HG21	1.81	0.62
1:B:646:MET:HB3	1:B:662:MET:HE3	1.81	0.61
1:C:376:SER:O	1:C:381:GLY:N	2.33	0.61
1:C:607:PHE:CE2	1:C:640:ILE:HD12	2.26	0.61
1:A:769:TYR:O	1:A:773:VAL:HG23	2.00	0.61
1:A:636:GLU:OE2	1:A:673:ARG:NH1	2.29	0.61
1:B:430:GLU:HG2	1:B:444:ARG:HD3	1.82	0.61
1:A:216:ALA:HB2	1:A:231:MET:HE1	1.82	0.61
1:A:442:PHE:CD2	1:A:602:LEU:HD21	2.36	0.61
1:C:771:LYS:O	1:C:774:LEU:HB3	2.00	0.61
1:B:521:HIS:CG	1:B:522:PRO:HD2	2.36	0.61
1:A:181:ILE:HD11	1:A:356:LYS:HB3	1.83	0.61
1:A:271:VAL:HG22	1:A:294:ILE:HB	1.81	0.61
1:B:745:ASN:ND2	1:B:759:SER:OG	2.33	0.61
1:B:89:VAL:HA	1:B:150:ASP:HB3	1.82	0.60
1:B:498:VAL:HG21	1:B:515:ILE:HG21	1.82	0.60
1:A:172:PHE:CE1	1:A:174:ASP:HA	2.36	0.60
1:A:219:PHE:HE2	1:A:273:VAL:HG21	1.66	0.60
1:A:128:ASP:HB2	1:A:131:VAL:HG23	1.84	0.59
1:C:481:LEU:O	1:C:484:GLU:HB2	2.02	0.59
1:A:607:PHE:HE2	1:A:640:ILE:HD12	1.68	0.59
1:C:72:ASP:OD1	1:C:347:ARG:NH2	2.34	0.59
1:C:397:ASP:HB3	1:C:400:VAL:HG23	1.84	0.59
1:C:481:LEU:CD2	1:C:486:ILE:HD12	2.33	0.59
1:B:201:VAL:HG13	1:B:270:ASP:HB2	1.83	0.59
1:A:71:TYR:CE2	1:A:76:LYS:HD3	2.38	0.59
1:C:30:LYS:NZ	1:C:34:ILE:O	2.32	0.59
1:A:495:PRO:HA	1:A:515:ILE:HG21	1.85	0.58
1:A:519:SER:HA	1:A:524:TYR:CE1	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:ALA:HB3	1:B:738:THR:OG1	2.03	0.58
1:C:208:ALA:HB2	1:C:233:ASP:HB3	1.86	0.58
1:B:102:PRO:HG3	1:C:74:THR:HG22	1.85	0.57
1:C:713:ASN:O	1:C:716:SER:OG	2.22	0.57
1:A:679:GLU:HB3	1:A:682:MET:HE1	1.86	0.57
1:B:598:LEU:HD21	1:B:609:VAL:HG13	1.87	0.57
1:B:682:MET:SD	1:B:687:ALA:HA	2.45	0.57
1:B:720:ALA:O	1:B:724:ILE:HG13	2.04	0.57
1:C:498:VAL:HG21	1:C:515:ILE:HD13	1.87	0.57
1:C:597:GLY:N	1:C:612:ASP:OD1	2.30	0.56
1:C:42:CYS:HA	1:C:47:ASP:HB3	1.87	0.56
1:B:328:ASN:OD1	1:B:391:LEU:N	2.36	0.56
1:C:189:ASN:ND2	1:C:391:LEU:O	2.33	0.56
1:A:521:HIS:CG	1:A:522:PRO:HD2	2.39	0.56
1:B:470:THR:HG22	1:B:498:VAL:HG12	1.87	0.56
1:B:73:TYR:CZ	1:C:23:LEU:HD22	2.41	0.56
1:B:162:ARG:HG3	1:B:166:GLU:HG3	1.88	0.56
1:B:307:PRO:HA	1:B:319:ILE:HD13	1.86	0.56
1:A:580:VAL:HA	1:A:583:ILE:HD12	1.88	0.56
1:C:339:ILE:HA	1:C:408:VAL:HG21	1.88	0.56
1:B:366:LEU:HD13	1:B:403:TRP:CD2	2.41	0.55
1:C:401:LEU:HD21	1:C:432:LEU:HD22	1.88	0.55
1:C:425:TRP:HB3	1:C:429:ARG:NH2	2.21	0.55
1:C:612:ASP:OD2	1:C:615:VAL:HB	2.05	0.55
1:C:662:MET:O	1:C:665:ALA:HB3	2.05	0.55
1:B:486:ILE:HD13	1:B:761:VAL:HG22	1.87	0.55
1:C:702:LEU:HD11	1:C:706:ALA:HB2	1.88	0.55
1:B:734:GLY:HA2	1:B:736:PHE:CE1	2.41	0.55
1:C:495:PRO:HD3	1:C:517:HIS:HB2	1.86	0.55
1:C:88:ALA:O	1:C:150:ASP:HB3	2.05	0.55
1:A:334:LEU:HD21	1:A:395:PRO:HA	1.88	0.55
1:A:757:VAL:O	1:A:761:VAL:HG23	2.06	0.55
1:A:766:GLU:O	1:A:770:ILE:HG12	2.06	0.55
1:A:282:THR:OG1	1:A:285:MET:HG3	2.07	0.55
1:B:172:PHE:CE1	1:B:174:ASP:HA	2.42	0.55
1:A:607:PHE:CE2	1:A:640:ILE:HD12	2.42	0.55
1:B:399:ARG:HA	1:B:402:LEU:HD12	1.89	0.55
1:B:547:ARG:O	1:B:550:ALA:HB3	2.07	0.55
1:C:536:GLN:HA	1:C:540:ILE:O	2.07	0.54
1:A:691:GLU:OE2	1:A:695:ARG:NH1	2.39	0.54
1:B:297:ALA:HB1	1:B:304:GLU:H	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:VAL:O	1:A:74:THR:OG1	2.14	0.54
1:A:221:ALA:HB1	1:A:357:LEU:HD11	1.89	0.54
1:B:202:ARG:NH2	1:B:267:ARG:O	2.41	0.54
1:A:182:VAL:CG1	1:A:330:VAL:HG13	2.37	0.54
1:B:693:MET:HE3	1:B:702:LEU:HD22	1.90	0.54
1:A:693:MET:HG2	1:A:702:LEU:O	2.08	0.54
1:B:440:LYS:O	1:B:443:ILE:HG22	2.08	0.54
1:B:239:TYR:CZ	1:B:242:ARG:HB2	2.43	0.54
1:A:178:GLY:HA3	1:A:332:ASN:ND2	2.23	0.54
1:A:450:VAL:HG22	1:A:765:LEU:HG	1.89	0.53
1:B:371:VAL:HG21	1:B:384:PHE:HB2	1.89	0.53
1:B:338:SER:O	1:B:341:ARG:HB3	2.07	0.53
1:C:85:ASN:OD1	1:C:151:ILE:HG23	2.08	0.53
1:B:603:LEU:HB2	1:B:606:LYS:O	2.08	0.53
1:C:439:SER:HA	1:C:602:LEU:CD2	2.38	0.53
1:A:444:ARG:NH1	1:A:484:GLU:OE2	2.35	0.53
1:B:771:LYS:NZ	1:B:774:LEU:HD12	2.23	0.53
1:C:286:LEU:HD11	1:C:305:ILE:HD13	1.90	0.53
1:B:291:LYS:NZ	1:B:292:ASP:OD2	2.42	0.53
1:C:226:ARG:NH2	1:C:252:TYR:O	2.41	0.53
1:A:478:LEU:HA	1:A:481:LEU:HD12	1.90	0.53
1:B:128:ASP:HB2	1:B:131:VAL:HG23	1.91	0.53
1:B:607:PHE:CE2	1:B:640:ILE:HD12	2.25	0.52
1:A:690:PRO:HB3	1:A:705:GLY:N	2.24	0.52
1:B:354:GLU:OE1	1:B:354:GLU:N	2.37	0.52
1:B:449:ARG:HG2	1:B:449:ARG:HH11	1.75	0.52
1:C:486:ILE:HD13	1:C:761:VAL:HG22	1.91	0.52
1:C:443:ILE:CD1	1:C:758:ASN:HB3	2.31	0.52
1:A:498:VAL:HG23	1:A:515:ILE:HD13	1.92	0.52
1:C:16:THR:HG22	1:C:18:PHE:H	1.75	0.52
1:C:259:ALA:O	1:C:260:ARG:NH1	2.39	0.52
1:A:644:VAL:HB	1:A:678:ILE:HG23	1.91	0.52
1:C:162:ARG:HG3	1:C:166:GLU:HG3	1.92	0.52
1:A:646:MET:HB3	1:A:662:MET:HE3	1.93	0.52
1:C:440:LYS:O	1:C:443:ILE:HG22	2.10	0.51
1:A:470:THR:HG22	1:A:498:VAL:HG12	1.92	0.51
1:A:487:CYS:O	1:A:489:PRO:HD3	2.10	0.51
1:B:498:VAL:CG2	1:B:515:ILE:HD13	2.41	0.51
1:B:595:PRO:HB2	1:B:615:VAL:HG11	1.90	0.51
1:B:74:THR:HG22	1:C:102:PRO:HG3	1.91	0.51
1:B:376:SER:O	1:B:381:GLY:N	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:ALA:HB2	1:C:393:PRO:HD3	1.91	0.51
1:A:282:THR:HG23	1:A:285:MET:HE3	1.93	0.51
1:A:443:ILE:O	1:A:446:ALA:HB3	2.11	0.51
1:C:725:GLN:HG3	1:C:732:VAL:HB	1.92	0.51
1:B:170:PRO:HB3	1:B:351:ILE:HG13	1.93	0.51
1:C:88:ALA:O	1:C:150:ASP:CB	2.59	0.51
1:C:214:SER:HA	1:C:217:LYS:HD3	1.92	0.51
1:C:693:MET:HE3	1:C:702:LEU:HD22	1.92	0.51
1:A:463:ARG:NH2	1:A:563:GLY:O	2.44	0.51
1:B:663:LYS:HE2	1:B:667:GLU:OE2	2.11	0.51
1:B:668:ILE:O	1:B:671:SER:HB2	2.11	0.51
1:C:605:ASP:CG	1:C:606:LYS:H	2.19	0.51
1:B:219:PHE:HE2	1:B:273:VAL:HG21	1.76	0.51
1:A:187:LEU:HD11	1:A:271:VAL:HG21	1.93	0.51
1:B:600:PHE:HB2	1:B:733:ILE:HG12	1.92	0.50
1:C:292:ASP:CG	1:C:388:ARG:HH22	2.19	0.50
1:A:281:LEU:HD21	1:A:286:LEU:HD21	1.92	0.50
1:B:38:SER:HB2	1:C:109:ILE:HD12	1.92	0.50
1:B:583:ILE:HG23	1:B:587:ILE:HD12	1.92	0.50
1:A:728:GLY:C	1:A:730:ALA:H	2.19	0.50
1:C:470:THR:HG22	1:C:498:VAL:HG12	1.93	0.50
1:B:356:LYS:O	1:B:360:VAL:HG23	2.11	0.50
1:C:155:GLU:O	1:C:159:ILE:HG13	2.11	0.50
1:C:519:SER:HA	1:C:524:TYR:CE1	2.46	0.50
1:C:556:ALA:O	1:C:560:VAL:HG23	2.11	0.50
1:A:577:ALA:O	1:A:580:VAL:HG12	2.11	0.50
1:B:443:ILE:O	1:B:446:ALA:HB3	2.12	0.50
1:B:662:MET:O	1:B:665:ALA:HB3	2.12	0.50
1:B:101:LYS:HB2	1:B:123:GLU:HG2	1.93	0.50
1:B:726:GLN:HG2	1:C:688:VAL:HG23	1.93	0.50
1:C:756:ILE:O	1:C:760:VAL:HG23	2.11	0.50
1:B:401:LEU:HG	1:B:432:LEU:HD23	1.94	0.50
1:B:431:SER:O	1:B:435:LEU:HD13	2.12	0.50
1:A:481:LEU:HD23	1:A:486:ILE:HD12	1.94	0.50
1:B:598:LEU:HD23	1:B:599:ASN:N	2.27	0.49
1:A:482:VAL:HG11	1:A:510:LEU:HD11	1.93	0.49
1:B:266:LEU:HD21	1:B:272:PHE:HD1	1.75	0.49
1:A:205:VAL:HB	1:A:231:MET:HG3	1.92	0.49
1:A:219:PHE:CE2	1:A:273:VAL:HG21	2.47	0.49
1:A:746:VAL:HG12	1:A:747:LEU:O	2.12	0.49
1:B:187:LEU:HD11	1:B:271:VAL:HG21	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:ARG:O	1:C:540:ILE:HB	2.11	0.49
1:C:668:ILE:O	1:C:671:SER:HB2	2.13	0.49
1:A:554:TYR:CZ	1:A:582:PRO:HB3	2.47	0.49
1:B:491:LEU:O	1:B:492:LEU:HD23	2.12	0.49
1:C:498:VAL:CG2	1:C:515:ILE:HD13	2.43	0.49
1:A:366:LEU:HD13	1:A:403:TRP:CG	2.47	0.49
1:C:644:VAL:HB	1:C:678:ILE:HG23	1.95	0.49
1:C:663:LYS:HE2	1:C:667:GLU:OE2	2.12	0.49
1:C:691:GLU:OE2	1:C:695:ARG:NH1	2.45	0.49
1:A:748:GLN:O	1:A:751:THR:OG1	2.29	0.49
1:B:470:THR:O	1:B:501:LYS:NZ	2.41	0.49
1:B:726:GLN:OE1	1:C:689:ASN:ND2	2.39	0.49
1:B:695:ARG:HE	1:B:696:LEU:HD21	1.78	0.49
1:C:182:VAL:CG1	1:C:330:VAL:HG13	2.43	0.49
1:A:467:PRO:HA	1:A:492:LEU:HB2	1.95	0.49
1:B:556:ALA:O	1:B:559:MET:HB2	2.12	0.49
1:C:296:PHE:HB3	1:C:298:MET:HE2	1.94	0.49
1:C:307:PRO:HB3	1:C:319:ILE:HG21	1.95	0.49
1:B:548:LEU:HD22	1:B:554:TYR:CE1	2.49	0.48
1:C:308:ASP:OD1	1:C:311:ARG:NH2	2.39	0.48
1:A:266:LEU:HD21	1:A:272:PHE:HD1	1.78	0.48
1:A:442:PHE:HD2	1:A:602:LEU:HD21	1.75	0.48
1:A:539:GLY:O	1:A:540:ILE:HD13	2.13	0.48
1:A:486:ILE:CD1	1:A:761:VAL:HG22	2.42	0.48
1:B:726:GLN:HG2	1:C:688:VAL:CG2	2.43	0.48
1:C:547:ARG:O	1:C:550:ALA:HB3	2.13	0.48
1:A:338:SER:HB3	1:A:404:VAL:HB	1.95	0.48
1:A:772:GLU:OE2	1:A:775:LYS:HD3	2.13	0.48
1:B:498:VAL:HG21	1:B:515:ILE:HD13	1.95	0.48
1:C:430:GLU:HG2	1:C:444:ARG:HD3	1.95	0.48
1:C:524:TYR:C	1:C:524:TYR:CD2	2.91	0.48
1:B:36:VAL:HG13	1:C:35:GLU:O	2.13	0.48
1:C:521:HIS:CG	1:C:522:PRO:HD2	2.48	0.48
1:A:612:ASP:OD2	1:A:615:VAL:HB	2.13	0.48
1:B:751:THR:HG22	1:B:752:THR:O	2.14	0.48
1:C:89:VAL:HA	1:C:150:ASP:HB3	1.95	0.48
1:C:148:LEU:HB3	1:C:151:ILE:CD1	2.44	0.48
1:C:266:LEU:HD21	1:C:272:PHE:HD1	1.78	0.48
1:C:492:LEU:HA	1:C:516:VAL:O	2.13	0.48
1:A:685:ASP:OD1	1:A:686:THR:N	2.47	0.48
1:B:443:ILE:CD1	1:B:758:ASN:HB3	2.38	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:ARG:N	1:B:582:PRO:HD2	2.28	0.48
1:B:600:PHE:HB2	1:B:733:ILE:CG1	2.44	0.48
1:B:684:ALA:O	1:B:687:ALA:HB3	2.14	0.48
1:A:278:ALA:HA	1:A:304:GLU:HA	1.95	0.48
1:A:374:LYS:HE3	1:A:398:THR:CG2	2.44	0.47
1:A:510:LEU:HA	1:A:510:LEU:HD12	1.35	0.47
1:B:325:ASP:OD2	1:B:325:ASP:N	2.42	0.47
1:A:576:TYR:CE1	1:A:614:THR:HG21	2.49	0.47
1:A:743:SER:OG	1:A:763:THR:O	2.33	0.47
1:A:467:PRO:HG2	1:A:570:SER:HB3	1.95	0.47
1:B:602:LEU:N	1:B:602:LEU:HD12	2.28	0.47
1:C:442:PHE:CD2	1:C:602:LEU:HD21	2.47	0.47
1:C:609:VAL:HG11	1:C:631:ALA:HB1	1.97	0.47
1:C:746:VAL:HG12	1:C:747:LEU:O	2.15	0.47
1:B:246:MET:HE2	1:B:251:GLU:OE2	2.14	0.47
1:B:711:PHE:CE2	1:B:717:SER:HA	2.49	0.47
1:A:152:LYS:NZ	1:A:155:GLU:OE1	2.40	0.47
1:B:683:GLN:OE1	1:C:722:LYS:HE2	2.15	0.47
1:C:571:GLY:HA2	1:C:574:ILE:HG13	1.97	0.47
1:C:734:GLY:HA2	1:C:736:PHE:CE1	2.50	0.47
1:A:659:PRO:HB3	1:A:681:ASP:OD2	2.14	0.47
1:B:164:LYS:HG2	1:B:171:VAL:HB	1.97	0.46
1:B:379:TYR:OH	1:B:395:PRO:HD2	2.15	0.46
1:B:648:SER:O	1:B:683:GLN:HA	2.15	0.46
1:C:338:SER:O	1:C:341:ARG:HB3	2.15	0.46
1:C:559:MET:HE2	1:C:565:ALA:HB2	1.97	0.46
1:A:723:LEU:HD23	1:A:723:LEU:HA	1.56	0.46
1:B:425:TRP:CE3	1:B:425:TRP:HA	2.49	0.46
1:C:329:GLN:NE2	1:C:331:ASN:HD22	2.13	0.46
1:C:663:LYS:O	1:C:667:GLU:HG3	2.15	0.46
1:B:239:TYR:CE1	1:B:242:ARG:HB2	2.51	0.46
1:C:86:GLY:HA3	1:C:96:GLY:O	2.15	0.46
1:A:413:MET:HE1	1:A:425:TRP:HZ2	1.79	0.46
1:B:402:LEU:O	1:B:406:PRO:HG2	2.15	0.46
1:C:349:THR:C	1:C:350:GLN:HG3	2.41	0.46
1:A:397:ASP:HB3	1:A:400:VAL:HG23	1.97	0.46
1:A:409:ALA:O	1:A:413:MET:HG3	2.15	0.46
1:A:435:LEU:HD12	1:A:435:LEU:HA	1.66	0.46
1:A:478:LEU:O	1:A:481:LEU:HB2	2.16	0.46
1:A:619:PRO:HD2	1:A:713:ASN:HA	1.97	0.46
1:A:81:ALA:HB2	1:A:143:PHE:CE1	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:756:ILE:O	1:B:760:VAL:HG23	2.15	0.46
1:C:148:LEU:HB3	1:C:151:ILE:HD11	1.97	0.46
1:C:291:LYS:NZ	1:C:292:ASP:OD2	2.48	0.46
1:A:536:GLN:HA	1:A:540:ILE:O	2.16	0.46
1:C:609:VAL:C	1:C:610:LEU:HD12	2.41	0.46
1:B:155:GLU:O	1:B:159:ILE:HG13	2.15	0.46
1:C:285:MET:O	1:C:289:MET:HG3	2.16	0.46
1:C:547:ARG:NH2	1:A:574:ILE:HA	2.31	0.46
1:B:211:SER:OG	1:B:275:LEU:HD22	2.16	0.45
1:B:478:LEU:HD23	1:B:478:LEU:HA	1.76	0.45
1:A:87:THR:HA	1:A:94:ASN:OD1	2.16	0.45
1:A:756:ILE:O	1:A:760:VAL:HG23	2.16	0.45
1:B:683:GLN:CD	1:C:722:LYS:HE2	2.41	0.45
1:A:519:SER:HA	1:A:524:TYR:CD1	2.51	0.45
1:B:219:PHE:CE2	1:B:273:VAL:HG21	2.51	0.45
1:B:292:ASP:OD1	1:B:316:ASP:HB2	2.15	0.45
1:B:386:PHE:HA	1:B:390:TYR:HD2	1.81	0.45
1:B:559:MET:HE2	1:B:565:ALA:HB2	1.98	0.45
1:C:231:MET:HE3	1:C:231:MET:HB2	1.73	0.45
1:C:523:LYS:HE3	1:C:564:GLU:OE1	2.16	0.45
1:B:50:LEU:HD13	1:C:25:TYR:HB2	1.98	0.45
1:C:600:PHE:HB2	1:C:733:ILE:CG1	2.47	0.45
1:A:472:THR:O	1:A:476:LYS:HG3	2.16	0.45
1:B:147:ASN:HB2	1:B:340:PHE:CZ	2.51	0.45
1:B:757:VAL:O	1:B:761:VAL:HG23	2.16	0.45
1:C:70:VAL:O	1:C:74:THR:OG1	2.30	0.45
1:A:556:ALA:O	1:A:560:VAL:HG23	2.16	0.45
1:B:233:ASP:CG	1:B:242:ARG:HH22	2.24	0.45
1:B:296:PHE:HB3	1:B:298:MET:HE2	1.99	0.45
1:B:649:TYR:CD2	1:C:714:LEU:HD23	2.52	0.45
1:B:688:VAL:HG12	1:B:709:LEU:HD21	1.98	0.45
1:A:338:SER:O	1:A:341:ARG:HB3	2.16	0.45
1:A:597:GLY:N	1:A:612:ASP:OD1	2.44	0.45
1:C:366:LEU:HD13	1:C:403:TRP:CD2	2.51	0.45
1:A:147:ASN:HB2	1:A:340:PHE:CZ	2.52	0.45
1:B:97:PRO:HB3	1:B:124:VAL:O	2.17	0.45
1:C:637:TYR:HD2	1:C:638:PHE:CE1	2.35	0.45
1:A:498:VAL:CG2	1:A:515:ILE:HD13	2.47	0.45
1:B:574:ILE:HG22	1:B:578:ASP:HB2	1.98	0.45
1:C:175:ASP:O	1:C:211:SER:HB3	2.17	0.45
1:A:154:PRO:HB3	1:A:247:ASN:ND2	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:523:LYS:O	1:C:526:SER:HB3	2.16	0.45
1:C:628:ALA:HB2	1:C:710:VAL:HG21	1.98	0.45
1:A:477:ALA:HB2	1:A:753:VAL:HG13	1.99	0.45
1:B:181:ILE:HG23	1:B:360:VAL:HG22	1.99	0.44
1:A:71:TYR:CZ	1:A:76:LYS:HD3	2.51	0.44
1:B:46:LYS:HE3	1:C:18:PHE:HE1	1.82	0.44
1:B:433:GLU:OE2	1:B:444:ARG:HD2	2.17	0.44
1:A:379:TYR:OH	1:A:396:PHE:HD1	2.00	0.44
1:A:598:LEU:HD21	1:A:609:VAL:HG13	2.00	0.44
1:B:103:VAL:HG23	1:C:60:CYS:SG	2.57	0.44
1:C:29:GLY:O	1:C:31:PRO:HD3	2.18	0.44
1:C:198:MET:HB3	1:C:198:MET:HE3	1.81	0.44
1:C:373:ASP:CB	1:C:476:LYS:HD2	2.47	0.44
1:C:669:ALA:HB1	1:C:678:ILE:HD13	1.99	0.44
1:B:76:LYS:O	1:B:78:ASN:N	2.50	0.44
1:A:179:THR:O	1:A:183:SER:OG	2.16	0.44
1:A:725:GLN:HG3	1:A:732:VAL:HB	1.99	0.44
1:B:349:THR:O	1:B:350:GLN:HG3	2.18	0.44
1:C:589:VAL:C	1:C:741:ARG:HG3	2.43	0.44
1:B:685:ASP:OD1	1:B:686:THR:N	2.51	0.44
1:C:366:LEU:HD13	1:C:403:TRP:CE2	2.53	0.44
1:C:751:THR:HG22	1:C:752:THR:O	2.18	0.44
1:A:448:ASN:O	1:A:452:GLN:HG3	2.17	0.44
1:C:78:ASN:ND2	1:C:118:ASP:OD2	2.51	0.44
1:C:81:ALA:HB3	1:C:146:ILE:HD12	2.00	0.44
1:C:432:LEU:O	1:C:435:LEU:HB2	2.18	0.44
1:A:345:ASP:OD2	1:A:428:TYR:OH	2.14	0.44
1:A:429:ARG:O	1:A:432:LEU:HB2	2.18	0.44
1:B:407:GLU:OE2	1:B:410:LYS:NZ	2.36	0.43
1:B:716:SER:HA	1:C:716:SER:HA	2.00	0.43
1:A:170:PRO:HG3	1:A:350:GLN:C	2.43	0.43
1:A:197:LYS:O	1:A:201:VAL:HG23	2.17	0.43
1:A:239:TYR:CE1	1:A:242:ARG:HB2	2.54	0.43
1:B:443:ILE:CD1	1:B:758:ASN:HD22	2.31	0.43
1:A:132:PHE:CE1	1:A:159:ILE:HD13	2.54	0.43
1:A:771:LYS:O	1:A:774:LEU:HB3	2.18	0.43
1:B:170:PRO:HD3	1:B:348:SER:O	2.19	0.43
1:C:523:LYS:HE3	1:C:564:GLU:CD	2.42	0.43
1:A:213:ASN:O	1:A:253:PHE:HE2	2.01	0.43
1:B:87:THR:HA	1:B:94:ASN:OD1	2.18	0.43
1:C:329:GLN:OE1	1:C:395:PRO:HG2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:MET:HE2	1:A:289:MET:HB3	1.96	0.43
1:A:734:GLY:HA2	1:A:736:PHE:CE1	2.54	0.43
1:B:341:ARG:NE	1:B:345:ASP:OD2	2.51	0.43
1:C:181:ILE:HG23	1:C:360:VAL:CG2	2.48	0.43
1:C:757:VAL:O	1:C:761:VAL:HG23	2.19	0.43
1:A:107:LYS:NZ	1:A:174:ASP:OD2	2.48	0.43
1:B:466:PHE:HD2	1:B:474:VAL:CG1	2.31	0.43
1:C:532:TYR:HE1	1:C:541:ASN:C	2.26	0.43
1:A:173:HIS:ND1	1:A:176:GLN:HG3	2.33	0.43
1:B:294:ILE:HG22	1:B:296:PHE:CE2	2.54	0.43
1:B:507:ILE:HD12	1:B:507:ILE:HA	1.78	0.43
1:B:636:GLU:OE2	1:B:673:ARG:NH1	2.31	0.43
1:C:282:THR:OG1	1:C:285:MET:HE3	2.18	0.43
1:C:577:ALA:O	1:C:580:VAL:HG12	2.19	0.43
1:A:600:PHE:HB2	1:A:733:ILE:HG12	2.01	0.43
1:B:561:ASN:OD1	1:B:741:ARG:NH2	2.49	0.43
1:B:719:ILE:HA	1:C:684:ALA:HB2	2.01	0.43
1:C:519:SER:HA	1:C:524:TYR:CD1	2.53	0.43
1:A:249:TYR:O	1:A:252:TYR:CD2	2.72	0.43
1:A:282:THR:O	1:A:286:LEU:HG	2.19	0.43
1:A:527:PHE:CE1	1:A:562:GLN:HG3	2.54	0.43
1:A:663:LYS:O	1:A:667:GLU:HG3	2.19	0.43
1:C:298:MET:HE3	1:C:298:MET:HB2	1.69	0.42
1:C:647:LEU:HD21	1:C:709:LEU:HD12	2.00	0.42
1:C:181:ILE:HG23	1:C:360:VAL:HG22	2.01	0.42
1:C:481:LEU:HD11	1:C:760:VAL:HG21	2.01	0.42
1:B:409:ALA:O	1:B:413:MET:HG3	2.20	0.42
1:B:128:ASP:HB2	1:B:131:VAL:CG2	2.49	0.42
1:B:753:VAL:O	1:B:757:VAL:HG12	2.20	0.42
1:B:297:ALA:HB1	1:B:304:GLU:N	2.33	0.42
1:B:752:THR:O	1:B:756:ILE:HG13	2.19	0.42
1:A:430:GLU:CD	1:A:448:ASN:HD21	2.26	0.42
1:B:231:MET:HE3	1:B:231:MET:HB2	1.55	0.42
1:B:248:LYS:HB3	1:B:248:LYS:HE3	1.87	0.42
1:C:512:ASP:OD1	1:C:512:ASP:N	2.50	0.42
1:C:737:LEU:HD12	1:C:737:LEU:HA	1.74	0.42
1:A:80:VAL:CG2	1:A:344:LEU:HD11	2.50	0.42
1:A:149:GLU:OE1	1:A:174:ASP:HB3	2.20	0.42
1:A:205:VAL:HG21	1:A:231:MET:HE2	2.01	0.42
1:A:374:LYS:O	1:A:377:ALA:HB3	2.20	0.42
1:A:475:LEU:O	1:A:478:LEU:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:ALA:HA	1:A:615:VAL:HG21	2.02	0.42
1:B:75:ALA:O	1:B:76:LYS:C	2.60	0.42
1:C:297:ALA:HB1	1:C:304:GLU:H	1.84	0.42
1:C:435:LEU:HD22	1:C:435:LEU:HA	1.86	0.42
1:A:111:PHE:HE1	1:A:340:PHE:CD2	2.37	0.42
1:A:668:ILE:O	1:A:671:SER:HB2	2.20	0.42
1:C:205:VAL:HG22	1:C:273:VAL:HB	2.02	0.42
1:A:499:LYS:HE2	1:A:499:LYS:HB3	1.89	0.42
1:B:80:VAL:HG13	1:B:145:GLY:O	2.20	0.42
1:B:410:LYS:CE	1:B:425:TRP:HE1	2.33	0.42
1:B:523:LYS:HE3	1:B:564:GLU:OE1	2.20	0.42
1:A:647:LEU:O	1:A:662:MET:HE2	2.19	0.42
1:B:170:PRO:HA	1:B:350:GLN:HA	2.02	0.41
1:A:75:ALA:O	1:A:76:LYS:C	2.62	0.41
1:B:87:THR:HA	1:B:94:ASN:HA	2.02	0.41
1:B:658:THR:HB	1:B:659:PRO:HD3	2.01	0.41
1:C:443:ILE:HD13	1:C:443:ILE:HG21	1.74	0.41
1:A:172:PHE:HE1	1:A:174:ASP:HA	1.80	0.41
1:A:675:ASP:OD1	1:A:676:LEU:HG	2.20	0.41
1:B:472:THR:O	1:B:476:LYS:HG3	2.20	0.41
1:C:656:GLU:HB2	1:C:660:ARG:NH2	2.35	0.41
1:A:16:THR:HG22	1:A:18:PHE:H	1.86	0.41
1:A:88:ALA:HB3	1:A:150:ASP:C	2.45	0.41
1:A:510:LEU:HG	1:A:513:VAL:HG13	2.01	0.41
1:A:629:LEU:HD23	1:A:629:LEU:HA	1.80	0.41
1:A:664:LYS:O	1:A:668:ILE:HG13	2.19	0.41
1:B:491:LEU:HB2	1:B:515:ILE:HG12	2.01	0.41
1:B:607:PHE:O	1:B:608:LEU:HD12	2.19	0.41
1:B:690:PRO:HB3	1:B:705:GLY:N	2.36	0.41
1:C:56:VAL:C	1:C:59:PRO:HD2	2.45	0.41
1:C:658:THR:N	1:C:659:PRO:CD	2.83	0.41
1:A:711:PHE:CG	1:A:717:SER:HB3	2.56	0.41
1:A:764:ALA:O	1:A:767:ALA:HB3	2.20	0.41
1:B:443:ILE:HD11	1:B:758:ASN:HD22	1.84	0.41
1:C:487:CYS:O	1:C:489:PRO:HD3	2.19	0.41
1:A:56:VAL:C	1:A:59:PRO:HD2	2.45	0.41
1:A:202:ARG:HA	1:A:228:ASN:O	2.21	0.41
1:A:159:ILE:HD13	1:A:159:ILE:HG21	1.89	0.41
1:A:324:SER:HB3	1:A:329:GLN:NE2	2.36	0.41
1:C:61:LYS:O	1:C:64:ALA:HB3	2.20	0.41
1:C:461:LEU:HA	1:C:461:LEU:HD23	1.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:SER:C	1:A:655:ALA:N	2.76	0.41
1:B:338:SER:HB3	1:B:404:VAL:HB	2.01	0.41
1:B:510:LEU:HD12	1:B:510:LEU:HA	1.72	0.41
1:C:213:ASN:O	1:C:217:LYS:HG3	2.20	0.41
1:C:439:SER:N	1:C:731:GLU:OE1	2.54	0.41
1:C:461:LEU:HD22	1:C:486:ILE:O	2.21	0.41
1:A:26:HIS:NE2	1:A:33:LYS:HD3	2.35	0.41
1:A:126:ALA:HB1	1:A:131:VAL:HB	2.02	0.41
1:A:371:VAL:HG21	1:A:384:PHE:HB2	2.01	0.41
1:A:401:LEU:HD21	1:A:432:LEU:HD22	2.03	0.41
1:A:432:LEU:O	1:A:435:LEU:HB2	2.21	0.41
1:B:56:VAL:C	1:B:59:PRO:HD2	2.46	0.41
1:B:634:ILE:HG22	1:B:635:VAL:N	2.36	0.41
1:A:443:ILE:O	1:A:447:ILE:HG13	2.20	0.41
1:A:602:LEU:HD12	1:A:602:LEU:N	2.36	0.41
1:B:380:GLY:C	1:B:382:LYS:H	2.29	0.40
1:B:609:VAL:C	1:B:610:LEU:HD12	2.46	0.40
1:C:498:VAL:HG23	1:C:499:LYS:N	2.36	0.40
1:A:325:ASP:OD2	1:A:325:ASP:N	2.35	0.40
1:B:277:VAL:O	1:B:304:GLU:HG3	2.21	0.40
1:B:293:PRO:HD3	1:B:314:ARG:NH2	2.36	0.40
1:C:677:MET:HE3	1:C:677:MET:HB2	2.01	0.40
1:A:205:VAL:CG2	1:A:231:MET:HE2	2.51	0.40
1:B:35:GLU:O	1:C:36:VAL:HG13	2.21	0.40
1:B:271:VAL:HG22	1:B:294:ILE:HD12	2.03	0.40
1:C:499:LYS:HB3	1:C:499:LYS:HE2	1.81	0.40
1:A:239:TYR:CZ	1:A:242:ARG:HB2	2.56	0.40
1:A:559:MET:HB3	1:A:559:MET:HE2	1.68	0.40
1:B:771:LYS:HD2	1:B:771:LYS:HA	1.80	0.40
1:C:449:ARG:HG2	1:C:449:ARG:HH11	1.86	0.40
1:C:619:PRO:HA	1:C:623:GLN:OE1	2.21	0.40
1:A:399:ARG:O	1:A:400:VAL:C	2.64	0.40
1:B:439:SER:N	1:B:731:GLU:OE1	2.55	0.40
1:B:664:LYS:O	1:B:668:ILE:HG13	2.21	0.40
1:B:682:MET:HG3	1:B:687:ALA:HB2	2.02	0.40
1:C:605:ASP:OD1	1:C:605:ASP:N	2.55	0.40
1:A:181:ILE:HG23	1:A:360:VAL:CG2	2.51	0.40
1:A:576:TYR:C	1:A:576:TYR:CD2	3.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	761/791 (96%)	731 (96%)	30 (4%)	0	100	100
1	B	761/791 (96%)	731 (96%)	30 (4%)	0	100	100
1	C	761/791 (96%)	738 (97%)	23 (3%)	0	100	100
All	All	2283/2373 (96%)	2200 (96%)	83 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	617/642 (96%)	603 (98%)	14 (2%)	44	62
1	B	617/642 (96%)	595 (96%)	22 (4%)	31	54
1	C	617/642 (96%)	607 (98%)	10 (2%)	55	68
All	All	1851/1926 (96%)	1805 (98%)	46 (2%)	43	61

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	34	ILE
1	B	66[A]	ASP
1	B	66[B]	ASP
1	B	306	THR
1	B	422	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	425	TRP
1	B	441	VAL
1	B	443	ILE
1	B	453	ASN
1	B	482	VAL
1	B	510	LEU
1	B	513	VAL
1	B	547	ARG
1	B	574	ILE
1	B	594	ILE
1	B	640	ILE
1	B	709	LEU
1	B	721	TYR
1	B	726	GLN
1	B	738	THR
1	B	740	VAL
1	B	774	LEU
1	C	34	ILE
1	C	306	THR
1	C	435	LEU
1	C	443	ILE
1	C	482	VAL
1	C	574	ILE
1	C	709	LEU
1	C	721	TYR
1	C	726	GLN
1	C	774	LEU
1	A	34	ILE
1	A	66[A]	ASP
1	A	66[B]	ASP
1	A	130	ASP
1	A	306	THR
1	A	426	ASP
1	A	435	LEU
1	A	444	ARG
1	A	482	VAL
1	A	510	LEU
1	A	574	ILE
1	A	634	ILE
1	A	709	LEU
1	A	721	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11)

such sidechains are listed below:

Mol	Chain	Res	Type
1	B	453	ASN
1	B	758	ASN
1	C	235	GLN
1	C	329	GLN
1	C	511	ASN
1	A	168	ASN
1	A	176	GLN
1	A	328	ASN
1	A	453	ASN
1	A	630	GLN
1	A	758	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 [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	761/791 (96%)	-0.15	10 (1%) 75 50	62, 92, 121, 142	2 (0%)
1	B	761/791 (96%)	-0.13	5 (0%) 84 63	63, 100, 132, 164	2 (0%)
1	C	761/791 (96%)	-0.14	6 (0%) 82 60	68, 109, 143, 163	2 (0%)
All	All	2283/2373 (96%)	-0.14	21 (0%) 81 58	62, 100, 136, 164	6 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	143	PHE	3.1
1	A	487	CYS	3.1
1	A	114	PHE	3.0
1	A	483	GLU	2.9
1	A	80	VAL	2.8
1	C	114	PHE	2.8
1	A	125	ALA	2.6
1	B	116	GLY	2.5
1	C	31	PRO	2.4
1	B	639	GLY	2.4
1	A	138	VAL	2.3
1	C	119	VAL	2.3
1	A	113	GLN	2.3
1	A	111	PHE	2.3
1	B	604	GLU	2.3
1	C	113	GLN	2.2
1	B	72	ASP	2.2
1	B	182	VAL	2.2
1	A	37	ILE	2.2
1	C	762	PHE	2.2
1	C	178	GLY	2.1

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.