



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:52 PM UTC

PDB ID : 1U15 / pdb_00001u15
Title : Crystal structure of a duck-delta-crystallin-1 double loop mutant (DLM)
Authors : Tsai, M.; Sampaleanu, L.M.; Greene, C.; Creagh, L.; Haynes, C.; Howell, P.L.
Deposited on : 2004-07-14
Resolution : 2.50 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

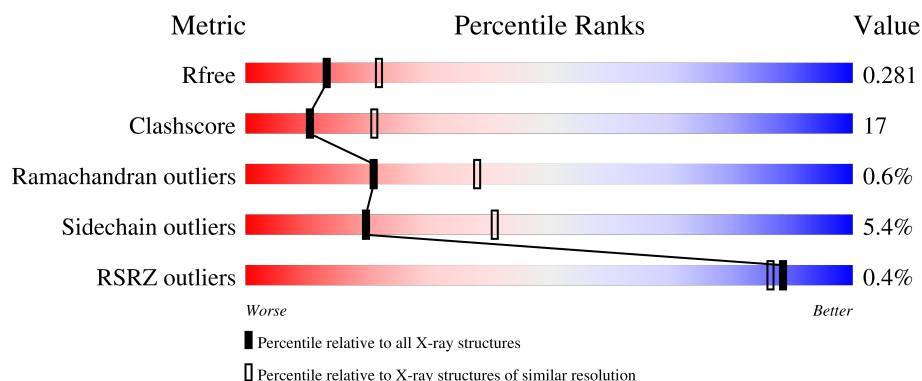
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	472	62% 28% • 5%
1	B	472	64% 28% • 5%
1	C	472	62% 29% • 5%
1	D	472	63% 29% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14536 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 Delta crystallin I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3475	2201	586	677	11			
1	B	450	Total	C	N	O	S	0	0	0
			3486	2207	590	678	11			
1	C	448	Total	C	N	O	S	0	0	0
			3472	2199	587	675	11			
1	D	450	Total	C	N	O	S	0	0	0
			3486	2207	590	678	11			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLU	GLN	engineered mutation	UNP P24057
A	23	LYS	MET	engineered mutation	UNP P24057
A	25	ASN	SER	engineered mutation	UNP P24057
A	26	SER	THR	engineered mutation	UNP P24057
A	29	ALA	SER	engineered mutation	UNP P24057
A	30	TYR	THR	engineered mutation	UNP P24057
A	31	ASP	GLU	engineered mutation	UNP P24057
A	74	TRP	LEU	engineered mutation	UNP P24057
A	79	PHE	ILE	engineered mutation	UNP P24057
A	82	LYS	THR	engineered mutation	UNP P24057
A	89	HIS	GLN	engineered mutation	UNP P24057
A	467	HIS	-	expression tag	UNP P24057
A	468	HIS	-	expression tag	UNP P24057
A	469	HIS	-	expression tag	UNP P24057
A	470	HIS	-	expression tag	UNP P24057
A	471	HIS	-	expression tag	UNP P24057
A	472	HIS	-	expression tag	UNP P24057
B	22	GLU	GLN	engineered mutation	UNP P24057
B	23	LYS	MET	engineered mutation	UNP P24057
B	25	ASN	SER	engineered mutation	UNP P24057
B	26	SER	THR	engineered mutation	UNP P24057

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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	ALA	SER	engineered mutation	UNP P24057
B	30	TYR	THR	engineered mutation	UNP P24057
B	31	ASP	GLU	engineered mutation	UNP P24057
B	74	TRP	LEU	engineered mutation	UNP P24057
B	79	PHE	ILE	engineered mutation	UNP P24057
B	82	LYS	THR	engineered mutation	UNP P24057
B	89	HIS	GLN	engineered mutation	UNP P24057
B	467	HIS	-	expression tag	UNP P24057
B	468	HIS	-	expression tag	UNP P24057
B	469	HIS	-	expression tag	UNP P24057
B	470	HIS	-	expression tag	UNP P24057
B	471	HIS	-	expression tag	UNP P24057
B	472	HIS	-	expression tag	UNP P24057
C	22	GLU	GLN	engineered mutation	UNP P24057
C	23	LYS	MET	engineered mutation	UNP P24057
C	25	ASN	SER	engineered mutation	UNP P24057
C	26	SER	THR	engineered mutation	UNP P24057
C	29	ALA	SER	engineered mutation	UNP P24057
C	30	TYR	THR	engineered mutation	UNP P24057
C	31	ASP	GLU	engineered mutation	UNP P24057
C	74	TRP	LEU	engineered mutation	UNP P24057
C	79	PHE	ILE	engineered mutation	UNP P24057
C	82	LYS	THR	engineered mutation	UNP P24057
C	89	HIS	GLN	engineered mutation	UNP P24057
C	467	HIS	-	expression tag	UNP P24057
C	468	HIS	-	expression tag	UNP P24057
C	469	HIS	-	expression tag	UNP P24057
C	470	HIS	-	expression tag	UNP P24057
C	471	HIS	-	expression tag	UNP P24057
C	472	HIS	-	expression tag	UNP P24057
D	22	GLU	GLN	engineered mutation	UNP P24057
D	23	LYS	MET	engineered mutation	UNP P24057
D	25	ASN	SER	engineered mutation	UNP P24057
D	26	SER	THR	engineered mutation	UNP P24057
D	29	ALA	SER	engineered mutation	UNP P24057
D	30	TYR	THR	engineered mutation	UNP P24057
D	31	ASP	GLU	engineered mutation	UNP P24057
D	74	TRP	LEU	engineered mutation	UNP P24057
D	79	PHE	ILE	engineered mutation	UNP P24057
D	82	LYS	THR	engineered mutation	UNP P24057
D	89	HIS	GLN	engineered mutation	UNP P24057
D	467	HIS	-	expression tag	UNP P24057

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Chain	Residue	Modelled	Actual	Comment	Reference
D	468	HIS	-	expression tag	UNP P24057
D	469	HIS	-	expression tag	UNP P24057
D	470	HIS	-	expression tag	UNP P24057
D	471	HIS	-	expression tag	UNP P24057
D	472	HIS	-	expression tag	UNP P24057

- Molecule 2 is water.

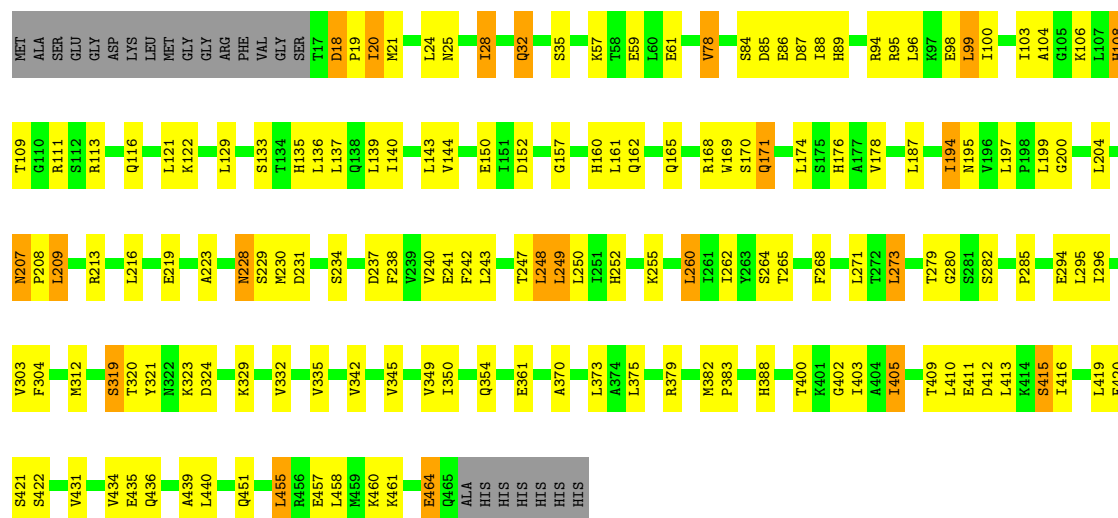
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	169	Total O 169 169	0	0
2	B	128	Total O 128 128	0	0
2	C	173	Total O 173 173	0	0
2	D	147	Total O 147 147	0	0

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.

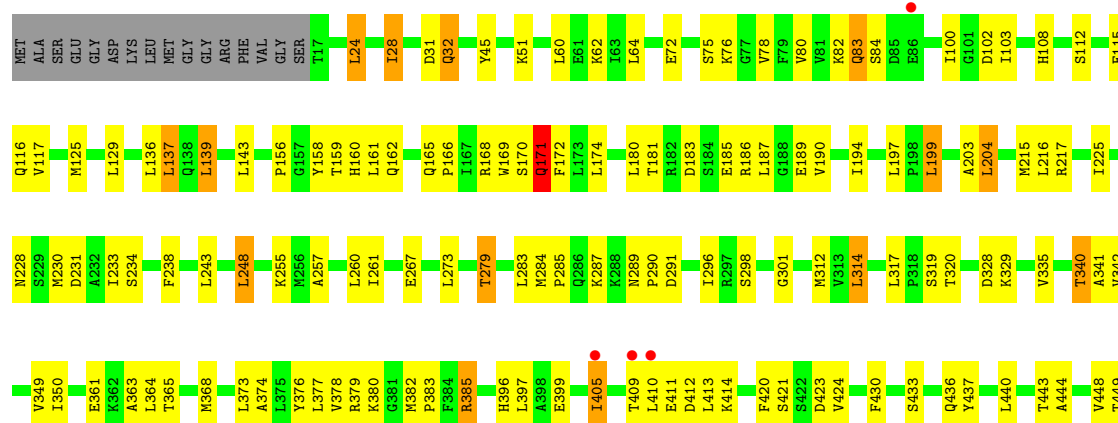
• Molecule 1: Delta crystallin I

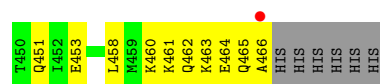
Chain A: 



• Molecule 1: Delta crystallin I

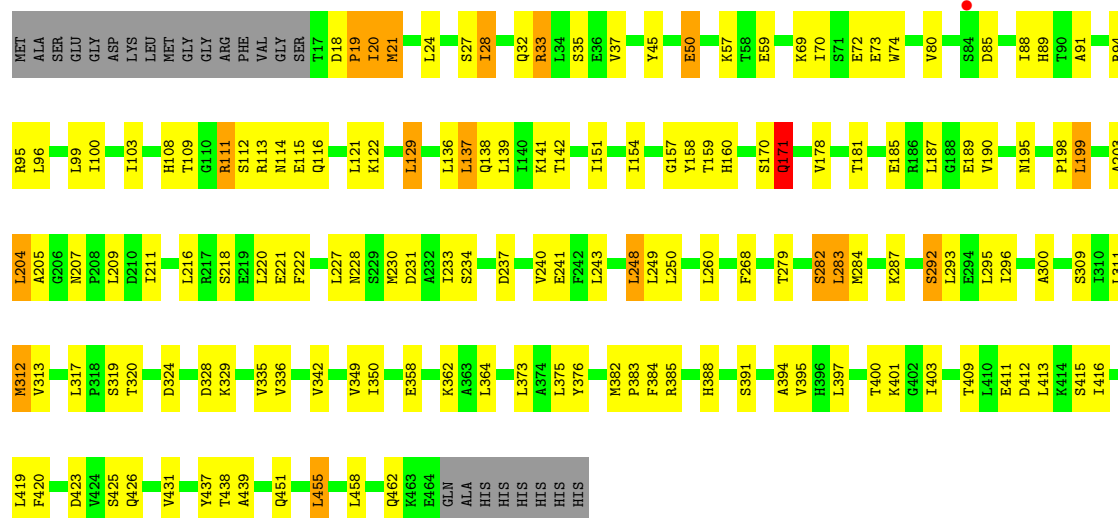
Chain B: 





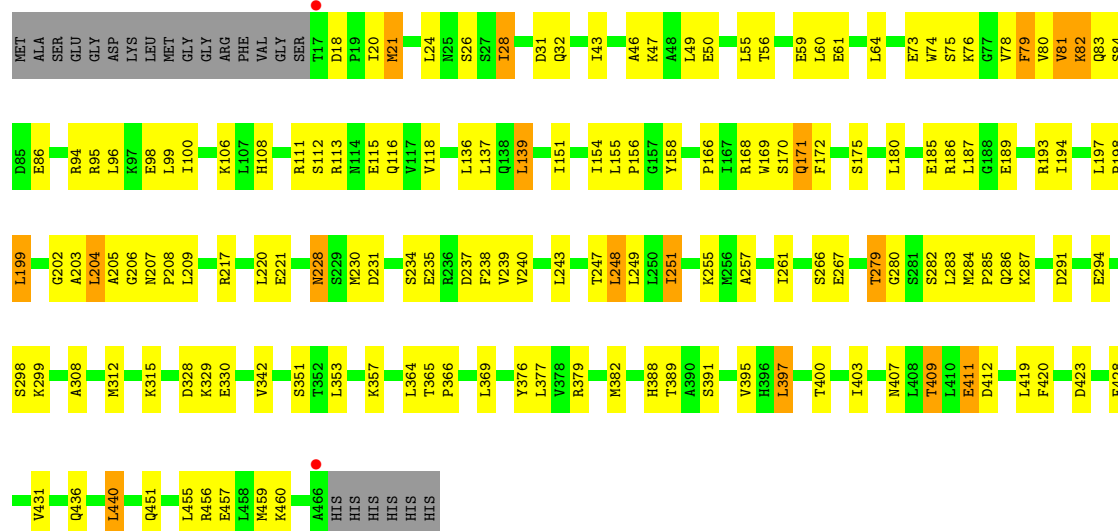
• Molecule 1: Delta crystallin I

Chain C: 62% 29% 5%



• Molecule 1: Delta crystallin I

Chain D: 63% 29% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.70Å 98.80Å 107.40Å 90.00° 101.50° 90.00°	Depositor
Resolution (Å)	35.19 – 2.50 35.19 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.3 (35.19-2.50) 98.2 (35.19-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.281 0.220 , 0.281	Depositor DCC
R_{free} test set	6627 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14536	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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	0.52	0/3518	0.97	15/4750 (0.3%)
1	B	0.51	0/3529	0.99	7/4764 (0.1%)
1	C	0.52	0/3515	0.98	16/4745 (0.3%)
1	D	0.53	0/3529	0.94	7/4764 (0.1%)
All	All	0.52	0/14091	0.97	45/19023 (0.2%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	292	SER	N-CA-C	-7.15	103.56	111.36
1	C	227	LEU	N-CA-C	6.65	119.54	111.82
1	B	171	GLN	N-CA-C	-6.48	104.14	111.07
1	A	197	LEU	N-CA-C	6.40	120.78	109.58
1	A	32	GLN	N-CA-C	-6.39	104.74	112.54
1	D	411	GLU	N-CA-C	-6.28	104.44	111.28
1	A	200	GLY	N-CA-C	-6.20	106.58	115.64
1	C	27	SER	N-CA-C	-5.98	106.97	114.56
1	C	437	TYR	N-CA-C	5.90	118.89	110.68
1	B	32	GLN	N-CA-C	-5.85	105.41	112.54
1	A	157	GLY	N-CA-C	-5.84	100.80	111.25
1	B	233	ILE	N-CA-C	5.82	116.59	110.72
1	D	251	ILE	N-CA-C	-5.80	104.85	110.42
1	C	157	GLY	N-CA-C	-5.80	100.86	110.95
1	A	319	SER	N-CA-C	-5.79	101.95	110.52
1	C	234	SER	N-CA-C	5.72	120.42	113.38
1	A	410	LEU	N-CA-C	-5.69	105.17	111.71
1	A	18	ASP	CA-C-N	5.67	125.14	119.24
1	A	18	ASP	C-N-CA	5.67	125.14	119.24
1	A	207	ASN	N-CA-C	-5.66	102.52	109.65
1	C	70	ILE	N-CA-C	-5.66	104.84	111.00
1	C	50	GLU	N-CA-C	-5.65	105.04	111.14
1	C	431	VAL	N-CA-C	-5.57	104.94	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	311	LEU	N-CA-C	-5.55	104.92	110.97
1	D	431	VAL	N-CA-C	-5.52	105.14	110.72
1	C	158	TYR	N-CA-C	5.51	118.71	109.95
1	A	242	PHE	N-CA-C	-5.46	105.33	111.28
1	A	99	LEU	N-CA-C	5.44	119.08	112.23
1	D	266	SER	N-CA-C	-5.42	105.53	111.82
1	D	234	SER	N-CA-C	5.34	120.07	113.50
1	B	158	TYR	N-CA-C	5.34	118.27	109.72
1	B	314	LEU	N-CA-C	5.32	119.03	112.54
1	D	351	SER	N-CA-C	5.28	117.04	111.28
1	A	415	SER	N-CA-C	-5.23	106.16	112.54
1	C	284	MET	CA-C-N	5.22	126.36	119.84
1	C	284	MET	C-N-CA	5.22	126.36	119.84
1	A	229	SER	N-CA-C	5.19	117.61	111.33
1	B	284	MET	CA-C-N	5.16	125.23	119.87
1	B	284	MET	C-N-CA	5.16	125.23	119.87
1	C	384	PHE	N-CA-C	5.15	119.81	111.37
1	C	171	GLN	N-CA-C	-5.14	105.68	111.28
1	A	160	HIS	N-CA-C	-5.14	106.59	112.86
1	C	32	GLN	N-CA-C	-5.13	106.97	113.18
1	D	158	TYR	N-CA-C	5.13	117.92	109.72
1	A	194	ILE	N-CA-C	-5.02	104.81	111.09

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	3475	0	3595	128	0
1	B	3486	0	3611	142	0
1	C	3472	0	3598	121	0
1	D	3486	0	3611	126	0
2	A	169	0	0	12	0
2	B	128	0	0	9	0
2	C	173	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	147	0	0	10	0
All	All	14536	0	14415	475	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 17.

All (475) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:LEU:HB3	2:C:636:HOH:O	1.25	1.24
1:B:24:LEU:HD13	2:C:636:HOH:O	1.32	1.22
1:B:24:LEU:CD1	2:C:636:HOH:O	1.86	1.14
1:C:382:MET:HE3	1:C:419:LEU:HD12	1.31	1.12
1:D:409:THR:HG22	1:D:412:ASP:H	0.91	1.05
1:D:409:THR:HG22	1:D:412:ASP:N	1.70	1.05
1:A:409:THR:HG22	1:A:411:GLU:H	1.21	1.01
1:B:279:THR:HG22	1:B:289:ASN:HD22	1.24	0.99
1:B:409:THR:HG22	1:B:411:GLU:H	1.26	0.98
1:D:379:ARG:HH22	1:D:436:GLN:HE21	1.10	0.96
1:B:405:ILE:HD12	1:B:405:ILE:H	1.28	0.96
1:B:165:GLN:NE2	2:B:599:HOH:O	1.93	0.96
1:C:171:GLN:HE22	1:C:451:GLN:HE22	1.14	0.95
1:C:426:GLN:HG2	2:C:632:HOH:O	1.68	0.93
1:A:25:ASN:HD21	1:A:323:LYS:HZ1	1.13	0.92
1:B:379:ARG:HH21	1:B:436:GLN:HE21	1.07	0.92
1:C:375:LEU:HD12	2:C:602:HOH:O	1.71	0.89
1:C:33:ARG:HB3	1:C:33:ARG:HH21	1.39	0.88
1:D:171:GLN:HE21	1:D:171:GLN:HA	1.38	0.87
1:A:228:ASN:HB3	2:A:482:HOH:O	1.73	0.87
1:C:228:ASN:HD22	1:C:231:ASP:H	1.19	0.86
1:C:114:ASN:HB3	1:C:233:ILE:HD12	1.60	0.83
1:A:20:ILE:HD12	1:A:20:ILE:H	1.42	0.83
1:B:379:ARG:NH2	1:B:436:GLN:HE21	1.75	0.82
1:B:171:GLN:HE21	1:B:171:GLN:HA	1.43	0.82
1:B:83:GLN:CA	1:B:83:GLN:HE21	1.94	0.79
1:A:25:ASN:HD21	1:A:323:LYS:NZ	1.79	0.79
1:B:199:LEU:HD13	1:B:216:LEU:HD13	1.64	0.79
1:C:283:LEU:H	1:C:283:LEU:HD22	1.47	0.79
1:A:59:GLU:HG2	1:A:103:ILE:HD11	1.65	0.78
1:D:379:ARG:HH22	1:D:436:GLN:NE2	1.81	0.78
1:A:409:THR:HG22	1:A:411:GLU:N	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:THR:HG22	1:C:411:GLU:H	1.48	0.78
1:B:385:ARG:HB2	2:B:532:HOH:O	1.84	0.77
1:C:199:LEU:HD13	1:C:216:LEU:HD22	1.67	0.77
1:C:33:ARG:HB3	1:C:33:ARG:NH2	2.00	0.75
1:A:231:ASP:HB3	2:A:482:HOH:O	1.87	0.74
1:C:295:LEU:CB	2:C:636:HOH:O	2.00	0.74
1:A:108:HIS:HB2	2:A:586:HOH:O	1.88	0.73
2:B:550:HOH:O	1:D:315:LYS:HE3	1.87	0.73
1:C:409:THR:HG22	1:C:411:GLU:N	2.05	0.72
1:B:301:GLY:HA2	1:C:312:MET:HG2	1.72	0.72
1:A:228:ASN:HD22	1:A:231:ASP:H	1.35	0.72
1:A:171:GLN:HA	1:A:171:GLN:HE21	1.55	0.71
1:C:228:ASN:HD21	1:C:230:MET:HB2	1.56	0.71
1:B:385:ARG:HH11	1:B:385:ARG:CG	2.03	0.71
1:A:57:LYS:O	1:A:61:GLU:HG3	1.89	0.71
1:A:165:GLN:HE21	1:C:205:ALA:HB3	1.56	0.71
1:C:113:ARG:HH21	1:C:116:GLN:HE22	1.39	0.71
1:A:165:GLN:HE21	1:C:205:ALA:CB	2.04	0.70
1:B:83:GLN:HE21	1:B:83:GLN:HA	1.55	0.70
1:A:28:ILE:O	1:A:32:GLN:HG3	1.91	0.70
1:B:112:SER:O	1:B:115:GLU:HG2	1.90	0.70
1:A:388:HIS:NE2	1:B:283:LEU:HD21	2.07	0.70
1:C:113:ARG:NH2	1:C:116:GLN:HE22	1.89	0.70
1:C:228:ASN:ND2	1:C:231:ASP:H	1.88	0.70
1:A:171:GLN:HE22	1:A:451:GLN:HE22	1.38	0.69
1:B:78:VAL:HG12	1:B:78:VAL:O	1.93	0.69
1:C:108:HIS:HD2	1:C:111:ARG:HD2	1.57	0.69
1:A:108:HIS:CD2	1:A:111:ARG:HE	2.11	0.68
1:A:113:ARG:HA	1:A:116:GLN:HE21	1.56	0.68
1:D:81:VAL:HG12	1:D:82:LYS:H	1.59	0.68
1:D:94:ARG:O	1:D:98:GLU:HG3	1.92	0.68
1:B:228:ASN:HD22	1:B:231:ASP:H	1.41	0.68
1:A:25:ASN:ND2	1:A:323:LYS:NZ	2.42	0.68
1:A:20:ILE:HD12	1:A:20:ILE:N	2.08	0.68
1:C:109:THR:HG22	1:C:209:LEU:HD11	1.76	0.68
1:A:282:SER:O	1:A:285:PRO:HD3	1.93	0.67
1:B:397:LEU:HD23	1:B:397:LEU:O	1.93	0.67
1:C:283:LEU:HD22	1:C:283:LEU:N	2.09	0.67
1:C:113:ARG:HH21	1:C:116:GLN:NE2	1.93	0.67
1:C:283:LEU:HD21	1:D:388:HIS:NE2	2.09	0.67
1:B:72:GLU:HB3	1:B:76:LYS:NZ	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LEU:HD13	1:B:180:LEU:HD13	1.78	0.66
1:D:20:ILE:HD12	1:D:20:ILE:H	1.60	0.65
1:B:340:THR:HG21	2:B:510:HOH:O	1.96	0.65
1:D:82:LYS:C	1:D:84:SER:H	2.02	0.65
1:A:165:GLN:NE2	1:C:205:ALA:HB3	2.10	0.65
1:B:283:LEU:HD22	1:B:283:LEU:H	1.61	0.65
1:B:62:LYS:NZ	1:B:62:LYS:HB3	2.12	0.65
1:B:405:ILE:H	1:B:405:ILE:CD1	2.01	0.65
1:A:255:LYS:HD3	2:A:488:HOH:O	1.96	0.64
1:B:197:LEU:HD22	1:B:217:ARG:HA	1.78	0.64
1:B:181:THR:HG21	1:B:458:LEU:HD13	1.79	0.64
1:D:95:ARG:NH1	1:D:99:LEU:HG	2.12	0.64
1:A:108:HIS:HD2	1:A:111:ARG:HE	1.44	0.64
1:B:405:ILE:HD12	1:B:405:ILE:N	2.06	0.64
1:A:133:SER:O	1:A:137:LEU:HD23	1.98	0.64
1:A:135:HIS:HE1	2:A:564:HOH:O	1.79	0.64
1:A:106:LYS:HE2	1:C:383:PRO:HB3	1.80	0.64
1:C:20:ILE:N	1:C:20:ILE:HD12	2.13	0.64
1:C:69:LYS:O	1:C:73:GLU:HG3	1.97	0.64
1:D:329:LYS:CD	2:D:617:HOH:O	2.44	0.64
1:A:207:ASN:ND2	1:A:209:LEU:H	1.95	0.63
1:B:83:GLN:HE21	1:B:83:GLN:N	1.97	0.62
1:C:112:SER:O	1:C:115:GLU:HG2	1.99	0.62
1:A:460:LYS:O	1:A:464:GLU:HG3	1.99	0.62
1:A:152:ASP:HB2	2:A:635:HOH:O	2.00	0.62
1:A:329:LYS:HG3	2:A:560:HOH:O	1.98	0.62
1:B:194:ILE:HG12	1:B:238:PHE:HB2	1.82	0.62
1:B:341:ALA:HB1	1:C:24:LEU:HD21	1.82	0.61
1:A:162:GLN:HB3	1:B:287:LYS:HD2	1.83	0.61
1:C:28:ILE:O	1:C:28:ILE:HD13	2.01	0.61
1:D:409:THR:N	1:D:412:ASP:HB2	2.15	0.61
1:D:409:THR:O	1:D:412:ASP:HB2	2.00	0.61
1:B:385:ARG:NH1	1:B:385:ARG:HG3	2.15	0.60
1:B:273:LEU:HD22	1:B:349:VAL:HG13	1.82	0.60
1:C:50:GLU:OE1	1:C:57:LYS:HE3	2.01	0.60
1:A:20:ILE:H	1:A:20:ILE:CD1	2.13	0.60
1:B:296:ILE:HG12	1:B:342:VAL:HG13	1.83	0.60
1:B:117:VAL:HG12	2:B:501:HOH:O	2.02	0.60
1:B:186:ARG:O	1:B:190:VAL:HG23	2.01	0.60
1:D:203:ALA:O	1:D:204:LEU:HB3	2.02	0.60
1:D:239:VAL:O	1:D:243:LEU:HG	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:LEU:HD22	1:B:440:LEU:H	1.66	0.60
1:B:301:GLY:CA	1:C:312:MET:HG2	2.32	0.59
1:D:94:ARG:HG2	1:D:94:ARG:HH11	1.67	0.59
1:A:87:ASP:OD2	1:A:89:HIS:HB2	2.01	0.59
1:C:328:ASP:OD1	1:C:329:LYS:N	2.35	0.59
1:A:219:GLU:HG2	2:A:619:HOH:O	2.02	0.59
1:C:412:ASP:O	1:C:415:SER:HB3	2.03	0.59
1:D:154:ILE:HG22	1:D:364:LEU:HD11	1.82	0.59
1:D:315:LYS:HD3	1:D:315:LYS:C	2.28	0.59
1:A:94:ARG:O	1:A:98:GLU:HG3	2.03	0.59
1:A:312:MET:HE2	1:B:312:MET:HA	1.85	0.59
1:D:379:ARG:NH2	1:D:436:GLN:HE21	1.92	0.59
1:B:420:PHE:HE2	1:B:424:VAL:HG21	1.68	0.58
1:B:421:SER:HB2	1:B:423:ASP:OD2	2.03	0.58
1:B:279:THR:HG22	1:B:289:ASN:ND2	2.07	0.58
1:D:28:ILE:HD13	1:D:28:ILE:O	2.03	0.58
1:D:329:LYS:HD2	2:D:617:HOH:O	2.02	0.58
1:B:385:ARG:CG	1:B:385:ARG:NH1	2.66	0.58
1:C:207:ASN:ND2	1:C:211:ILE:H	2.01	0.57
1:A:296:ILE:HG12	1:A:342:VAL:HG13	1.86	0.57
1:B:28:ILE:O	1:B:32:GLN:HG3	2.04	0.57
1:D:409:THR:H	1:D:412:ASP:HB2	1.69	0.57
1:D:139:LEU:HD13	1:D:180:LEU:HD13	1.87	0.57
1:D:56:THR:HG23	1:D:59:GLU:OE2	2.04	0.57
1:D:108:HIS:HD2	1:D:111:ARG:HB3	1.69	0.57
1:A:59:GLU:CG	1:A:103:ILE:HD11	2.35	0.57
1:A:176:HIS:HE1	1:A:255:LYS:HG2	1.70	0.57
1:B:171:GLN:HE22	1:B:451:GLN:HE22	1.52	0.57
1:B:279:THR:HB	1:B:291:ASP:OD1	2.03	0.57
1:A:440:LEU:HD22	1:A:440:LEU:H	1.69	0.57
1:B:376:TYR:CZ	1:B:380:LYS:HD2	2.39	0.57
1:D:171:GLN:HA	1:D:171:GLN:NE2	2.14	0.56
1:D:171:GLN:HE22	1:D:451:GLN:HE22	1.53	0.56
1:D:197:LEU:HD12	1:D:198:PRO:HD2	1.87	0.56
1:D:353:LEU:HD12	1:D:353:LEU:C	2.30	0.56
1:C:108:HIS:CD2	1:C:111:ARG:HD2	2.38	0.56
1:C:319:SER:HB3	1:C:320:THR:HG22	1.87	0.56
1:D:185:GLU:O	1:D:189:GLU:HG3	2.05	0.56
1:D:357:LYS:HG3	2:D:542:HOH:O	2.04	0.56
1:D:377:LEU:HD13	1:D:382:MET:SD	2.46	0.56
1:A:237:ASP:O	1:A:241:GLU:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:VAL:O	1:D:82:LYS:HG2	2.04	0.56
1:A:228:ASN:ND2	1:A:231:ASP:H	2.01	0.56
1:D:28:ILE:O	1:D:32:GLN:HG3	2.05	0.56
1:A:382:MET:HE3	1:A:419:LEU:HD12	1.88	0.55
1:C:409:THR:HB	1:C:412:ASP:OD2	2.06	0.55
1:B:186:ARG:NH2	1:B:248:LEU:HD13	2.22	0.55
1:D:409:THR:HB	1:D:412:ASP:OD2	2.06	0.55
1:D:409:THR:CG2	1:D:412:ASP:H	1.87	0.55
1:A:174:LEU:O	1:A:178:VAL:HG23	2.07	0.55
1:B:169:TRP:O	1:B:172:PHE:HB3	2.07	0.55
1:C:108:HIS:HB2	2:C:643:HOH:O	2.06	0.55
1:A:59:GLU:HG2	1:A:103:ILE:CD1	2.36	0.55
1:B:420:PHE:CE2	1:B:424:VAL:HG21	2.42	0.55
1:B:243:LEU:HD22	1:B:335:VAL:HG21	1.89	0.55
2:A:482:HOH:O	1:C:178:VAL:HG11	2.07	0.55
1:B:45:TYR:HA	1:B:216:LEU:HD21	1.89	0.55
1:B:83:GLN:CA	1:B:83:GLN:NE2	2.67	0.55
1:D:112:SER:O	1:D:115:GLU:HG2	2.07	0.54
1:B:340:THR:HG22	2:B:513:HOH:O	2.07	0.54
1:D:95:ARG:HH12	1:D:99:LEU:HG	1.73	0.54
1:A:96:LEU:HD23	1:A:104:ALA:HB1	1.89	0.54
1:A:457:GLU:OE2	1:A:457:GLU:HA	2.07	0.53
1:A:96:LEU:O	1:A:100:ILE:HG12	2.08	0.53
1:B:203:ALA:O	1:B:204:LEU:HB3	2.07	0.53
1:D:397:LEU:O	1:D:400:THR:HB	2.09	0.53
1:C:283:LEU:H	1:C:283:LEU:CD2	2.20	0.53
1:A:403:ILE:HD12	1:A:403:ILE:O	2.09	0.53
1:C:45:TYR:CE2	1:C:111:ARG:HB2	2.43	0.53
1:B:143:LEU:HD23	1:B:350:ILE:HG21	1.91	0.53
1:B:341:ALA:CB	1:C:24:LEU:HD21	2.38	0.53
1:C:151:ILE:HA	1:C:170:SER:OG	2.09	0.53
1:A:24:LEU:HD21	1:D:299:LYS:HE3	1.91	0.53
1:A:121:LEU:HD12	1:A:121:LEU:O	2.09	0.53
1:C:391:SER:O	1:C:395:VAL:HG23	2.09	0.52
1:B:72:GLU:HB3	1:B:76:LYS:HZ3	1.72	0.52
1:C:243:LEU:HD22	1:C:335:VAL:HG21	1.90	0.52
1:C:18:ASP:HB3	1:C:21:MET:HB2	1.91	0.52
1:D:409:THR:HG23	1:D:411:GLU:H	1.75	0.52
1:B:129:LEU:HD11	1:B:187:LEU:HD22	1.92	0.52
1:B:430:PHE:O	1:B:433:SER:HB3	2.10	0.52
1:D:228:ASN:HD22	1:D:231:ASP:H	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:ILE:HB	2:D:607:HOH:O	2.09	0.52
1:A:375:LEU:O	1:A:379:ARG:HG2	2.10	0.51
1:B:458:LEU:O	1:B:462:GLN:HG3	2.10	0.51
1:D:382:MET:HE3	1:D:419:LEU:HD12	1.93	0.51
1:A:265:THR:HA	1:B:162:GLN:NE2	2.26	0.51
1:B:108:HIS:HE1	1:B:116:GLN:NE2	2.09	0.51
1:A:329:LYS:HE3	2:A:560:HOH:O	2.09	0.51
1:B:60:LEU:O	1:B:64:LEU:HG	2.11	0.51
1:A:440:LEU:H	1:A:440:LEU:CD2	2.24	0.51
1:A:403:ILE:HD12	1:A:403:ILE:C	2.36	0.50
1:D:20:ILE:HD12	1:D:20:ILE:N	2.25	0.50
1:D:206:GLY:HA3	2:D:523:HOH:O	2.11	0.50
1:D:369:LEU:HD13	1:D:428:PHE:HA	1.92	0.50
1:B:314:LEU:HA	1:B:317:LEU:CD1	2.40	0.50
1:C:401:LYS:O	1:C:403:ILE:HG23	2.11	0.50
1:B:283:LEU:HD22	1:B:283:LEU:N	2.26	0.50
1:B:314:LEU:HA	1:B:317:LEU:HD12	1.92	0.50
1:B:28:ILE:O	1:B:28:ILE:HD13	2.11	0.50
1:B:317:LEU:O	1:D:255:LYS:HG3	2.12	0.50
1:A:375:LEU:HB3	1:A:379:ARG:NH1	2.27	0.50
1:B:28:ILE:HA	1:B:31:ASP:OD2	2.12	0.49
1:D:403:ILE:HD12	1:D:407:ASN:HB3	1.93	0.49
1:C:309:SER:O	1:C:313:VAL:HG23	2.12	0.49
1:B:125:MET:HE2	1:B:194:ILE:HD13	1.94	0.49
1:D:328:ASP:OD1	1:D:329:LYS:N	2.45	0.49
1:D:43:ILE:O	1:D:47:LYS:HG3	2.12	0.49
1:D:220:LEU:O	1:D:221:GLU:HB2	2.12	0.49
1:D:391:SER:O	1:D:395:VAL:HG23	2.12	0.49
1:B:374:ALA:O	1:B:378:VAL:HG23	2.13	0.49
1:D:217:ARG:HG2	1:D:217:ARG:HH11	1.78	0.49
1:D:409:THR:CG2	1:D:411:GLU:HB3	2.41	0.49
1:A:431:VAL:O	1:A:434:VAL:HG22	2.12	0.49
1:B:230:MET:HE3	1:B:320:THR:CG2	2.43	0.49
1:C:88:ILE:HG23	1:C:89:HIS:CD2	2.48	0.49
1:B:383:PRO:HB3	1:D:106:LYS:HE3	1.95	0.49
1:B:449:THR:O	1:B:453:GLU:HG3	2.13	0.49
1:D:61:GLU:HG2	2:D:597:HOH:O	2.11	0.49
1:D:228:ASN:HD21	1:D:230:MET:HB2	1.77	0.49
1:B:361:GLU:HA	1:B:364:LEU:HD12	1.95	0.49
1:D:28:ILE:HD13	1:D:28:ILE:C	2.37	0.49
1:D:28:ILE:HA	1:D:31:ASP:OD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:LYS:C	1:D:84:SER:N	2.71	0.48
1:A:373:LEU:HD11	1:A:420:PHE:HE2	1.78	0.48
1:C:207:ASN:ND2	1:C:209:LEU:H	2.10	0.48
1:C:283:LEU:HB2	2:C:539:HOH:O	2.12	0.48
1:B:165:GLN:HE21	1:D:205:ALA:HB3	1.78	0.48
1:C:160:HIS:HA	1:D:294:GLU:OE1	2.12	0.48
1:A:273:LEU:HD13	1:A:349:VAL:HG13	1.95	0.48
1:B:228:ASN:ND2	1:D:175:SER:HB3	2.29	0.48
1:C:199:LEU:CD1	1:C:216:LEU:HD22	2.41	0.48
1:D:50:GLU:HA	1:D:55:LEU:HB2	1.96	0.48
1:B:413:LEU:HD13	1:B:420:PHE:CD2	2.48	0.48
1:C:142:THR:HG22	1:C:350:ILE:HG22	1.95	0.48
1:D:155:LEU:HB2	1:D:156:PRO:HD2	1.95	0.48
1:C:59:GLU:HG2	1:C:103:ILE:CD1	2.43	0.48
1:B:373:LEU:O	1:B:376:TYR:HB3	2.13	0.48
1:D:365:THR:HB	1:D:366:PRO:HD2	1.96	0.48
1:B:72:GLU:HA	1:B:75:SER:OG	2.13	0.48
1:C:94:ARG:HG2	1:C:94:ARG:HH11	1.79	0.48
1:D:60:LEU:O	1:D:64:LEU:HG	2.14	0.48
1:D:207:ASN:N	2:D:523:HOH:O	2.47	0.48
1:A:265:THR:HA	1:B:162:GLN:HE22	1.78	0.47
1:A:320:THR:HG22	1:A:321:TYR:N	2.29	0.47
1:B:385:ARG:HH11	1:B:385:ARG:HG3	1.70	0.47
1:D:197:LEU:HD22	1:D:217:ARG:HA	1.96	0.47
1:A:122:LYS:HE3	2:A:503:HOH:O	2.14	0.47
1:A:379:ARG:HH22	1:A:436:GLN:HE21	1.60	0.47
1:A:195:ASN:ND2	1:A:223:ALA:HB2	2.30	0.47
1:C:96:LEU:O	1:C:100:ILE:HG12	2.14	0.47
1:D:94:ARG:HG2	1:D:94:ARG:NH1	2.30	0.47
1:C:312:MET:HE2	1:D:312:MET:HA	1.96	0.47
1:A:161:LEU:HD21	1:A:262:ILE:HD13	1.96	0.47
1:A:249:LEU:HD12	1:A:249:LEU:O	2.14	0.47
1:B:168:ARG:HD2	1:B:443:THR:O	2.15	0.47
1:B:361:GLU:O	1:B:364:LEU:HB2	2.15	0.47
1:D:108:HIS:CD2	1:D:111:ARG:HE	2.33	0.47
1:A:78:VAL:HG13	1:A:78:VAL:O	2.15	0.47
1:C:121:LEU:HD12	1:C:121:LEU:HA	1.76	0.47
1:A:409:THR:CG2	1:A:411:GLU:HB3	2.45	0.47
1:A:243:LEU:CD2	1:A:335:VAL:HG21	2.44	0.47
1:A:295:LEU:HD21	1:D:24:LEU:HB3	1.96	0.47
1:D:112:SER:HB3	1:D:202:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:LEU:O	1:B:414:LYS:HB2	2.15	0.46
1:B:465:GLN:O	1:B:466:ALA:HB2	2.15	0.46
1:D:409:THR:H	1:D:412:ASP:CB	2.28	0.46
1:A:409:THR:HG21	1:A:411:GLU:HB3	1.98	0.46
1:A:455:LEU:HD12	1:A:458:LEU:HD12	1.98	0.46
1:B:243:LEU:CD2	1:B:335:VAL:HG21	2.45	0.46
1:C:413:LEU:HB3	1:C:420:PHE:CD1	2.51	0.46
1:A:171:GLN:HA	1:A:171:GLN:NE2	2.27	0.46
1:B:225:ILE:HD11	1:D:440:LEU:HD23	1.97	0.46
1:B:461:LYS:HA	1:B:464:GLU:HG2	1.96	0.46
1:A:78:VAL:O	1:A:78:VAL:CG1	2.63	0.46
1:A:213:ARG:HA	1:A:216:LEU:HD12	1.97	0.46
1:B:273:LEU:HD12	1:B:290:PRO:HA	1.97	0.46
1:B:396:HIS:O	1:B:399:GLU:HB2	2.16	0.46
1:A:248:LEU:HG	1:C:240:VAL:HG11	1.98	0.46
1:B:125:MET:HE2	1:B:194:ILE:CD1	2.46	0.46
2:B:503:HOH:O	1:D:193:ARG:HD2	2.14	0.46
1:C:438:THR:O	1:C:439:ALA:C	2.58	0.46
1:A:194:ILE:HG12	1:A:238:PHE:HB2	1.97	0.46
1:B:383:PRO:HB3	1:D:106:LYS:CE	2.45	0.46
1:B:437:TYR:O	1:B:444:ALA:CB	2.64	0.46
1:C:312:MET:CE	1:D:312:MET:HA	2.46	0.46
1:A:409:THR:HB	1:A:412:ASP:CG	2.40	0.46
1:B:83:GLN:HA	1:B:83:GLN:NE2	2.27	0.46
1:C:185:GLU:O	1:C:189:GLU:HG3	2.16	0.46
1:D:235:GLU:OE2	1:D:237:ASP:N	2.49	0.46
1:C:122:LYS:HE3	2:C:552:HOH:O	2.16	0.46
1:C:159:THR:O	1:C:160:HIS:HB2	2.15	0.46
1:C:220:LEU:O	1:C:221:GLU:HB2	2.16	0.46
1:D:81:VAL:HG12	1:D:82:LYS:N	2.27	0.46
1:D:95:ARG:HD3	2:D:543:HOH:O	2.16	0.46
1:A:228:ASN:HD21	1:A:230:MET:HB2	1.81	0.45
1:B:298:SER:HB3	1:C:324:ASP:HA	1.98	0.45
1:C:203:ALA:O	1:C:204:LEU:HB3	2.16	0.45
1:C:388:HIS:CE1	1:D:283:LEU:HD13	2.51	0.45
1:A:109:THR:HG22	1:A:209:LEU:HD11	1.97	0.45
1:B:51:LYS:HD2	1:B:215:MET:SD	2.56	0.45
1:B:80:VAL:HG12	2:B:556:HOH:O	2.15	0.45
1:A:129:LEU:HD22	1:A:187:LEU:HD22	1.98	0.45
1:B:137:LEU:HB3	1:B:463:LYS:HE3	1.97	0.45
1:C:204:LEU:N	1:C:204:LEU:HD23	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ARG:HA	1:C:116:GLN:HE21	1.82	0.45
1:B:377:LEU:HD13	1:B:382:MET:SD	2.57	0.45
1:D:217:ARG:HG2	1:D:217:ARG:NH1	2.32	0.45
1:A:370:ALA:CB	1:B:283:LEU:HB3	2.46	0.45
1:B:166:PRO:HD3	1:B:368:MET:HE2	1.99	0.45
1:C:195:ASN:OD1	1:C:222:PHE:HA	2.17	0.45
1:C:455:LEU:HA	1:C:455:LEU:HD12	1.77	0.45
1:D:279:THR:HB	1:D:291:ASP:OD1	2.17	0.45
1:C:137:LEU:HD12	1:C:137:LEU:HA	1.77	0.45
1:A:260:LEU:O	1:A:264:SER:HB3	2.17	0.44
1:A:279:THR:HG22	1:A:280:GLY:N	2.32	0.44
1:B:257:ALA:O	1:B:261:ILE:HG13	2.17	0.44
1:C:250:LEU:HB3	1:C:300:ALA:HA	1.98	0.44
1:D:74:TRP:C	1:D:76:LYS:H	2.25	0.44
1:A:129:LEU:CD2	1:A:187:LEU:HD22	2.47	0.44
1:A:240:VAL:HG11	1:C:248:LEU:HG	1.99	0.44
1:C:112:SER:N	1:C:115:GLU:OE2	2.44	0.44
1:A:457:GLU:O	1:A:461:LYS:HG2	2.18	0.44
1:B:437:TYR:CE2	1:D:208:PRO:HB3	2.52	0.44
1:C:20:ILE:N	1:C:20:ILE:CD1	2.79	0.44
1:A:121:LEU:HD11	1:A:332:VAL:HG11	2.00	0.44
1:A:413:LEU:O	1:A:416:ILE:HB	2.17	0.44
1:B:234:SER:HB3	1:B:320:THR:O	2.18	0.44
1:C:59:GLU:HG2	1:C:103:ILE:HD11	2.00	0.44
1:D:197:LEU:HD11	1:D:199:LEU:HB2	1.99	0.44
1:A:28:ILE:O	1:A:28:ILE:HD13	2.17	0.44
1:A:35:SER:HA	1:A:88:ILE:HD11	1.99	0.44
1:B:170:SER:O	1:B:174:LEU:HG	2.16	0.44
1:B:248:LEU:HG	1:D:240:VAL:HG11	1.99	0.44
1:B:397:LEU:HD23	1:B:397:LEU:C	2.42	0.44
1:C:85:ASP:OD1	1:C:91:ALA:HA	2.17	0.44
1:C:114:ASN:CB	1:C:233:ILE:HD12	2.38	0.44
1:B:62:LYS:HB3	1:B:62:LYS:HZ2	1.83	0.44
1:B:255:LYS:HD2	2:D:595:HOH:O	2.16	0.44
1:B:413:LEU:HD13	1:B:420:PHE:CE2	2.53	0.44
1:C:129:LEU:HA	1:C:129:LEU:HD12	1.80	0.44
1:D:207:ASN:ND2	1:D:209:LEU:H	2.15	0.44
1:D:456:ARG:HA	1:D:459:MET:HE3	2.00	0.44
1:A:271:LEU:C	1:A:271:LEU:HD12	2.43	0.44
1:A:440:LEU:HD22	1:A:440:LEU:N	2.32	0.44
1:C:37:VAL:HG22	2:C:567:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:THR:CA	1:D:412:ASP:HB2	2.47	0.44
1:A:304:PHE:CE2	1:D:308:ALA:HB1	2.53	0.44
1:B:82:LYS:C	1:B:84:SER:H	2.26	0.44
1:A:108:HIS:HD2	1:A:111:ARG:HH21	1.66	0.43
1:A:382:MET:HA	1:A:383:PRO:HD3	1.89	0.43
1:C:190:VAL:HG22	1:C:241:GLU:HB3	1.99	0.43
1:C:20:ILE:HD12	1:C:20:ILE:H	1.81	0.43
1:C:358:GLU:HG2	1:C:362:LYS:HE3	2.00	0.43
1:C:409:THR:CG2	1:C:411:GLU:H	2.25	0.43
1:D:376:TYR:OH	1:D:423:ASP:OD1	2.32	0.43
1:A:209:LEU:HD21	1:C:375:LEU:HD22	2.01	0.43
1:A:370:ALA:HB3	1:B:283:LEU:HB3	2.00	0.43
1:B:166:PRO:HB3	1:B:364:LEU:CD2	2.48	0.43
1:B:440:LEU:HD22	1:B:440:LEU:N	2.32	0.43
1:C:109:THR:HG22	1:C:209:LEU:CD1	2.47	0.43
1:B:62:LYS:HB3	1:B:62:LYS:HZ3	1.81	0.43
1:B:228:ASN:HD21	1:B:230:MET:HB2	1.84	0.43
1:C:283:LEU:N	1:C:283:LEU:CD2	2.80	0.43
1:C:394:ALA:HA	1:C:416:ILE:CD1	2.49	0.43
1:B:24:LEU:HD12	2:C:636:HOH:O	1.86	0.43
1:B:159:THR:O	1:B:160:HIS:HB2	2.19	0.43
1:C:80:VAL:HG12	2:C:596:HOH:O	2.19	0.43
1:C:423:ASP:C	1:C:425:SER:N	2.77	0.43
1:B:365:THR:O	1:B:368:MET:HB2	2.19	0.43
1:D:75:SER:O	1:D:76:LYS:HG3	2.18	0.43
1:D:169:TRP:O	1:D:172:PHE:HB3	2.19	0.43
1:A:208:PRO:HG2	1:A:209:LEU:HG	2.00	0.42
1:A:247:THR:OG1	1:A:303:VAL:HG12	2.18	0.42
1:D:168:ARG:O	1:D:169:TRP:C	2.63	0.42
1:C:89:HIS:ND1	1:C:113:ARG:HD2	2.34	0.42
1:D:186:ARG:CZ	1:D:248:LEU:HD13	2.48	0.42
1:C:100:ILE:O	1:C:103:ILE:HG22	2.19	0.42
1:B:100:ILE:HD12	1:B:103:ILE:HG23	2.01	0.42
1:C:292:SER:O	1:C:296:ILE:HG13	2.20	0.42
1:D:194:ILE:HG12	1:D:238:PHE:HB2	2.02	0.42
1:A:345:VAL:O	1:A:349:VAL:HG23	2.19	0.42
1:B:287:LYS:HE2	2:B:492:HOH:O	2.18	0.42
1:C:181:THR:HG21	1:C:458:LEU:HD13	2.00	0.42
1:C:409:THR:O	1:C:412:ASP:HB2	2.18	0.42
1:D:228:ASN:ND2	1:D:231:ASP:H	2.17	0.42
1:D:284:MET:HE1	1:D:287:LYS:HZ3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:THR:C	1:A:402:GLY:H	2.28	0.42
1:B:440:LEU:H	1:B:440:LEU:CD2	2.33	0.42
1:C:35:SER:HB2	1:C:74:TRP:CD1	2.55	0.42
1:D:330:GLU:HB2	2:D:492:HOH:O	2.18	0.42
1:B:460:LYS:O	1:B:464:GLU:HG2	2.20	0.42
1:A:219:GLU:CG	2:A:619:HOH:O	2.65	0.42
1:B:319:SER:HA	1:B:320:THR:HA	1.83	0.42
1:B:373:LEU:HD11	1:B:420:PHE:CE2	2.54	0.42
1:B:437:TYR:O	1:B:444:ALA:HB3	2.20	0.41
1:C:293:LEU:HD21	1:C:349:VAL:HG11	2.01	0.41
1:C:373:LEU:O	1:C:376:TYR:HB3	2.20	0.41
1:C:397:LEU:O	1:C:400:THR:HB	2.20	0.41
1:D:82:LYS:O	1:D:84:SER:N	2.49	0.41
1:D:187:LEU:HA	1:D:187:LEU:HD23	1.77	0.41
1:A:252:HIS:NE2	1:C:237:ASP:OD1	2.53	0.41
1:D:78:VAL:O	1:D:80:VAL:N	2.52	0.41
1:A:95:ARG:HG3	1:A:99:LEU:HD12	2.02	0.41
1:A:143:LEU:HD23	1:A:350:ILE:HG21	2.01	0.41
1:A:400:THR:C	1:A:402:GLY:N	2.77	0.41
1:B:82:LYS:C	1:B:84:SER:N	2.79	0.41
1:B:156:PRO:HG2	1:B:363:ALA:HB1	2.02	0.41
1:A:140:ILE:O	1:A:144:VAL:HG23	2.21	0.41
1:A:375:LEU:HB3	1:A:379:ARG:HH12	1.85	0.41
1:C:94:ARG:HG2	1:C:94:ARG:NH1	2.35	0.41
1:C:218:SER:OG	2:C:623:HOH:O	2.21	0.41
1:C:313:VAL:O	1:C:317:LEU:HD11	2.21	0.41
1:D:279:THR:CG2	1:D:280:GLY:N	2.83	0.41
1:A:405:ILE:HD13	1:A:405:ILE:HA	1.84	0.41
1:A:421:SER:O	1:A:422:SER:C	2.63	0.41
1:B:197:LEU:HD22	1:B:217:ARG:CA	2.48	0.41
1:C:95:ARG:NH2	1:C:99:LEU:HD21	2.36	0.41
1:C:154:ILE:HG22	1:C:364:LEU:HD11	2.02	0.41
1:A:18:ASP:HA	1:A:19:PRO:HD3	1.88	0.41
1:C:409:THR:CG2	1:C:411:GLU:HB3	2.50	0.41
1:A:234:SER:HB3	1:A:320:THR:O	2.21	0.41
1:B:328:ASP:OD1	1:B:329:LYS:N	2.54	0.41
1:C:113:ARG:HD3	1:C:116:GLN:NE2	2.35	0.41
1:C:282:SER:OG	1:D:388:HIS:HE1	2.03	0.41
1:D:73:GLU:O	1:D:79:PHE:N	2.44	0.41
1:D:377:LEU:HD21	1:D:420:PHE:CE2	2.56	0.41
1:B:185:GLU:O	1:B:189:GLU:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:GLU:O	1:B:412:ASP:C	2.61	0.41
1:C:141:LYS:HE3	1:C:141:LYS:HB2	1.94	0.41
1:D:166:PRO:HB3	1:D:364:LEU:HD22	2.03	0.41
1:D:457:GLU:O	1:D:460:LYS:HB3	2.21	0.41
1:A:268:PHE:CG	1:B:267:GLU:HG2	2.55	0.41
1:A:324:ASP:HA	1:D:298:SER:HB3	2.02	0.41
1:A:434:VAL:HG23	1:A:435:GLU:N	2.36	0.41
1:A:439:ALA:O	1:A:440:LEU:C	2.64	0.41
1:D:18:ASP:HB3	1:D:21:MET:HB2	2.02	0.41
1:D:46:ALA:O	1:D:49:LEU:N	2.54	0.41
1:A:150:GLU:OE2	1:A:169:TRP:NE1	2.50	0.41
1:B:171:GLN:HA	1:B:171:GLN:NE2	2.22	0.41
1:D:95:ARG:HD2	1:D:98:GLU:OE1	2.21	0.41
1:D:96:LEU:O	1:D:100:ILE:HG12	2.21	0.41
1:A:373:LEU:HD11	1:A:420:PHE:CE2	2.55	0.40
1:C:122:LYS:HD2	1:C:198:PRO:HG3	2.02	0.40
1:D:84:SER:O	1:D:86:GLU:OE2	2.39	0.40
1:D:151:ILE:HA	1:D:170:SER:OG	2.21	0.40
1:B:444:ALA:O	1:B:448:VAL:HG23	2.21	0.40
1:C:268:PHE:CG	1:D:267:GLU:HG2	2.57	0.40
1:A:84:SER:O	1:A:86:GLU:OE2	2.39	0.40
1:A:208:PRO:HB2	1:C:375:LEU:HD13	2.03	0.40
1:A:294:GLU:OE1	1:B:160:HIS:HA	2.21	0.40
1:A:412:ASP:O	1:A:415:SER:OG	2.36	0.40
1:B:72:GLU:HB3	1:B:76:LYS:HZ2	1.86	0.40
1:B:180:LEU:O	1:B:183:ASP:HB2	2.22	0.40
1:D:257:ALA:O	1:D:261:ILE:HG13	2.20	0.40
1:A:25:ASN:ND2	1:A:323:LYS:HZ3	2.15	0.40
1:A:168:ARG:C	1:A:170:SER:N	2.75	0.40
1:C:19:PRO:HB2	1:C:20:ILE:HD12	2.03	0.40
1:D:113:ARG:HA	1:D:116:GLN:HE21	1.87	0.40
1:D:247:THR:O	1:D:251:ILE:HG12	2.21	0.40
1:D:282:SER:O	1:D:285:PRO:HD3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	447/472 (95%)	426 (95%)	18 (4%)	3 (1%)	18	34
1	B	448/472 (95%)	432 (96%)	14 (3%)	2 (0%)	30	49
1	C	446/472 (94%)	429 (96%)	15 (3%)	2 (0%)	30	49
1	D	448/472 (95%)	425 (95%)	19 (4%)	4 (1%)	14	27
All	All	1789/1888 (95%)	1712 (96%)	66 (4%)	11 (1%)	21	38

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	204	LEU
1	D	204	LEU
1	A	85	ASP
1	A	204	LEU
1	C	204	LEU
1	D	26	SER
1	D	79	PHE
1	A	464	GLU
1	B	102	ASP
1	D	83	GLN
1	C	19	PRO

5.3.2 Protein sidechains [i](#)

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	390/409 (95%)	369 (95%)	21 (5%)	20	41
1	B	391/409 (96%)	375 (96%)	16 (4%)	27	53
1	C	390/409 (95%)	363 (93%)	27 (7%)	14	30
1	D	391/409 (96%)	370 (95%)	21 (5%)	20	41
All	All	1562/1636 (96%)	1477 (95%)	85 (5%)	20	41

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	21	MET
1	A	28	ILE
1	A	78	VAL
1	A	108	HIS
1	A	136	LEU
1	A	139	LEU
1	A	171	GLN
1	A	199	LEU
1	A	209	LEU
1	A	228	ASN
1	A	248	LEU
1	A	249	LEU
1	A	250	LEU
1	A	260	LEU
1	A	273	LEU
1	A	319	SER
1	A	354	GLN
1	A	361	GLU
1	A	405	ILE
1	A	455	LEU
1	B	24	LEU
1	B	28	ILE
1	B	83	GLN
1	B	136	LEU
1	B	137	LEU
1	B	139	LEU
1	B	161	LEU
1	B	171	GLN
1	B	199	LEU
1	B	248	LEU
1	B	260	LEU
1	B	279	THR

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Mol	Chain	Res	Type
1	B	285	PRO
1	B	340	THR
1	B	385	ARG
1	B	405	ILE
1	C	20	ILE
1	C	21	MET
1	C	28	ILE
1	C	33	ARG
1	C	72	GLU
1	C	111	ARG
1	C	129	LEU
1	C	136	LEU
1	C	137	LEU
1	C	138	GLN
1	C	139	LEU
1	C	171	GLN
1	C	187	LEU
1	C	199	LEU
1	C	248	LEU
1	C	249	LEU
1	C	260	LEU
1	C	279	THR
1	C	282	SER
1	C	283	LEU
1	C	287	LYS
1	C	312	MET
1	C	336	VAL
1	C	342	VAL
1	C	385	ARG
1	C	455	LEU
1	C	462	GLN
1	D	21	MET
1	D	28	ILE
1	D	81	VAL
1	D	82	LYS
1	D	118	VAL
1	D	136	LEU
1	D	137	LEU
1	D	139	LEU
1	D	171	GLN
1	D	199	LEU
1	D	228	ASN

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Mol	Chain	Res	Type
1	D	248	LEU
1	D	249	LEU
1	D	279	THR
1	D	286	GLN
1	D	342	VAL
1	D	389	THR
1	D	397	LEU
1	D	409	THR
1	D	440	LEU
1	D	455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	108	HIS
1	A	114	ASN
1	A	116	GLN
1	A	127	ASN
1	A	135	HIS
1	A	165	GLN
1	A	171	GLN
1	A	176	HIS
1	A	207	ASN
1	A	228	ASN
1	A	289	ASN
1	A	344	GLN
1	A	354	GLN
1	A	359	ASN
1	A	407	ASN
1	A	436	GLN
1	A	465	GLN
1	B	83	GLN
1	B	114	ASN
1	B	116	GLN
1	B	127	ASN
1	B	165	GLN
1	B	171	GLN
1	B	207	ASN
1	B	228	ASN
1	B	286	GLN
1	B	289	ASN

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Mol	Chain	Res	Type
1	B	359	ASN
1	B	407	ASN
1	B	436	GLN
1	C	108	HIS
1	C	114	ASN
1	C	116	GLN
1	C	127	ASN
1	C	135	HIS
1	C	165	GLN
1	C	171	GLN
1	C	207	ASN
1	C	228	ASN
1	C	386	GLN
1	C	388	HIS
1	C	407	ASN
1	D	32	GLN
1	D	83	GLN
1	D	108	HIS
1	D	114	ASN
1	D	116	GLN
1	D	127	ASN
1	D	135	HIS
1	D	165	GLN
1	D	171	GLN
1	D	207	ASN
1	D	228	ASN
1	D	286	GLN
1	D	344	GLN
1	D	386	GLN
1	D	407	ASN
1	D	436	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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	449/472 (95%)	-0.09	0 100 100	20, 37, 60, 82	0
1	B	450/472 (95%)	0.14	5 (1%) 78 75	24, 42, 67, 82	0
1	C	448/472 (94%)	-0.13	1 (0%) 91 89	19, 35, 59, 79	0
1	D	450/472 (95%)	0.01	2 (0%) 88 86	20, 40, 68, 79	0
All	All	1797/1888 (95%)	-0.02	8 (0%) 88 86	19, 39, 65, 82	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	17	THR	3.4
1	B	466	ALA	3.0
1	D	466	ALA	2.5
1	C	84	SER	2.2
1	B	409	THR	2.1
1	B	410	LEU	2.1
1	B	405	ILE	2.1
1	B	86	GLU	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.