Full wwPDB X-ray Structure Validation Report (i)

Mar 3, 2025 – 06:10 PM JST

PDB ID	:	8YMA
Title	:	CRYSTAL STRUCTURE OF A NOVEL PU PLASTIC DEGRADATION ENZYME FROM THERMAEROBACTER MARIANENSIS
Authors	:	Li, Z.S.; Wang, H.; Gao, J.; Chen, Y.Y.; Wei, H.L.; Han, X.; Wei, R.; Bornscheuer, U.T.; Liu, W.D.
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 (i) 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 (i)) were used in the production of this report:

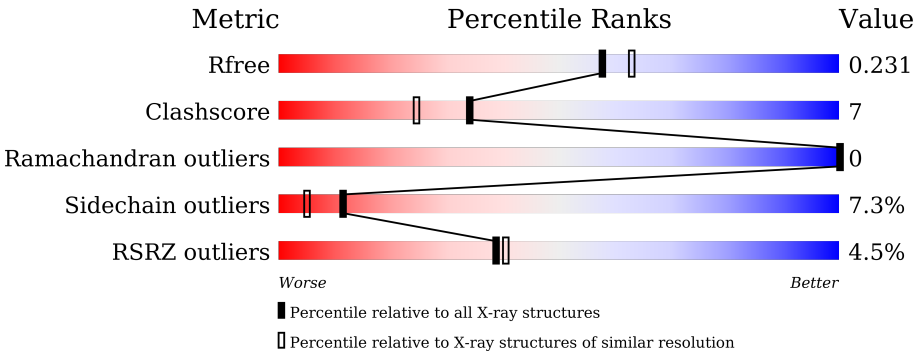
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	164625	3436 (2.08-2.04)
Clashscore	180529	3661 (2.08-2.04)
Ramachandran outliers	177936	3649 (2.08-2.04)
Sidechain outliers	177891	3649 (2.08-2.04)
RSRZ outliers	164620	3436 (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 <=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% 82% 11% • 6%
1	B	527	4% 79% 15% • 6%
1	C	527	5% 74% 18% • 6%
1	D	527	6% 79% 13% • 6%

2 Entry composition (i)

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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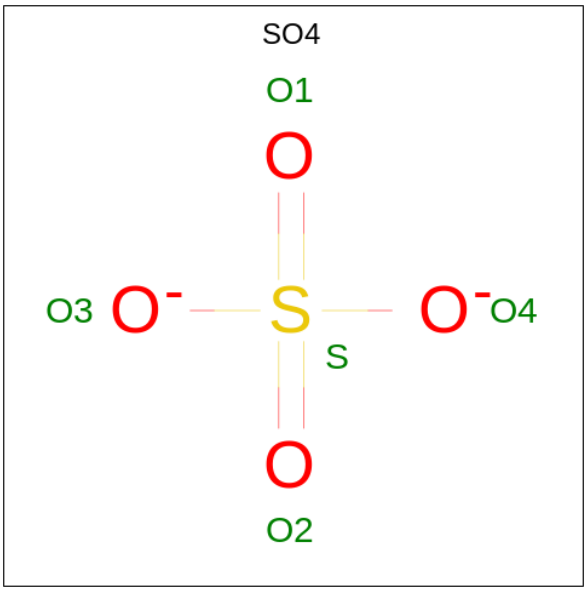
Chain	Residue	Modelled	Actual	Comment	Reference
C	11	GLY	-	expression tag	UNP E6SHQ4
C	12	ALA	-	expression tag	UNP E6SHQ4
C	13	GLY	-	expression tag	UNP E6SHQ4
C	14	ALA	-	expression tag	UNP E6SHQ4
C	15	GLY	-	expression tag	UNP E6SHQ4
C	16	ALA	-	expression tag	UNP E6SHQ4
D	-6	MET	-	initiating methionine	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 (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

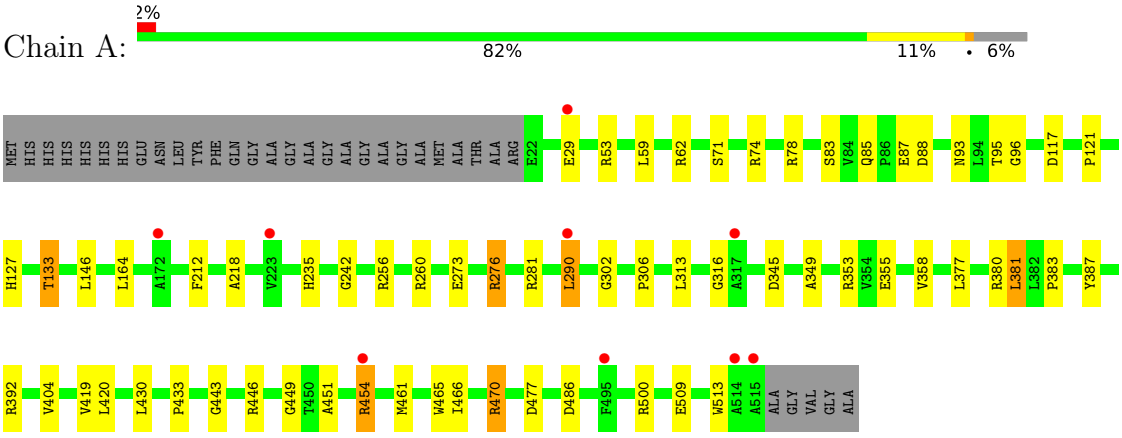
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	116	Total O 116 116	0	0
3	B	117	Total O 117 117	0	0
3	C	126	Total O 126 126	0	0
3	D	120	Total O 120 120	0	0

3 Residue-property plots

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

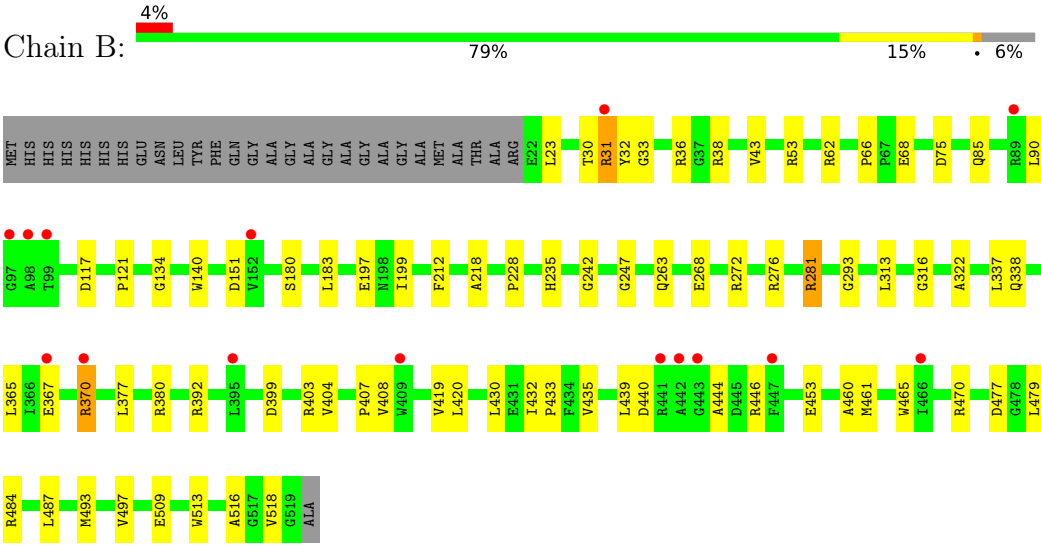
• Molecule 1: Carboxylic ester hydrolase

Chain A:



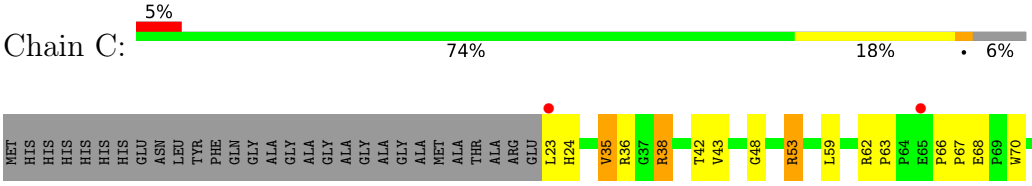
• Molecule 1: Carboxylic ester hydrolase

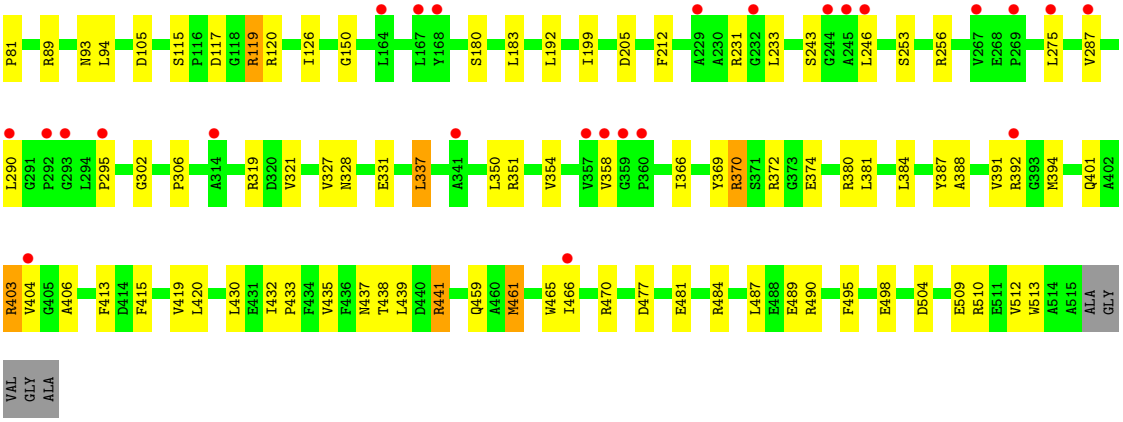
Chain B:



• Molecule 1: Carboxylic ester hydrolase

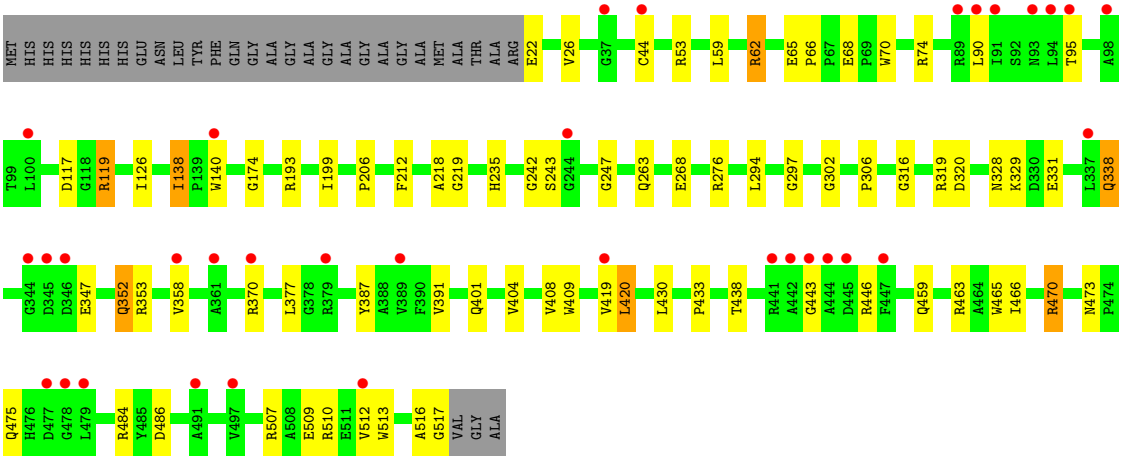
Chain C:





• Molecule 1: Carboxylic ester hydrolase

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	7697 reflections (5.03%)	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]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.55	0/3805	0.79	0/5204
1	B	0.58	0/3857	0.83	0/5270
1	C	0.57	0/3817	0.79	0/5218
1	D	0.57	0/3822	0.82	0/5226
All	All	0.57	0/15301	0.81	0/20918

There are no bond length outliers.

There are no bond angle outliers.

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	42	0
1	B	3755	0	3661	52	0
1	C	3715	0	3625	77	0
1	D	3720	0	3619	50	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	220	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 7.

All (220) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:377:LEU:HD13	1:B:380:ARG:NH2	2.20	0.56
1:B:479:LEU:HD22	1:B:493:MET:HE2	1.88	0.56
1:C:337:LEU:HD11	1:C:420:LEU:HD13	1.87	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:C:490:ARG:HD2	1:C:504:ASP:CG	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:87:GLU:O	1:A:88:ASP:C	2.47	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
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: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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:GLY:C	3:D:641:HOH:O	2.52	0.47
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: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
1:B:460:ALA:HB1	1:B:479:LEU:HD21	1.98	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:C:24:HIS:C	1:C:38:ARG:HD3	2.35	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:435:VAL:HG23	1:C:461:MET:HE1	1.97	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: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:D:516:ALA:O	1:D:517:GLY:C	2.56	0.44
1:A:276:ARG:CG	1:A:276:ARG:NH1	2.61	0.44
1:C:433:PRO:HB2	1:C:439:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:372:ARG:HH12	1:C:509:GLU:CD	2.21	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
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:B:30:THR:HG1	1:B:33:GLY:H	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	11 4
1	B	363/383 (95%)	344 (95%)	19 (5%)	19 12
1	C	359/383 (94%)	326 (91%)	33 (9%)	7 3
1	D	357/383 (93%)	331 (93%)	26 (7%)	11 5
All	All	1434/1532 (94%)	1329 (93%)	105 (7%)	11 5

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
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	212	PHE
1	A	235	HIS
1	A	273	GLU
1	A	276	ARG
1	A	281	ARG
1	A	290	LEU
1	A	313	LEU
1	A	345	ASP
1	A	355	GLU
1	A	358	VAL
1	A	381	LEU
1	A	454	ARG
1	A	461	MET

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Mol	Chain	Res	Type
1	A	465	TRP
1	A	470	ARG
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	212	PHE
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	461	MET
1	B	465	TRP
1	B	477	ASP
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	212	PHE
1	C	243	SER
1	C	246	LEU
1	C	275	LEU
1	C	321	VAL

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Mol	Chain	Res	Type
1	C	337	LEU
1	C	358	VAL
1	C	370	ARG
1	C	374	GLU
1	C	394	MET
1	C	403	ARG
1	C	441	ARG
1	C	459	GLN
1	C	461	MET
1	C	465	TRP
1	C	477	ASP
1	C	481	GLU
1	C	484	ARG
1	C	489	GLU
1	C	498	GLU
1	D	22	GLU
1	D	26	VAL
1	D	44	CYS
1	D	62	ARG
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	276	ARG
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	463	ARG
1	D	465	TRP
1	D	470	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	D	473	ASN

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

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	0.66	0	6,6,6	0.15	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 (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, 95^{th} 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%)	0.44	9 (1%)	67	69	33, 49, 74, 91	0
1	B	498/527 (94%)	0.50	19 (3%)	44	46	27, 49, 72, 108	0
1	C	493/527 (93%)	0.55	27 (5%)	32	33	29, 49, 84, 137	0
1	D	496/527 (94%)	0.52	34 (6%)	24	25	31, 49, 80, 109	0
All	All	1981/2108 (93%)	0.50	89 (4%)	39	40	27, 49, 78, 137	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	94	LEU	7.7
1	D	443	GLY	6.7
1	D	94	LEU	6.4
1	D	478	GLY	5.4
1	D	90	LEU	4.7
1	B	447	PHE	4.7
1	D	442	ALA	4.3
1	D	444	ALA	4.2
1	A	515	ALA	3.9
1	D	447	PHE	3.8
1	D	93	ASN	3.8
1	C	246	LEU	3.7
1	C	244	GLY	3.5
1	C	295	PRO	3.4
1	B	443	GLY	3.4
1	C	404	VAL	3.3
1	C	392	ARG	3.2
1	D	91	ILE	3.2
1	B	442	ALA	3.1
1	C	360	PRO	3.0
1	D	419	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	514	ALA	2.9
1	D	95	THR	2.9
1	B	480	PRO	2.8
1	D	445	ASP	2.8
1	C	357	VAL	2.8
1	A	172	ALA	2.7
1	C	245	ALA	2.7
1	D	37	GLY	2.7
1	A	290	LEU	2.7
1	D	497	VAL	2.7
1	D	370	ARG	2.7
1	A	29	GLU	2.7
1	C	168	TYR	2.7
1	B	97	GLY	2.7
1	D	89	ARG	2.7
1	D	140	TRP	2.7
1	C	287	VAL	2.6
1	C	292	PRO	2.6
1	B	367	GLU	2.6
1	A	495	PHE	2.6
1	C	466	ILE	2.6
1	D	479	LEU	2.6
1	B	95	THR	2.5
1	D	379	ARG	2.5
1	B	482	TRP	2.5
1	D	100	LEU	2.5
1	B	31	ARG	2.5
1	D	344	GLY	2.5
1	D	477	ASP	2.5
1	D	44	CYS	2.5
1	C	314	ALA	2.5
1	C	164	LEU	2.4
1	C	229	ALA	2.4
1	D	98	ALA	2.4
1	D	491	ALA	2.4
1	B	441	ARG	2.4
1	D	441	ARG	2.4
1	B	152	VAL	2.3
1	C	293	GLY	2.3
1	D	337	LEU	2.3
1	C	341	ALA	2.3
1	D	361	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	358	VAL	2.3
1	C	167	LEU	2.2
1	C	267	VAL	2.2
1	B	409	TRP	2.2
1	C	65	GLU	2.2
1	A	454	ARG	2.2
1	C	290	LEU	2.2
1	A	317	ALA	2.2
1	B	466	ILE	2.1
1	C	23	LEU	2.1
1	C	232	GLY	2.1
1	D	389	VAL	2.1
1	B	370	ARG	2.1
1	B	98	ALA	2.1
1	D	358	VAL	2.1
1	D	345	ASP	2.1
1	D	244	GLY	2.1
1	D	346	ASP	2.1
1	B	395	LEU	2.1
1	B	99	THR	2.1
1	C	269	PRO	2.0
1	B	89	ARG	2.0
1	A	223	VAL	2.0
1	D	512	VAL	2.0
1	C	275	LEU	2.0
1	C	359	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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, 95^{th} 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(Å^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.