



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:22 PM UTC

PDB ID : 8YMA / pdb_00008yma
Title : CRYSTAL STRUCTURE OF A NOVEL PU PLASTIC DEGRADATION ENZYME FROM THERMAEROBACTER MARIANENSIS
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Deposited on : 2024-03-08
Resolution : 2.07 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

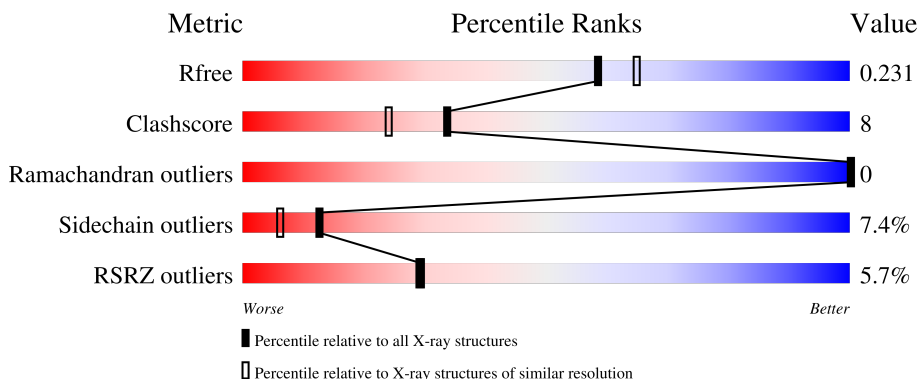
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	527	2% 80% 13% 6%
1	B	527	6% 78% 15% 6%
1	C	527	6% 73% 18% 6%
1	D	527	7% 78% 14% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15377 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 Carboxylic ester hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3703	2356	673	665	9			
1	B	498	Total	C	N	O	S	0	0	0
			3755	2384	684	678	9			
1	C	493	Total	C	N	O	S	0	0	0
			3715	2363	676	667	9			
1	D	496	Total	C	N	O	S	0	0	0
			3720	2368	673	670	9			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP E6SHQ4
A	-5	HIS	-	expression tag	UNP E6SHQ4
A	-4	HIS	-	expression tag	UNP E6SHQ4
A	-3	HIS	-	expression tag	UNP E6SHQ4
A	-2	HIS	-	expression tag	UNP E6SHQ4
A	-1	HIS	-	expression tag	UNP E6SHQ4
A	0	HIS	-	expression tag	UNP E6SHQ4
A	1	GLU	-	expression tag	UNP E6SHQ4
A	2	ASN	-	expression tag	UNP E6SHQ4
A	3	LEU	-	expression tag	UNP E6SHQ4
A	4	TYR	-	expression tag	UNP E6SHQ4
A	5	PHE	-	expression tag	UNP E6SHQ4
A	6	GLN	-	expression tag	UNP E6SHQ4
A	7	GLY	-	expression tag	UNP E6SHQ4
A	8	ALA	-	expression tag	UNP E6SHQ4
A	9	GLY	-	expression tag	UNP E6SHQ4
A	10	ALA	-	expression tag	UNP E6SHQ4
A	11	GLY	-	expression tag	UNP E6SHQ4
A	12	ALA	-	expression tag	UNP E6SHQ4
A	13	GLY	-	expression tag	UNP E6SHQ4
A	14	ALA	-	expression tag	UNP E6SHQ4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	-	expression tag	UNP E6SHQ4
A	16	ALA	-	expression tag	UNP E6SHQ4
B	-6	MET	-	initiating methionine	UNP E6SHQ4
B	-5	HIS	-	expression tag	UNP E6SHQ4
B	-4	HIS	-	expression tag	UNP E6SHQ4
B	-3	HIS	-	expression tag	UNP E6SHQ4
B	-2	HIS	-	expression tag	UNP E6SHQ4
B	-1	HIS	-	expression tag	UNP E6SHQ4
B	0	HIS	-	expression tag	UNP E6SHQ4
B	1	GLU	-	expression tag	UNP E6SHQ4
B	2	ASN	-	expression tag	UNP E6SHQ4
B	3	LEU	-	expression tag	UNP E6SHQ4
B	4	TYR	-	expression tag	UNP E6SHQ4
B	5	PHE	-	expression tag	UNP E6SHQ4
B	6	GLN	-	expression tag	UNP E6SHQ4
B	7	GLY	-	expression tag	UNP E6SHQ4
B	8	ALA	-	expression tag	UNP E6SHQ4
B	9	GLY	-	expression tag	UNP E6SHQ4
B	10	ALA	-	expression tag	UNP E6SHQ4
B	11	GLY	-	expression tag	UNP E6SHQ4
B	12	ALA	-	expression tag	UNP E6SHQ4
B	13	GLY	-	expression tag	UNP E6SHQ4
B	14	ALA	-	expression tag	UNP E6SHQ4
B	15	GLY	-	expression tag	UNP E6SHQ4
B	16	ALA	-	expression tag	UNP E6SHQ4
C	-6	MET	-	initiating methionine	UNP E6SHQ4
C	-5	HIS	-	expression tag	UNP E6SHQ4
C	-4	HIS	-	expression tag	UNP E6SHQ4
C	-3	HIS	-	expression tag	UNP E6SHQ4
C	-2	HIS	-	expression tag	UNP E6SHQ4
C	-1	HIS	-	expression tag	UNP E6SHQ4
C	0	HIS	-	expression tag	UNP E6SHQ4
C	1	GLU	-	expression tag	UNP E6SHQ4
C	2	ASN	-	expression tag	UNP E6SHQ4
C	3	LEU	-	expression tag	UNP E6SHQ4
C	4	TYR	-	expression tag	UNP E6SHQ4
C	5	PHE	-	expression tag	UNP E6SHQ4
C	6	GLN	-	expression tag	UNP E6SHQ4
C	7	GLY	-	expression tag	UNP E6SHQ4
C	8	ALA	-	expression tag	UNP E6SHQ4
C	9	GLY	-	expression tag	UNP E6SHQ4
C	10	ALA	-	expression tag	UNP E6SHQ4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	11	GLY	-	expression tag	UNP E6SHQ4
C	12	ALA	-	expression tag	UNP E6SHQ4
C	13	GLY	-	expression tag	UNP E6SHQ4
C	14	ALA	-	expression tag	UNP E6SHQ4
C	15	GLY	-	expression tag	UNP E6SHQ4
C	16	ALA	-	expression tag	UNP E6SHQ4
D	-6	MET	-	initiating methionine	UNP E6SHQ4
D	-5	HIS	-	expression tag	UNP E6SHQ4
D	-4	HIS	-	expression tag	UNP E6SHQ4
D	-3	HIS	-	expression tag	UNP E6SHQ4
D	-2	HIS	-	expression tag	UNP E6SHQ4
D	-1	HIS	-	expression tag	UNP E6SHQ4
D	0	HIS	-	expression tag	UNP E6SHQ4
D	1	GLU	-	expression tag	UNP E6SHQ4
D	2	ASN	-	expression tag	UNP E6SHQ4
D	3	LEU	-	expression tag	UNP E6SHQ4
D	4	TYR	-	expression tag	UNP E6SHQ4
D	5	PHE	-	expression tag	UNP E6SHQ4
D	6	GLN	-	expression tag	UNP E6SHQ4
D	7	GLY	-	expression tag	UNP E6SHQ4
D	8	ALA	-	expression tag	UNP E6SHQ4
D	9	GLY	-	expression tag	UNP E6SHQ4
D	10	ALA	-	expression tag	UNP E6SHQ4
D	11	GLY	-	expression tag	UNP E6SHQ4
D	12	ALA	-	expression tag	UNP E6SHQ4
D	13	GLY	-	expression tag	UNP E6SHQ4
D	14	ALA	-	expression tag	UNP E6SHQ4
D	15	GLY	-	expression tag	UNP E6SHQ4
D	16	ALA	-	expression tag	UNP E6SHQ4

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		

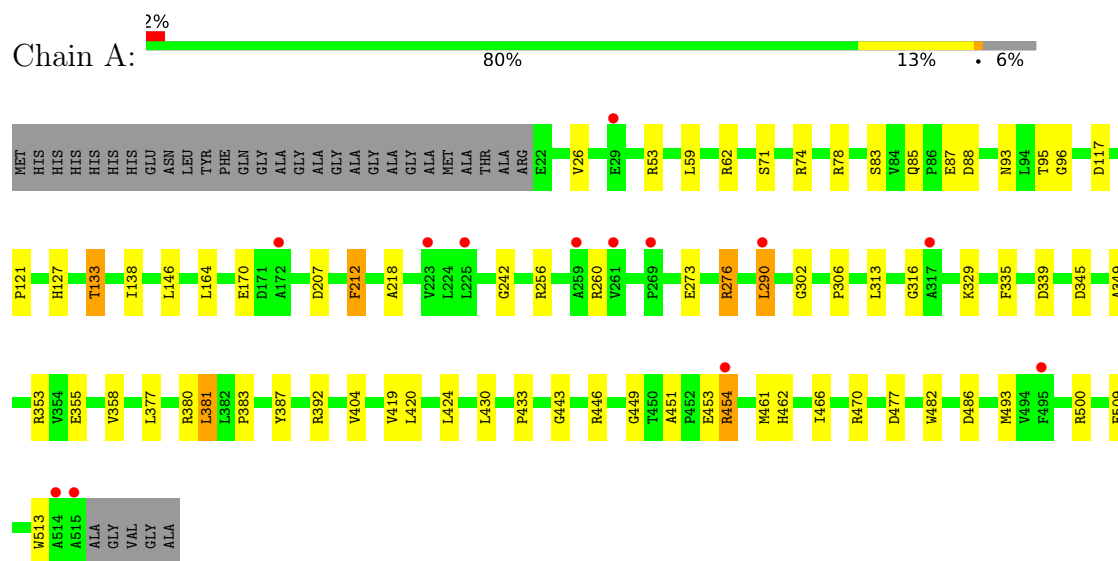
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	116	Total	O	0	0
			116	116		
3	B	117	Total	O	0	0
			117	117		
3	C	126	Total	O	0	0
			126	126		
3	D	120	Total	O	0	0
			120	120		

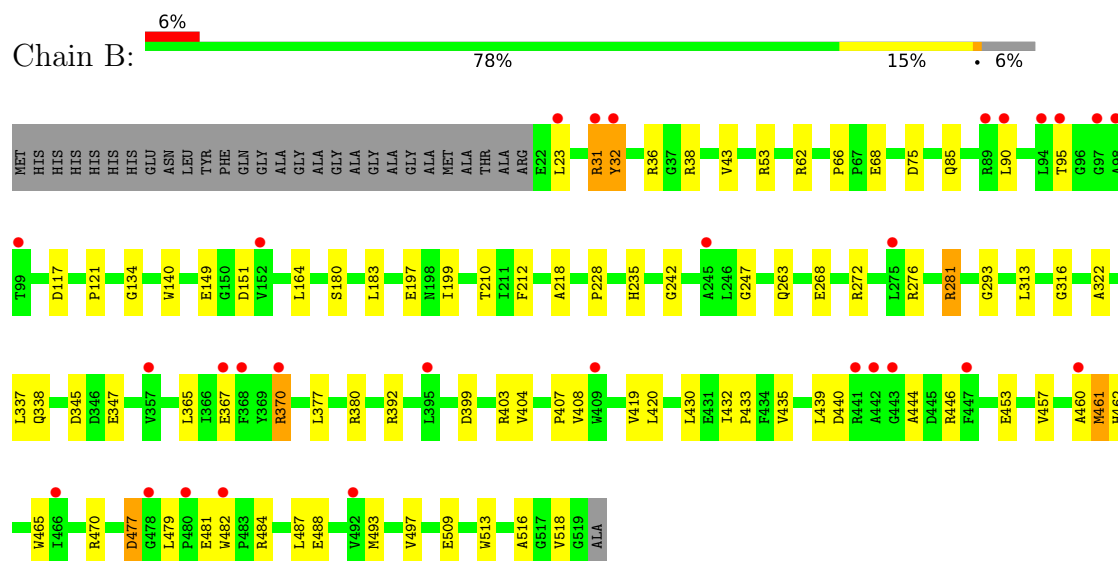
3 Residue-property plots [i](#)

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.

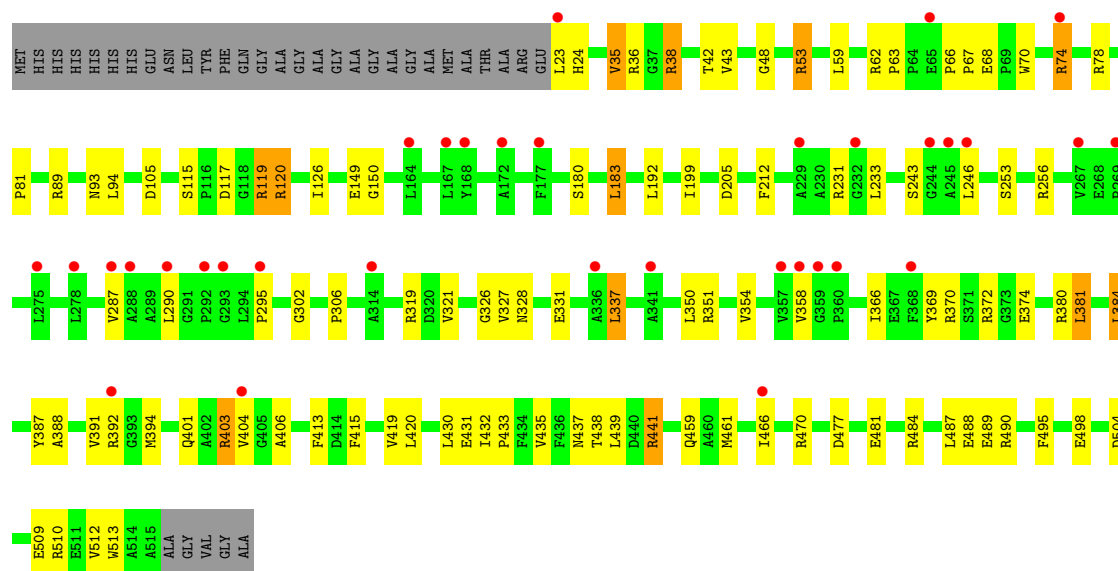
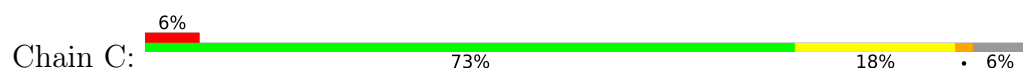
- Molecule 1: Carboxylic ester hydrolase



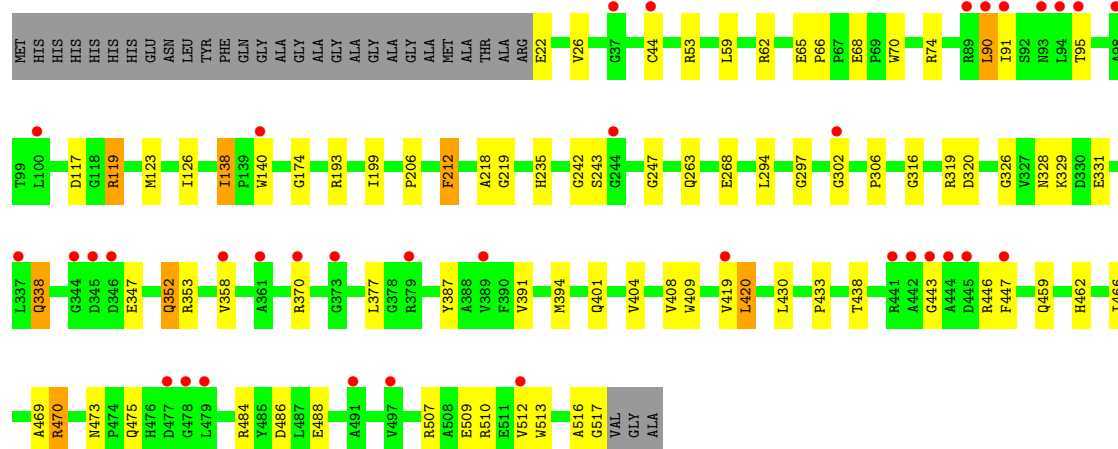
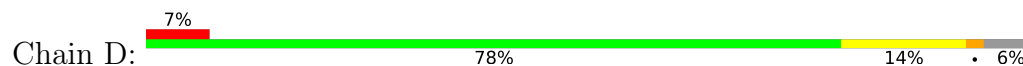
- Molecule 1: Carboxylic ester hydrolase



- Molecule 1: Carboxylic ester hydrolase



• Molecule 1: Carboxylic ester hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	81.83Å 81.83Å 667.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.59 – 2.07 48.59 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.59-2.07) 100.0 (48.59-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.182 , 0.227 0.196 , 0.231	Depositor DCC
R_{free} test set	7699 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.287 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15377	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.77	0/3805	1.05	6/5204 (0.1%)
1	B	0.79	0/3857	1.10	6/5270 (0.1%)
1	C	0.80	1/3817 (0.0%)	1.06	1/5218 (0.0%)
1	D	0.77	0/3822	1.07	3/5226 (0.1%)
All	All	0.78	1/15301 (0.0%)	1.07	16/20918 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	120	ARG	C-N	7.68	1.43	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	212	PHE	CA-CB-CG	7.47	121.27	113.80
1	A	212	PHE	CA-CB-CG	7.17	120.97	113.80
1	C	212	PHE	CA-CB-CG	7.15	120.95	113.80
1	B	212	PHE	CA-CB-CG	6.89	120.69	113.80
1	A	453	GLU	N-CA-C	-5.97	105.25	112.54
1	A	335	PHE	CA-CB-CG	-5.96	107.84	113.80
1	B	477	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	339	ASP	CA-CB-CG	5.72	118.32	112.60
1	B	488	GLU	CB-CG-CD	5.67	122.23	112.60
1	D	462	HIS	CA-CB-CG	5.65	119.45	113.80
1	B	462	HIS	CA-CB-CG	5.58	119.39	113.80
1	A	207	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	32	TYR	CB-CA-C	5.44	119.82	110.79
1	A	462	HIS	CA-CB-CG	5.29	119.09	113.80
1	B	210	THR	CA-CB-OG1	-5.25	101.73	109.60
1	D	447	PHE	CA-CB-CG	5.23	119.03	113.80

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	3703	0	3597	43	0
1	B	3755	0	3661	53	0
1	C	3715	0	3625	79	0
1	D	3720	0	3619	52	0
2	C	5	0	0	0	0
3	A	116	0	0	5	0
3	B	117	0	0	5	0
3	C	126	0	0	3	0
3	D	120	0	0	7	0
All	All	15377	0	14502	226	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 8.

All (226) 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:119:ARG:HH11	1:C:119:ARG:CG	1.64	1.10
1:A:451:ALA:O	1:A:454:ARG:HG3	1.53	1.08
1:C:119:ARG:NH1	1:C:119:ARG:HG3	1.55	1.03
1:A:454:ARG:HG3	1:A:454:ARG:HH11	0.89	1.03
1:A:121:PRO:HG2	1:A:470:ARG:HG2	1.39	1.02
1:C:388:ALA:HA	1:C:392:ARG:CD	1.90	1.00
1:C:38:ARG:HG3	1:C:38:ARG:HH11	1.29	0.98
1:A:454:ARG:HG3	1:A:454:ARG:NH1	1.70	0.95
1:A:454:ARG:HH11	1:A:454:ARG:CG	1.79	0.95
1:C:387:TYR:O	1:C:392:ARG:HG3	1.68	0.94
1:C:119:ARG:HH11	1:C:119:ARG:HG3	0.77	0.94
1:C:388:ALA:HA	1:C:392:ARG:HD3	1.50	0.93
1:D:193:ARG:HH11	1:D:193:ARG:HG2	1.34	0.90
1:A:454:ARG:HD3	3:A:610:HOH:O	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:GLY:HA2	3:B:679:HOH:O	1.73	0.88
1:C:38:ARG:HH11	1:C:38:ARG:CG	1.87	0.88
1:D:370:ARG:HG3	1:D:377:LEU:HD13	1.55	0.86
1:A:276:ARG:CG	1:A:276:ARG:HH11	1.91	0.83
1:D:140:TRP:HZ2	1:D:443:GLY:HA3	1.44	0.81
1:C:53:ARG:HD2	1:C:68:GLU:HG2	1.64	0.79
1:A:276:ARG:HH11	1:A:276:ARG:HG2	1.47	0.78
1:C:470:ARG:HH11	1:C:470:ARG:HG2	1.48	0.77
1:A:451:ALA:O	1:A:454:ARG:CG	2.31	0.76
1:C:388:ALA:HA	1:C:392:ARG:HD2	1.68	0.76
1:C:403:ARG:HH11	1:C:487:LEU:CD1	1.99	0.75
1:A:260:ARG:HD2	1:A:290:LEU:HD21	1.69	0.74
1:B:276:ARG:HG3	1:B:276:ARG:HH11	1.52	0.74
1:B:31:ARG:HD3	1:B:32:TYR:CZ	2.23	0.73
1:C:387:TYR:CE1	1:C:392:ARG:HG2	2.23	0.72
1:D:62:ARG:HD2	3:D:614:HOH:O	1.91	0.71
1:A:83:SER:O	1:A:85:GLN:HG3	1.91	0.70
1:D:70:TRP:CE2	1:D:74:ARG:HG3	2.26	0.70
1:D:70:TRP:NE1	1:D:74:ARG:HG3	2.05	0.70
1:C:403:ARG:HH11	1:C:487:LEU:HD13	1.54	0.70
1:D:193:ARG:HG2	1:D:193:ARG:NH1	2.07	0.70
1:B:151:ASP:HB3	1:B:470:ARG:HH21	1.57	0.69
1:B:90:LEU:HD21	1:B:337:LEU:HB2	1.74	0.68
1:A:451:ALA:O	1:A:454:ARG:NH1	2.27	0.67
1:D:466:ILE:O	1:D:470:ARG:HG3	1.94	0.67
1:C:180:SER:HA	1:C:183:LEU:HD13	1.78	0.66
1:A:127:HIS:NE2	3:A:602:HOH:O	2.29	0.65
1:C:470:ARG:HG2	1:C:470:ARG:NH1	2.10	0.65
1:D:370:ARG:HG3	1:D:377:LEU:CD1	2.26	0.65
1:D:326:GLY:HA2	1:D:394:MET:HE3	1.79	0.64
1:C:350:LEU:HB3	1:C:381:LEU:HD12	1.79	0.64
1:C:53:ARG:HG3	1:C:66:PRO:O	1.97	0.63
1:C:53:ARG:CG	1:C:66:PRO:O	2.46	0.63
1:B:365:LEU:HD11	1:B:518:VAL:HG11	1.81	0.62
1:C:35:VAL:HG12	1:C:74:ARG:HH11	1.64	0.62
1:B:276:ARG:HG3	1:B:276:ARG:NH1	2.15	0.62
1:B:516:ALA:HB3	1:B:518:VAL:HG12	1.81	0.61
1:C:372:ARG:HH12	1:C:509:GLU:CG	2.14	0.61
1:B:134:GLY:HA3	3:B:607:HOH:O	2.00	0.60
1:A:316:GLY:HA2	1:A:404:VAL:HG11	1.82	0.60
1:C:38:ARG:HG3	1:C:38:ARG:NH1	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:O	1:A:260:ARG:HG3	2.02	0.59
1:B:31:ARG:NH1	1:B:197:GLU:OE2	2.35	0.59
1:C:490:ARG:HD2	1:C:504:ASP:CG	2.26	0.59
1:C:62:ARG:HD2	1:C:63:PRO:HD2	1.83	0.59
1:C:403:ARG:HD3	1:C:487:LEU:CD1	2.32	0.59
1:A:454:ARG:NH1	1:A:454:ARG:CG	2.48	0.59
1:B:90:LEU:HD22	1:B:338:GLN:HG2	1.85	0.58
1:C:419:VAL:HG12	1:C:420:LEU:HG	1.85	0.58
1:B:121:PRO:HG2	1:B:470:ARG:HG2	1.86	0.57
1:D:473:ASN:HD21	1:D:475:GLN:HB3	1.70	0.57
1:A:87:GLU:O	1:A:88:ASP:C	2.47	0.57
1:A:377:LEU:HG	1:A:381:LEU:HD22	1.86	0.56
1:D:70:TRP:CD1	1:D:74:ARG:HG3	2.40	0.56
1:B:316:GLY:HA2	1:B:404:VAL:HG11	1.87	0.56
1:C:372:ARG:HH12	1:C:509:GLU:HG3	1.69	0.56
1:B:479:LEU:HD22	1:B:493:MET:HE2	1.88	0.56
1:B:377:LEU:HD13	1:B:380:ARG:NH2	2.20	0.56
1:C:337:LEU:HD11	1:C:420:LEU:HD13	1.87	0.55
1:C:326:GLY:HA2	1:C:394:MET:HE3	1.89	0.55
1:D:507:ARG:HA	1:D:510:ARG:HH11	1.71	0.55
1:C:388:ALA:CA	1:C:392:ARG:HD3	2.31	0.55
1:D:140:TRP:CZ2	1:D:443:GLY:HA3	2.35	0.55
1:A:392:ARG:NH1	3:A:603:HOH:O	2.39	0.55
1:B:482:TRP:CE2	1:B:493:MET:HB2	2.43	0.54
1:B:377:LEU:HA	1:B:380:ARG:CZ	2.37	0.54
1:C:510:ARG:NH1	3:C:702:HOH:O	2.31	0.54
1:D:90:LEU:HD13	1:D:338:GLN:HG2	1.90	0.54
1:D:53:ARG:HD2	3:D:605:HOH:O	2.08	0.54
1:C:387:TYR:CD1	1:C:392:ARG:CG	2.91	0.53
1:A:164:LEU:HD12	3:A:667:HOH:O	2.07	0.53
1:A:449:GLY:O	1:A:454:ARG:NE	2.42	0.53
1:C:403:ARG:NH1	1:C:487:LEU:HD13	2.24	0.53
1:B:403:ARG:HG3	1:B:487:LEU:HD11	1.91	0.52
1:C:381:LEU:O	1:C:384:LEU:HB3	2.10	0.52
1:D:74:ARG:NH1	3:D:609:HOH:O	2.42	0.52
1:B:399:ASP:HB3	1:B:403:ARG:HH21	1.74	0.52
1:D:174:GLY:C	3:D:641:HOH:O	2.52	0.52
1:D:68:GLU:HG3	3:D:703:HOH:O	2.09	0.52
1:D:95:THR:HB	1:D:140:TRP:CH2	2.43	0.52
1:A:88:ASP:HB3	1:A:133:THR:HG21	1.91	0.52
1:C:319:ARG:HA	1:C:406:ALA:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:PRO:HD2	3:B:670:HOH:O	2.10	0.51
1:D:138:ILE:HG23	1:D:140:TRP:HE3	1.75	0.51
1:D:53:ARG:HG3	1:D:66:PRO:O	2.10	0.51
1:D:247:GLY:O	1:D:297:GLY:HA3	2.10	0.51
1:B:392:ARG:NH2	1:B:513:TRP:CZ3	2.79	0.51
1:C:403:ARG:HD3	1:C:487:LEU:HD11	1.93	0.50
1:C:24:HIS:C	1:C:38:ARG:HD3	2.35	0.50
1:C:35:VAL:HG12	1:C:74:ARG:NH1	2.27	0.50
1:D:316:GLY:HA2	1:D:404:VAL:HG11	1.92	0.50
1:B:95:THR:HB	1:B:140:TRP:HH2	1.77	0.50
1:B:377:LEU:HD13	1:B:380:ARG:HH21	1.77	0.50
1:D:409:TRP:CZ2	1:D:484:ARG:HG2	2.46	0.50
1:A:349:ALA:HB1	1:A:353:ARG:HH12	1.77	0.50
1:C:387:TYR:CD1	1:C:392:ARG:HG2	2.46	0.50
1:A:146:LEU:HD23	1:A:466:ILE:HD11	1.95	0.49
1:C:53:ARG:HG2	1:C:66:PRO:O	2.12	0.49
1:C:431:GLU:HB2	1:C:461:MET:HE1	1.95	0.49
1:B:140:TRP:HE1	1:B:444:ALA:HB2	1.77	0.49
1:D:401:GLN:HA	1:D:404:VAL:HG22	1.95	0.49
1:A:276:ARG:HH11	1:A:276:ARG:HG3	1.76	0.49
1:C:435:VAL:HG23	1:C:461:MET:HE3	1.95	0.49
1:D:319:ARG:HA	1:D:404:VAL:HG21	1.94	0.49
1:C:192:LEU:HB2	1:C:233:LEU:HD13	1.94	0.49
1:D:516:ALA:O	1:D:517:GLY:C	2.56	0.49
1:B:408:VAL:O	1:B:484:ARG:HG2	2.13	0.48
1:C:89:ARG:O	1:C:93:ASN:HB2	2.12	0.48
1:B:513:TRP:CE3	1:B:518:VAL:HG13	2.47	0.48
1:C:372:ARG:HH12	1:C:509:GLU:CD	2.21	0.48
1:A:446:ARG:NH1	3:A:608:HOH:O	2.45	0.48
1:B:377:LEU:CD1	1:B:380:ARG:NH2	2.77	0.48
1:C:38:ARG:CG	1:C:38:ARG:NH1	2.58	0.48
1:D:430:LEU:O	1:D:433:PRO:HD2	2.14	0.47
1:B:218:ALA:HB3	1:B:242:GLY:HA3	1.96	0.47
1:D:486:ASP:HB2	3:D:670:HOH:O	2.14	0.47
1:A:146:LEU:CD2	1:A:466:ILE:HD11	2.45	0.47
1:B:461:MET:HE3	1:B:461:MET:HB2	1.69	0.47
1:D:193:ARG:NH1	1:D:193:ARG:CG	2.72	0.47
1:B:433:PRO:HB2	1:B:439:LEU:HD23	1.95	0.47
1:C:253:SER:HA	1:C:256:ARG:NH2	2.30	0.46
1:C:370:ARG:O	1:C:380:ARG:HD2	2.14	0.46
1:A:387:TYR:O	1:A:392:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:ALA:HB1	1:B:479:LEU:HD21	1.98	0.46
1:D:123:MET:HE3	1:D:469:ALA:HB2	1.97	0.46
1:D:53:ARG:HD3	1:D:65:GLU:HB2	1.98	0.46
1:A:430:LEU:O	1:A:433:PRO:HD2	2.16	0.46
1:B:23:LEU:HD23	1:B:38:ARG:HH21	1.81	0.46
1:C:53:ARG:HG2	1:C:67:PRO:HA	1.98	0.46
1:C:231:ARG:O	3:C:701:HOH:O	2.21	0.46
1:B:419:VAL:HG11	1:B:446:ARG:O	2.16	0.45
1:C:302:GLY:HA2	1:C:306:PRO:HA	1.99	0.45
1:C:438:THR:O	1:C:441:ARG:HB2	2.16	0.45
1:D:509:GLU:O	1:D:513:TRP:HD1	1.99	0.45
1:A:349:ALA:HB1	1:A:353:ARG:NH1	2.31	0.45
1:D:219:GLY:HA2	1:D:243:SER:O	2.17	0.45
1:D:218:ALA:HB3	1:D:242:GLY:HA3	1.97	0.45
1:A:302:GLY:HA2	1:A:306:PRO:HA	1.97	0.45
1:C:287:VAL:HG13	1:C:295:PRO:HG3	1.99	0.45
1:A:419:VAL:HG12	1:A:420:LEU:HG	1.99	0.45
1:B:85:GLN:O	1:B:281:ARG:NH2	2.50	0.45
1:C:432:ILE:HB	1:C:433:PRO:HD3	1.98	0.45
1:D:119:ARG:HE	1:D:119:ARG:HB3	1.66	0.45
1:B:31:ARG:HH11	1:B:197:GLU:CD	2.25	0.45
1:C:199:ILE:HD12	1:C:199:ILE:HA	1.86	0.45
1:B:392:ARG:NH2	1:B:513:TRP:HZ3	2.14	0.45
1:C:387:TYR:CD1	1:C:392:ARG:HG3	2.52	0.45
1:C:290:LEU:HD22	1:C:295:PRO:HB3	1.98	0.44
1:A:93:ASN:O	1:D:66:PRO:HD2	2.18	0.44
1:C:430:LEU:O	1:C:433:PRO:HD2	2.18	0.44
1:C:369:TYR:CE2	1:C:384:LEU:HD23	2.53	0.44
1:A:276:ARG:CG	1:A:276:ARG:NH1	2.61	0.44
1:A:482:TRP:HB2	1:A:493:MET:HE2	1.99	0.44
1:C:433:PRO:HB2	1:C:439:LEU:HD23	2.00	0.44
1:D:512:VAL:HG23	3:D:607:HOH:O	2.18	0.44
1:C:354:VAL:HG13	1:C:384:LEU:HD11	2.00	0.44
1:B:90:LEU:HD12	1:B:90:LEU:HA	1.82	0.43
1:B:36:ARG:HH21	1:B:75:ASP:HB2	1.82	0.43
1:B:90:LEU:HD11	1:B:337:LEU:HB3	2.00	0.43
1:C:437:ASN:ND2	3:C:704:HOH:O	2.38	0.43
1:A:387:TYR:CE1	1:A:392:ARG:HG2	2.53	0.43
1:D:199:ILE:HG22	1:D:206:PRO:HG3	2.01	0.43
1:D:419:VAL:HG23	1:D:420:LEU:HD22	2.01	0.43
1:C:401:GLN:HA	1:C:404:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:509:GLU:HA	1:C:512:VAL:HG22	2.00	0.43
1:B:430:LEU:O	1:B:433:PRO:HD2	2.19	0.43
1:B:247:GLY:HA2	3:B:696:HOH:O	2.18	0.43
1:A:509:GLU:O	1:A:513:TRP:HD1	2.02	0.43
1:B:453:GLU:HB3	1:B:497:VAL:HG22	2.00	0.43
1:D:352:GLN:OE1	1:D:353:ARG:HG3	2.19	0.43
1:A:95:THR:HG23	1:A:443:GLY:HA3	2.01	0.42
1:C:23:LEU:HB3	1:C:38:ARG:HD2	2.01	0.42
1:C:150:GLY:HA3	1:C:466:ILE:HD12	2.01	0.42
1:A:449:GLY:O	1:A:454:ARG:CZ	2.67	0.42
1:C:48:GLY:O	1:C:74:ARG:NH2	2.53	0.42
1:C:461:MET:HG2	1:C:495:PHE:CD1	2.54	0.42
1:D:409:TRP:CE2	1:D:484:ARG:HG2	2.54	0.42
1:D:419:VAL:HG11	1:D:446:ARG:O	2.20	0.42
1:A:380:ARG:O	1:A:383:PRO:HD2	2.20	0.42
1:B:235:HIS:HE1	3:B:621:HOH:O	2.02	0.42
1:C:119:ARG:HB3	1:C:205:ASP:HB2	2.02	0.41
1:A:218:ALA:HB3	1:A:242:GLY:HA3	2.01	0.41
1:B:53:ARG:HD2	1:B:68:GLU:HG2	2.02	0.41
1:B:509:GLU:O	1:B:513:TRP:HD1	2.03	0.41
1:C:287:VAL:HG13	1:C:295:PRO:CG	2.50	0.41
1:D:138:ILE:HG23	1:D:140:TRP:CE3	2.56	0.41
1:B:199:ILE:HD12	1:B:199:ILE:HA	1.86	0.41
1:B:370:ARG:O	1:B:380:ARG:NE	2.53	0.41
1:A:95:THR:HG22	1:A:96:GLY:N	2.36	0.41
1:B:53:ARG:HG3	1:B:66:PRO:O	2.20	0.41
1:D:302:GLY:HA2	1:D:306:PRO:HA	2.01	0.41
1:C:328:ASN:O	1:C:331:GLU:HG2	2.21	0.41
1:D:59:LEU:HD23	1:D:59:LEU:HA	1.77	0.41
1:B:377:LEU:CD1	1:B:380:ARG:HH21	2.34	0.41
1:B:432:ILE:O	1:B:435:VAL:HG22	2.20	0.41
1:C:413:PHE:CZ	1:C:415:PHE:HB3	2.55	0.41
1:B:322:ALA:HB2	1:B:407:PRO:HG2	2.03	0.41
1:C:81:PRO:HG2	1:C:105:ASP:O	2.20	0.41
1:C:351:ARG:HG2	1:C:366:ILE:HD13	2.03	0.41
1:C:509:GLU:O	1:C:513:TRP:HD1	2.04	0.41
1:B:180:SER:HA	1:B:183:LEU:HG	2.03	0.41
1:B:513:TRP:HE3	1:B:518:VAL:HG13	1.86	0.41
1:D:328:ASN:O	1:D:331:GLU:HG2	2.22	0.40
1:D:466:ILE:O	1:D:470:ARG:CG	2.65	0.40
1:A:449:GLY:O	1:A:454:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ASP:O	1:C:120:ARG:NH1	2.52	0.40
1:D:329:LYS:HB3	1:D:329:LYS:HE2	1.80	0.40
1:D:387:TYR:HA	1:D:391:VAL:HB	2.03	0.40
1:C:35:VAL:HG13	1:C:70:TRP:HZ2	1.87	0.40
1:C:327:VAL:HG21	1:C:391:VAL:HG22	2.04	0.40
1:C:387:TYR:HA	1:C:391:VAL:HB	2.04	0.40
1:D:319:ARG:HA	1:D:404:VAL:CG2	2.52	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	492/527 (93%)	483 (98%)	9 (2%)	0	100	100
1	B	496/527 (94%)	487 (98%)	9 (2%)	0	100	100
1	C	491/527 (93%)	481 (98%)	10 (2%)	0	100	100
1	D	494/527 (94%)	486 (98%)	8 (2%)	0	100	100
All	All	1973/2108 (94%)	1937 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	355/383 (93%)	328 (92%)	27 (8%)	12	6
1	B	363/383 (95%)	341 (94%)	22 (6%)	17	9
1	C	359/383 (94%)	327 (91%)	32 (9%)	9	4
1	D	357/383 (93%)	332 (93%)	25 (7%)	14	7
All	All	1434/1532 (94%)	1328 (93%)	106 (7%)	13	6

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	53	ARG
1	A	59	LEU
1	A	62	ARG
1	A	71	SER
1	A	74	ARG
1	A	78	ARG
1	A	117	ASP
1	A	133	THR
1	A	138	ILE
1	A	170	GLU
1	A	212	PHE
1	A	273	GLU
1	A	276	ARG
1	A	290	LEU
1	A	313	LEU
1	A	329	LYS
1	A	345	ASP
1	A	355	GLU
1	A	358	VAL
1	A	381	LEU
1	A	424	LEU
1	A	454	ARG
1	A	461	MET
1	A	477	ASP
1	A	486	ASP
1	A	500	ARG
1	B	31	ARG
1	B	43	VAL
1	B	62	ARG
1	B	117	ASP
1	B	149	GLU
1	B	164	LEU

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Mol	Chain	Res	Type
1	B	263	GLN
1	B	268	GLU
1	B	272	ARG
1	B	281	ARG
1	B	313	LEU
1	B	345	ASP
1	B	347	GLU
1	B	367	GLU
1	B	370	ARG
1	B	420	LEU
1	B	440	ASP
1	B	457	VAL
1	B	461	MET
1	B	465	TRP
1	B	477	ASP
1	B	481	GLU
1	C	35	VAL
1	C	36	ARG
1	C	38	ARG
1	C	42	THR
1	C	43	VAL
1	C	53	ARG
1	C	59	LEU
1	C	74	ARG
1	C	78	ARG
1	C	94	LEU
1	C	115	SER
1	C	119	ARG
1	C	126	ILE
1	C	149	GLU
1	C	183	LEU
1	C	243	SER
1	C	246	LEU
1	C	321	VAL
1	C	337	LEU
1	C	358	VAL
1	C	374	GLU
1	C	381	LEU
1	C	384	LEU
1	C	403	ARG
1	C	441	ARG
1	C	459	GLN

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Mol	Chain	Res	Type
1	C	477	ASP
1	C	481	GLU
1	C	484	ARG
1	C	488	GLU
1	C	489	GLU
1	C	498	GLU
1	D	22	GLU
1	D	26	VAL
1	D	44	CYS
1	D	90	LEU
1	D	91	ILE
1	D	117	ASP
1	D	119	ARG
1	D	126	ILE
1	D	138	ILE
1	D	212	PHE
1	D	235	HIS
1	D	263	GLN
1	D	268	GLU
1	D	294	LEU
1	D	320	ASP
1	D	338	GLN
1	D	347	GLU
1	D	352	GLN
1	D	358	VAL
1	D	408	VAL
1	D	420	LEU
1	D	438	THR
1	D	459	GLN
1	D	470	ARG
1	D	488	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	263	GLN
1	C	352	GLN
1	D	473	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	C	601	-	4,4,4	0.49	0	6,6,6	0.10	0

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 ⓘ

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	494/527 (93%)	0.56	13 (2%) 57 59	33, 49, 74, 91	0
1	B	498/527 (94%)	0.61	29 (5%) 29 28	27, 49, 72, 108	0
1	C	493/527 (93%)	0.66	34 (6%) 23 22	29, 49, 84, 137	0
1	D	496/527 (94%)	0.63	36 (7%) 21 21	31, 49, 80, 109	0
All	All	1981/2108 (93%)	0.61	112 (5%) 29 29	27, 49, 78, 137	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	94	LEU	7.9
1	D	443	GLY	6.9
1	D	94	LEU	6.6
1	D	478	GLY	5.6
1	B	447	PHE	4.9
1	D	90	LEU	4.9
1	D	442	ALA	4.5
1	D	444	ALA	4.4
1	A	515	ALA	4.1
1	D	447	PHE	4.0
1	C	246	LEU	3.9
1	D	93	ASN	3.9
1	C	244	GLY	3.7
1	C	295	PRO	3.6
1	B	443	GLY	3.5
1	C	404	VAL	3.5
1	B	442	ALA	3.3
1	D	91	ILE	3.3
1	C	392	ARG	3.2
1	C	360	PRO	3.2
1	A	514	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	419	VAL	3.1
1	D	95	THR	3.0
1	B	480	PRO	3.0
1	C	357	VAL	2.9
1	A	172	ALA	2.9
1	C	245	ALA	2.9
1	D	445	ASP	2.9
1	D	37	GLY	2.9
1	D	140	TRP	2.9
1	A	290	LEU	2.8
1	D	497	VAL	2.8
1	C	168	TYR	2.8
1	B	97	GLY	2.8
1	C	287	VAL	2.8
1	A	495	PHE	2.8
1	C	292	PRO	2.8
1	D	370	ARG	2.7
1	A	29	GLU	2.7
1	D	89	ARG	2.7
1	B	482	TRP	2.7
1	D	479	LEU	2.7
1	C	466	ILE	2.7
1	B	95	THR	2.7
1	D	100	LEU	2.7
1	B	367	GLU	2.7
1	D	344	GLY	2.6
1	C	314	ALA	2.6
1	D	379	ARG	2.6
1	D	44	CYS	2.6
1	C	229	ALA	2.6
1	D	98	ALA	2.6
1	D	491	ALA	2.6
1	C	164	LEU	2.6
1	B	31	ARG	2.6
1	D	477	ASP	2.6
1	C	293	GLY	2.5
1	B	152	VAL	2.5
1	B	441	ARG	2.5
1	C	341	ALA	2.5
1	D	337	LEU	2.5
1	D	361	ALA	2.4
1	D	441	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	358	VAL	2.4
1	B	409	TRP	2.4
1	C	167	LEU	2.4
1	C	267	VAL	2.4
1	A	317	ALA	2.3
1	C	290	LEU	2.3
1	C	23	LEU	2.3
1	C	232	GLY	2.3
1	C	65	GLU	2.3
1	B	466	ILE	2.3
1	D	389	VAL	2.3
1	A	454	ARG	2.3
1	B	98	ALA	2.3
1	D	358	VAL	2.2
1	D	244	GLY	2.2
1	B	395	LEU	2.2
1	B	370	ARG	2.2
1	B	99	THR	2.2
1	C	269	PRO	2.2
1	D	345	ASP	2.2
1	A	223	VAL	2.2
1	D	512	VAL	2.2
1	C	359	GLY	2.2
1	C	275	LEU	2.2
1	D	346	ASP	2.2
1	C	177	PHE	2.1
1	C	336	ALA	2.1
1	A	225	LEU	2.1
1	B	275	LEU	2.1
1	B	357	VAL	2.1
1	B	89	ARG	2.1
1	B	460	ALA	2.1
1	B	368	PHE	2.1
1	C	368	PHE	2.1
1	A	261	VAL	2.1
1	B	492	VAL	2.1
1	B	90	LEU	2.1
1	A	269	PRO	2.1
1	D	373	GLY	2.1
1	A	259	ALA	2.1
1	C	172	ALA	2.1
1	B	23	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	478	GLY	2.0
1	D	302	GLY	2.0
1	B	245	ALA	2.0
1	C	288	ALA	2.0
1	C	278	LEU	2.0
1	C	74	ARG	2.0
1	B	32	TYR	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	SO4	C	601	5/5	0.92	0.08	38,46,53,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.