



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:04 PM UTC

PDB ID : 1R52 / pdb_00001r52
Title : Crystal structure of the bifunctional chorismate synthase from *Saccharomyces cerevisiae*
Authors : Quevillon-Cheruel, S.; Leulliot, N.; Meyer, P.; Graille, M.; Bremang, M.; Blondeau, K.; Sorel, I.; Poupon, A.; Janin, J.; van Tilbeurgh, H.
Deposited on : 2003-10-09
Resolution : 2.89 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

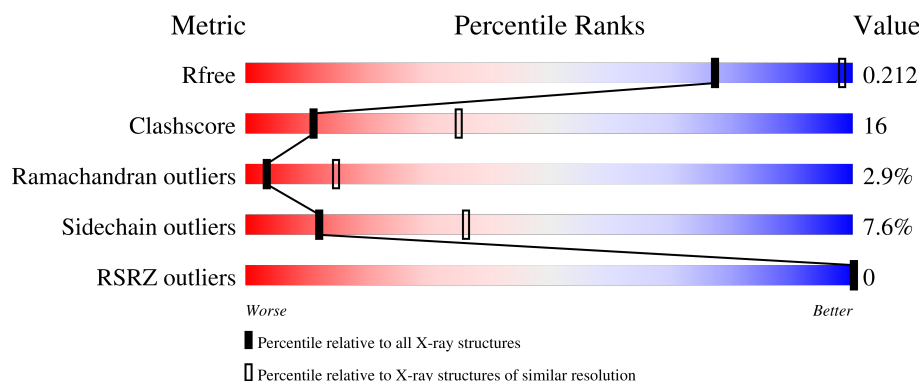
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 $\leq 5\%$. 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	382	
1	B	382	
1	C	382	
1	D	382	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8636 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 Chorismate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	45	0	0
			2138	1347	371	405	15			
1	B	282	Total	C	N	O	S	44	0	0
			2130	1340	373	402	15			
1	C	283	Total	C	N	O	S	46	0	0
			2139	1345	374	405	15			
1	D	282	Total	C	N	O	S	41	0	0
			2131	1341	373	402	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	377	HIS	-	expression tag	UNP P28777
A	378	HIS	-	expression tag	UNP P28777
A	379	HIS	-	expression tag	UNP P28777
A	380	HIS	-	expression tag	UNP P28777
A	381	HIS	-	expression tag	UNP P28777
A	382	HIS	-	expression tag	UNP P28777
B	377	HIS	-	expression tag	UNP P28777
B	378	HIS	-	expression tag	UNP P28777
B	379	HIS	-	expression tag	UNP P28777
B	380	HIS	-	expression tag	UNP P28777
B	381	HIS	-	expression tag	UNP P28777
B	382	HIS	-	expression tag	UNP P28777
C	377	HIS	-	expression tag	UNP P28777
C	378	HIS	-	expression tag	UNP P28777
C	379	HIS	-	expression tag	UNP P28777
C	380	HIS	-	expression tag	UNP P28777
C	381	HIS	-	expression tag	UNP P28777
C	382	HIS	-	expression tag	UNP P28777
D	377	HIS	-	expression tag	UNP P28777
D	378	HIS	-	expression tag	UNP P28777
D	379	HIS	-	expression tag	UNP P28777

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Chain	Residue	Modelled	Actual	Comment	Reference
D	380	HIS	-	expression tag	UNP P28777
D	381	HIS	-	expression tag	UNP P28777
D	382	HIS	-	expression tag	UNP P28777

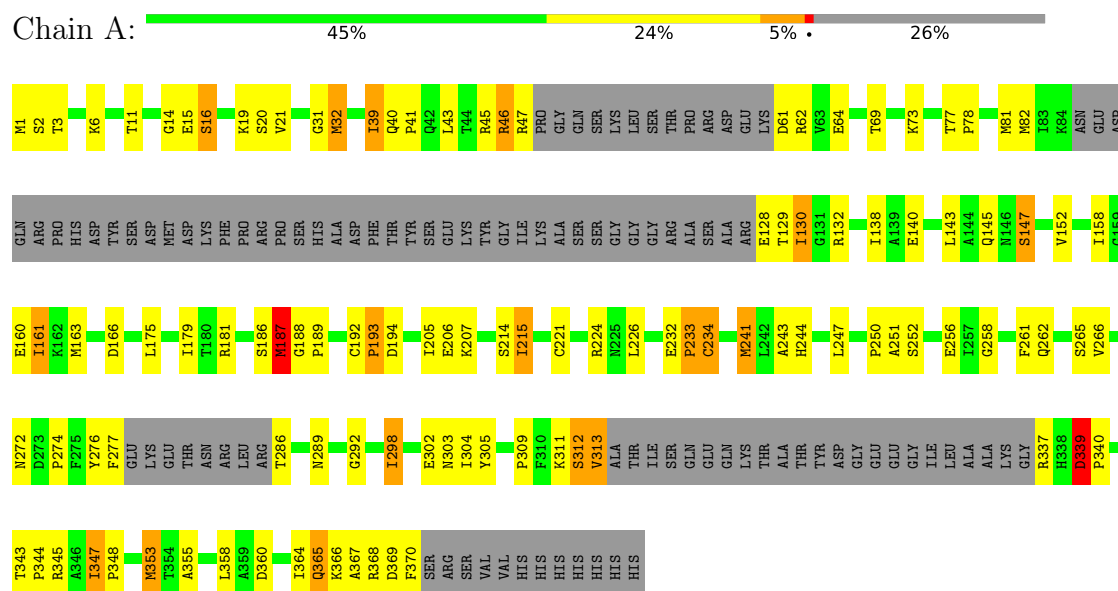
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	25	Total	O	0	0
			25	25		
2	B	26	Total	O	0	0
			26	26		
2	C	27	Total	O	0	0
			27	27		
2	D	20	Total	O	0	0
			20	20		

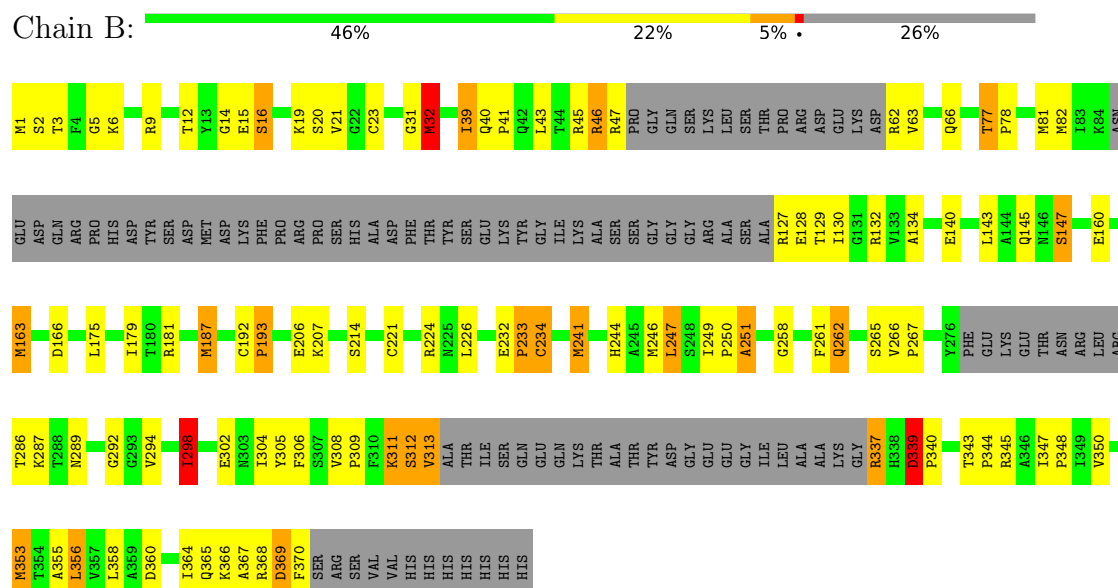
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

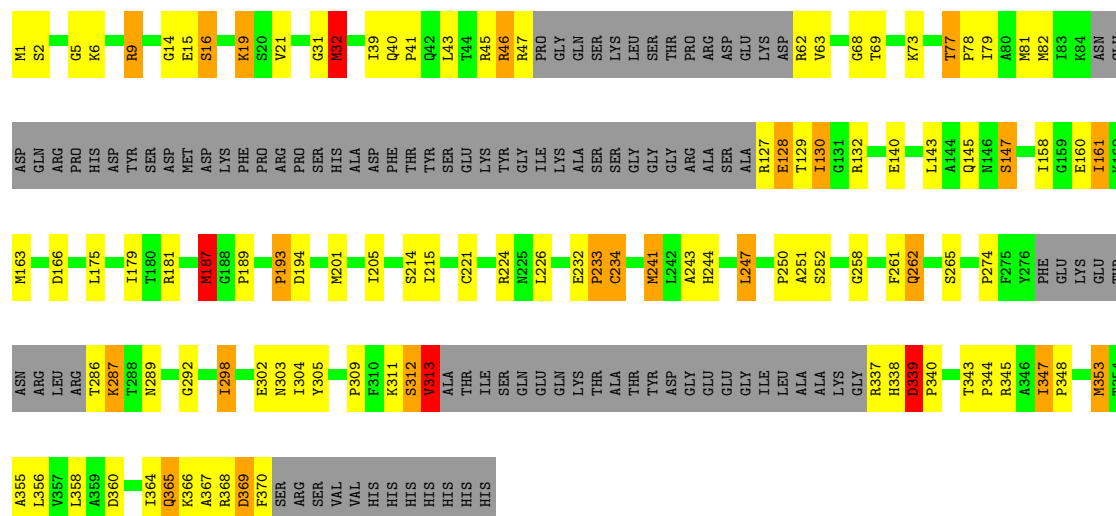
• Molecule 1: Chorismate synthase



• Molecule 1: Chorismate synthase



Chain C: 48% 19% 6% 26%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.82Å 75.60Å 91.33Å 114.44° 108.43° 89.98°	Depositor
Resolution (Å)	29.75 – 2.89 29.75 – 2.89	Depositor EDS
% Data completeness (in resolution range)	89.6 (29.75-2.89) 89.7 (29.75-2.89)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.52 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.188 , 0.224 0.176 , 0.212	Depositor DCC
R_{free} test set	1344 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-h-l 0.467 for -h,k,-k-l 0.467 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8636	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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	1.45	16/2172 (0.7%)	1.27	8/2927 (0.3%)
1	B	1.43	18/2163 (0.8%)	1.28	11/2914 (0.4%)
1	C	1.46	14/2173 (0.6%)	1.36	13/2928 (0.4%)
1	D	1.45	14/2165 (0.6%)	1.30	14/2917 (0.5%)
All	All	1.45	62/8673 (0.7%)	1.30	46/11686 (0.4%)

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	286	THR	CB-OG1	13.89	1.66	1.43
1	A	187	MET	SD-CE	11.52	2.08	1.79
1	D	187	MET	SD-CE	11.43	2.08	1.79
1	B	353	MET	SD-CE	-11.14	1.51	1.79
1	D	19	LYS	C-O	-11.12	1.11	1.24
1	C	19	LYS	C-O	-10.85	1.11	1.24
1	C	61	ASP	CB-CG	-10.67	1.25	1.52
1	A	353	MET	SD-CE	-10.54	1.53	1.79
1	C	187	MET	SD-CE	10.42	2.05	1.79
1	D	353	MET	SD-CE	-9.96	1.54	1.79
1	D	286	THR	CB-OG1	9.42	1.58	1.43
1	C	353	MET	SD-CE	-9.40	1.56	1.79
1	C	313	VAL	CB-CG1	9.37	1.83	1.52
1	A	19	LYS	C-O	-8.57	1.13	1.24
1	B	286	THR	CB-OG1	-8.20	1.30	1.43
1	D	347	ILE	CA-CB	7.51	1.57	1.54
1	B	355	ALA	CA-CB	-7.46	1.41	1.53
1	A	61	ASP	CB-CG	-7.21	1.34	1.52
1	C	337	ARG	CB-CG	-7.14	1.31	1.52
1	B	187	MET	SD-CE	7.06	1.97	1.79
1	D	355	ALA	CA-CB	-7.00	1.42	1.53
1	B	19	LYS	C-O	-6.94	1.15	1.24
1	A	47	ARG	CB-CG	-6.89	1.31	1.52
1	A	241	MET	SD-CE	6.42	1.95	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	32	MET	SD-CE	6.41	1.95	1.79
1	B	32	MET	SD-CE	6.36	1.95	1.79
1	B	241	MET	SD-CE	6.34	1.95	1.79
1	B	77	THR	CA-CB	6.14	1.63	1.53
1	A	19	LYS	CB-CG	-6.13	1.34	1.52
1	C	241	MET	SD-CE	6.10	1.94	1.79
1	A	276	TYR	CB-CG	-6.08	1.38	1.51
1	A	347	ILE	CA-CB	6.05	1.57	1.54
1	B	241	MET	CG-SD	6.02	1.95	1.80
1	A	215	ILE	CA-CB	-5.92	1.48	1.55
1	D	241	MET	CG-SD	5.89	1.95	1.80
1	C	298	ILE	C-O	-5.88	1.18	1.24
1	C	339	ASP	CA-C	5.84	1.60	1.52
1	A	252	SER	C-O	-5.83	1.16	1.23
1	D	201	MET	SD-CE	-5.68	1.65	1.79
1	A	241	MET	CG-SD	5.63	1.94	1.80
1	C	355	ALA	CA-CB	-5.62	1.44	1.53
1	B	339	ASP	CA-C	5.60	1.59	1.52
1	D	9	ARG	NE-CZ	5.57	1.39	1.33
1	B	163	MET	SD-CE	-5.50	1.65	1.79
1	B	9	ARG	NE-CZ	5.48	1.39	1.33
1	D	286	THR	CB-CG2	-5.47	1.34	1.52
1	D	77	THR	CA-CB	5.41	1.61	1.53
1	A	339	ASP	CA-C	5.40	1.59	1.52
1	B	294	VAL	CA-C	5.39	1.59	1.52
1	A	355	ALA	CA-CB	-5.35	1.44	1.53
1	A	138	ILE	CA-CB	-5.34	1.48	1.54
1	B	356	LEU	C-O	-5.34	1.18	1.24
1	B	134	ALA	CA-CB	-5.29	1.45	1.53
1	B	298	ILE	C-O	-5.27	1.18	1.24
1	C	77	THR	CA-CB	5.26	1.61	1.53
1	B	47	ARG	CB-CG	-5.22	1.36	1.52
1	D	252	SER	C-O	-5.22	1.17	1.23
1	D	339	ASP	CA-C	5.18	1.59	1.52
1	B	251	ALA	CA-CB	-5.18	1.44	1.53
1	C	62	ARG	CB-CG	-5.03	1.37	1.52
1	C	221	CYS	CA-C	-5.01	1.46	1.52
1	A	152	VAL	C-O	-5.00	1.18	1.24

All (46) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	313	VAL	CA-CB-CG2	-15.99	83.22	110.40
1	C	313	VAL	CA-CB-CG1	-15.75	83.62	110.40
1	C	276	TYR	CB-CG-CD1	-10.76	104.66	120.80
1	C	276	TYR	CB-CG-CD2	9.66	135.28	120.80
1	D	337	ARG	CA-CB-CG	-9.15	95.80	114.10
1	C	61	ASP	CA-CB-CG	8.96	121.56	112.60
1	B	337	ARG	CA-CB-CG	8.96	132.02	114.10
1	D	128	GLU	N-CA-C	8.91	122.06	108.52
1	C	313	VAL	CG1-CB-CG2	-8.79	91.47	110.80
1	B	128	GLU	N-CA-C	8.78	121.86	108.52
1	C	286	THR	CA-CB-OG1	-7.70	98.05	109.60
1	A	277	PHE	CA-CB-CG	6.36	120.16	113.80
1	A	61	ASP	CA-CB-CG	6.30	118.90	112.60
1	B	312	SER	N-CA-C	6.09	118.71	111.71
1	C	62	ARG	CA-CB-CG	6.08	126.25	114.10
1	A	312	SER	N-CA-C	6.01	118.62	111.71
1	D	312	SER	N-CA-C	5.80	118.38	111.71
1	D	286	THR	CA-CB-CG2	5.75	120.27	110.50
1	B	337	ARG	CB-CG-CD	5.74	124.50	111.30
1	D	286	THR	CA-CB-OG1	-5.71	101.03	109.60
1	D	47	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	B	224	ARG	CG-CD-NE	-5.42	100.07	112.00
1	C	47	ARG	NE-CZ-NH2	5.42	124.07	119.20
1	B	5	GLY	CA-C-O	-5.41	118.55	122.45
1	A	19	LYS	N-CA-C	-5.38	100.33	108.67
1	B	47	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	C	337	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	A	62	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	D	127	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	B	62	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	C	127	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	D	337	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	C	62	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	B	337	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	D	62	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	A	337	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	B	127	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	A	47	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	A	266	VAL	CB-CA-C	-5.19	105.03	110.53
1	D	265	SER	CA-CB-OG	-5.18	100.74	111.10
1	D	313	VAL	CB-CA-C	-5.16	101.60	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	GLU	N-CA-C	5.15	121.77	110.80
1	D	5	GLY	CA-C-O	-5.10	118.78	122.45
1	D	63	VAL	CB-CA-C	-5.09	103.03	110.62
1	B	308	VAL	CA-C-O	5.07	122.58	119.94
1	D	338	HIS	CA-C-O	5.07	121.53	118.33

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	2138	0	2151	85	0
1	B	2130	0	2151	76	0
1	C	2139	0	2161	82	0
1	D	2131	0	2157	85	0
2	A	25	0	0	2	0
2	B	26	0	0	0	0
2	C	27	0	0	0	0
2	D	20	0	0	2	0
All	All	8636	0	8620	272	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 (272) 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:187:MET:SD	1:C:187:MET:CE	2.05	1.44
1:A:187:MET:SD	1:A:187:MET:CE	2.08	1.41
1:D:187:MET:SD	1:D:187:MET:CE	2.08	1.40
1:B:368:ARG:HD3	2:D:385:HOH:O	1.68	0.92
1:A:367:ALA:HB2	1:C:367:ALA:HB2	1.61	0.81
1:D:9:ARG:HD3	2:D:388:HOH:O	1.80	0.81
1:B:367:ALA:HB2	1:D:367:ALA:HB2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:MET:HE1	1:B:193:PRO:HD2	1.63	0.79
1:C:163:MET:HE1	1:C:193:PRO:HD2	1.64	0.79
1:B:369:ASP:O	1:D:366:LYS:NZ	2.16	0.77
1:B:175:LEU:HD23	1:B:179:ILE:HB	1.68	0.75
1:B:366:LYS:NZ	1:D:369:ASP:O	2.18	0.74
2:A:402:HOH:O	1:C:368:ARG:HD3	1.92	0.70
1:A:233:PRO:HD3	1:A:298:ILE:HG22	1.75	0.69
1:A:262:GLN:HG2	2:A:403:HOH:O	1.92	0.69
1:B:233:PRO:HD3	1:B:298:ILE:HG22	1.74	0.69
1:B:233:PRO:O	1:B:234:CYS:HB2	1.92	0.68
1:D:233:PRO:HD3	1:D:298:ILE:HG22	1.75	0.68
1:A:143:LEU:O	1:A:147:SER:OG	2.12	0.68
1:C:312:SER:O	1:C:313:VAL:CB	2.42	0.67
1:C:233:PRO:O	1:C:234:CYS:HB2	1.94	0.67
1:D:175:LEU:HD23	1:D:179:ILE:HB	1.76	0.66
1:A:132:ARG:HD3	1:A:353:MET:HE3	1.77	0.66
1:C:175:LEU:HD23	1:C:179:ILE:HB	1.78	0.66
1:A:64:GLU:CD	1:D:19:LYS:HZ2	2.04	0.65
1:A:175:LEU:HD23	1:A:179:ILE:HB	1.79	0.65
1:D:163:MET:HE1	1:D:193:PRO:HD2	1.78	0.65
1:A:365:GLN:HE21	1:A:366:LYS:N	1.95	0.65
1:B:250:PRO:O	1:B:251:ALA:HB3	1.96	0.65
1:C:233:PRO:HD3	1:C:298:ILE:HG22	1.77	0.65
1:A:311:LYS:HE2	1:A:313:VAL:O	1.98	0.64
1:D:43:LEU:O	1:D:46:ARG:HG2	1.97	0.64
1:D:365:GLN:HE21	1:D:366:LYS:N	1.96	0.64
1:D:39:ILE:HG12	1:D:81:MET:HE1	1.80	0.64
1:C:43:LEU:O	1:C:46:ARG:HG2	1.98	0.64
1:A:1:MET:HE3	1:B:6:LYS:HE2	1.80	0.64
1:A:166:ASP:HA	1:A:262:GLN:NE2	2.14	0.62
1:D:45:ARG:NH1	1:D:181:ARG:HD3	2.15	0.61
1:C:309:PRO:HD3	1:D:261:PHE:CZ	2.35	0.61
1:C:312:SER:O	1:C:313:VAL:HB	2.00	0.61
1:D:353:MET:HE2	1:D:353:MET:HA	1.81	0.61
1:D:214:SER:HA	1:D:340:PRO:HB3	1.82	0.61
1:A:233:PRO:O	1:A:234:CYS:HB2	2.00	0.60
1:D:166:ASP:HA	1:D:262:GLN:NE2	2.16	0.60
1:C:128:GLU:HG3	1:C:130:ILE:HG12	1.82	0.60
1:D:233:PRO:O	1:D:234:CYS:HB2	2.01	0.60
1:B:39:ILE:HG12	1:B:81:MET:HE1	1.84	0.60
1:D:166:ASP:HA	1:D:262:GLN:HE22	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:MET:HE1	1:A:193:PRO:HD2	1.83	0.59
1:A:289:ASN:ND2	1:A:302:GLU:HB3	2.16	0.59
1:A:214:SER:HA	1:A:340:PRO:HB3	1.84	0.59
1:B:360:ASP:O	1:B:364:ILE:HG13	2.02	0.59
1:A:45:ARG:NH1	1:A:181:ARG:HD3	2.18	0.58
1:A:272:ASN:HD21	1:B:313:VAL:HG21	1.67	0.58
1:A:43:LEU:O	1:A:46:ARG:HG2	2.03	0.58
1:C:272:ASN:HD21	1:D:313:VAL:HG21	1.68	0.58
1:A:2:SER:OG	1:D:78:PRO:HG3	2.04	0.57
1:A:244:HIS:HB2	1:B:244:HIS:HB2	1.85	0.57
1:B:214:SER:HA	1:B:340:PRO:HB3	1.85	0.57
1:B:311:LYS:HE2	1:B:313:VAL:O	2.04	0.57
1:A:309:PRO:HD3	1:B:261:PHE:CZ	2.39	0.57
1:A:261:PHE:CZ	1:B:309:PRO:HD3	2.40	0.56
1:C:214:SER:HA	1:C:340:PRO:HB3	1.87	0.56
1:A:370:PHE:HA	1:C:366:LYS:NZ	2.20	0.56
1:B:339:ASP:HB3	1:B:340:PRO:C	2.30	0.56
1:A:1:MET:HG2	1:A:3:THR:H	1.71	0.56
1:A:129:THR:O	1:A:132:ARG:HB2	2.05	0.56
1:A:292:GLY:O	1:A:304:ILE:HA	2.05	0.56
1:B:43:LEU:O	1:B:46:ARG:HG2	2.05	0.56
1:C:39:ILE:HG12	1:C:81:MET:HE1	1.87	0.55
1:B:339:ASP:HB3	1:B:340:PRO:CA	2.36	0.55
1:B:353:MET:HE2	1:B:356:LEU:HD12	1.89	0.55
1:B:40:GLN:N	1:B:41:PRO:HD2	2.22	0.55
1:D:292:GLY:O	1:D:304:ILE:HA	2.07	0.55
1:B:221:CYS:O	1:B:305:TYR:HA	2.08	0.54
1:D:163:MET:CE	1:D:193:PRO:HD2	2.36	0.54
1:A:64:GLU:CD	1:D:19:LYS:NZ	2.65	0.54
1:A:166:ASP:HA	1:A:262:GLN:HE21	1.73	0.54
1:A:40:GLN:N	1:A:41:PRO:HD2	2.23	0.54
1:D:353:MET:HE2	1:D:356:LEU:HD12	1.89	0.54
1:A:366:LYS:NZ	1:C:370:PHE:HA	2.22	0.54
1:A:39:ILE:HG12	1:A:81:MET:HE1	1.90	0.53
1:C:31:GLY:O	1:C:32:MET:C	2.50	0.53
1:D:311:LYS:HE2	1:D:313:VAL:O	2.07	0.53
1:B:166:ASP:HA	1:B:262:GLN:NE2	2.23	0.53
1:B:313:VAL:HG12	1:B:337:ARG:O	2.09	0.53
1:D:274:PRO:HA	1:D:287:LYS:HB3	1.91	0.53
1:C:292:GLY:O	1:C:304:ILE:HA	2.09	0.53
1:D:128:GLU:HG3	1:D:130:ILE:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LYS:HE2	1:D:1:MET:CE	2.39	0.53
1:C:39:ILE:HG21	1:C:81:MET:HE1	1.91	0.53
1:B:132:ARG:HD3	1:B:353:MET:HE3	1.91	0.52
1:C:68:GLY:HA3	1:C:79:ILE:HG12	1.90	0.52
1:C:258:GLY:HA2	1:C:305:TYR:CZ	2.44	0.52
1:A:6:LYS:HE2	1:B:1:MET:HE3	1.92	0.52
1:D:143:LEU:O	1:D:147:SER:OG	2.27	0.52
1:A:226:LEU:HD11	1:A:358:LEU:HD22	1.92	0.52
1:C:368:ARG:HG3	1:C:368:ARG:HH11	1.74	0.52
1:D:353:MET:CE	1:D:356:LEU:HD12	2.40	0.52
1:C:258:GLY:HA2	1:C:305:TYR:CE1	2.44	0.51
1:D:250:PRO:O	1:D:251:ALA:HB3	2.11	0.51
1:D:258:GLY:HA2	1:D:305:TYR:CZ	2.45	0.51
1:D:345:ARG:O	1:D:348:PRO:HD2	2.11	0.51
1:A:221:CYS:O	1:A:305:TYR:HA	2.09	0.51
1:C:1:MET:CE	1:D:6:LYS:HE2	2.41	0.51
1:A:250:PRO:O	1:A:251:ALA:HB3	2.10	0.51
1:D:40:GLN:N	1:D:41:PRO:HD2	2.25	0.51
1:B:233:PRO:O	1:B:234:CYS:CB	2.59	0.51
1:C:339:ASP:HB3	1:C:340:PRO:CA	2.41	0.51
1:D:14:GLY:CA	1:D:21:VAL:HG12	2.40	0.51
1:A:160:GLU:HG2	1:B:265:SER:HB2	1.92	0.51
1:C:353:MET:HE2	1:C:353:MET:HA	1.93	0.50
1:A:365:GLN:HE21	1:A:365:GLN:C	2.20	0.50
1:C:272:ASN:HD21	1:D:313:VAL:CG2	2.24	0.50
1:C:143:LEU:O	1:C:147:SER:OG	2.26	0.50
1:C:339:ASP:HB3	1:C:340:PRO:C	2.36	0.50
1:A:6:LYS:HE2	1:B:1:MET:CE	2.42	0.50
1:A:39:ILE:HG21	1:A:81:MET:HE1	1.94	0.50
1:C:244:HIS:HB2	1:D:244:HIS:HB2	1.94	0.50
1:A:15:GLU:O	1:A:16:SER:CB	2.60	0.49
1:A:128:GLU:HG3	1:A:130:ILE:HG12	1.94	0.49
1:A:339:ASP:HB3	1:A:340:PRO:CA	2.42	0.49
1:B:1:MET:HG2	1:B:3:THR:H	1.77	0.49
1:B:343:THR:HB	1:B:344:PRO:HD3	1.95	0.49
1:C:15:GLU:O	1:C:16:SER:CB	2.60	0.49
1:C:45:ARG:NH1	1:C:181:ARG:HD3	2.27	0.49
1:D:233:PRO:HD3	1:D:298:ILE:CG2	2.43	0.49
1:A:343:THR:HB	1:A:344:PRO:HD3	1.95	0.49
1:B:175:LEU:CD2	1:B:179:ILE:HB	2.41	0.49
1:B:370:PHE:CZ	1:D:366:LYS:HD3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PRO:HG3	1:D:2:SER:OG	2.12	0.49
1:C:272:ASN:ND2	1:D:313:VAL:HG21	2.28	0.48
1:D:15:GLU:O	1:D:16:SER:CB	2.61	0.48
1:D:368:ARG:HG3	1:D:368:ARG:HH11	1.77	0.48
1:A:256:GLU:HG2	1:B:261:PHE:CZ	2.48	0.48
1:A:339:ASP:HB3	1:A:340:PRO:C	2.38	0.48
1:A:31:GLY:O	1:A:32:MET:C	2.57	0.48
1:B:292:GLY:O	1:B:304:ILE:HA	2.14	0.48
1:B:339:ASP:HB3	1:B:340:PRO:HA	1.96	0.48
1:B:345:ARG:O	1:B:348:PRO:HD2	2.14	0.48
1:A:1:MET:CE	1:B:6:LYS:HE2	2.43	0.48
1:C:163:MET:CE	1:C:193:PRO:HD2	2.40	0.48
1:D:221:CYS:O	1:D:305:TYR:HA	2.14	0.48
1:D:339:ASP:HB3	1:D:340:PRO:CA	2.44	0.48
1:B:15:GLU:O	1:B:16:SER:CB	2.61	0.48
1:D:77:THR:HB	1:D:78:PRO:HD2	1.96	0.48
1:C:187:MET:HA	1:C:187:MET:HE2	1.96	0.47
1:C:243:ALA:CB	1:D:247:LEU:HD13	2.45	0.47
1:D:226:LEU:HD11	1:D:358:LEU:HD22	1.95	0.47
1:B:143:LEU:O	1:B:147:SER:OG	2.31	0.47
1:A:360:ASP:O	1:A:364:ILE:HG13	2.15	0.47
1:D:339:ASP:HB3	1:D:340:PRO:HA	1.96	0.47
1:B:129:THR:O	1:B:132:ARG:HB2	2.15	0.47
1:B:258:GLY:HA2	1:B:305:TYR:CZ	2.50	0.47
1:C:6:LYS:HE2	1:D:1:MET:HE2	1.97	0.47
1:D:129:THR:O	1:D:132:ARG:HB2	2.15	0.47
1:C:206:GLU:O	1:C:207:LYS:C	2.57	0.47
1:A:274:PRO:O	1:A:286:THR:HA	2.15	0.47
1:D:68:GLY:HA3	1:D:79:ILE:HG12	1.97	0.47
1:A:370:PHE:CZ	1:C:366:LYS:HD3	2.50	0.47
1:B:366:LYS:HD3	1:D:370:PHE:CZ	2.49	0.47
1:B:140:GLU:OE2	1:B:181:ARG:NH2	2.48	0.46
1:C:250:PRO:O	1:C:251:ALA:HB3	2.15	0.46
1:C:343:THR:HB	1:C:344:PRO:HD3	1.96	0.46
1:A:64:GLU:OE1	1:D:19:LYS:NZ	2.48	0.46
1:B:39:ILE:HG21	1:B:81:MET:HE1	1.97	0.46
1:D:343:THR:HB	1:D:344:PRO:HD3	1.96	0.46
1:D:289:ASN:ND2	1:D:302:GLU:HB3	2.30	0.46
1:A:163:MET:HE2	1:A:192:CYS:SG	2.56	0.46
1:B:366:LYS:NZ	1:D:370:PHE:HA	2.31	0.46
1:B:31:GLY:O	1:B:32:MET:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:GLN:N	1:C:41:PRO:HD2	2.30	0.46
1:D:15:GLU:O	1:D:16:SER:HB3	2.16	0.46
1:B:77:THR:HB	1:B:78:PRO:HD2	1.98	0.45
1:A:130:ILE:HG12	1:A:130:ILE:H	1.62	0.45
1:A:366:LYS:NZ	1:C:369:ASP:O	2.26	0.45
1:A:1:MET:N	1:B:232:GLU:HB3	2.32	0.45
1:A:158:ILE:HG21	1:A:205:ILE:HG13	1.98	0.45
1:A:258:GLY:HA2	1:A:305:TYR:CZ	2.52	0.45
1:B:14:GLY:CA	1:B:21:VAL:HG12	2.47	0.45
1:C:1:MET:HG2	1:C:3:THR:H	1.82	0.45
1:C:1:MET:HE3	1:D:6:LYS:HE2	1.99	0.45
1:A:265:SER:HB2	1:B:160:GLU:HG2	1.99	0.45
1:D:368:ARG:HG3	1:D:368:ARG:NH1	2.32	0.45
1:C:247:LEU:HD13	1:D:243:ALA:HB2	1.99	0.45
1:B:370:PHE:HA	1:D:366:LYS:NZ	2.32	0.45
1:C:289:ASN:ND2	1:C:302:GLU:HB3	2.31	0.45
1:D:360:ASP:O	1:D:364:ILE:HG13	2.16	0.44
1:A:311:LYS:HE2	1:A:313:VAL:C	2.42	0.44
1:B:163:MET:CE	1:B:193:PRO:HD2	2.40	0.44
1:B:226:LEU:HD11	1:B:358:LEU:HD22	1.99	0.44
1:A:206:GLU:O	1:A:207:LYS:C	2.60	0.44
1:C:1:MET:CE	1:D:6:LYS:CE	2.96	0.44
1:C:261:PHE:CZ	1:D:309:PRO:HD3	2.52	0.44
1:B:249:ILE:CG2	1:B:250:PRO:HD2	2.47	0.44
1:D:31:GLY:O	1:D:32:MET:C	2.60	0.44
1:A:345:ARG:O	1:A:348:PRO:HD2	2.17	0.44
1:D:289:ASN:ND2	1:D:303:ASN:O	2.50	0.44
1:D:158:ILE:HG21	1:D:205:ILE:HG13	1.98	0.44
1:D:161:ILE:HD13	1:D:161:ILE:N	2.33	0.44
1:C:289:ASN:ND2	1:C:303:ASN:O	2.51	0.43
1:A:272:ASN:HD21	1:B:313:VAL:CG2	2.29	0.43
1:D:339:ASP:HB3	1:D:340:PRO:C	2.43	0.43
1:C:2:SER:O	1:C:11:THR:HA	2.19	0.43
1:C:194:ASP:OD1	1:C:194:ASP:C	2.61	0.43
1:A:194:ASP:OD1	1:A:194:ASP:C	2.62	0.43
1:C:232:GLU:HB3	1:D:1:MET:N	2.33	0.43
1:C:339:ASP:HB3	1:C:340:PRO:HA	2.00	0.43
1:D:14:GLY:HA3	1:D:21:VAL:HG12	2.00	0.43
1:C:233:PRO:O	1:C:234:CYS:CB	2.65	0.43
1:D:258:GLY:HA2	1:D:305:TYR:CE1	2.54	0.43
1:C:243:ALA:HB2	1:D:247:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:VAL:HB	1:C:338:HIS:O	2.18	0.42
1:A:261:PHE:CE1	1:B:309:PRO:HD3	2.53	0.42
1:C:353:MET:HE2	1:C:356:LEU:HD12	2.00	0.42
1:A:298:ILE:HG21	1:A:298:ILE:HD13	1.67	0.42
1:B:206:GLU:O	1:B:207:LYS:C	2.60	0.42
1:A:69:THR:HA	1:A:73:LYS:O	2.19	0.42
1:A:77:THR:HB	1:A:78:PRO:HD2	2.01	0.42
1:B:289:ASN:ND2	1:B:302:GLU:HB3	2.34	0.42
1:A:2:SER:O	1:A:11:THR:HA	2.20	0.42
1:A:289:ASN:ND2	1:A:303:ASN:O	2.53	0.42
1:C:265:SER:HB2	1:D:160:GLU:HG2	2.02	0.42
1:D:39:ILE:HG21	1:D:81:MET:HE1	2.00	0.42
1:A:232:GLU:HB3	1:B:1:MET:N	2.34	0.42
1:B:66:GLN:HE22	1:C:82:MET:CE	2.32	0.42
1:D:194:ASP:C	1:D:194:ASP:OD1	2.61	0.42
1:C:158:ILE:HG21	1:C:205:ILE:HG13	2.01	0.42
1:A:368:ARG:HG3	1:A:368:ARG:HH11	1.84	0.42
1:B:246:MET:SD	1:B:350:VAL:HG13	2.60	0.42
1:C:163:MET:HG2	1:C:164:ASN:N	2.34	0.42
1:A:132:ARG:CD	1:A:353:MET:HE3	2.47	0.42
1:A:366:LYS:HD3	1:C:370:PHE:CE2	2.55	0.42
1:A:368:ARG:HG3	1:A:368:ARG:NH1	2.34	0.42
1:B:43:LEU:CD1	1:B:63:VAL:HG21	2.49	0.42
1:B:266:VAL:HA	1:B:267:PRO:HD3	1.90	0.42
1:A:140:GLU:OE2	1:A:181:ARG:NH2	2.52	0.42
1:C:77:THR:HB	1:C:78:PRO:HD2	2.01	0.42
1:C:166:ASP:HA	1:C:262:GLN:NE2	2.34	0.42
1:C:215:ILE:C	1:C:312:SER:HB3	2.45	0.42
1:D:175:LEU:CD2	1:D:179:ILE:HB	2.49	0.42
1:C:129:THR:O	1:C:132:ARG:HB2	2.20	0.41
1:C:214:SER:OG	1:C:312:SER:HB2	2.20	0.41
1:A:14:GLY:HA3	1:A:21:VAL:HB	2.03	0.41
1:B:339:ASP:CB	1:B:340:PRO:HA	2.50	0.41
1:A:161:ILE:N	1:A:161:ILE:HD13	2.35	0.41
1:B:2:SER:OG	1:C:78:PRO:HG3	2.20	0.41
1:C:368:ARG:HG3	1:C:368:ARG:NH1	2.34	0.41
1:C:6:LYS:CE	1:D:1:MET:CE	2.99	0.41
1:A:339:ASP:HB3	1:A:340:PRO:HA	2.03	0.41
1:C:132:ARG:HD3	1:C:353:MET:HE3	2.03	0.41
1:A:15:GLU:O	1:A:16:SER:HB3	2.21	0.41
1:B:221:CYS:HB3	1:B:306:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ALA:HB2	1:B:247:LEU:HD13	2.02	0.41
1:C:221:CYS:O	1:C:305:TYR:HA	2.19	0.41
1:C:272:ASN:HD21	1:D:313:VAL:CB	2.33	0.41
1:D:69:THR:HA	1:D:73:LYS:O	2.20	0.41
1:D:140:GLU:OE2	1:D:181:ARG:NH2	2.54	0.41
1:A:132:ARG:HD3	1:A:353:MET:CE	2.46	0.41
1:B:12:THR:HG22	1:B:23:CYS:HB3	2.03	0.41
1:C:1:MET:N	1:D:232:GLU:HB3	2.36	0.41
1:A:186:SER:C	1:A:188:GLY:H	2.27	0.40
1:B:163:MET:HE2	1:B:192:CYS:SG	2.62	0.40
1:C:346:ALA:O	1:C:347:ILE:C	2.62	0.40
1:C:353:MET:CE	1:C:356:LEU:HD12	2.51	0.40
1:C:358:LEU:HD23	1:C:358:LEU:HA	1.95	0.40
1:B:298:ILE:HG21	1:B:298:ILE:HD13	1.68	0.40
1:A:364:ILE:HD13	1:A:364:ILE:HG21	1.91	0.40
1:C:69:THR:HA	1:C:73:LYS:O	2.21	0.40
1:B:45:ARG:NH1	1:B:181:ARG:HD3	2.37	0.40
1:B:78:PRO:HG3	1:C:2:SER:OG	2.21	0.40
1:B:353:MET:HE2	1:B:353:MET:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	273/382 (72%)	249 (91%)	16 (6%)	8 (3%)	3	15
1	B	272/382 (71%)	250 (92%)	14 (5%)	8 (3%)	3	15
1	C	273/382 (72%)	247 (90%)	18 (7%)	8 (3%)	3	15
1	D	272/382 (71%)	248 (91%)	16 (6%)	8 (3%)	3	15
All	All	1090/1528 (71%)	994 (91%)	64 (6%)	32 (3%)	3	15

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	147	SER
1	A	234	CYS
1	A	339	ASP
1	B	16	SER
1	B	147	SER
1	B	234	CYS
1	B	339	ASP
1	C	16	SER
1	C	147	SER
1	C	234	CYS
1	C	339	ASP
1	D	16	SER
1	D	147	SER
1	D	234	CYS
1	D	339	ASP
1	A	32	MET
1	B	32	MET
1	C	32	MET
1	D	32	MET
1	A	233	PRO
1	B	287	LYS
1	C	233	PRO
1	A	20	SER
1	B	20	SER
1	D	233	PRO
1	D	287	LYS
1	B	233	PRO
1	C	287	LYS
1	D	189	PRO
1	A	189	PRO
1	C	189	PRO

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	234/318 (74%)	215 (92%)	19 (8%)	11	33
1	B	233/318 (73%)	215 (92%)	18 (8%)	12	35
1	C	235/318 (74%)	219 (93%)	16 (7%)	14	42
1	D	234/318 (74%)	216 (92%)	18 (8%)	12	35
All	All	936/1272 (74%)	865 (92%)	71 (8%)	12	36

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ILE
1	A	46	ARG
1	A	82	MET
1	A	130	ILE
1	A	145	GLN
1	A	161	ILE
1	A	187	MET
1	A	193	PRO
1	A	215	ILE
1	A	224	ARG
1	A	241	MET
1	A	247	LEU
1	A	298	ILE
1	A	312	SER
1	A	313	VAL
1	A	339	ASP
1	A	347	ILE
1	A	365	GLN
1	A	369	ASP
1	B	39	ILE
1	B	46	ARG
1	B	82	MET
1	B	130	ILE
1	B	145	GLN
1	B	187	MET
1	B	193	PRO
1	B	241	MET
1	B	247	LEU
1	B	262	GLN
1	B	298	ILE
1	B	311	LYS
1	B	312	SER
1	B	313	VAL

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Mol	Chain	Res	Type
1	B	339	ASP
1	B	347	ILE
1	B	365	GLN
1	B	369	ASP
1	C	39	ILE
1	C	46	ARG
1	C	82	MET
1	C	130	ILE
1	C	145	GLN
1	C	187	MET
1	C	215	ILE
1	C	224	ARG
1	C	241	MET
1	C	247	LEU
1	C	262	GLN
1	C	312	SER
1	C	339	ASP
1	C	347	ILE
1	C	365	GLN
1	C	369	ASP
1	D	46	ARG
1	D	82	MET
1	D	130	ILE
1	D	145	GLN
1	D	161	ILE
1	D	187	MET
1	D	193	PRO
1	D	215	ILE
1	D	224	ARG
1	D	241	MET
1	D	247	LEU
1	D	262	GLN
1	D	298	ILE
1	D	312	SER
1	D	313	VAL
1	D	347	ILE
1	D	365	GLN
1	D	369	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	148	ASN
1	A	262	GLN
1	A	272	ASN
1	A	365	GLN
1	B	17	HIS
1	B	66	GLN
1	B	145	GLN
1	B	272	ASN
1	B	365	GLN
1	C	148	ASN
1	C	262	GLN
1	C	272	ASN
1	C	365	GLN
1	D	17	HIS
1	D	66	GLN
1	D	145	GLN
1	D	148	ASN
1	D	262	GLN
1	D	365	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	283/382 (74%)	-1.73	0 100 100	10, 31, 54, 67	9 (3%)
1	B	282/382 (73%)	-1.72	0 100 100	9, 31, 54, 67	9 (3%)
1	C	283/382 (74%)	-1.73	0 100 100	9, 31, 54, 66	10 (3%)
1	D	282/382 (73%)	-1.70	0 100 100	10, 31, 54, 67	8 (2%)
All	All	1130/1528 (73%)	-1.72	0 100 100	9, 31, 55, 67	36 (3%)

There are no RSRZ outliers to report.

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.