



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:42 AM UTC

PDB ID : 2OVL / pdb_00002ovl
Title : Crystal structure of a racemase from *Streptomyces coelicolor* A3(2)
Authors : Rao, K.N.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center
for Structural Genomics (NYSGXRC)
Deposited on : 2007-02-14
Resolution : 2.13 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

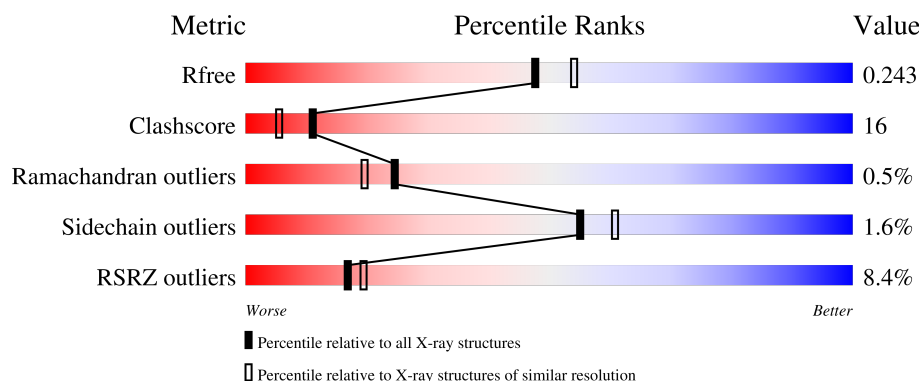
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	371	 5% 73% 21% . .
1	B	371	 5% 71% 23% . .
1	C	371	 10% 67% 29% . .
1	D	371	 11% 68% 21% . 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11225 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 Putative racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	Se	0	0	0
			2749	1738	492	506	2	11			
1	B	357	Total	C	N	O	S	Se	0	0	0
			2749	1738	492	506	2	11			
1	C	357	Total	C	N	O	S	Se	0	0	0
			2749	1738	492	506	2	11			
1	D	334	Total	C	N	O	S	Se	0	0	0
			2577	1631	462	474	2	8			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	cloning artifact	UNP Q9RKF7
A	2	SER	-	cloning artifact	UNP Q9RKF7
A	3	LEU	-	cloning artifact	UNP Q9RKF7
A	28	MSE	MET	modified residue	UNP Q9RKF7
A	29	MSE	MET	modified residue	UNP Q9RKF7
A	63	MSE	MET	modified residue	UNP Q9RKF7
A	87	MSE	MET	modified residue	UNP Q9RKF7
A	167	MSE	MET	modified residue	UNP Q9RKF7
A	195	MSE	MET	modified residue	UNP Q9RKF7
A	200	MSE	MET	modified residue	UNP Q9RKF7
A	294	MSE	MET	modified residue	UNP Q9RKF7
A	318	MSE	MET	modified residue	UNP Q9RKF7
A	329	MSE	MET	modified residue	UNP Q9RKF7
A	333	MSE	MET	modified residue	UNP Q9RKF7
A	364	GLU	-	cloning artifact	UNP Q9RKF7
A	365	GLY	-	cloning artifact	UNP Q9RKF7
A	366	HIS	-	cloning artifact	UNP Q9RKF7
A	367	HIS	-	cloning artifact	UNP Q9RKF7
A	368	HIS	-	cloning artifact	UNP Q9RKF7
A	369	HIS	-	cloning artifact	UNP Q9RKF7
A	370	HIS	-	cloning artifact	UNP Q9RKF7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	371	HIS	-	cloning artifact	UNP Q9RKF7
B	1	MSE	-	cloning artifact	UNP Q9RKF7
B	2	SER	-	cloning artifact	UNP Q9RKF7
B	3	LEU	-	cloning artifact	UNP Q9RKF7
B	28	MSE	MET	modified residue	UNP Q9RKF7
B	29	MSE	MET	modified residue	UNP Q9RKF7
B	63	MSE	MET	modified residue	UNP Q9RKF7
B	87	MSE	MET	modified residue	UNP Q9RKF7
B	167	MSE	MET	modified residue	UNP Q9RKF7
B	195	MSE	MET	modified residue	UNP Q9RKF7
B	200	MSE	MET	modified residue	UNP Q9RKF7
B	294	MSE	MET	modified residue	UNP Q9RKF7
B	318	MSE	MET	modified residue	UNP Q9RKF7
B	329	MSE	MET	modified residue	UNP Q9RKF7
B	333	MSE	MET	modified residue	UNP Q9RKF7
B	364	GLU	-	cloning artifact	UNP Q9RKF7
B	365	GLY	-	cloning artifact	UNP Q9RKF7
B	366	HIS	-	cloning artifact	UNP Q9RKF7
B	367	HIS	-	cloning artifact	UNP Q9RKF7
B	368	HIS	-	cloning artifact	UNP Q9RKF7
B	369	HIS	-	cloning artifact	UNP Q9RKF7
B	370	HIS	-	cloning artifact	UNP Q9RKF7
B	371	HIS	-	cloning artifact	UNP Q9RKF7
C	1	MSE	-	cloning artifact	UNP Q9RKF7
C	2	SER	-	cloning artifact	UNP Q9RKF7
C	3	LEU	-	cloning artifact	UNP Q9RKF7
C	28	MSE	MET	modified residue	UNP Q9RKF7
C	29	MSE	MET	modified residue	UNP Q9RKF7
C	63	MSE	MET	modified residue	UNP Q9RKF7
C	87	MSE	MET	modified residue	UNP Q9RKF7
C	167	MSE	MET	modified residue	UNP Q9RKF7
C	195	MSE	MET	modified residue	UNP Q9RKF7
C	200	MSE	MET	modified residue	UNP Q9RKF7
C	294	MSE	MET	modified residue	UNP Q9RKF7
C	318	MSE	MET	modified residue	UNP Q9RKF7
C	329	MSE	MET	modified residue	UNP Q9RKF7
C	333	MSE	MET	modified residue	UNP Q9RKF7
C	364	GLU	-	cloning artifact	UNP Q9RKF7
C	365	GLY	-	cloning artifact	UNP Q9RKF7
C	366	HIS	-	cloning artifact	UNP Q9RKF7
C	367	HIS	-	cloning artifact	UNP Q9RKF7
C	368	HIS	-	cloning artifact	UNP Q9RKF7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	369	HIS	-	cloning artifact	UNP Q9RKF7
C	370	HIS	-	cloning artifact	UNP Q9RKF7
C	371	HIS	-	cloning artifact	UNP Q9RKF7
D	1	MSE	-	cloning artifact	UNP Q9RKF7
D	2	SER	-	cloning artifact	UNP Q9RKF7
D	3	LEU	-	cloning artifact	UNP Q9RKF7
D	28	MSE	MET	modified residue	UNP Q9RKF7
D	29	MSE	MET	modified residue	UNP Q9RKF7
D	63	MSE	MET	modified residue	UNP Q9RKF7
D	87	MSE	MET	modified residue	UNP Q9RKF7
D	167	MSE	MET	modified residue	UNP Q9RKF7
D	195	MSE	MET	modified residue	UNP Q9RKF7
D	200	MSE	MET	modified residue	UNP Q9RKF7
D	294	MSE	MET	modified residue	UNP Q9RKF7
D	318	MSE	MET	modified residue	UNP Q9RKF7
D	329	MSE	MET	modified residue	UNP Q9RKF7
D	333	MSE	MET	modified residue	UNP Q9RKF7
D	364	GLU	-	cloning artifact	UNP Q9RKF7
D	365	GLY	-	cloning artifact	UNP Q9RKF7
D	366	HIS	-	cloning artifact	UNP Q9RKF7
D	367	HIS	-	cloning artifact	UNP Q9RKF7
D	368	HIS	-	cloning artifact	UNP Q9RKF7
D	369	HIS	-	cloning artifact	UNP Q9RKF7
D	370	HIS	-	cloning artifact	UNP Q9RKF7
D	371	HIS	-	cloning artifact	UNP Q9RKF7

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0

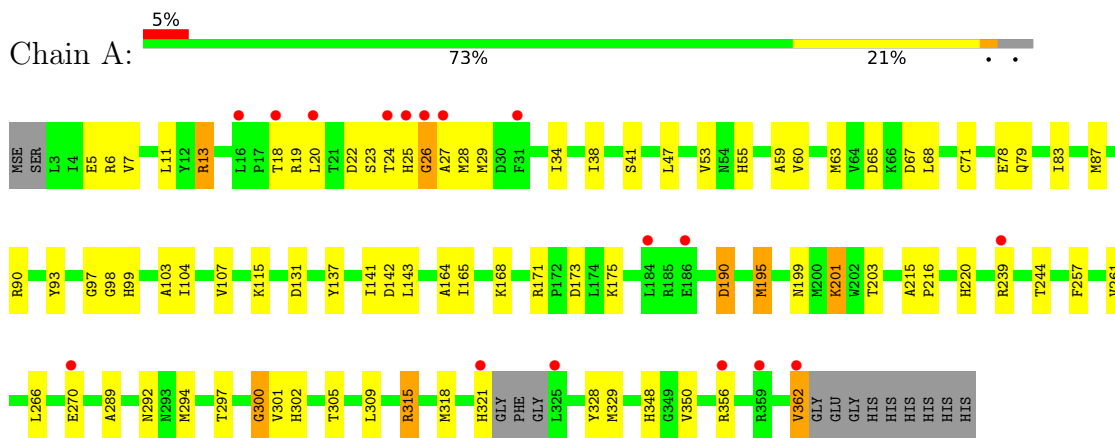
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	130	Total 130	O 130	0	0
3	B	107	Total 107	O 107	0	0
3	C	85	Total 85	O 85	0	0
3	D	75	Total 75	O 75	0	0

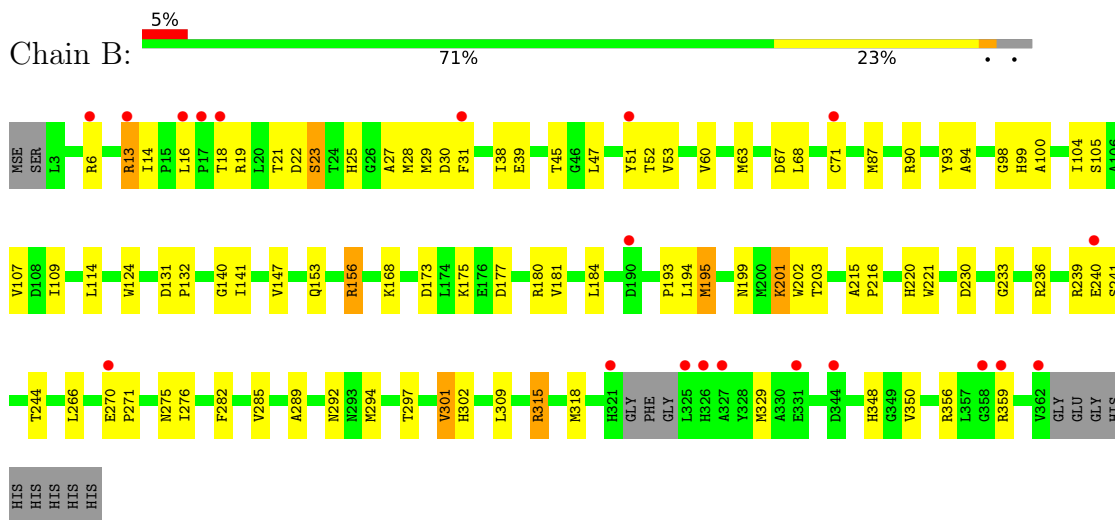
3 Residue-property plots [i](#)

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.

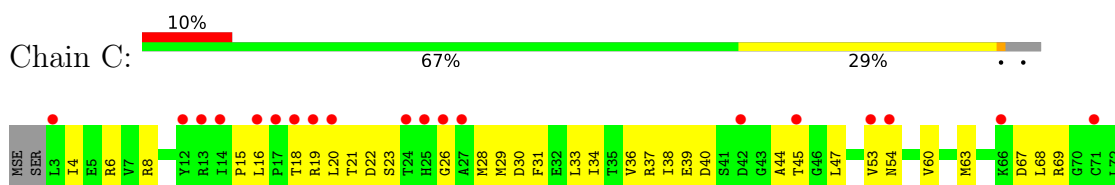
• Molecule 1: Putative racemase

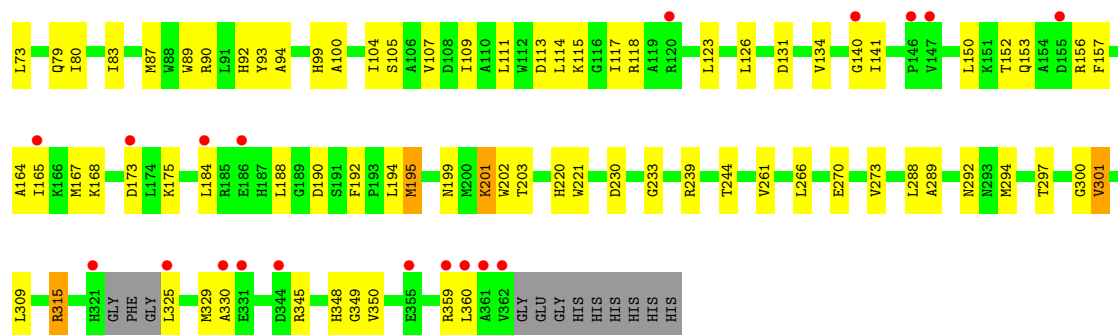


• Molecule 1: Putative racemase

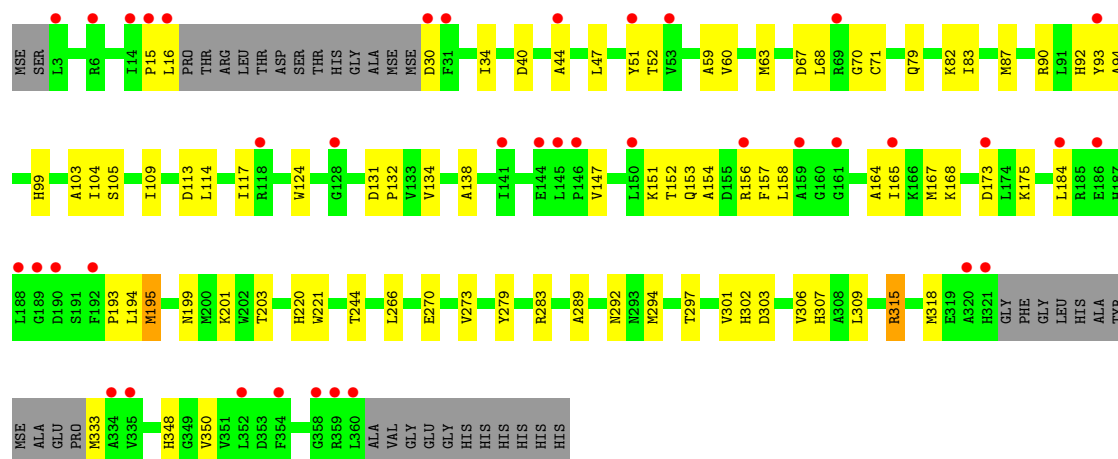


• Molecule 1: Putative racemase





● Molecule 1: Putative racemase



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	177.60Å 177.60Å 111.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.05 – 2.13 32.05 – 2.13	Depositor EDS
% Data completeness (in resolution range)	97.4 (32.05-2.13) 97.3 (32.05-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.243 0.215 , 0.243	Depositor DCC
R_{free} test set	2431 reflections (2.43%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11225	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
NA

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	0.41	0/2802	0.90	9/3794 (0.2%)
1	B	0.40	0/2802	0.91	7/3794 (0.2%)
1	C	0.37	0/2802	0.88	7/3794 (0.2%)
1	D	0.37	0/2628	0.90	5/3561 (0.1%)
All	All	0.39	0/11034	0.90	28/14943 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	THR	N-CA-C	-7.94	100.29	110.53
1	B	23	SER	N-CA-C	7.39	119.33	111.28
1	D	203	THR	N-CA-C	-7.22	100.38	110.35
1	A	201	LYS	N-CA-C	7.02	119.01	111.36
1	A	190	ASP	N-CA-C	6.98	118.53	111.07
1	C	201	LYS	N-CA-C	6.79	118.33	111.07
1	D	134	VAL	N-CA-C	6.72	115.21	107.89
1	B	201	LYS	N-CA-C	6.65	118.19	111.07
1	C	203	THR	N-CA-C	-6.52	101.14	110.59
1	B	202	TRP	N-CA-C	6.45	119.26	110.55
1	B	203	THR	N-CA-C	-6.41	101.30	110.59
1	C	202	TRP	N-CA-C	6.23	118.75	110.53
1	C	190	ASP	N-CA-C	6.21	118.13	111.36
1	D	201	LYS	N-CA-C	6.10	118.01	111.36
1	C	244	THR	N-CA-C	-6.08	100.83	109.96
1	A	65	ASP	N-CA-C	5.95	117.76	111.28
1	A	300	GLY	N-CA-C	5.74	120.12	112.65
1	A	244	THR	N-CA-C	-5.70	101.41	109.96
1	D	244	THR	N-CA-C	-5.61	101.55	109.96
1	C	134	VAL	N-CA-C	5.59	113.98	107.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	241	SER	N-CA-C	5.44	119.64	112.89
1	B	244	THR	N-CA-C	-5.31	101.99	109.96
1	A	97	GLY	N-CA-C	-5.24	104.66	111.52
1	D	92	HIS	N-CA-C	5.21	116.77	111.14
1	C	300	GLY	N-CA-C	5.13	119.33	112.65
1	A	142	ASP	N-CA-C	5.02	118.48	111.56
1	A	55	HIS	N-CA-C	5.01	116.81	109.24
1	B	240	GLU	N-CA-C	5.01	120.38	113.97

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	2749	0	2711	78	0
1	B	2749	0	2711	89	0
1	C	2749	0	2711	111	0
1	D	2577	0	2543	79	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	130	0	0	3	0
3	B	107	0	0	1	0
3	C	85	0	0	0	0
3	D	75	0	0	0	0
All	All	11225	0	10676	352	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 16.

All (352) 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:68:LEU:HD13	1:C:87:MSE:HE3	1.30	1.13
1:B:68:LEU:HD13	1:B:87:MSE:HE3	1.27	1.13
1:D:60:VAL:HA	1:D:63:MSE:HE2	1.27	1.12
1:A:13:ARG:HH11	1:A:13:ARG:HB2	1.12	1.11
1:B:60:VAL:HA	1:B:63:MSE:HE3	1.30	1.10
1:A:60:VAL:HA	1:A:63:MSE:HE2	1.25	1.10
1:D:68:LEU:HD13	1:D:87:MSE:HE3	1.14	1.09
1:A:68:LEU:HD13	1:A:87:MSE:HE3	1.32	1.08
1:D:289:ALA:HA	1:D:294:MSE:HE3	1.35	1.06
1:C:289:ALA:HA	1:C:294:MSE:HE3	1.34	1.06
1:B:194:LEU:C	1:B:195:MSE:HE3	1.83	1.03
1:A:289:ALA:HA	1:A:294:MSE:HE3	1.36	1.03
1:D:270:GLU:HG2	1:D:297:THR:HG23	1.44	0.98
1:C:60:VAL:HA	1:C:63:MSE:HE3	1.44	0.98
1:B:276:ILE:HD11	1:B:285:VAL:HG21	1.45	0.98
1:C:194:LEU:C	1:C:195:MSE:HE3	1.87	0.97
1:B:289:ALA:HA	1:B:294:MSE:HE3	1.44	0.96
1:A:292:ASN:HB2	1:A:294:MSE:HE2	1.47	0.96
1:C:195:MSE:HE2	1:C:220:HIS:HB3	1.46	0.96
1:D:292:ASN:HB2	1:D:294:MSE:HE2	1.49	0.94
1:B:348:HIS:HD2	1:B:350:VAL:H	1.12	0.94
1:A:164:ALA:HB1	1:A:195:MSE:HE1	1.51	0.92
1:C:87:MSE:HE2	1:C:104:ILE:HG12	1.53	0.91
1:C:348:HIS:HD2	1:C:350:VAL:H	1.13	0.91
1:C:19:ARG:NH1	1:C:29:MSE:HB3	1.86	0.91
1:D:348:HIS:HD2	1:D:350:VAL:H	1.20	0.90
1:B:292:ASN:HB2	1:B:294:MSE:HE2	1.55	0.89
1:B:60:VAL:HA	1:B:63:MSE:CE	2.03	0.88
1:A:13:ARG:HB2	1:A:13:ARG:NH1	1.87	0.88
1:A:87:MSE:HE1	1:A:104:ILE:HA	1.56	0.87
1:B:195:MSE:HE2	1:B:220:HIS:CB	2.04	0.87
1:A:131:ASP:HB3	1:A:315:ARG:HH22	1.38	0.87
1:D:63:MSE:HE3	1:D:103:ALA:HB2	1.57	0.87
1:A:348:HIS:HD2	1:A:350:VAL:H	1.17	0.87
1:B:87:MSE:HE1	1:B:104:ILE:HA	1.57	0.87
1:B:87:MSE:HE2	1:B:104:ILE:HG12	1.57	0.86
1:D:270:GLU:HG2	1:D:297:THR:CG2	2.06	0.85
1:B:131:ASP:HB3	1:B:315:ARG:HH22	1.43	0.84
1:C:68:LEU:HD13	1:C:87:MSE:CE	2.07	0.84
1:B:68:LEU:HD13	1:B:87:MSE:CE	2.07	0.84
1:D:87:MSE:HE2	1:D:104:ILE:HG12	1.58	0.83
1:C:131:ASP:HB3	1:C:315:ARG:HH22	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:MSE:HE3	1:A:103:ALA:HB2	1.59	0.83
1:C:292:ASN:HB2	1:C:294:MSE:HE2	1.60	0.83
1:B:348:HIS:CD2	1:B:350:VAL:H	1.99	0.81
1:B:63:MSE:HE1	1:B:99:HIS:HB3	1.63	0.81
1:A:68:LEU:HD13	1:A:87:MSE:CE	2.11	0.81
1:D:68:LEU:CD1	1:D:87:MSE:HE3	2.06	0.80
1:A:87:MSE:HE2	1:A:104:ILE:HG12	1.63	0.80
1:C:195:MSE:HE2	1:C:220:HIS:CB	2.10	0.80
1:A:60:VAL:HA	1:A:63:MSE:CE	2.10	0.79
1:B:195:MSE:HE2	1:B:220:HIS:HB3	1.63	0.79
1:D:303:ASP:HA	1:D:333:MSE:HE2	1.62	0.79
1:C:63:MSE:HE1	1:C:99:HIS:HB3	1.64	0.78
1:D:131:ASP:HB3	1:D:315:ARG:HH22	1.48	0.78
1:D:68:LEU:HD22	1:D:87:MSE:HG2	1.66	0.78
1:A:292:ASN:CB	1:A:294:MSE:HE2	2.14	0.78
1:C:289:ALA:HA	1:C:294:MSE:CE	2.14	0.78
1:B:195:MSE:CE	1:B:220:HIS:HB2	2.14	0.77
1:C:93:TYR:HH	1:D:51:TYR:HE1	1.30	0.77
1:A:22:ASP:H	1:A:26:GLY:HA2	1.50	0.76
1:B:16:LEU:HD13	1:B:30:ASP:HA	1.67	0.76
1:A:20:LEU:HD13	1:A:141:ILE:HD12	1.65	0.76
1:D:87:MSE:CE	1:D:104:ILE:HA	2.14	0.76
1:D:195:MSE:HE2	1:D:220:HIS:CB	2.16	0.75
1:C:87:MSE:HE1	1:C:104:ILE:HA	1.68	0.75
1:A:270:GLU:HG2	1:A:297:THR:CG2	2.16	0.75
1:B:87:MSE:CE	1:B:104:ILE:HA	2.17	0.74
1:C:18:THR:HG22	1:C:19:ARG:H	1.51	0.74
1:D:87:MSE:HE1	1:D:104:ILE:HA	1.68	0.74
1:A:87:MSE:CE	1:A:104:ILE:HA	2.18	0.74
1:D:292:ASN:CB	1:D:294:MSE:HE2	2.19	0.73
1:B:194:LEU:CA	1:B:195:MSE:HE3	2.18	0.73
1:D:195:MSE:HE2	1:D:220:HIS:HB3	1.70	0.73
1:C:68:LEU:CD1	1:C:87:MSE:HE3	2.14	0.73
1:A:68:LEU:CD1	1:A:87:MSE:HE3	2.14	0.73
1:B:68:LEU:CD1	1:B:87:MSE:HE3	2.12	0.72
1:D:68:LEU:HD13	1:D:87:MSE:CE	2.07	0.72
1:B:329:MSE:HE3	1:B:350:VAL:HG13	1.71	0.71
1:B:195:MSE:HE2	1:B:220:HIS:HB2	1.70	0.71
1:B:16:LEU:HD11	1:B:31:PHE:CD2	2.24	0.71
1:D:105:SER:O	1:D:109:ILE:HG12	1.91	0.71
1:B:276:ILE:CD1	1:B:285:VAL:HG21	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:MSE:HE3	1:C:350:VAL:HG13	1.72	0.71
1:B:14:ILE:HD12	1:B:31:PHE:HE1	1.55	0.71
1:A:13:ARG:HH11	1:A:13:ARG:CB	1.98	0.69
1:A:63:MSE:HE1	1:A:99:HIS:O	1.93	0.69
1:C:194:LEU:CA	1:C:195:MSE:HE3	2.23	0.69
1:B:13:ARG:HG3	1:B:13:ARG:HH11	1.57	0.69
1:C:348:HIS:CD2	1:C:350:VAL:H	2.05	0.68
1:B:28:MSE:HG2	1:B:53:VAL:CG1	2.23	0.68
1:D:60:VAL:HA	1:D:63:MSE:CE	2.15	0.68
1:B:28:MSE:HG2	1:B:53:VAL:HG11	1.76	0.68
1:B:173:ASP:OD2	1:B:175:LYS:HB3	1.94	0.68
1:D:194:LEU:CA	1:D:195:MSE:HE3	2.24	0.67
1:C:18:THR:HG22	1:C:19:ARG:N	2.08	0.67
1:B:14:ILE:HD12	1:B:31:PHE:CE1	2.28	0.67
1:C:63:MSE:HE1	1:C:99:HIS:CB	2.24	0.67
1:B:195:MSE:CE	1:B:220:HIS:CB	2.71	0.66
1:B:194:LEU:N	1:B:195:MSE:HE3	2.11	0.66
1:D:194:LEU:N	1:D:195:MSE:HE3	2.11	0.66
1:B:194:LEU:C	1:B:195:MSE:CE	2.67	0.66
1:B:47:LEU:O	1:B:348:HIS:HE1	1.78	0.65
1:A:270:GLU:HG2	1:A:297:THR:HG23	1.76	0.65
1:C:173:ASP:OD2	1:C:175:LYS:HB3	1.96	0.65
1:A:11:LEU:HG	1:A:362:VAL:HG13	1.79	0.65
1:A:23:SER:OG	1:A:201:LYS:HB2	1.96	0.65
1:A:137:TYR:HB2	1:A:195:MSE:HE3	1.78	0.65
1:A:168:LYS:NZ	1:A:199:ASN:HD21	1.94	0.65
1:A:87:MSE:CE	1:A:104:ILE:HG12	2.27	0.65
1:D:194:LEU:C	1:D:195:MSE:HE3	2.22	0.65
1:C:87:MSE:CE	1:C:104:ILE:HA	2.26	0.64
1:C:131:ASP:HB3	1:C:315:ARG:NH2	2.11	0.64
1:C:36:VAL:HG12	1:C:38:ILE:CD1	2.28	0.64
1:C:195:MSE:CE	1:C:220:HIS:CB	2.76	0.64
1:A:348:HIS:CD2	1:A:350:VAL:H	2.08	0.64
1:B:67:ASP:O	1:B:90:ARG:HD3	1.98	0.64
1:A:165:ILE:C	1:A:195:MSE:HE2	2.23	0.64
1:D:67:ASP:O	1:D:90:ARG:HD3	1.98	0.64
1:C:60:VAL:CA	1:C:63:MSE:HE3	2.24	0.64
1:C:270:GLU:HG3	1:C:297:THR:HG23	1.80	0.64
1:A:20:LEU:HB3	1:A:141:ILE:HB	1.80	0.63
1:D:279:TYR:O	1:D:283:ARG:HG3	1.97	0.63
1:B:270:GLU:HG2	1:B:297:THR:CG2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HG	1:A:362:VAL:CG1	2.28	0.63
1:D:109:ILE:HD11	1:D:273:VAL:HG22	1.80	0.62
1:D:113:ASP:O	1:D:117:ILE:HG12	1.99	0.62
1:C:109:ILE:HD11	1:C:273:VAL:HG22	1.82	0.62
1:D:302:HIS:CD2	1:D:333:MSE:HE3	2.35	0.62
1:C:105:SER:O	1:C:109:ILE:HG12	2.00	0.61
1:C:93:TYR:OH	1:D:51:TYR:HE1	1.81	0.61
1:C:194:LEU:N	1:C:195:MSE:HE3	2.16	0.61
1:C:36:VAL:HG12	1:C:38:ILE:HD11	1.83	0.61
1:A:300:GLY:HA2	1:A:321:HIS:HE1	1.64	0.61
1:B:292:ASN:CB	1:B:294:MSE:HE2	2.29	0.61
1:D:193:PRO:C	1:D:195:MSE:HE3	2.25	0.61
1:A:47:LEU:O	1:A:348:HIS:HE1	1.85	0.59
1:C:141:ILE:N	1:C:141:ILE:HD12	2.16	0.59
1:D:195:MSE:HE2	1:D:220:HIS:HB2	1.84	0.59
1:D:173:ASP:OD1	1:D:175:LYS:HB3	2.02	0.59
1:D:348:HIS:CD2	1:D:350:VAL:H	2.12	0.59
1:A:309:LEU:O	1:A:315:ARG:HG2	2.03	0.59
1:B:195:MSE:HE3	1:B:195:MSE:N	2.16	0.59
1:C:26:GLY:HA2	1:C:28:MSE:HE2	1.84	0.59
1:C:315:ARG:HD2	1:C:315:ARG:O	2.02	0.58
1:B:18:THR:O	1:B:19:ARG:HB2	2.03	0.58
1:D:147:VAL:O	1:D:151:LYS:HG3	2.04	0.58
1:B:153:GLN:HG3	1:B:156:ARG:HH12	1.69	0.58
1:B:87:MSE:CE	1:B:104:ILE:HG12	2.32	0.58
1:A:131:ASP:HB3	1:A:315:ARG:NH2	2.14	0.57
1:C:34:ILE:N	1:C:34:ILE:HD12	2.19	0.57
1:C:292:ASN:CB	1:C:294:MSE:HE2	2.31	0.57
1:B:289:ALA:HA	1:B:294:MSE:CE	2.27	0.57
1:C:118:ARG:HG2	1:C:118:ARG:HH11	1.70	0.57
1:C:195:MSE:HE3	1:C:195:MSE:N	2.19	0.57
1:D:47:LEU:O	1:D:348:HIS:HE1	1.87	0.57
1:C:40:ASP:OD2	1:C:118:ARG:HD2	2.05	0.56
1:C:69:ARG:HH11	1:C:73:LEU:HD11	1.69	0.56
1:A:292:ASN:HB2	1:A:294:MSE:CE	2.30	0.56
1:C:309:LEU:O	1:C:315:ARG:HG2	2.06	0.56
1:D:154:ALA:O	1:D:158:LEU:HG	2.05	0.56
1:B:23:SER:OG	1:B:201:LYS:HB2	2.06	0.56
1:D:79:GLN:O	1:D:83:ILE:HG12	2.05	0.55
1:C:79:GLN:O	1:C:83:ILE:HG12	2.07	0.55
1:C:325:LEU:N	1:C:325:LEU:HD12	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:405:HOH:O	1:B:25:HIS:HE1	1.89	0.55
1:B:22:ASP:OD2	1:B:25:HIS:HD2	1.89	0.55
1:C:195:MSE:CE	1:C:220:HIS:HB2	2.37	0.55
1:C:168:LYS:HD2	1:C:199:ASN:ND2	2.22	0.55
1:C:194:LEU:C	1:C:195:MSE:CE	2.73	0.55
1:B:131:ASP:HB3	1:B:315:ARG:NH2	2.20	0.54
1:D:193:PRO:C	1:D:195:MSE:CE	2.81	0.54
1:B:21:THR:N	1:B:141:ILE:HG22	2.23	0.54
1:C:6:ARG:CZ	1:C:8:ARG:HD3	2.38	0.54
1:B:13:ARG:HG3	1:B:13:ARG:NH1	2.21	0.53
1:D:15:PRO:O	1:D:16:LEU:C	2.51	0.53
1:C:22:ASP:H	1:C:26:GLY:HA3	1.73	0.53
1:D:303:ASP:HA	1:D:333:MSE:CE	2.35	0.53
1:B:195:MSE:HE1	1:B:220:HIS:HB2	1.90	0.53
1:A:7:VAL:HG13	1:A:38:ILE:CD1	2.39	0.53
1:C:19:ARG:CZ	1:C:29:MSE:HB3	2.37	0.53
1:D:194:LEU:C	1:D:195:MSE:CE	2.82	0.53
1:A:220:HIS:HE1	3:A:440:HOH:O	1.91	0.53
1:C:47:LEU:O	1:C:348:HIS:HE1	1.92	0.53
1:C:195:MSE:CE	1:C:220:HIS:HB3	2.30	0.52
1:D:315:ARG:HD2	1:D:315:ARG:O	2.08	0.52
1:B:309:LEU:O	1:B:315:ARG:HG2	2.09	0.52
1:B:87:MSE:SE	1:B:107:VAL:HG11	2.59	0.52
1:B:141:ILE:N	1:B:141:ILE:HD12	2.25	0.52
1:C:80:ILE:N	1:C:80:ILE:HD12	2.25	0.52
1:D:63:MSE:HE1	1:D:99:HIS:C	2.35	0.52
1:A:87:MSE:SE	1:A:107:VAL:HG11	2.60	0.52
1:B:105:SER:O	1:B:109:ILE:HG13	2.10	0.51
1:C:37:ARG:C	1:C:38:ILE:HD12	2.35	0.51
1:C:315:ARG:HG2	1:C:315:ARG:HH11	1.76	0.51
1:B:51:TYR:N	1:B:51:TYR:CD2	2.77	0.51
1:D:157:PHE:HB3	1:D:165:ILE:HD11	1.92	0.51
1:D:315:ARG:HG2	1:D:315:ARG:HH11	1.74	0.51
1:C:21:THR:N	1:C:141:ILE:HG22	2.26	0.51
1:C:345:ARG:NH1	1:C:349:GLY:O	2.43	0.51
1:C:16:LEU:HG	1:C:30:ASP:HA	1.92	0.51
1:D:195:MSE:CE	1:D:220:HIS:CB	2.87	0.51
1:B:21:THR:HG22	1:B:27:ALA:HA	1.92	0.51
1:B:71:CYS:SG	1:B:90:ARG:HD2	2.51	0.50
1:D:114:LEU:C	1:D:114:LEU:HD23	2.36	0.50
1:A:71:CYS:SG	1:A:90:ARG:HD2	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:MSE:HE1	1:D:99:HIS:O	2.11	0.50
1:A:143:LEU:HD11	1:A:171:ARG:HG2	1.93	0.50
1:D:195:MSE:CE	1:D:220:HIS:HB2	2.42	0.49
1:A:34:ILE:N	1:A:34:ILE:HD12	2.27	0.49
1:B:124:TRP:CH2	1:B:132:PRO:HD3	2.47	0.49
1:D:70:GLY:HA3	1:D:90:ARG:HH12	1.77	0.49
1:C:150:LEU:HG	1:C:184:LEU:HD21	1.94	0.49
1:C:114:LEU:HD23	1:C:118:ARG:HG3	1.94	0.49
1:C:167:MSE:SE	1:C:184:LEU:HD22	2.63	0.49
1:A:67:ASP:O	1:A:90:ARG:HD3	2.12	0.49
1:C:80:ILE:HD13	1:C:115:LYS:HE2	1.94	0.49
1:D:16:LEU:HD12	1:D:16:LEU:H	1.77	0.49
1:D:309:LEU:O	1:D:315:ARG:HG2	2.12	0.49
1:A:266:LEU:C	1:A:266:LEU:HD12	2.38	0.48
1:D:138:ALA:HB3	1:D:165:ILE:CD1	2.43	0.48
1:B:63:MSE:HE1	1:B:99:HIS:CB	2.40	0.48
1:C:38:ILE:HD12	1:C:38:ILE:N	2.28	0.48
1:A:79:GLN:O	1:A:83:ILE:HG12	2.14	0.48
1:C:348:HIS:CD2	1:C:350:VAL:HB	2.48	0.48
1:A:63:MSE:HE1	1:A:99:HIS:C	2.39	0.48
1:D:87:MSE:HE2	1:D:104:ILE:HA	1.94	0.48
1:D:93:TYR:O	1:D:94:ALA:HB3	2.14	0.48
1:B:16:LEU:HD11	1:B:31:PHE:CE2	2.48	0.48
1:C:23:SER:HB2	1:C:201:LYS:HB2	1.96	0.48
1:A:165:ILE:O	1:A:195:MSE:HE2	2.15	0.47
1:C:53:VAL:O	1:C:54:ASN:HB2	2.14	0.47
1:A:5:GLU:O	1:A:6:ARG:HG3	2.14	0.47
1:A:78:GLU:OE1	1:A:115:LYS:NZ	2.48	0.47
1:D:168:LYS:HD2	1:D:199:ASN:ND2	2.29	0.47
1:C:18:THR:CG2	1:C:19:ARG:N	2.78	0.47
1:A:98:GLY:HA3	1:B:98:GLY:HA3	1.97	0.47
1:B:270:GLU:HG2	1:B:297:THR:HG23	1.95	0.47
1:C:18:THR:CG2	1:C:19:ARG:H	2.23	0.47
1:C:168:LYS:NZ	1:C:199:ASN:HD21	2.13	0.47
1:A:173:ASP:OD1	1:A:175:LYS:HB3	2.14	0.46
1:A:164:ALA:CB	1:A:195:MSE:HE1	2.35	0.46
1:B:266:LEU:C	1:B:266:LEU:HD12	2.40	0.46
1:C:113:ASP:O	1:C:117:ILE:HG13	2.15	0.46
1:A:315:ARG:HD2	1:A:315:ARG:O	2.16	0.46
1:D:164:ALA:O	1:D:165:ILE:HD13	2.16	0.46
1:A:53:VAL:O	1:A:53:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:TYR:O	1:C:94:ALA:HB3	2.16	0.46
1:B:230:ASP:OD2	1:B:233:GLY:HA3	2.16	0.45
1:D:15:PRO:HA	1:D:30:ASP:HB3	1.98	0.45
1:D:153:GLN:HG2	1:D:157:PHE:CE2	2.52	0.45
1:C:80:ILE:CD1	1:C:115:LYS:HE2	2.47	0.45
1:D:131:ASP:HB3	1:D:315:ARG:NH2	2.23	0.45
1:C:164:ALA:O	1:C:165:ILE:HD13	2.16	0.45
1:C:188:LEU:HD13	1:C:192:PHE:CD2	2.52	0.45
1:D:16:LEU:H	1:D:16:LEU:CD1	2.29	0.45
1:D:71:CYS:SG	1:D:90:ARG:HD2	2.56	0.45
1:C:80:ILE:HG13	1:C:111:LEU:HB3	1.98	0.45
1:C:359:ARG:HH12	1:C:360:LEU:HD21	1.82	0.45
1:C:153:GLN:HA	1:C:156:ARG:CZ	2.47	0.45
1:B:38:ILE:O	1:B:45:THR:HA	2.17	0.44
1:D:168:LYS:HD2	1:D:199:ASN:HD21	1.83	0.44
1:D:194:LEU:N	1:D:195:MSE:CE	2.78	0.44
1:C:301:VAL:HG23	1:C:301:VAL:O	2.17	0.44
1:A:266:LEU:HD12	1:A:266:LEU:O	2.17	0.44
1:D:309:LEU:HD12	1:D:318:MSE:HB2	1.99	0.44
1:A:168:LYS:HZ2	1:A:199:ASN:HD21	1.66	0.44
1:A:13:ARG:HH12	1:A:362:VAL:HG11	1.83	0.44
1:D:315:ARG:HD2	1:D:315:ARG:C	2.42	0.44
1:A:239:ARG:HD3	3:A:479:HOH:O	2.17	0.44
1:C:266:LEU:HD12	1:C:266:LEU:C	2.43	0.44
1:A:5:GLU:OE2	1:A:41:SER:HA	2.17	0.44
1:C:20:LEU:HB3	1:C:141:ILE:CG2	2.48	0.44
1:A:329:MSE:HE3	1:A:350:VAL:HG13	2.00	0.43
1:C:315:ARG:HD2	1:C:315:ARG:C	2.42	0.43
1:A:168:LYS:HD2	1:A:199:ASN:ND2	2.33	0.43
1:C:80:ILE:HD13	1:C:115:LYS:CE	2.48	0.43
1:C:19:ARG:HH12	1:C:29:MSE:HB3	1.80	0.43
1:B:271:PRO:HG2	1:B:282:PHE:CE1	2.54	0.43
1:C:140:GLY:C	1:C:141:ILE:HD12	2.43	0.43
1:C:261:VAL:HG11	1:C:292:ASN:ND2	2.33	0.43
1:A:5:GLU:C	1:A:6:ARG:HG3	2.43	0.43
1:C:152:THR:HG22	1:C:156:ARG:NH1	2.34	0.43
1:D:34:ILE:N	1:D:34:ILE:HD12	2.33	0.43
1:A:165:ILE:N	1:A:195:MSE:HE2	2.33	0.43
1:C:118:ARG:HG2	1:C:118:ARG:NH1	2.32	0.43
1:D:59:ALA:O	1:D:63:MSE:HG3	2.18	0.43
1:A:19:ARG:CZ	1:A:29:MSE:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLY:O	1:A:28:MSE:N	2.52	0.42
1:B:236:ARG:HA	1:B:239:ARG:HH11	1.83	0.42
1:C:67:ASP:O	1:C:90:ARG:HD3	2.19	0.42
1:D:167:MSE:SE	1:D:184:LEU:HD23	2.69	0.42
1:B:6:ARG:HB2	1:B:39:GLU:HB3	2.00	0.42
1:D:221:TRP:CD1	1:D:221:TRP:C	2.97	0.42
1:B:93:TYR:O	1:B:94:ALA:HB3	2.19	0.42
1:C:168:LYS:HD2	1:C:199:ASN:HD21	1.84	0.42
1:A:18:THR:HG22	1:A:19:ARG:N	2.34	0.42
1:C:23:SER:CB	1:C:201:LYS:HB2	2.49	0.42
1:D:306:VAL:HG13	1:D:307:HIS:N	2.34	0.42
1:C:16:LEU:HD21	1:C:31:PHE:CD2	2.55	0.42
1:C:21:THR:HA	1:C:26:GLY:O	2.20	0.42
1:B:194:LEU:N	1:B:195:MSE:CE	2.79	0.42
1:C:150:LEU:HG	1:C:184:LEU:HD11	2.02	0.42
1:D:40:ASP:OD2	1:D:44:ALA:HB3	2.18	0.42
1:A:328:TYR:CD1	1:A:356:ARG:NH1	2.88	0.42
1:B:168:LYS:NZ	1:B:199:ASN:HD21	2.18	0.42
1:C:38:ILE:O	1:C:45:THR:HA	2.20	0.42
1:C:39:GLU:HA	1:C:44:ALA:O	2.20	0.41
1:A:215:ALA:N	1:A:216:PRO:CD	2.83	0.41
1:C:93:TYR:CE2	1:D:52:THR:HA	2.55	0.41
1:C:230:ASP:OD2	1:C:233:GLY:HA3	2.20	0.41
1:A:300:GLY:HA2	1:A:321:HIS:CE1	2.51	0.41
1:B:193:PRO:C	1:B:195:MSE:CE	2.94	0.41
1:B:215:ALA:N	1:B:216:PRO:CD	2.83	0.41
1:B:301:VAL:HG23	1:B:301:VAL:O	2.20	0.41
1:C:4:ILE:HG23	1:C:38:ILE:HG23	2.03	0.41
1:C:221:TRP:CD1	1:C:221:TRP:C	2.99	0.41
1:A:19:ARG:HA	1:A:19:ARG:HD3	1.84	0.41
1:C:15:PRO:HA	1:C:30:ASP:HB3	2.02	0.41
1:D:152:THR:HG22	1:D:156:ARG:NH1	2.35	0.41
1:B:63:MSE:SE	1:B:100:ALA:HA	2.71	0.41
1:B:275:ASN:OD1	1:B:275:ASN:C	2.63	0.41
1:C:87:MSE:SE	1:C:107:VAL:HG11	2.71	0.41
1:A:302:HIS:HA	1:A:305:THR:HB	2.03	0.41
1:B:23:SER:CB	1:B:201:LYS:HB2	2.51	0.41
1:B:195:MSE:CE	1:B:195:MSE:N	2.83	0.41
1:C:123:LEU:HD23	1:C:126:LEU:HD23	2.02	0.41
1:C:157:PHE:CD2	1:C:165:ILE:HD12	2.56	0.41
1:B:276:ILE:O	1:B:276:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ARG:CZ	1:C:239:ARG:HB3	2.51	0.41
1:D:266:LEU:C	1:D:266:LEU:HD12	2.46	0.41
1:A:257:PHE:O	1:A:261:VAL:HG23	2.21	0.41
1:B:140:GLY:C	1:B:141:ILE:HD12	2.45	0.41
1:B:184:LEU:HD12	1:B:184:LEU:HA	1.78	0.41
1:B:177:ASP:O	1:B:181:VAL:HG23	2.21	0.41
1:B:220:HIS:O	1:B:221:TRP:HB3	2.21	0.40
1:C:63:MSE:SE	1:C:100:ALA:HA	2.71	0.40
1:A:25:HIS:O	1:A:26:GLY:C	2.62	0.40
1:A:93:TYR:CE2	1:B:52:THR:HA	2.56	0.40
1:B:13:ARG:NH1	1:B:13:ARG:CG	2.84	0.40
1:B:220:HIS:HE1	3:B:480:HOH:O	2.04	0.40
1:D:124:TRP:CH2	1:D:132:PRO:HD3	2.57	0.40
1:A:59:ALA:O	1:A:63:MSE:HG3	2.22	0.40
1:A:68:LEU:HD22	1:A:87:MSE:HG2	2.04	0.40
1:B:147:VAL:HG22	1:B:180:ARG:HG2	2.03	0.40
1:C:33:LEU:HD13	1:C:325:LEU:HD21	2.02	0.40
1:A:309:LEU:HD12	1:A:318:MSE:SE	2.72	0.40
1:B:302:HIS:HB2	1:B:318:MSE:HE3	2.03	0.40
1:B:356:ARG:O	1:B:359:ARG:HB3	2.22	0.40
1:C:69:ARG:NH1	1:C:73:LEU:HD11	2.36	0.40
1:C:89:TRP:HA	1:C:92:HIS:HB2	2.04	0.40
1:D:157:PHE:CD2	1:D:165:ILE:HD12	2.57	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	353/371 (95%)	340 (96%)	10 (3%)	3 (1%)	16 9
1	B	353/371 (95%)	338 (96%)	14 (4%)	1 (0%)	36 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	353/371 (95%)	336 (95%)	15 (4%)	2 (1%)	21	15
1	D	328/371 (88%)	314 (96%)	13 (4%)	1 (0%)	36	33
All	All	1387/1484 (94%)	1328 (96%)	52 (4%)	7 (0%)	24	19

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	GLY
1	A	27	ALA
1	C	330	ALA
1	C	301	VAL
1	A	301	VAL
1	D	301	VAL
1	B	301	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	283/281 (101%)	277 (98%)	6 (2%)	47	51
1	B	283/281 (101%)	277 (98%)	6 (2%)	47	51
1	C	283/281 (101%)	280 (99%)	3 (1%)	65	71
1	D	265/281 (94%)	262 (99%)	3 (1%)	65	71
All	All	1114/1124 (99%)	1096 (98%)	18 (2%)	55	61

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	24	THR
1	A	190	ASP
1	A	195	MSE
1	A	315	ARG

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Mol	Chain	Res	Type
1	A	362	VAL
1	B	13	ARG
1	B	29	MSE
1	B	114	LEU
1	B	156	ARG
1	B	195	MSE
1	B	315	ARG
1	C	195	MSE
1	C	288	LEU
1	C	315	ARG
1	D	82	LYS
1	D	195	MSE
1	D	315	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	199	ASN
1	A	220	HIS
1	A	348	HIS
1	B	25	HIS
1	B	55	HIS
1	B	199	ASN
1	B	292	ASN
1	B	348	HIS
1	C	54	ASN
1	C	153	GLN
1	C	199	ASN
1	C	252	HIS
1	C	258	HIS
1	C	292	ASN
1	C	348	HIS
1	D	54	ASN
1	D	187	HIS
1	D	199	ASN
1	D	292	ASN
1	D	302	HIS
1	D	348	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	346/371 (93%)	0.24	17 (4%) 35 40	15, 25, 46, 64	0
1	B	346/371 (93%)	0.28	20 (5%) 29 33	16, 27, 46, 59	0
1	C	346/371 (93%)	0.68	38 (10%) 10 12	20, 35, 55, 65	0
1	D	326/371 (87%)	0.71	39 (11%) 9 10	19, 33, 52, 61	0
All	All	1364/1484 (91%)	0.47	114 (8%) 17 19	15, 30, 51, 65	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	25	HIS	7.9
1	D	16	LEU	7.2
1	A	25	HIS	6.1
1	B	31	PHE	5.6
1	D	51	TYR	5.2
1	A	26	GLY	5.1
1	D	31	PHE	5.0
1	C	26	GLY	5.0
1	D	320	ALA	4.7
1	D	321	HIS	4.5
1	C	321	HIS	4.4
1	C	362	VAL	4.4
1	A	321	HIS	4.3
1	D	145	LEU	4.3
1	D	128	GLY	4.2
1	A	27	ALA	4.2
1	D	165	ILE	4.1
1	C	27	ALA	3.9
1	C	330	ALA	3.9
1	D	359	ARG	3.7
1	D	141	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	335	VAL	3.4
1	C	3	LEU	3.4
1	C	360	LEU	3.4
1	C	24	THR	3.3
1	A	362	VAL	3.3
1	B	325	LEU	3.3
1	D	53	VAL	3.2
1	C	325	LEU	3.2
1	A	24	THR	3.2
1	C	186	GLU	3.2
1	D	144	GLU	3.1
1	D	360	LEU	3.1
1	B	362	VAL	3.0
1	C	359	ARG	3.0
1	B	17	PRO	3.0
1	D	334	ALA	2.9
1	A	18	THR	2.9
1	B	190	ASP	2.9
1	D	146	PRO	2.9
1	D	358	GLY	2.9
1	D	156	ARG	2.8
1	A	325	LEU	2.8
1	D	159	ALA	2.8
1	D	188	LEU	2.8
1	B	6	ARG	2.7
1	A	186	GLU	2.7
1	B	344	ASP	2.7
1	B	16	LEU	2.7
1	C	361	ALA	2.6
1	A	31	PHE	2.6
1	D	161	GLY	2.6
1	D	15	PRO	2.6
1	D	184	LEU	2.6
1	D	30	ASP	2.6
1	A	356	ARG	2.6
1	C	53	VAL	2.6
1	C	17	PRO	2.6
1	B	270	GLU	2.6
1	C	18	THR	2.6
1	D	14	ILE	2.5
1	C	45	THR	2.5
1	B	71	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	327	ALA	2.5
1	C	184	LEU	2.5
1	D	190	ASP	2.4
1	B	51	TYR	2.4
1	C	71	CYS	2.4
1	D	3	LEU	2.4
1	A	270	GLU	2.4
1	D	352	LEU	2.4
1	C	331	GLU	2.4
1	C	173	ASP	2.4
1	D	173	ASP	2.4
1	D	354	PHE	2.4
1	B	359	ARG	2.4
1	C	344	ASP	2.3
1	C	16	LEU	2.3
1	C	19	ARG	2.3
1	D	118	ARG	2.3
1	B	321	HIS	2.3
1	C	14	ILE	2.3
1	C	155	ASP	2.3
1	C	54	ASN	2.3
1	D	44	ALA	2.3
1	D	150	LEU	2.3
1	A	16	LEU	2.2
1	C	12	TYR	2.2
1	A	239	ARG	2.2
1	B	358	GLY	2.2
1	A	184	LEU	2.2
1	C	120	ARG	2.2
1	C	66	LYS	2.2
1	C	146	PRO	2.2
1	C	42	ASP	2.2
1	D	93	TYR	2.2
1	B	240	GLU	2.1
1	C	165	ILE	2.1
1	A	359	ARG	2.1
1	B	13	ARG	2.1
1	C	147	VAL	2.1
1	D	69	ARG	2.1
1	D	192	PHE	2.1
1	C	355	GLU	2.1
1	D	189	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	331	GLU	2.0
1	C	20	LEU	2.0
1	C	13	ARG	2.0
1	D	6	ARG	2.0
1	B	326	HIS	2.0
1	C	140	GLY	2.0
1	D	186	GLU	2.0
1	A	20	LEU	2.0
1	B	18	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	D	400	1/1	0.82	0.10	46,46,46,46	0
2	NA	A	400	1/1	0.88	0.14	48,48,48,48	0
2	NA	C	400	1/1	0.90	0.10	48,48,48,48	0
2	NA	B	400	1/1	0.90	0.09	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.