



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 06:58 PM EDT

PDB ID : 7UTF
Title : Structure-Function characterization of an aldo-keto reductase involved in detoxification of the mycotoxin, deoxynivalenol
Authors : Abraham, N.; Schroeter, K.L.; Kimber, M.S.; Seah, S.Y.K.
Deposited on : 2022-04-26
Resolution : 2.50 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

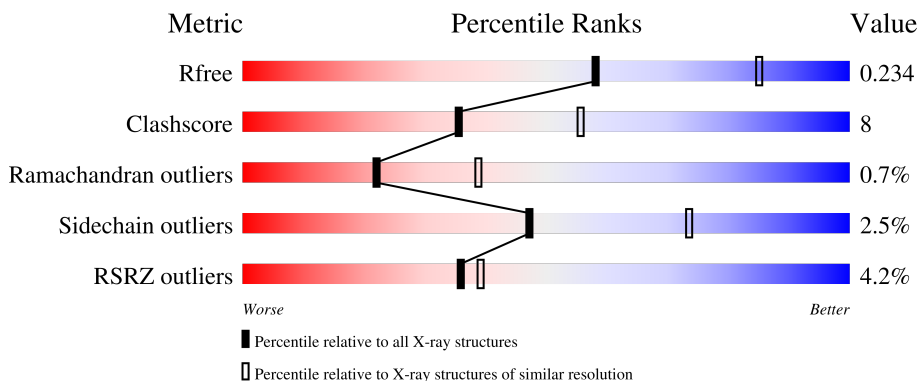
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	363	 2% 71% 16% • 12%
1	B	363	 % 72% 15% • 12%
1	C	363	 7% 68% 19% • 12%
1	D	363	 3% 74% 13% • 12%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 10584 atoms, of which 5 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putative oxidoreductase, aryl-alcohol dehydrogenase like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	321	Total 2476	C 1560	N 441	O 464	S 11	0	0	0
1	B	318	Total 2442	C 1538	N 434	O 459	S 11	0	0	0
1	C	318	Total 2454	C 1548	N 435	O 460	S 11	0	0	0
1	D	318	Total 2449	C 1544	N 434	O 460	S 11	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP J0WHR2
A	-19	GLY	-	expression tag	UNP J0WHR2
A	-18	SER	-	expression tag	UNP J0WHR2
A	-17	SER	-	expression tag	UNP J0WHR2
A	-16	HIS	-	expression tag	UNP J0WHR2
A	-15	HIS	-	expression tag	UNP J0WHR2
A	-14	HIS	-	expression tag	UNP J0WHR2
A	-13	HIS	-	expression tag	UNP J0WHR2
A	-12	HIS	-	expression tag	UNP J0WHR2
A	-11	HIS	-	expression tag	UNP J0WHR2
A	-10	SER	-	expression tag	UNP J0WHR2
A	-9	SER	-	expression tag	UNP J0WHR2
A	-8	GLY	-	expression tag	UNP J0WHR2
A	-7	LEU	-	expression tag	UNP J0WHR2
A	-6	VAL	-	expression tag	UNP J0WHR2
A	-5	PRO	-	expression tag	UNP J0WHR2
A	-4	ARG	-	expression tag	UNP J0WHR2
A	-3	GLY	-	expression tag	UNP J0WHR2
A	-2	SER	-	expression tag	UNP J0WHR2
A	-1	HIS	-	expression tag	UNP J0WHR2

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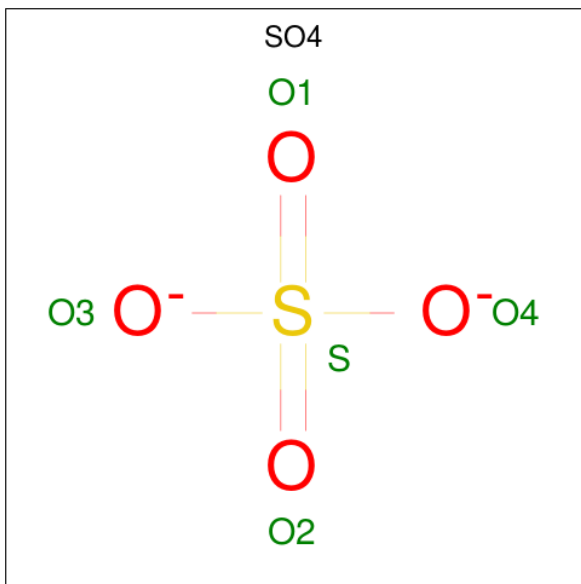
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	initiating methionine	UNP J0WHR2
B	-19	GLY	-	expression tag	UNP J0WHR2
B	-18	SER	-	expression tag	UNP J0WHR2
B	-17	SER	-	expression tag	UNP J0WHR2
B	-16	HIS	-	expression tag	UNP J0WHR2
B	-15	HIS	-	expression tag	UNP J0WHR2
B	-14	HIS	-	expression tag	UNP J0WHR2
B	-13	HIS	-	expression tag	UNP J0WHR2
B	-12	HIS	-	expression tag	UNP J0WHR2
B	-11	HIS	-	expression tag	UNP J0WHR2
B	-10	SER	-	expression tag	UNP J0WHR2
B	-9	SER	-	expression tag	UNP J0WHR2
B	-8	GLY	-	expression tag	UNP J0WHR2
B	-7	LEU	-	expression tag	UNP J0WHR2
B	-6	VAL	-	expression tag	UNP J0WHR2
B	-5	PRO	-	expression tag	UNP J0WHR2
B	-4	ARG	-	expression tag	UNP J0WHR2
B	-3	GLY	-	expression tag	UNP J0WHR2
B	-2	SER	-	expression tag	UNP J0WHR2
B	-1	HIS	-	expression tag	UNP J0WHR2
C	-20	MET	-	initiating methionine	UNP J0WHR2
C	-19	GLY	-	expression tag	UNP J0WHR2
C	-18	SER	-	expression tag	UNP J0WHR2
C	-17	SER	-	expression tag	UNP J0WHR2
C	-16	HIS	-	expression tag	UNP J0WHR2
C	-15	HIS	-	expression tag	UNP J0WHR2
C	-14	HIS	-	expression tag	UNP J0WHR2
C	-13	HIS	-	expression tag	UNP J0WHR2
C	-12	HIS	-	expression tag	UNP J0WHR2
C	-11	HIS	-	expression tag	UNP J0WHR2
C	-10	SER	-	expression tag	UNP J0WHR2
C	-9	SER	-	expression tag	UNP J0WHR2
C	-8	GLY	-	expression tag	UNP J0WHR2
C	-7	LEU	-	expression tag	UNP J0WHR2
C	-6	VAL	-	expression tag	UNP J0WHR2
C	-5	PRO	-	expression tag	UNP J0WHR2
C	-4	ARG	-	expression tag	UNP J0WHR2
C	-3	GLY	-	expression tag	UNP J0WHR2
C	-2	SER	-	expression tag	UNP J0WHR2
C	-1	HIS	-	expression tag	UNP J0WHR2
D	-20	MET	-	initiating methionine	UNP J0WHR2
D	-19	GLY	-	expression tag	UNP J0WHR2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	SER	-	expression tag	UNP J0WHR2
D	-17	SER	-	expression tag	UNP J0WHR2
D	-16	HIS	-	expression tag	UNP J0WHR2
D	-15	HIS	-	expression tag	UNP J0WHR2
D	-14	HIS	-	expression tag	UNP J0WHR2
D	-13	HIS	-	expression tag	UNP J0WHR2
D	-12	HIS	-	expression tag	UNP J0WHR2
D	-11	HIS	-	expression tag	UNP J0WHR2
D	-10	SER	-	expression tag	UNP J0WHR2
D	-9	SER	-	expression tag	UNP J0WHR2
D	-8	GLY	-	expression tag	UNP J0WHR2
D	-7	LEU	-	expression tag	UNP J0WHR2
D	-6	VAL	-	expression tag	UNP J0WHR2
D	-5	PRO	-	expression tag	UNP J0WHR2
D	-4	ARG	-	expression tag	UNP J0WHR2
D	-3	GLY	-	expression tag	UNP J0WHR2
D	-2	SER	-	expression tag	UNP J0WHR2
D	-1	HIS	-	expression tag	UNP J0WHR2

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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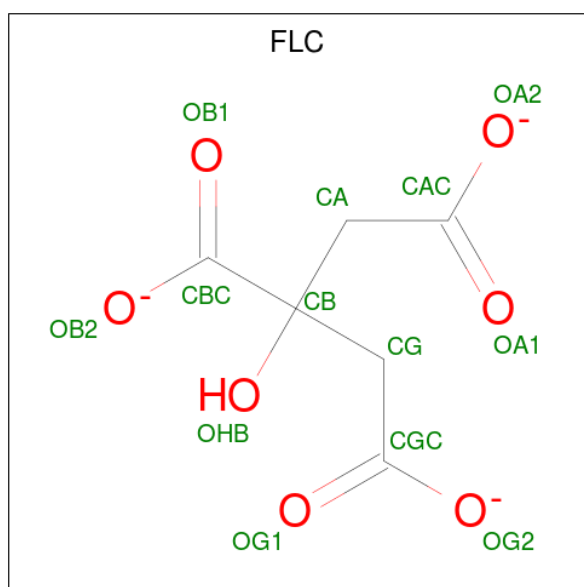
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B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

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

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7^-$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			18	6	5	7		

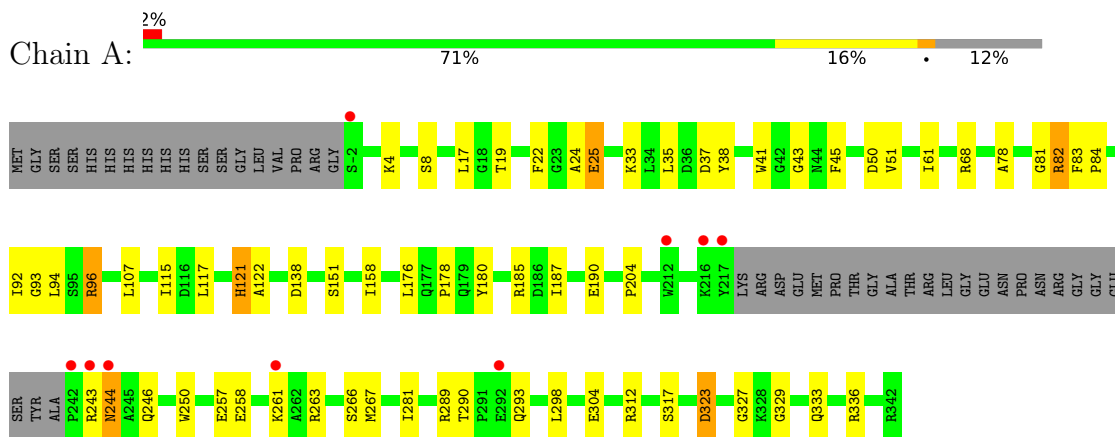
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total	O	0	0
			139	139		
4	B	153	Total	O	0	0
			153	153		
4	C	110	Total	O	0	0
			110	110		
4	D	173	Total	O	0	0
			173	173		

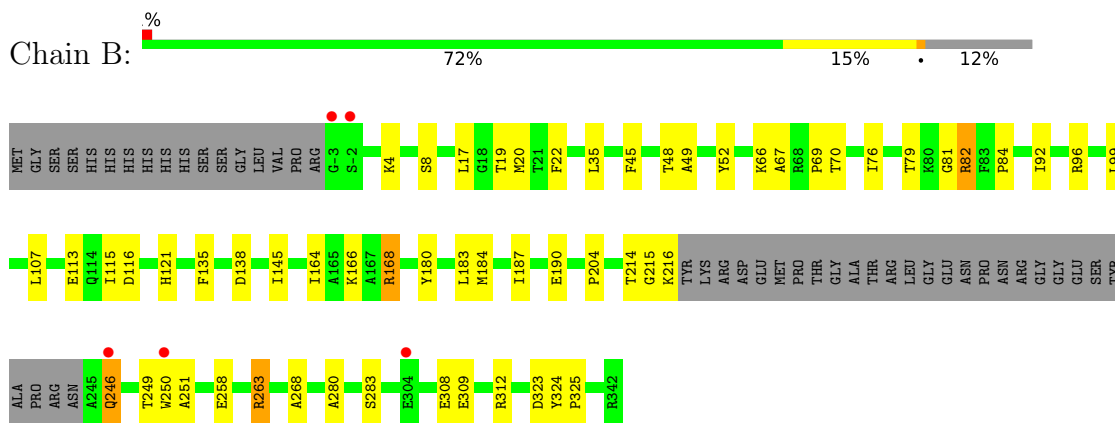
3 Residue-property plots [i](#)

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

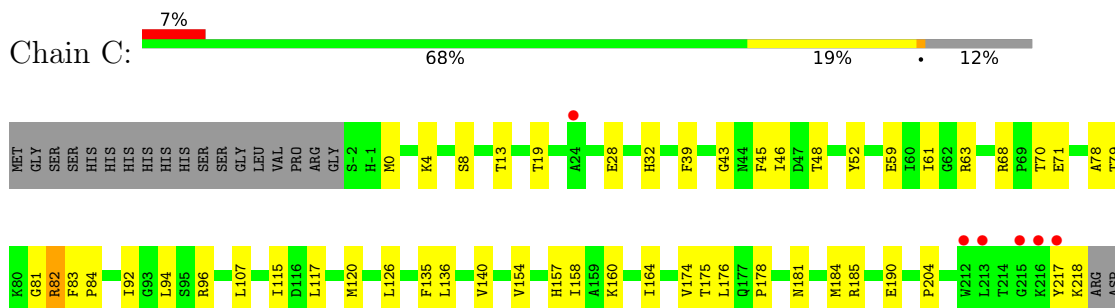
- Molecule 1: Putative oxidoreductase, aryl-alcohol dehydrogenase like protein

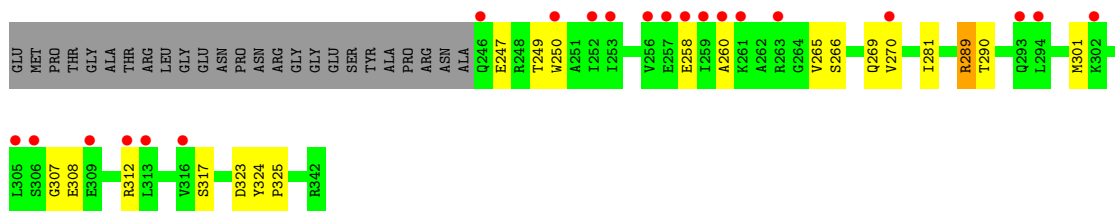


- Molecule 1: Putative oxidoreductase, aryl-alcohol dehydrogenase like protein

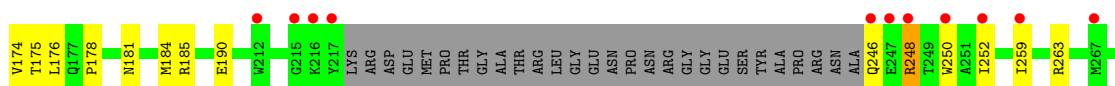
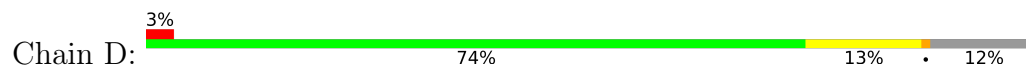


- Molecule 1: Putative oxidoreductase, aryl-alcohol dehydrogenase like protein





- Molecule 1: Putative oxidoreductase, aryl-alcohol dehydrogenase like protein



4 Data and refinement statistics i

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.45Å 159.45Å 163.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.45 – 2.50 48.19 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.45-2.50) 82.6 (48.19-2.10)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.34 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.185 , 0.234 0.185 , 0.234	Depositor DCC
R_{free} test set	6143 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtrriage
Anisotropy	0.210	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.021 for -h,l,k 0.000 for -l,-k,-h	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10584	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.37 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.0925e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: FLC, 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	0.24	0/2530	0.48	0/3425
1	B	0.24	0/2494	0.47	0/3376
1	C	0.24	0/2507	0.47	0/3393
1	D	0.24	0/2502	0.47	0/3387
All	All	0.24	0/10033	0.47	0/13581

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 [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	2476	0	2445	44	0
1	B	2442	0	2412	41	0
1	C	2454	0	2426	48	0
1	D	2449	0	2416	32	0
2	A	40	0	0	1	0
2	B	50	0	0	2	0
2	C	40	0	0	3	0
2	D	40	0	0	0	0
3	A	13	5	5	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	139	0	0	3	0
4	B	153	0	0	6	0
4	C	110	0	0	4	0
4	D	173	0	0	3	0
All	All	10579	5	9704	160	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 (160) 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)
3:A:409:FLC:OHB	3:A:409:FLC:OG1	1.91	0.87
1:D:263:ARG:NH2	1:D:304:GLU:O	2.12	0.82
1:B:308:GLU:OE2	1:B:312:ARG:NH1	2.18	0.76
1:A:289:ARG:HD2	1:A:290:THR:HG23	1.68	0.74
1:C:307:GLY:N	2:C:407:SO4:O3	2.20	0.73
2:A:404:SO4:O4	4:A:501:HOH:O	2.07	0.72
1:D:342:ARG:NH1	4:D:501:HOH:O	2.22	0.72
1:A:4:LYS:HE3	1:A:8:SER:O	1.90	0.71
1:D:248:ARG:NH1	1:D:320:GLN:OE1	2.26	0.69
1:A:336:ARG:HD3	1:C:126:LEU:HD12	1.75	0.67
1:B:280:ALA:N	2:B:407:SO4:O4	2.21	0.66
1:D:96:ARG:NH1	4:D:503:HOH:O	2.29	0.65
1:C:19:THR:HG21	1:C:61:ILE:HD11	1.77	0.64
1:A:83:PHE:HB3	1:A:84:PRO:HD2	1.80	0.64
1:B:4:LYS:HE3	1:B:8:SER:O	1.98	0.63
1:A:243:ARG:HG2	1:B:250:TRP:CZ2	2.33	0.63
1:A:258:GLU:HG2	1:A:312:ARG:HH22	1.63	0.63
1:D:246:GLN:O	1:D:250:TRP:HD1	1.81	0.63
1:D:19:THR:HG21	1:D:61:ILE:HD11	1.79	0.63
1:D:311:ALA:O	1:D:315:GLU:HG3	1.99	0.62
1:A:289:ARG:O	1:A:289:ARG:HG2	1.98	0.62
1:B:204:PRO:HD2	1:B:283:SER:O	1.99	0.62
1:A:257:GLU:HB3	1:A:267:MET:SD	2.41	0.61
1:C:174:VAL:HG23	1:C:175:THR:HG23	1.81	0.61
1:B:263:ARG:HD2	1:B:309:GLU:OE1	2.00	0.61
1:D:83:PHE:HB3	1:D:84:PRO:HD2	1.83	0.60
1:A:33:LYS:HE2	1:A:37:ASP:OD1	2.02	0.60
1:B:82:ARG:HB3	1:B:121:HIS:HB3	1.83	0.59
1:B:48:THR:O	1:B:79:THR:HA	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:PRO:HG3	1:C:92:ILE:HD12	1.85	0.59
1:D:181:ASN:HD21	1:D:184:MET:CE	2.15	0.59
1:B:17:LEU:CD2	1:B:35:LEU:HD23	2.33	0.58
1:A:289:ARG:HD2	1:A:290:THR:CG2	2.33	0.58
2:C:408:SO4:O3	4:C:501:HOH:O	2.16	0.58
1:C:96:ARG:HD2	4:C:511:HOH:O	2.03	0.57
1:B:246:GLN:HG3	1:B:250:TRP:HE1	1.70	0.57
1:B:17:LEU:HD23	1:B:35:LEU:HD23	1.87	0.56
1:A:244:ASN:N	1:A:244:ASN:OD1	2.39	0.55
1:A:336:ARG:CD	1:C:126:LEU:HD12	2.36	0.55
1:C:96:ARG:HH12	1:C:135:PHE:HA	1.70	0.55
1:C:70:THR:HB	2:C:401:SO4:O1	2.07	0.55
1:B:99:LEU:HB3	1:B:135:PHE:CE2	2.41	0.54
1:C:260:ALA:HB2	1:C:270:VAL:HG21	1.89	0.54
1:B:66:LYS:HE3	4:B:587:HOH:O	2.08	0.54
1:C:4:LYS:HE3	1:C:8:SER:O	2.08	0.54
1:C:181:ASN:HD21	1:C:184:MET:CE	2.21	0.54
1:C:82:ARG:HB2	1:C:94:LEU:HD21	1.89	0.54
1:A:51:VAL:HG11	1:A:83:PHE:HB2	1.90	0.54
1:C:260:ALA:HB1	1:C:265:VAL:O	2.08	0.53
1:A:263:ARG:NH1	1:A:304:GLU:O	2.39	0.52
1:A:185:ARG:HD3	1:A:317:SER:O	2.10	0.52
1:C:204:PRO:HG3	1:C:281:ILE:HD12	1.91	0.52
1:B:82:ARG:HB3	1:B:121:HIS:CB	2.39	0.52
1:B:84:PRO:HG2	1:D:342:ARG:HG2	1.90	0.52
1:A:176:LEU:O	1:A:178:PRO:HD3	2.10	0.51
1:C:218:LYS:HD2	1:C:250:TRP:CH2	2.45	0.51
1:A:122:ALA:HA	1:A:151:SER:O	2.11	0.51
1:C:28:GLU:CD	1:C:63:ARG:HE	2.13	0.51
1:C:28:GLU:OE1	1:C:63:ARG:NH2	2.41	0.51
1:C:258:GLU:OE1	1:C:312:ARG:NH1	2.43	0.51
1:C:289:ARG:HG3	1:C:290:THR:HG23	1.92	0.51
1:D:17:LEU:HD23	1:D:35:LEU:HD23	1.93	0.50
1:C:96:ARG:NH1	4:C:511:HOH:O	2.45	0.50
1:C:154:VAL:O	1:C:158:ILE:HG12	2.11	0.50
1:D:94:LEU:HD22	1:D:120:MET:SD	2.51	0.50
1:B:20:MET:HE2	4:B:632:HOH:O	2.11	0.50
1:C:48:THR:O	1:C:79:THR:HA	2.11	0.49
1:A:33:LYS:HE2	1:A:37:ASP:CG	2.33	0.49
1:A:78:ALA:HB2	1:A:117:LEU:HB3	1.94	0.49
1:D:174:VAL:HG23	1:D:175:THR:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:MET:HA	4:C:529:HOH:O	2.12	0.49
1:D:181:ASN:HD21	1:D:184:MET:HE3	1.78	0.48
1:D:259:ILE:HD13	1:D:309:GLU:HB3	1.94	0.48
1:A:25:GLU:OE1	1:A:25:GLU:N	2.46	0.48
1:C:68:ARG:HH21	1:C:71:GLU:CD	2.17	0.48
1:C:59:GLU:O	1:C:63:ARG:HG2	2.13	0.48
1:B:92:ILE:HD11	4:B:604:HOH:O	2.13	0.48
1:D:81:GLY:O	1:D:82:ARG:CB	2.61	0.48
1:D:181:ASN:HD21	1:D:184:MET:HE2	1.76	0.48
1:B:96:ARG:NH2	1:B:138:ASP:OD2	2.47	0.47
1:D:38:TYR:CZ	1:D:43:GLY:HA3	2.50	0.47
1:B:115:ILE:O	1:B:145:ILE:HA	2.16	0.46
1:C:176:LEU:O	1:C:178:PRO:HD3	2.16	0.46
1:B:184:MET:CE	1:D:324:TYR:HB3	2.45	0.46
1:A:81:GLY:O	1:A:82:ARG:CB	2.63	0.46
1:A:329:GLY:O	1:A:333:GLN:HG3	2.16	0.46
1:C:120:MET:HA	1:C:120:MET:HE2	1.97	0.46
1:C:136:LEU:O	1:C:140:VAL:HG23	2.16	0.46
1:B:19:THR:HG22	1:B:22:PHE:CE2	2.51	0.46
1:C:39:PHE:CE1	1:C:46:ILE:HD11	2.51	0.46
1:C:83:PHE:HB3	1:C:84:PRO:CD	2.45	0.46
1:B:76:ILE:HA	1:B:116:ASP:OD2	2.16	0.46
1:B:107:LEU:HD23	1:B:115:ILE:HG13	1.97	0.46
1:D:185:ARG:NH1	1:D:318:ALA:HA	2.31	0.45
1:A:17:LEU:HD23	1:A:35:LEU:HD23	1.99	0.45
1:A:107:LEU:HD23	1:A:115:ILE:HG13	1.98	0.45
1:D:82:ARG:HB3	1:D:121:HIS:HB3	1.97	0.45
1:C:324:TYR:HA	1:C:325:PRO:HA	1.77	0.45
1:D:176:LEU:O	1:D:178:PRO:HD3	2.16	0.45
1:C:13:THR:HG21	1:C:43:GLY:HA2	1.97	0.45
1:A:82:ARG:HB3	1:A:121:HIS:CB	2.47	0.45
1:A:323:ASP:HA	1:A:327:GLY:HA3	1.99	0.45
1:C:78:ALA:HA	1:C:117:LEU:O	2.17	0.44
1:C:185:ARG:HD3	1:C:317:SER:O	2.17	0.44
1:D:56:LYS:HD2	1:D:59:GLU:OE1	2.17	0.44
1:B:180:TYR:CD1	1:B:187:ILE:HD11	2.51	0.44
1:C:160:LYS:O	1:C:164:ILE:HG13	2.17	0.44
1:A:19:THR:HG21	1:A:61:ILE:HD11	1.99	0.44
1:B:183:LEU:HD22	1:B:249:THR:HG23	1.99	0.44
1:D:71:GLU:OE1	1:D:71:GLU:N	2.46	0.44
1:D:154:VAL:HG22	1:D:157:HIS:ND1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:VAL:HB	1:C:269:GLN:OE1	2.17	0.44
1:A:96:ARG:NH2	1:A:138:ASP:OD2	2.49	0.44
1:A:261:LYS:HD3	1:B:308:GLU:CG	2.48	0.44
1:B:113:GLU:HG2	4:B:514:HOH:O	2.17	0.44
1:B:215:GLY:O	1:B:216:LYS:HB2	2.17	0.44
1:A:24:ALA:HB1	1:A:25:GLU:OE1	2.18	0.44
1:C:81:GLY:O	1:C:82:ARG:CB	2.66	0.44
1:D:82:ARG:HB3	1:D:121:HIS:CB	2.48	0.44
1:A:41:TRP:CG	1:A:298:LEU:HD13	2.54	0.43
1:A:250:TRP:CD1	1:B:251:ALA:HA	2.54	0.43
1:C:308:GLU:CD	1:C:312:ARG:HH21	2.22	0.43
1:A:94:LEU:HD12	4:A:589:HOH:O	2.19	0.43
1:D:252:ILE:HD11	1:D:317:SER:HA	2.00	0.43
1:D:329:GLY:O	1:D:333:GLN:HG3	2.18	0.43
1:C:154:VAL:HG22	1:C:157:HIS:ND1	2.33	0.43
1:C:181:ASN:HD21	1:C:184:MET:HE2	1.83	0.43
1:A:38:TYR:CZ	1:A:43:GLY:HA3	2.54	0.42
1:A:92:ILE:HG12	1:A:93:GLY:N	2.33	0.42
1:B:67:ALA:O	1:B:69:PRO:HD3	2.19	0.42
1:C:154:VAL:HG22	1:C:157:HIS:CE1	2.54	0.42
1:A:4:LYS:NZ	4:A:513:HOH:O	2.50	0.42
1:A:204:PRO:HG3	1:A:281:ILE:HD12	2.01	0.42
1:A:290:THR:OG1	1:A:293:GLN:HG2	2.19	0.42
1:B:81:GLY:O	1:B:82:ARG:CB	2.65	0.42
1:C:154:VAL:O	1:C:157:HIS:HB2	2.20	0.42
1:A:243:ARG:HG2	1:B:250:TRP:CH2	2.53	0.42
1:B:70:THR:N	2:B:401:SO4:O1	2.46	0.42
1:A:68:ARG:HD3	3:A:409:FLC:OB2	2.20	0.42
1:B:49:ALA:HB3	1:B:52:TYR:CE1	2.55	0.42
1:C:218:LYS:HB2	1:C:250:TRP:CH2	2.55	0.42
1:B:324:TYR:CD1	1:B:325:PRO:HA	2.54	0.42
1:D:288:ALA:CB	1:D:294:LEU:HD13	2.49	0.41
1:D:288:ALA:HB3	1:D:294:LEU:HD13	2.02	0.41
1:B:258:GLU:HG2	4:B:559:HOH:O	2.20	0.41
1:B:49:ALA:HB3	1:B:52:TYR:CD1	2.56	0.41
1:B:166:LYS:NZ	4:B:520:HOH:O	2.53	0.41
1:B:214:THR:HG22	1:B:268:ALA:HB2	2.02	0.41
1:C:107:LEU:HD23	1:C:115:ILE:HG13	2.01	0.41
1:B:81:GLY:O	1:B:82:ARG:HB2	2.20	0.41
1:C:266:SER:OG	1:C:269:GLN:HG3	2.21	0.41
1:A:19:THR:HG22	1:A:22:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:LYS:HE3	1:D:4:LYS:HB3	1.76	0.41
1:D:337:LYS:HE3	4:D:584:HOH:O	2.21	0.41
1:B:164:ILE:O	1:B:168:ARG:HG3	2.21	0.41
1:C:39:PHE:HE1	1:C:46:ILE:HD11	1.86	0.41
1:A:50:ASP:OD1	1:A:51:VAL:N	2.54	0.41
1:A:158:ILE:HD11	1:A:176:LEU:HD22	2.03	0.41
1:A:180:TYR:CD1	1:A:187:ILE:HD11	2.56	0.40
1:C:218:LYS:CB	1:C:250:TRP:HH2	2.35	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	317/363 (87%)	299 (94%)	16 (5%)	2 (1%)	25	43
1	B	314/363 (86%)	301 (96%)	11 (4%)	2 (1%)	25	43
1	C	314/363 (86%)	300 (96%)	11 (4%)	3 (1%)	15	28
1	D	314/363 (86%)	300 (96%)	12 (4%)	2 (1%)	25	43
All	All	1259/1452 (87%)	1200 (95%)	50 (4%)	9 (1%)	22	39

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	B	82	ARG
1	C	82	ARG
1	D	82	ARG
1	C	190	GLU
1	D	190	GLU
1	A	190	GLU

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Mol	Chain	Res	Type
1	B	190	GLU
1	C	52	TYR

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	249/282 (88%)	241 (97%)	8 (3%)	39 65
1	B	245/282 (87%)	240 (98%)	5 (2%)	55 79
1	C	247/282 (88%)	239 (97%)	8 (3%)	39 65
1	D	246/282 (87%)	242 (98%)	4 (2%)	62 84
All	All	987/1128 (88%)	962 (98%)	25 (2%)	47 73

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	45	PHE
1	A	96	ARG
1	A	121	HIS
1	A	244	ASN
1	A	246	GLN
1	A	266	SER
1	A	323	ASP
1	B	45	PHE
1	B	168	ARG
1	B	246	GLN
1	B	263	ARG
1	B	323	ASP
1	C	0	MET
1	C	32	HIS
1	C	45	PHE
1	C	217	TYR
1	C	247	GLU
1	C	249	THR

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Mol	Chain	Res	Type
1	C	289	ARG
1	C	323	ASP
1	D	45	PHE
1	D	96	ARG
1	D	152	ASN
1	D	248	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	GLN
1	D	179	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

35 ligands are 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	A	401	-	4,4,4	0.14	0	6,6,6	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	D	401	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	C	407	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	408	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	404	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	402	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	A	403	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	407	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	402	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	402	-	4,4,4	0.14	0	6,6,6	0.05	0
3	FLC	A	409	-	12,12,12	1.04	0	17,17,17	1.97	5 (29%)
2	SO4	A	407	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	408	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	405	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	410	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	D	406	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	A	405	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	405	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	404	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	404	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	404	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	408	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	403	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	407	-	4,4,4	0.15	0	6,6,6	0.04	0
2	SO4	C	401	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	402	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	403	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	409	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	405	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	408	-	4,4,4	0.12	0	6,6,6	0.08	0
2	SO4	A	406	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	403	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	406	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	C	406	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	401	-	4,4,4	0.14	0	6,6,6	0.05	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FLC	A	409	-	-	4/16/16/16	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	409	FLC	OB2-CBC-CB	4.52	120.89	113.05
3	A	409	FLC	CB-CA-CAC	-3.14	106.20	113.81
3	A	409	FLC	CB-CG-CGC	-2.54	107.67	113.81
3	A	409	FLC	CG-CB-CA	2.25	115.03	109.16
3	A	409	FLC	OG2-CGC-CG	2.12	121.16	114.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	409	FLC	CA-CB-CG-CGC
3	A	409	FLC	CBC-CB-CG-CGC
3	A	409	FLC	OHB-CB-CG-CGC
3	A	409	FLC	CAC-CA-CB-CBC

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	407	SO4	1	0
3	A	409	FLC	2	0
2	A	404	SO4	1	0
2	B	407	SO4	1	0
2	C	401	SO4	1	0
2	C	408	SO4	1	0
2	B	401	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	321/363 (88%)	-0.21	9 (2%) 53 56	34, 49, 91, 130	0
1	B	318/363 (87%)	-0.26	5 (1%) 72 74	35, 53, 87, 135	0
1	C	318/363 (87%)	0.14	27 (8%) 10 10	42, 67, 111, 170	0
1	D	318/363 (87%)	-0.16	12 (3%) 40 43	34, 51, 96, 142	0
All	All	1275/1452 (87%)	-0.12	53 (4%) 36 39	34, 55, 100, 170	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	217	TYR	6.0
1	C	217	TYR	5.2
1	C	215	GLY	5.1
1	A	217	TYR	4.9
1	B	-2	SER	4.9
1	C	250	TRP	4.8
1	C	261	LYS	4.7
1	C	256	VAL	4.4
1	D	246	GLN	4.1
1	D	248	ARG	4.0
1	D	250	TRP	3.8
1	C	212	TRP	3.8
1	C	216	LYS	3.5
1	C	252	ILE	3.3
1	D	212	TRP	3.3
1	C	253	ILE	3.3
1	C	24	ALA	3.2
1	C	312	ARG	3.2
1	C	213	LEU	3.1
1	C	257	GLU	3.1
1	D	247	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	246	GLN	3.0
1	C	305	LEU	2.9
1	A	242	PRO	2.8
1	C	316	VAL	2.8
1	A	243	ARG	2.8
1	A	292	GLU	2.7
1	C	306	SER	2.6
1	C	270	VAL	2.5
1	A	212	TRP	2.5
1	C	302	LYS	2.5
1	D	-2	SER	2.5
1	D	215	GLY	2.5
1	B	246	GLN	2.5
1	C	260	ALA	2.4
1	A	216	LYS	2.4
1	A	261	LYS	2.4
1	A	-2	SER	2.4
1	C	258	GLU	2.3
1	D	259	ILE	2.3
1	C	294	LEU	2.3
1	C	309	GLU	2.3
1	C	263	ARG	2.2
1	D	216	LYS	2.2
1	D	252	ILE	2.2
1	A	244	ASN	2.1
1	B	-3	GLY	2.1
1	B	250	TRP	2.1
1	D	267	MET	2.1
1	B	304	GLU	2.0
1	C	259	ILE	2.0
1	C	313	LEU	2.0
1	C	293	GLN	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, 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(Å ²)	Q<0.9
2	SO4	B	407	5/5	0.79	0.21	66,71,91,99	5
2	SO4	C	401	5/5	0.79	0.18	118,120,123,128	5
2	SO4	C	407	5/5	0.79	0.27	94,102,112,121	5
2	SO4	B	405	5/5	0.81	0.16	90,93,96,111	5
2	SO4	D	408	5/5	0.83	0.13	103,107,110,117	5
2	SO4	B	404	5/5	0.85	0.22	95,99,110,115	0
2	SO4	C	406	5/5	0.85	0.16	95,103,119,120	0
2	SO4	A	407	5/5	0.87	0.19	91,94,109,110	5
2	SO4	A	404	5/5	0.87	0.17	74,77,112,117	5
2	SO4	D	407	5/5	0.88	0.14	89,99,122,123	0
2	SO4	C	408	5/5	0.88	0.32	105,115,123,157	0
3	FLC	A	409	13/13	0.88	0.24	49,76,87,87	18
2	SO4	C	404	5/5	0.89	0.20	83,90,100,101	5
2	SO4	B	410	5/5	0.89	0.26	102,104,148,194	5
2	SO4	D	401	5/5	0.89	0.27	85,86,90,92	5
2	SO4	B	401	5/5	0.90	0.12	86,91,95,97	5
2	SO4	B	408	5/5	0.90	0.21	110,112,121,130	5
2	SO4	A	406	5/5	0.92	0.17	76,80,114,116	0
2	SO4	B	409	5/5	0.93	0.11	91,95,106,106	5
2	SO4	A	408	5/5	0.93	0.08	70,74,96,104	5
2	SO4	D	402	5/5	0.93	0.06	87,88,101,109	0
2	SO4	D	403	5/5	0.94	0.13	82,82,84,87	5
2	SO4	B	406	5/5	0.94	0.13	59,62,73,96	0
2	SO4	A	401	5/5	0.94	0.09	94,98,117,120	0
2	SO4	C	403	5/5	0.94	0.15	56,56,62,68	5
2	SO4	B	402	5/5	0.95	0.15	58,59,62,66	5
2	SO4	C	402	5/5	0.95	0.14	50,60,71,72	5
2	SO4	D	405	5/5	0.95	0.17	56,57,62,76	5
2	SO4	A	405	5/5	0.96	0.09	60,69,83,87	0
2	SO4	A	403	5/5	0.96	0.18	72,72,78,79	5
2	SO4	B	403	5/5	0.96	0.15	70,76,81,85	5
2	SO4	D	406	5/5	0.97	0.10	65,74,81,90	0
2	SO4	D	404	5/5	0.97	0.10	49,55,61,70	5
2	SO4	A	402	5/5	0.98	0.08	44,48,54,59	0
2	SO4	C	405	5/5	0.98	0.09	72,84,87,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.