Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2021 – 07:30 AM EDT

PDB ID	:	1L7J
Title	:	X-ray structure of galactose mutarotase from Lactococcus lactis (apo)
Authors	:	Holden, H.M.; Thoden, J.B.
Deposited on	:	2002-03-15
Resolution	:	1.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

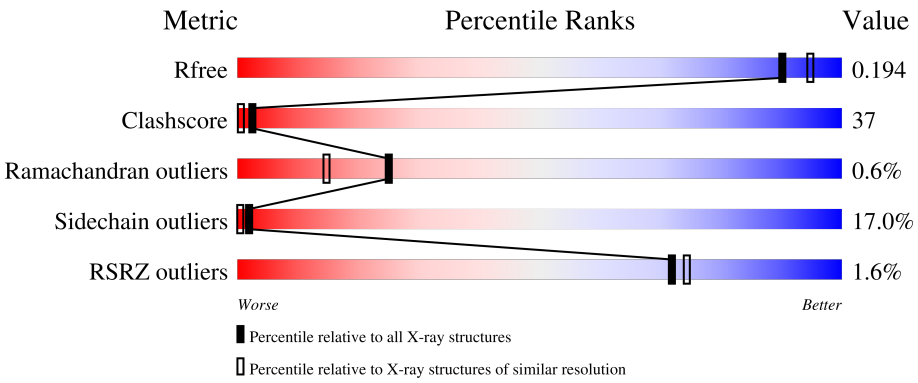
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	347	3%; 35%; 41%; 18%; • •
1	B	347	46%; 37%; 14%; • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6065 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 galactose mutarotase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	338	2650	1673	447	527	3	0	3	0
1	B	338	2645	1667	446	529	3	0	2	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	GLU	engineered mutation	UNP Q9ZB17
A	340	LEU	-	expression tag	UNP Q9ZB17
A	341	GLU	-	expression tag	UNP Q9ZB17
A	342	HIS	-	expression tag	UNP Q9ZB17
A	343	HIS	-	expression tag	UNP Q9ZB17
A	344	HIS	-	expression tag	UNP Q9ZB17
A	345	HIS	-	expression tag	UNP Q9ZB17
A	346	HIS	-	expression tag	UNP Q9ZB17
A	347	HIS	-	expression tag	UNP Q9ZB17
B	2	SER	GLU	engineered mutation	UNP Q9ZB17
B	340	LEU	-	expression tag	UNP Q9ZB17
B	341	GLU	-	expression tag	UNP Q9ZB17
B	342	HIS	-	expression tag	UNP Q9ZB17
B	343	HIS	-	expression tag	UNP Q9ZB17
B	344	HIS	-	expression tag	UNP Q9ZB17
B	345	HIS	-	expression tag	UNP Q9ZB17
B	346	HIS	-	expression tag	UNP Q9ZB17
B	347	HIS	-	expression tag	UNP Q9ZB17

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	376	376	376	0	0

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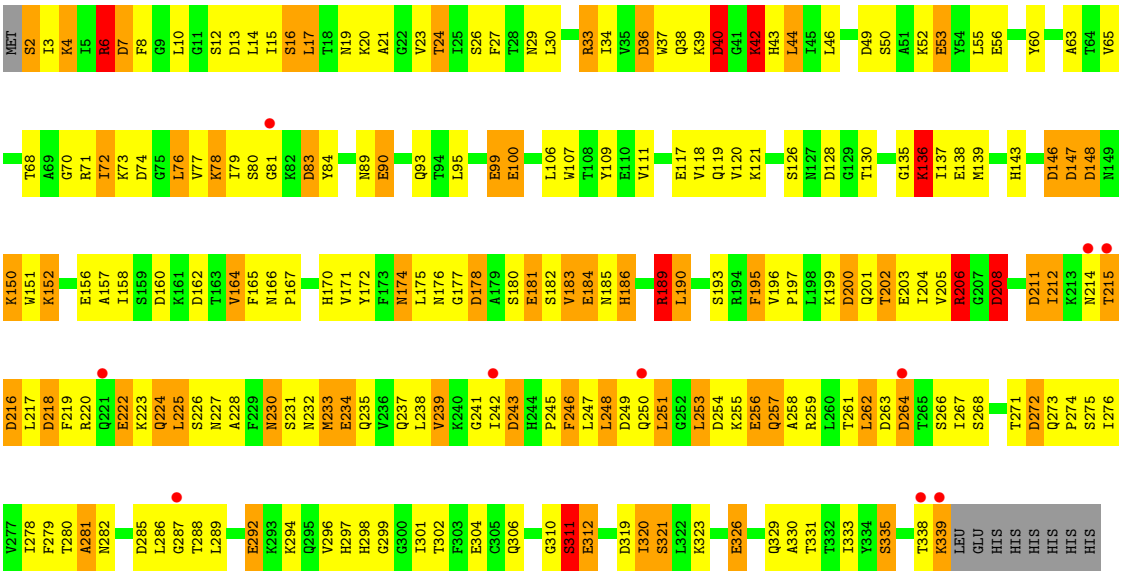
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	B	394	394	394	0	0

3 Residue-property plots (i)

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.

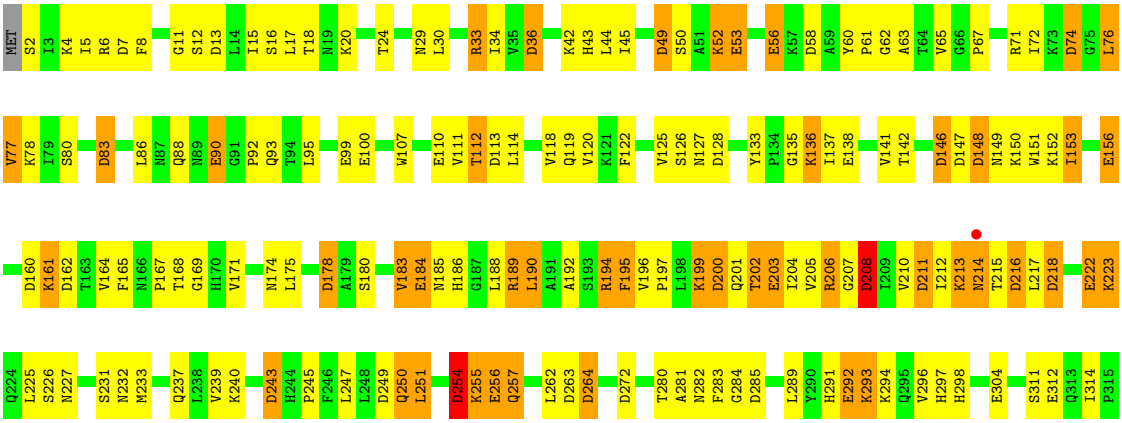
- Molecule 1: galactose mutarotase

Chain A:



- Molecule 1: galactose mutarotase

Chain B:



E316
D319
I320
S321
L322
K323
E326
K327
I333
L336
H337
T338
K339
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	42.50Å 76.10Å 206.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 51.70 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.6 (30.00-1.90) 89.7 (51.70-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 1.79Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.189 , 0.267 0.195 , 0.194	Depositor DCC
R_{free} test set	5844 reflections (10.21%)	wwPDB-VP
Wilson B-factor (Å^2)	13.4	Xtriage
Anisotropy	0.815	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 145.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6065	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	1.00	13/2714 (0.5%)	1.49	53/3672 (1.4%)
1	B	1.02	15/2705 (0.6%)	1.50	56/3661 (1.5%)
All	All	1.01	28/5419 (0.5%)	1.50	109/7333 (1.5%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	GLU	CD-OE2	7.80	1.34	1.25
1	B	304	GLU	CD-OE2	7.22	1.33	1.25
1	B	138	GLU	CD-OE2	6.38	1.32	1.25
1	A	117	GLU	CD-OE2	6.33	1.32	1.25
1	B	203	GLU	CD-OE2	6.29	1.32	1.25
1	B	316	GLU	CD-OE2	6.22	1.32	1.25
1	B	53	GLU	CD-OE2	6.09	1.32	1.25
1	B	292	GLU	CD-OE2	6.05	1.32	1.25
1	A	56	GLU	CD-OE2	6.04	1.32	1.25
1	A	326	GLU	CD-OE2	6.00	1.32	1.25
1	A	304	GLU	CD-OE2	6.00	1.32	1.25
1	B	184	GLU	CD-OE2	5.75	1.31	1.25
1	B	156	GLU	CD-OE2	5.73	1.31	1.25
1	A	184	GLU	CD-OE2	5.64	1.31	1.25
1	A	234	GLU	CD-OE2	5.60	1.31	1.25
1	B	99	GLU	CD-OE2	5.55	1.31	1.25
1	A	53	GLU	CD-OE2	5.53	1.31	1.25
1	B	110	GLU	CD-OE2	5.40	1.31	1.25
1	A	90	GLU	CD-OE1	-5.40	1.19	1.25
1	B	256	GLU	CD-OE2	5.38	1.31	1.25
1	B	56	GLU	CD-OE2	5.33	1.31	1.25
1	A	222	GLU	CD-OE2	5.25	1.31	1.25
1	B	90	GLU	CD-OE2	5.21	1.31	1.25
1	A	292	GLU	CD-OE2	5.20	1.31	1.25
1	B	326	GLU	CD-OE2	5.12	1.31	1.25
1	A	100	GLU	CD-OE2	5.05	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	100	GLU	CD-OE2	5.01	1.31	1.25
1	A	138	GLU	CD-OE2	5.00	1.31	1.25

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	33	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	B	249	ASP	CB-CG-OD2	-9.52	109.73	118.30
1	A	136	LYS	N-CA-CB	-9.18	94.08	110.60
1	B	194	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	B	148	ASP	CB-CG-OD2	-8.56	110.60	118.30
1	A	146	ASP	CB-CG-OD1	8.55	125.99	118.30
1	A	200	ASP	CB-CG-OD2	-8.13	110.98	118.30
1	A	146	ASP	CB-CG-OD2	-7.94	111.15	118.30
1	B	208	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	A	216	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	B	136	LYS	N-CA-CB	-7.57	96.97	110.60
1	A	206	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	36	ASP	CB-CG-OD1	7.36	124.93	118.30
1	A	208	ASP	CB-CG-OD2	-7.34	111.70	118.30
1	B	263	ASP	CB-CG-OD1	7.32	124.89	118.30
1	B	36	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	B	272	ASP	CB-CG-OD1	7.15	124.74	118.30
1	B	178	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	B	216	ASP	CB-CG-OD1	7.03	124.63	118.30
1	B	162	ASP	CB-CG-OD1	6.92	124.53	118.30
1	A	6	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	218	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	A	254	ASP	CB-CG-OD1	6.86	124.47	118.30
1	B	74	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	A	148	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	A	249	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	135	GLY	C-N-CA	6.79	138.66	121.70
1	B	13	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	A	206	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	40	ASP	CB-CG-OD1	6.73	124.36	118.30
1	A	74	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	A	189	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	B	128	ASP	CB-CG-OD1	6.66	124.30	118.30
1	B	113	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	B	83	ASP	CB-CG-OD1	6.64	124.28	118.30
1	B	319	ASP	CB-CG-OD2	-6.63	112.33	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	74	ASP	CB-CG-OD1	6.60	124.24	118.30
1	B	254	ASP	CB-CG-OD1	6.58	124.22	118.30
1	B	113	ASP	CB-CG-OD1	6.55	124.19	118.30
1	B	83	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	A	216	ASP	CB-CG-OD1	6.53	124.18	118.30
1	B	178	ASP	CB-CG-OD1	6.51	124.16	118.30
1	B	249	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	49	ASP	CB-CG-OD1	6.42	124.07	118.30
1	A	147	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	A	83	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	B	264	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	211	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	B	216	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	B	272	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	208	ASP	CB-CA-C	-6.26	97.87	110.40
1	B	211	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	A	178	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	264	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	B	243	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	B	148	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	162	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	A	218	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	B	7	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	A	319	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	B	254	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	B	128	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	A	249	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	A	147	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	13	ASP	CB-CG-OD1	5.95	123.65	118.30
1	B	146	ASP	CB-CA-C	-5.93	98.53	110.40
1	B	58	ASP	CB-CG-OD1	5.92	123.63	118.30
1	B	33	ARG	CD-NE-CZ	5.90	131.87	123.60
1	A	36	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	A	83	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	272	ASP	N-CA-CB	-5.83	100.11	110.60
1	B	218	ASP	CB-CG-OD1	5.82	123.53	118.30
1	B	147	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	272	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	272	ASP	CB-CG-OD1	5.75	123.48	118.30
1	B	7	ASP	CB-CG-OD1	5.74	123.46	118.30
1	B	49	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	13	ASP	CB-CG-OD1	5.66	123.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	146	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	B	263	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	A	148	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	162	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	B	211	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	147	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	264	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	160	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	264	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	218	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	42	LYS	CB-CA-C	-5.50	99.39	110.40
1	A	128	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	49	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	B	208	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	263	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	B	136	LYS	CB-CA-C	-5.40	99.60	110.40
1	A	214	ASN	C-N-CA	5.39	135.18	121.70
1	B	146	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	243	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	254	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	B	49	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	B	243	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	135	GLY	O-C-N	-5.15	114.46	122.70
1	A	160	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	200	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	60	TYR	CB-CG-CD2	5.09	124.05	121.00
1	A	135	GLY	C-N-CA	5.08	134.39	121.70
1	B	174	ASN	N-CA-CB	5.08	119.74	110.60
1	A	174	ASN	N-CA-CB	5.07	119.72	110.60
1	B	141	VAL	CA-CB-CG2	-5.07	103.30	110.90
1	A	7	ASP	CB-CG-OD2	-5.05	113.75	118.30

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	2650	0	2592	240	0
1	B	2645	0	2576	155	0
2	A	376	0	0	29	0
2	B	394	0	0	23	0
All	All	6065	0	5168	392	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 37.

All (392) 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:151:TRP:HH2	1:B:171:VAL:HG21	1.11	1.10
1:A:216:ASP:HB2	1:A:233:MET:HE2	1.26	1.09
1:A:46[A]:LEU:HD13	1:A:172:TYR:HB3	1.32	1.07
1:A:19:ASN:HD21	1:A:21:ALA:HB3	1.21	1.03
1:A:151:TRP:HH2	1:A:171:VAL:HG21	1.28	0.97
1:A:166:ASN:HD22	1:A:320:ILE:HD11	1.29	0.94
1:B:151:TRP:CH2	1:B:171:VAL:HG21	2.03	0.92
1:B:202:THR:HG21	1:B:204:ILE:HG12	1.51	0.92
1:A:166:ASN:ND2	1:A:320:ILE:HD11	1.84	0.91
1:B:184:GLU:HG3	1:B:226:SER:HB3	1.50	0.91
1:A:6:ARG:HG2	1:A:6:ARG:HH11	1.35	0.89
1:A:151:TRP:CH2	1:A:171:VAL:HG21	2.10	0.87
1:A:215:THR:HG23	1:A:233:MET:SD	2.16	0.84
1:A:6:ARG:HD3	1:A:14:LEU:HD23	1.60	0.84
1:A:46[A]:LEU:HD13	1:A:172:TYR:CB	2.07	0.84
1:A:195:PHE:CD2	1:A:212:ILE:HD12	2.13	0.84
1:A:183:VAL:HG13	1:A:225:LEU:HD23	1.61	0.81
1:B:216:ASP:HB2	1:B:233:MET:HE2	1.62	0.81
1:A:200:ASP:HB2	1:A:202:THR:HB	1.63	0.81
1:B:202:THR:CG2	1:B:204:ILE:HG12	2.11	0.79
1:A:223:LYS:HB2	2:A:656:HOH:O	1.82	0.79
1:A:33:ARG:HB3	1:A:63:ALA:HA	1.65	0.78
1:A:250:GLN:HB3	1:A:255:LYS:HE2	1.65	0.78
1:B:71:ARG:HG2	1:B:95:LEU:HD13	1.65	0.78
1:A:217:LEU:HG	1:A:233:MET:CE	2.14	0.77
1:B:202:THR:HG23	1:B:204:ILE:H	1.48	0.77
1:A:296:VAL:HG23	1:A:297:HIS:O	1.83	0.77
1:A:19:ASN:ND2	1:A:21:ALA:HB3	2.00	0.77
1:A:287:GLY:O	1:A:294:LYS:HG3	1.85	0.76
1:A:248:LEU:HD13	1:A:257:GLN:HG2	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LEU:HG	1:A:233:MET:HE1	1.69	0.74
1:A:216:ASP:HB2	1:A:233:MET:CE	2.13	0.74
1:A:321:SER:HB2	2:A:464:HOH:O	1.86	0.74
1:B:148:ASP:OD1	1:B:150:LYS:HE3	1.87	0.74
1:A:289:LEU:HD23	1:A:294:LYS:HA	1.69	0.74
1:A:7:ASP:HB2	2:A:515:HOH:O	1.87	0.74
1:A:37:TRP:O	1:A:44:LEU:HG	1.88	0.74
1:B:171:VAL:HG23	2:B:699:HOH:O	1.86	0.74
1:B:250:GLN:NE2	1:B:255:LYS:HE3	2.04	0.73
1:A:212:ILE:HD11	1:A:217:LEU:CB	2.19	0.73
1:B:146:ASP:HB2	1:B:150:LYS:H	1.52	0.73
1:A:216:ASP:CB	1:A:233:MET:HE2	2.14	0.72
1:B:239:VAL:HG13	2:B:604:HOH:O	1.88	0.72
1:A:247:LEU:HD22	2:A:394:HOH:O	1.87	0.72
1:B:86:LEU:HD13	1:B:133:TYR:CZ	2.23	0.72
1:A:78:LYS:HG3	1:A:83:ASP:OD1	1.90	0.72
1:A:248:LEU:HD21	1:A:276:ILE:HD12	1.70	0.72
1:A:248:LEU:HD11	1:A:276:ILE:CD1	2.20	0.71
1:B:202:THR:CG2	1:B:204:ILE:H	2.03	0.71
1:B:217:LEU:N	1:B:233:MET:HE1	2.05	0.71
1:A:20:LYS:HD2	1:A:147:ASP:OD2	1.90	0.70
1:A:136:LYS:NZ	2:A:402:HOH:O	2.24	0.70
1:B:208:ASP:HA	2:B:548:HOH:O	1.91	0.70
1:A:33:ARG:NH1	1:A:63:ALA:HB2	2.07	0.70
1:B:146:ASP:OD2	1:B:150:LYS:HB2	1.91	0.69
1:A:217:LEU:N	1:A:233:MET:HE1	2.07	0.69
1:B:71:ARG:CG	1:B:95:LEU:HD13	2.23	0.69
1:A:39:LYS:O	1:A:42:LYS:HB2	1.91	0.69
1:A:39:LYS:NZ	1:A:338:THR:HG21	2.08	0.69
1:B:33:ARG:NH1	1:B:63:ALA:HB2	2.08	0.69
1:A:17:LEU:HD13	1:A:118:VAL:HB	1.76	0.68
1:A:250:GLN:O	1:A:257:GLN:NE2	2.27	0.68
1:B:289:LEU:HD11	1:B:294:LYS:HG3	1.74	0.68
1:B:190:LEU:HD13	1:B:192:ALA:HB3	1.76	0.67
1:B:126:SER:HB3	1:B:137:ILE:HB	1.75	0.67
1:A:280:THR:HG22	1:A:301:ILE:HD12	1.75	0.67
1:A:151:TRP:HH2	1:A:171:VAL:CG2	2.07	0.67
1:A:232:ASN:O	1:A:237:GLN:NE2	2.28	0.66
1:B:189:ARG:NH2	1:B:256:GLU:O	2.29	0.66
1:B:33:ARG:CZ	1:B:63:ALA:HB2	2.25	0.66
1:B:34:ILE:CG2	1:B:171:VAL:HG22	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:VAL:HG23	1:B:168:THR:HG22	1.77	0.66
1:A:2:SER:N	2:A:659:HOH:O	2.28	0.65
1:A:248:LEU:HD11	1:A:276:ILE:HD12	1.76	0.65
1:A:6:ARG:NH2	2:A:361:HOH:O	2.28	0.65
1:A:242:ILE:HG22	1:A:278:ILE:O	1.97	0.65
1:A:71:ARG:NH1	1:A:90:GLU:OE1	2.29	0.65
1:A:6:ARG:NH1	1:A:7:ASP:O	2.29	0.65
1:B:112:THR:OG1	1:B:119:GLN:HB2	1.96	0.65
1:B:17:LEU:HD13	1:B:118:VAL:HB	1.78	0.64
1:A:39:LYS:HZ2	1:A:338:THR:HG21	1.61	0.64
1:A:212:ILE:HD11	1:A:217:LEU:HB2	1.77	0.64
1:B:65:VAL:CG2	1:B:168:THR:HG22	2.26	0.64
1:A:232:ASN:ND2	2:A:389:HOH:O	2.29	0.64
1:B:321:SER:OG	1:B:323:LYS:NZ	2.31	0.64
1:A:216:ASP:O	1:A:223:LYS:NZ	2.29	0.64
1:A:165:PHE:CE2	1:A:167:PRO:HG3	2.32	0.64
1:A:152:LYS:HG3	1:A:333:ILE:CG1	2.28	0.63
1:A:100:GLU:OE2	1:B:125:VAL:HG21	1.98	0.63
1:A:19:ASN:OD1	1:A:23:VAL:N	2.30	0.63
1:B:338:THR:HB	2:B:732:HOH:O	1.98	0.63
1:B:311:SER:OG	1:B:320:ILE:HD12	1.98	0.63
1:A:44:LEU:HD23	1:A:44:LEU:N	2.14	0.62
1:A:180:SER:HA	1:A:296:VAL:HG13	1.81	0.62
1:A:206:ARG:HD2	1:A:208:ASP:OD1	1.99	0.62
1:B:52:LYS:NZ	2:B:697:HOH:O	2.32	0.62
1:A:310:GLY:O	1:A:312:GLU:N	2.31	0.62
1:B:111:VAL:HG13	1:B:120:VAL:HG22	1.80	0.62
1:B:156:GLU:OE2	1:B:327:LYS:HE2	2.00	0.62
1:A:282:ASN:HA	1:A:297:HIS:CE1	2.35	0.61
1:A:222:GLU:HG2	2:A:715:HOH:O	1.99	0.61
1:A:183:VAL:O	1:A:225:LEU:HD23	2.00	0.61
1:B:339:LYS:HE3	2:B:735:HOH:O	1.99	0.61
1:A:10:LEU:HD11	1:A:52[B]:LYS:HG2	1.82	0.61
1:A:16:SER:HB3	1:A:26:SER:HB3	1.82	0.61
1:A:177:GLY:HA2	2:A:359:HOH:O	2.00	0.61
1:B:216:ASP:O	1:B:223:LYS:NZ	2.29	0.60
1:A:185:ASN:OD1	1:A:186:HIS:ND1	2.31	0.60
1:A:282:ASN:ND2	1:A:298:HIS:NE2	2.49	0.60
1:A:253:LEU:HD21	1:A:333:ILE:CD1	2.31	0.60
1:A:218:ASP:O	1:A:223:LYS:HD3	2.01	0.60
1:B:164:VAL:HB	1:B:320:ILE:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ILE:HG21	1:B:171:VAL:HG22	1.82	0.60
1:B:197:PRO:HD2	1:B:208:ASP:O	2.01	0.60
1:A:202:THR:HG22	1:A:204:ILE:H	1.66	0.60
1:A:231:SER:OG	1:A:232:ASN:N	2.30	0.60
1:A:212:ILE:HD11	1:A:217:LEU:HB3	1.84	0.59
1:A:83:ASP:HB2	2:A:469:HOH:O	2.02	0.59
1:A:239:VAL:HG21	1:A:243:ASP:HB3	1.84	0.59
1:B:194:ARG:NH2	2:B:705:HOH:O	2.30	0.59
1:A:78:LYS:HG2	1:A:81:GLY:O	2.02	0.59
1:B:2:SER:OG	1:B:18:THR:HB	2.02	0.58
1:A:6:ARG:HB3	2:A:352:HOH:O	2.03	0.58
1:A:273:GLN:HG3	1:A:306:GLN:HA	1.85	0.58
1:A:10:LEU:N	1:A:10:LEU:HD23	2.19	0.58
1:A:190:LEU:HD23	1:A:257:GLN:O	2.04	0.58
1:B:8:PHE:HB3	1:B:12:SER:OG	2.04	0.58
1:A:15:ILE:N	1:A:15:ILE:HD12	2.19	0.57
1:A:248:LEU:HD21	1:A:276:ILE:CD1	2.34	0.57
1:A:280:THR:CG2	1:A:301:ILE:HD12	2.33	0.57
1:B:199:LYS:HB3	1:B:206:ARG:HB3	1.85	0.57
1:B:212:ILE:C	1:B:215:THR:HG23	2.24	0.57
1:A:200:ASP:CB	1:A:202:THR:HB	2.34	0.57
1:A:190:LEU:HD23	1:A:258:ALA:HB2	1.86	0.57
1:B:18:THR:OG1	1:B:24:THR:HG22	2.05	0.57
1:A:152:LYS:HG3	1:A:333:ILE:HG12	1.86	0.57
1:B:207:GLY:HA2	1:B:314:ILE:CD1	2.34	0.57
1:A:230:ASN:ND2	2:A:531:HOH:O	2.37	0.56
1:A:36:ASP:OD1	1:A:37:TRP:N	2.31	0.56
1:B:149:ASN:HB3	1:B:336:LEU:HB3	1.87	0.56
1:A:323:LYS:HD2	1:A:326:GLU:OE1	2.05	0.56
1:B:33:ARG:HB3	1:B:63:ALA:HA	1.87	0.56
1:B:92:PRO:HG3	2:B:692:HOH:O	2.05	0.56
1:A:20:LYS:HB2	2:A:574:HOH:O	2.04	0.56
1:A:185:ASN:OD1	1:A:185:ASN:N	2.35	0.56
1:B:289:LEU:HD11	1:B:294:LYS:CG	2.34	0.56
1:A:282:ASN:HD22	1:A:298:HIS:CD2	2.24	0.56
1:A:256:GLU:HG2	1:A:268:SER:OG	2.05	0.56
1:B:74:ASP:HA	1:B:92:PRO:O	2.06	0.56
1:B:217:LEU:HG	1:B:233:MET:CE	2.36	0.56
1:B:199:LYS:HD2	1:B:200:ASP:OD2	2.06	0.56
1:B:255:LYS:HG3	1:B:257:GLN:HE22	1.71	0.56
1:B:5:ILE:HD13	1:B:15:ILE:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ARG:HD2	1:B:208:ASP:HB2	1.88	0.56
1:A:6:ARG:HH11	1:A:6:ARG:CG	2.13	0.55
1:A:166:ASN:HB2	1:A:320:ILE:HG12	1.86	0.55
1:A:232:ASN:HB2	1:A:237:GLN:NE2	2.21	0.55
1:A:261:THR:HG22	1:A:266:SER:HB2	1.88	0.55
1:A:272:ASP:OD2	1:A:330:ALA:HA	2.06	0.55
1:A:253:LEU:HD11	1:A:331:THR:HB	1.88	0.55
1:B:78:LYS:HD3	1:B:83:ASP:OD1	2.07	0.55
1:A:310:GLY:O	1:A:311:SER:C	2.45	0.55
1:B:196:VAL:HB	1:B:245:PRO:HG2	1.88	0.55
1:A:16:SER:C	1:A:17:LEU:HD23	2.26	0.55
1:A:193[A]:SER:OG	1:A:220:ARG:HD2	2.08	0.54
1:A:338:THR:HG22	1:A:338:THR:O	2.06	0.54
1:A:72:ILE:HD13	1:A:312:GLU:OE2	2.06	0.54
1:B:213:LYS:O	1:B:214:ASN:ND2	2.39	0.54
1:B:201:GLN:HG2	2:B:724:HOH:O	2.07	0.54
1:B:34:ILE:HG21	1:B:171:VAL:CG2	2.36	0.54
1:A:38:GLN:HA	1:A:42:LYS:O	2.08	0.53
1:A:174:ASN:ND2	1:A:299:GLY:O	2.32	0.53
1:A:189:ARG:O	1:A:258:ALA:HA	2.08	0.53
1:A:12:SER:HB3	1:A:106:LEU:HD21	1.90	0.53
1:A:199:LYS:HE3	1:A:200:ASP:OD2	2.07	0.53
1:A:227:ASN:N	1:A:227:ASN:HD22	2.05	0.53
1:B:188:LEU:HG	1:B:189:ARG:N	2.23	0.53
1:B:207:GLY:HA2	1:B:314:ILE:HG12	1.90	0.53
1:A:237:GLN:NE2	2:A:546:HOH:O	2.40	0.53
1:B:289:LEU:HD12	1:B:294:LYS:HA	1.90	0.53
1:A:217:LEU:H	1:A:233:MET:HE1	1.74	0.53
1:B:71:ARG:HG2	1:B:95:LEU:CD1	2.39	0.53
1:A:77:VAL:HA	2:A:495:HOH:O	2.08	0.53
1:A:232:ASN:CA	1:A:237:GLN:HE21	2.21	0.52
1:A:146:ASP:HB3	2:A:680:HOH:O	2.08	0.52
1:A:248:LEU:HD11	1:A:276:ILE:HD11	1.91	0.52
1:A:170:HIS:O	1:A:170:HIS:ND1	2.39	0.52
1:B:296:VAL:HG12	2:B:444:HOH:O	2.08	0.52
1:A:197:PRO:HG2	1:A:208:ASP:HB2	1.91	0.52
1:A:282:ASN:ND2	1:A:298:HIS:CD2	2.78	0.52
1:B:88:GLN:HA	1:B:93:GLN:O	2.10	0.52
1:A:190:LEU:CD2	1:A:258:ALA:HB2	2.40	0.52
1:A:130:THR:HG23	1:B:127:ASN:HB2	1.92	0.52
1:A:280:THR:O	1:A:298:HIS:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ASP:HB3	1:B:148:ASP:H	1.74	0.52
1:B:207:GLY:CA	1:B:314:ILE:HD11	2.40	0.52
1:B:250:GLN:HE21	1:B:255:LYS:HE3	1.74	0.51
1:A:17:LEU:HD23	1:A:17:LEU:N	2.26	0.51
1:B:161:LYS:NZ	2:B:689:HOH:O	2.43	0.51
1:B:165:PHE:CE2	1:B:167:PRO:HG3	2.46	0.51
1:B:282:ASN:HD22	1:B:298:HIS:CD2	2.28	0.51
1:B:86:LEU:HD13	1:B:133:TYR:CE2	2.45	0.51
1:A:203:GLU:OE2	1:A:243:ASP:OD2	2.29	0.51
1:B:36:ASP:HA	1:B:45:ILE:HD11	1.93	0.51
1:A:29:ASN:HB2	1:A:107:TRP:O	2.11	0.51
1:B:207:GLY:HA2	1:B:314:ILE:HD11	1.92	0.51
1:B:136:LYS:HE3	1:B:160:ASP:OD2	2.11	0.50
1:B:189:ARG:HB3	1:B:222:GLU:HG3	1.93	0.50
1:A:278:ILE:CG2	1:A:301:ILE:HD11	2.42	0.50
1:B:72:ILE:HG23	1:B:312:GLU:OE1	2.10	0.50
1:B:297:HIS:CD2	1:B:298:HIS:CE1	3.00	0.50
1:A:242:ILE:O	1:A:279:PHE:HA	2.12	0.50
1:B:33:ARG:HB2	1:B:62:GLY:O	2.12	0.50
1:A:241:GLY:HA2	2:A:428:HOH:O	2.11	0.50
1:B:291:HIS:O	1:B:292:GLU:HB2	2.10	0.50
1:B:2:SER:HB3	2:B:546:HOH:O	2.12	0.50
1:A:253:LEU:HD21	1:A:333:ILE:HD12	1.93	0.49
1:A:39:LYS:O	1:A:40:ASP:HB2	2.12	0.49
1:A:121:LYS:HD2	2:A:714:HOH:O	2.12	0.49
1:B:200:ASP:C	1:B:202:THR:H	2.14	0.49
1:B:216:ASP:HB2	1:B:233:MET:CE	2.37	0.49
1:B:338:THR:O	1:B:338:THR:HG22	2.10	0.49
1:A:205:VAL:HG12	1:A:206:ARG:N	2.27	0.49
1:B:180:SER:HA	1:B:296:VAL:HG13	1.94	0.49
1:A:171:VAL:O	1:A:302:THR:HG22	2.12	0.49
1:B:206:ARG:CD	1:B:208:ASP:HB2	2.42	0.49
1:B:217:LEU:H	1:B:233:MET:HE1	1.77	0.49
1:A:271:THR:OG1	1:A:272:ASP:N	2.45	0.49
1:B:212:ILE:O	1:B:215:THR:HG23	2.12	0.49
1:A:27:PHE:CZ	1:A:143:HIS:HB3	2.47	0.49
1:A:286:LEU:O	1:A:286:LEU:HD23	2.13	0.49
1:A:150:LYS:HG2	1:A:335:SER:HB2	1.94	0.49
1:A:227:ASN:N	1:A:227:ASN:ND2	2.61	0.48
1:A:261:THR:HG22	1:A:266:SER:CB	2.44	0.48
1:B:178:ASP:OD1	1:B:180:SER:OG	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:LYS:HE2	2:B:684:HOH:O	2.13	0.48
1:A:212:ILE:O	1:A:212:ILE:HG23	2.13	0.48
1:A:217:LEU:HG	1:A:233:MET:HE3	1.95	0.48
1:A:55:LEU:HD22	2:A:681:HOH:O	2.14	0.48
1:A:183:VAL:HG13	1:A:183:VAL:O	2.14	0.48
1:B:232:ASN:CA	1:B:237:GLN:HE21	2.26	0.48
1:A:182:SER:C	1:A:184:GLU:H	2.17	0.48
1:A:216:ASP:C	1:A:223:LYS:HZ1	2.13	0.48
1:B:175:LEU:HB2	1:B:186:HIS:NE2	2.28	0.48
1:A:39:LYS:HZ2	1:A:338:THR:CG2	2.27	0.48
1:A:241:GLY:HA3	1:A:282:ASN:ND2	2.28	0.48
1:A:14:LEU:HD11	1:A:26:SER:HB2	1.96	0.47
1:A:23:VAL:HG13	1:A:38:GLN:O	2.13	0.47
1:A:175:LEU:HB2	1:A:262:LEU:HD12	1.96	0.47
1:A:196:VAL:HB	1:A:245:PRO:HG2	1.95	0.47
1:B:339:LYS:HG3	2:B:675:HOH:O	2.14	0.47
1:A:76:LEU:HG	1:A:77:VAL:N	2.29	0.47
1:B:71:ARG:NE	1:B:90:GLU:OE1	2.42	0.47
1:A:176:ASN:HD22	1:A:181:GLU:HB2	1.80	0.47
1:B:152:LYS:HB2	1:B:333:ILE:HG12	1.97	0.47
1:B:207:GLY:N	1:B:314:ILE:HD11	2.28	0.47
1:A:10:LEU:HD23	1:A:10:LEU:H	1.79	0.47
1:A:272:ASP:HB2	1:A:331:THR:O	2.15	0.47
1:B:29:ASN:HB2	1:B:107:TRP:O	2.15	0.47
1:B:212:ILE:HD12	1:B:218:ASP:HA	1.96	0.47
1:B:169:GLY:C	2:B:699:HOH:O	2.54	0.47
1:B:194:ARG:HD3	2:B:663:HOH:O	2.15	0.47
1:B:282:ASN:ND2	1:B:298:HIS:CD2	2.82	0.47
1:A:152:LYS:HG3	1:A:333:ILE:HG13	1.96	0.46
1:A:289:LEU:CD2	1:A:294:LYS:N	2.79	0.46
1:A:78:LYS:HE2	1:A:83:ASP:OD1	2.15	0.46
1:A:89:ASN:ND2	1:A:95:LEU:O	2.48	0.46
1:B:206:ARG:HD2	1:B:208:ASP:CB	2.45	0.46
1:A:72:ILE:O	1:A:93:GLN:HG3	2.16	0.46
1:A:311:SER:HB2	2:A:607:HOH:O	2.14	0.46
1:A:38:GLN:HE21	1:A:38:GLN:HB2	1.48	0.46
1:A:80:SER:N	2:A:567:HOH:O	2.39	0.46
1:A:296:VAL:O	1:A:297:HIS:C	2.53	0.46
1:B:212:ILE:HA	1:B:215:THR:HG21	1.98	0.46
1:A:43:HIS:C	1:A:44:LEU:HD23	2.36	0.46
1:B:207:GLY:HA2	1:B:314:ILE:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ASP:O	1:B:338:THR:HA	2.16	0.46
1:A:182:SER:HA	1:A:298:HIS:O	2.16	0.46
1:A:248:LEU:HD13	1:A:257:GLN:CG	2.41	0.46
1:B:60:TYR:N	1:B:61:PRO:CD	2.79	0.46
1:B:239:VAL:O	1:B:240:LYS:HB2	2.17	0.45
1:A:278:ILE:HG23	1:A:301:ILE:HD11	1.98	0.45
1:B:194:ARG:HA	1:B:210:VAL:O	2.16	0.45
1:B:195:PHE:CD2	1:B:212:ILE:CG2	2.99	0.45
1:B:17:LEU:HD22	1:B:118:VAL:HG11	1.97	0.45
1:B:239:VAL:CG1	1:B:243:ASP:HB2	2.47	0.45
1:A:200:ASP:HB3	1:A:202:THR:H	1.81	0.45
1:A:3:ILE:O	1:A:4:LYS:HG2	2.16	0.45
1:A:50:SER:OG	1:A:53:GLU:HG3	2.17	0.45
1:A:224:GLN:HB2	2:A:675:HOH:O	2.17	0.45
1:A:256:GLU:CD	1:A:259:ARG:HE	2.20	0.45
1:A:274:PRO:HB2	2:A:704:HOH:O	2.15	0.45
1:B:29:ASN:HA	1:B:122:PHE:CE2	2.52	0.45
1:A:137:ILE:HG22	1:A:139:MET:HG2	1.99	0.45
1:A:109:TYR:CE2	1:B:11:GLY:HA2	2.52	0.45
1:A:156:GLU:HG2	1:A:329:GLN:HG2	1.98	0.45
1:A:239:VAL:CG2	1:A:243:ASP:HB3	2.47	0.45
1:B:227:ASN:ND2	2:B:406:HOH:O	2.50	0.45
1:A:157:ALA:C	1:A:158:ILE:HG13	2.37	0.45
1:A:297:HIS:NE2	1:A:298:HIS:CE1	2.85	0.44
1:B:202:THR:HG23	1:B:204:ILE:N	2.24	0.44
1:B:52:LYS:O	1:B:56:GLU:HB2	2.16	0.44
1:B:114:LEU:HD23	1:B:114:LEU:HA	1.64	0.44
1:A:73:LYS:HA	1:A:93:GLN:OE1	2.17	0.44
1:A:126:SER:HB3	1:A:137:ILE:HB	1.99	0.44
1:A:312:GLU:H	1:A:312:GLU:HG2	1.24	0.44
1:A:339:LYS:HE3	1:A:339:LYS:HB2	1.55	0.44
1:B:283:PHE:O	1:B:284:GLY:C	2.52	0.44
1:A:232:ASN:HA	1:A:237:GLN:HE21	1.82	0.44
1:B:178:ASP:OD1	1:B:293:LYS:HD3	2.17	0.44
1:A:77:VAL:HG23	1:A:84:TYR:HB2	1.99	0.44
1:A:178:ASP:HB3	1:A:181:GLU:OE1	2.18	0.44
1:A:232:ASN:HB2	1:A:237:GLN:HE21	1.81	0.44
1:A:296:VAL:O	1:A:299:GLY:N	2.51	0.44
1:A:72:ILE:HG13	2:A:366:HOH:O	2.16	0.44
1:A:285:ASP:HB2	2:A:476:HOH:O	2.18	0.44
1:B:183:VAL:HG13	1:B:225:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:LYS:H	1:B:255:LYS:HG2	1.50	0.44
1:B:206:ARG:HD2	1:B:208:ASP:OD2	2.18	0.43
1:B:251:LEU:HA	2:B:389:HOH:O	2.18	0.43
1:A:27:PHE:HB3	1:A:33:ARG:O	2.17	0.43
1:A:178:ASP:HB3	1:A:181:GLU:HG3	1.99	0.43
1:B:215:THR:HA	2:B:411:HOH:O	2.18	0.43
1:A:39:LYS:NZ	1:A:338:THR:CG2	2.80	0.43
1:A:274:PRO:HD2	1:A:306:GLN:O	2.19	0.43
1:B:111:VAL:HG22	1:B:120:VAL:HG13	2.01	0.43
1:A:34:ILE:HG23	1:A:34:ILE:O	2.17	0.43
1:A:36:ASP:HB2	2:A:358:HOH:O	2.17	0.43
1:A:152:LYS:CG	1:A:333:ILE:HG13	2.49	0.43
1:A:279:PHE:CZ	1:A:281:ALA:HA	2.53	0.43
1:B:52:LYS:HG3	1:B:53:GLU:N	2.33	0.43
1:B:185:ASN:OD1	1:B:186:HIS:ND1	2.51	0.43
1:B:189:ARG:NH2	1:B:256:GLU:HB3	2.33	0.43
1:A:44:LEU:N	1:A:44:LEU:CD2	2.80	0.43
1:A:195:PHE:HZ	1:A:235:GLN:HG3	1.84	0.43
1:B:49:ASP:HB3	2:B:358:HOH:O	2.19	0.43
1:A:70:GLY:HA2	2:A:638:HOH:O	2.18	0.43
1:B:232:ASN:HB2	1:B:237:GLN:NE2	2.34	0.43
1:A:176:ASN:ND2	1:A:181:GLU:HB2	2.34	0.43
1:A:289:LEU:CD2	1:A:294:LYS:HA	2.43	0.43
1:A:79:ILE:O	1:A:80:SER:C	2.56	0.42
1:B:232:ASN:HB2	1:B:237:GLN:HE21	1.84	0.42
1:B:280:THR:O	1:B:298:HIS:HA	2.19	0.42
1:A:10:LEU:HD11	1:A:52[B]:LYS:CG	2.49	0.42
1:A:228:ALA:O	1:A:231:SER:HB3	2.18	0.42
1:B:239:VAL:HG11	1:B:243:ASP:HB2	2.00	0.42
1:A:246:PHE:O	1:A:275:SER:HB2	2.19	0.42
1:A:289:LEU:HD22	1:A:294:LYS:N	2.34	0.42
1:B:142:THR:O	1:B:153:ILE:HA	2.20	0.42
1:A:176:ASN:OD1	1:A:262:LEU:HD11	2.20	0.42
1:A:225:LEU:HD12	1:A:225:LEU:HA	1.62	0.42
1:B:254:ASP:CG	1:B:255:LYS:HD3	2.40	0.42
1:A:10:LEU:HD11	1:A:52[A]:LYS:HG3	2.02	0.42
1:A:196:VAL:HG13	2:A:407:HOH:O	2.20	0.42
1:A:232:ASN:CB	1:A:237:GLN:HE21	2.33	0.42
1:A:323:LYS:HD3	1:A:326:GLU:OE2	2.20	0.42
1:B:6:ARG:NH2	2:B:556:HOH:O	2.52	0.42
1:B:33:ARG:CB	1:B:63:ALA:HA	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:HD11	1:A:164:VAL:HG13	2.02	0.42
1:A:286:LEU:HD23	1:A:286:LEU:C	2.39	0.42
1:B:36:ASP:CG	1:B:43:HIS:HD1	2.24	0.42
1:B:280:THR:O	1:B:281:ALA:C	2.56	0.42
1:A:39:LYS:NZ	1:A:338:THR:CB	2.82	0.41
1:A:197:PRO:HA	1:A:235:GLN:OE1	2.19	0.41
1:B:67:PRO:HG2	1:B:133:TYR:CE2	2.55	0.41
1:A:109:TYR:HA	1:A:121:LYS:O	2.20	0.41
1:B:67:PRO:HG2	1:B:133:TYR:CZ	2.54	0.41
1:B:262:LEU:HD12	1:B:262:LEU:HA	1.92	0.41
1:A:10:LEU:HD11	1:A:52[A]:LYS:CG	2.50	0.41
1:A:24:THR:O	1:A:37:TRP:HD1	2.04	0.41
1:B:207:GLY:CA	1:B:314:ILE:CD1	2.99	0.41
1:A:219:PHE:O	1:A:220:ARG:C	2.58	0.41
1:B:251:LEU:HD11	2:B:605:HOH:O	2.19	0.41
1:A:68:THR:CG2	1:A:164:VAL:HG23	2.50	0.41
1:A:246:PHE:CD1	1:A:246:PHE:N	2.89	0.41
1:A:251:LEU:HD11	1:A:274:PRO:HA	2.03	0.41
1:A:289:LEU:CD2	1:A:294:LYS:CA	2.98	0.41
1:A:111:VAL:HG22	1:A:120:VAL:HG22	2.02	0.41
1:A:190:LEU:HD23	1:A:190:LEU:HA	1.87	0.41
1:A:232:ASN:O	1:A:233:MET:C	2.56	0.41
1:A:235:GLN:O	1:A:238:LEU:HB3	2.20	0.41
1:A:273:GLN:HB3	1:A:274:PRO:HD2	2.03	0.41
1:B:76:LEU:HG	1:B:77:VAL:N	2.36	0.41
1:B:206:ARG:HG3	2:B:654:HOH:O	2.20	0.41
1:B:216:ASP:OD2	1:B:231:SER:HB2	2.22	0.40
1:A:164:VAL:HB	1:A:320:ILE:CG2	2.51	0.40
1:A:166:ASN:CB	1:A:320:ILE:CD1	3.00	0.40
1:A:248:LEU:HD22	1:A:257:GLN:HG2	2.02	0.40
1:A:273:GLN:HA	1:A:274:PRO:HD3	1.79	0.40
1:A:289:LEU:HD23	1:A:294:LYS:CA	2.46	0.40
1:B:212:ILE:HD12	1:B:217:LEU:O	2.21	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	339/347 (98%)	299 (88%)	36 (11%)	4 (1%)	13 4
1	B	338/347 (97%)	309 (91%)	29 (9%)	0	100 100
All	All	677/694 (98%)	608 (90%)	65 (10%)	4 (1%)	25 15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	THR
1	A	311	SER
1	A	40	ASP
1	A	281	ALA

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	294/300 (98%)	236 (80%)	58 (20%)	1 0
1	B	293/300 (98%)	251 (86%)	42 (14%)	3 1
All	All	587/600 (98%)	487 (83%)	100 (17%)	2 0

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	4	LYS

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Mol	Chain	Res	Type
1	A	6	ARG
1	A	8	PHE
1	A	16	SER
1	A	17	LEU
1	A	24	THR
1	A	30	LEU
1	A	33	ARG
1	A	42	LYS
1	A	44	LEU
1	A	65	VAL
1	A	72	ILE
1	A	76	LEU
1	A	78	LYS
1	A	99	GLU
1	A	119	GLN
1	A	136	LYS
1	A	148	ASP
1	A	150	LYS
1	A	152	LYS
1	A	164	VAL
1	A	181	GLU
1	A	183	VAL
1	A	186	HIS
1	A	189	ARG
1	A	190	LEU
1	A	195	PHE
1	A	201	GLN
1	A	202	THR
1	A	206	ARG
1	A	208	ASP
1	A	211	ASP
1	A	212	ILE
1	A	224	GLN
1	A	225	LEU
1	A	226	SER
1	A	230	ASN
1	A	233	MET
1	A	234	GLU
1	A	239	VAL
1	A	246	PHE
1	A	248	LEU
1	A	251	LEU

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Mol	Chain	Res	Type
1	A	253	LEU
1	A	256	GLU
1	A	257	GLN
1	A	262	LEU
1	A	264	ASP
1	A	267	ILE
1	A	288	THR
1	A	292	GLU
1	A	311	SER
1	A	312	GLU
1	A	320	ILE
1	A	321	SER
1	A	335	SER
1	A	339	LYS
1	B	4	LYS
1	B	16	SER
1	B	20	LYS
1	B	30	LEU
1	B	42	LYS
1	B	44	LEU
1	B	50	SER
1	B	52	LYS
1	B	76	LEU
1	B	77	VAL
1	B	80	SER
1	B	112	THR
1	B	153	ILE
1	B	161	LYS
1	B	183	VAL
1	B	189	ARG
1	B	190	LEU
1	B	195	PHE
1	B	199	LYS
1	B	200	ASP
1	B	202	THR
1	B	203	GLU
1	B	205	VAL
1	B	206	ARG
1	B	208	ASP
1	B	211	ASP
1	B	213	LYS
1	B	214	ASN

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Mol	Chain	Res	Type
1	B	222	GLU
1	B	223	LYS
1	B	247	LEU
1	B	250	GLN
1	B	251	LEU
1	B	254	ASP
1	B	255	LYS
1	B	257	GLN
1	B	285[A]	ASP
1	B	285[B]	ASP
1	B	293	LYS
1	B	321	SER
1	B	323	LYS
1	B	339	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	43	HIS
1	A	89	ASN
1	A	227	ASN
1	A	230	ASN
1	A	237	GLN
1	A	250	GLN
1	A	282	ASN
1	A	329	GLN
1	B	38	GLN
1	B	227	ASN
1	B	237	GLN
1	B	250	GLN
1	B	282	ASN
1	B	329	GLN

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 monosaccharides 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	338/347 (97%)	0.31	10 (2%)	50	53	11, 28, 54, 90	0
1	B	338/347 (97%)	-0.02	1 (0%)	94	94	9, 22, 45, 68	0
All	All	676/694 (97%)	0.15	11 (1%)	72	74	9, 24, 49, 90	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	215	THR	5.6
1	A	339	LYS	5.0
1	A	214	ASN	3.8
1	B	214	ASN	3.7
1	A	287	GLY	2.8
1	A	81	GLY	2.8
1	A	221	GLN	2.7
1	A	242	ILE	2.6
1	A	264	ASP	2.6
1	A	250	GLN	2.5
1	A	338	THR	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 monosaccharides 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.