



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2024 – 10:36 AM EST

PDB ID : 3MEN
Title : Crystal structure of acetylpolyamine aminohydrolase from Burkholderia pseudomallei, iodide soak
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2010-03-31
Resolution : 2.20 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 : 2.36
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) : 2.36

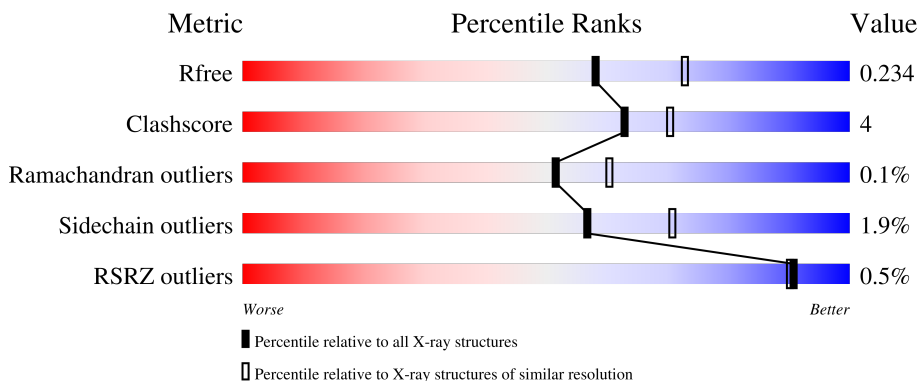
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	362	84% 10% 6%
1	B	362	89% 6% 6%
1	C	362	86% 6% 7%
1	D	362	85% 9% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	IOD	A	348	-	-	X	-
5	IOD	D	350	-	-	X	-

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 10859 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 Acetyl polyamine aminohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	339	2585	1636	470	469	10	0	1	0
1	B	342	2608	1650	475	472	11	0	2	0
1	C	337	2512	1591	455	457	9	0	0	0
1	D	339	2565	1626	466	463	10	0	2	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q3JUN4
A	-19	ALA	-	expression tag	UNP Q3JUN4
A	-18	HIS	-	expression tag	UNP Q3JUN4
A	-17	HIS	-	expression tag	UNP Q3JUN4
A	-16	HIS	-	expression tag	UNP Q3JUN4
A	-15	HIS	-	expression tag	UNP Q3JUN4
A	-14	HIS	-	expression tag	UNP Q3JUN4
A	-13	HIS	-	expression tag	UNP Q3JUN4
A	-12	MET	-	expression tag	UNP Q3JUN4
A	-11	GLY	-	expression tag	UNP Q3JUN4
A	-10	THR	-	expression tag	UNP Q3JUN4
A	-9	LEU	-	expression tag	UNP Q3JUN4
A	-8	GLU	-	expression tag	UNP Q3JUN4
A	-7	ALA	-	expression tag	UNP Q3JUN4
A	-6	GLN	-	expression tag	UNP Q3JUN4
A	-5	THR	-	expression tag	UNP Q3JUN4
A	-4	GLN	-	expression tag	UNP Q3JUN4
A	-3	GLY	-	expression tag	UNP Q3JUN4
A	-2	PRO	-	expression tag	UNP Q3JUN4
A	-1	GLY	-	expression tag	UNP Q3JUN4
A	0	SER	-	expression tag	UNP Q3JUN4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	expression tag	UNP Q3JUN4
B	-19	ALA	-	expression tag	UNP Q3JUN4
B	-18	HIS	-	expression tag	UNP Q3JUN4
B	-17	HIS	-	expression tag	UNP Q3JUN4
B	-16	HIS	-	expression tag	UNP Q3JUN4
B	-15	HIS	-	expression tag	UNP Q3JUN4
B	-14	HIS	-	expression tag	UNP Q3JUN4
B	-13	HIS	-	expression tag	UNP Q3JUN4
B	-12	MET	-	expression tag	UNP Q3JUN4
B	-11	GLY	-	expression tag	UNP Q3JUN4
B	-10	THR	-	expression tag	UNP Q3JUN4
B	-9	LEU	-	expression tag	UNP Q3JUN4
B	-8	GLU	-	expression tag	UNP Q3JUN4
B	-7	ALA	-	expression tag	UNP Q3JUN4
B	-6	GLN	-	expression tag	UNP Q3JUN4
B	-5	THR	-	expression tag	UNP Q3JUN4
B	-4	GLN	-	expression tag	UNP Q3JUN4
B	-3	GLY	-	expression tag	UNP Q3JUN4
B	-2	PRO	-	expression tag	UNP Q3JUN4
B	-1	GLY	-	expression tag	UNP Q3JUN4
B	0	SER	-	expression tag	UNP Q3JUN4
C	-20	MET	-	expression tag	UNP Q3JUN4
C	-19	ALA	-	expression tag	UNP Q3JUN4
C	-18	HIS	-	expression tag	UNP Q3JUN4
C	-17	HIS	-	expression tag	UNP Q3JUN4
C	-16	HIS	-	expression tag	UNP Q3JUN4
C	-15	HIS	-	expression tag	UNP Q3JUN4
C	-14	HIS	-	expression tag	UNP Q3JUN4
C	-13	HIS	-	expression tag	UNP Q3JUN4
C	-12	MET	-	expression tag	UNP Q3JUN4
C	-11	GLY	-	expression tag	UNP Q3JUN4
C	-10	THR	-	expression tag	UNP Q3JUN4
C	-9	LEU	-	expression tag	UNP Q3JUN4
C	-8	GLU	-	expression tag	UNP Q3JUN4
C	-7	ALA	-	expression tag	UNP Q3JUN4
C	-6	GLN	-	expression tag	UNP Q3JUN4
C	-5	THR	-	expression tag	UNP Q3JUN4
C	-4	GLN	-	expression tag	UNP Q3JUN4
C	-3	GLY	-	expression tag	UNP Q3JUN4
C	-2	PRO	-	expression tag	UNP Q3JUN4
C	-1	GLY	-	expression tag	UNP Q3JUN4
C	0	SER	-	expression tag	UNP Q3JUN4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	expression tag	UNP Q3JUN4
D	-19	ALA	-	expression tag	UNP Q3JUN4
D	-18	HIS	-	expression tag	UNP Q3JUN4
D	-17	HIS	-	expression tag	UNP Q3JUN4
D	-16	HIS	-	expression tag	UNP Q3JUN4
D	-15	HIS	-	expression tag	UNP Q3JUN4
D	-14	HIS	-	expression tag	UNP Q3JUN4
D	-13	HIS	-	expression tag	UNP Q3JUN4
D	-12	MET	-	expression tag	UNP Q3JUN4
D	-11	GLY	-	expression tag	UNP Q3JUN4
D	-10	THR	-	expression tag	UNP Q3JUN4
D	-9	LEU	-	expression tag	UNP Q3JUN4
D	-8	GLU	-	expression tag	UNP Q3JUN4
D	-7	ALA	-	expression tag	UNP Q3JUN4
D	-6	GLN	-	expression tag	UNP Q3JUN4
D	-5	THR	-	expression tag	UNP Q3JUN4
D	-4	GLN	-	expression tag	UNP Q3JUN4
D	-3	GLY	-	expression tag	UNP Q3JUN4
D	-2	PRO	-	expression tag	UNP Q3JUN4
D	-1	GLY	-	expression tag	UNP Q3JUN4
D	0	SER	-	expression tag	UNP Q3JUN4

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	9	Total I 9 9	0	0
5	B	9	Total I 9 9	0	0
5	C	8	Total I 8 8	0	0
5	D	9	Total I 9 9	0	0


- Molecule 6 is water.

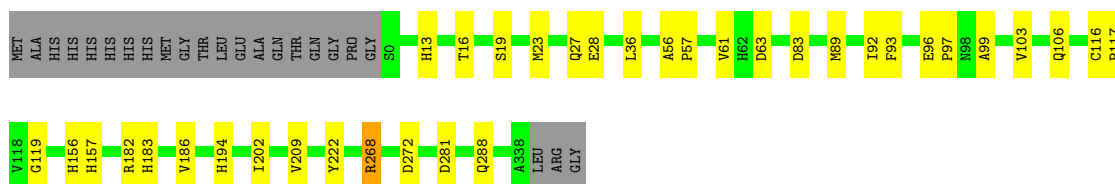
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	204	Total O 204 204	0	0
6	B	124	Total O 124 124	0	0
6	C	77	Total O 77 77	0	0
6	D	111	Total O 111 111	0	0

3 Residue-property plots [i](#)


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

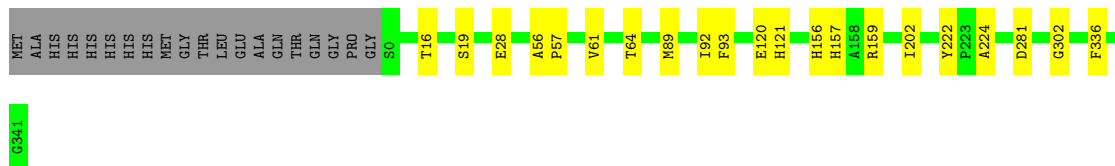
- Molecule 1: Acetylpolyamine aminohydrolase

Chain A: 




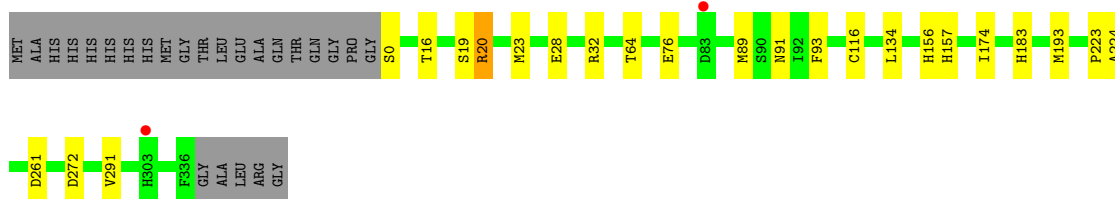
- Molecule 1: Acetylpolyamine aminohydrolase

Chain B: 




- Molecule 1: Acetylpolyamine aminohydrolase

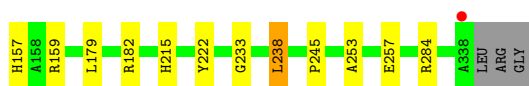
Chain C: 



- Molecule 1: Acetylpolyamine aminohydrolase

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	45.70Å 162.12Å 173.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 44.19 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-2.20) 98.1 (44.19-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.25 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.179 , 0.237 0.179 , 0.234	Depositor DCC
R_{free} test set	3315 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtrriage
Anisotropy	0.011	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10859	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: ZN, IOD, SO4, K

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	0.85	1/2664 (0.0%)	0.79	3/3632 (0.1%)
1	B	0.71	0/2690	0.75	2/3667 (0.1%)
1	C	0.65	1/2585 (0.0%)	0.73	1/3532 (0.0%)
1	D	0.70	0/2647	0.76	3/3613 (0.1%)
All	All	0.73	2/10586 (0.0%)	0.76	9/14444 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	116	CYS	CB-SG	-5.39	1.73	1.81
1	A	222	TYR	CD2-CE2	5.28	1.47	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ASP	CB-CG-OD1	8.19	125.67	118.30
1	D	159	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	A	268	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	B	281	ASP	CB-CG-OD1	6.09	123.78	118.30
1	D	32	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	D	238	LEU	CA-CB-CG	5.83	128.70	115.30
1	B	159	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	C	32	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	281	ASP	CB-CG-OD2	-5.02	113.78	118.30

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	2585	0	2422	27	0
1	B	2608	0	2445	13	0
1	C	2512	0	2323	23	0
1	D	2565	0	2390	31	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	1	0
3	B	10	0	0	1	0
3	C	5	0	0	1	0
3	D	10	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	9	0	0	5	0
5	B	9	0	0	1	0
5	C	8	0	0	2	0
5	D	9	0	0	9	0
6	A	204	0	0	3	0
6	B	124	0	0	2	0
6	C	77	0	0	0	0
6	D	111	0	0	2	0
All	All	10859	0	9580	85	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 4.

All (85) 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)
5:D:347:IOD:I	6:D:360:HOH:O	2.54	0.94
1:C:16:THR:HG21	1:C:89:MET:SD	2.08	0.93
1:C:89:MET:HE2	1:D:21:GLY:HA2	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:MET:HE3	1:D:18:PHE:HZ	1.39	0.88
5:B:348:IOD:I	6:B:424:HOH:O	2.63	0.86
1:A:16:THR:HG23	1:A:23:MET:CE	2.08	0.84
1:C:16:THR:CG2	1:C:89:MET:SD	2.65	0.83
5:A:349:IOD:I	6:A:480:HOH:O	2.66	0.82
1:D:157:HIS:NE2	3:D:401:SO4:O2	2.16	0.79
1:C:89:MET:HE3	1:D:18:PHE:CZ	2.19	0.76
1:A:16:THR:HG23	1:A:23:MET:HE3	1.67	0.76
1:C:19:SER:HB2	5:C:348:IOD:I	2.62	0.69
1:C:89:MET:CE	1:D:21:GLY:HA2	2.23	0.67
1:A:16:THR:HG23	1:A:23:MET:HE1	1.79	0.64
1:B:61:VAL:CG1	1:B:202:ILE:HD13	2.28	0.63
1:B:61:VAL:HG13	1:B:202:ILE:HD13	1.80	0.63
1:D:141:ARG:HG3	5:D:350:IOD:I	2.69	0.62
1:D:16:THR:HG21	1:D:89:MET:SD	2.42	0.60
1:A:16:THR:HG21	1:A:89:MET:SD	2.42	0.59
1:C:16:THR:HG22	1:C:89:MET:SD	2.41	0.59
1:D:284[B]:ARG:HH11	1:D:284[B]:ARG:CG	2.15	0.58
1:A:61:VAL:HG13	1:A:202:ILE:HD13	1.85	0.58
1:B:157:HIS:NE2	3:B:401:SO4:O2	2.39	0.56
1:D:253:ALA:O	1:D:257:GLU:HG3	2.07	0.55
1:D:16:THR:HG22	1:D:89:MET:CE	2.38	0.54
1:A:61:VAL:CG1	1:A:202:ILE:HD13	2.38	0.53
1:A:157:HIS:NE2	3:A:401:SO4:O2	2.41	0.53
1:A:16:THR:CG2	1:A:89:MET:SD	2.97	0.53
1:D:16:THR:CG2	1:D:89:MET:SD	2.97	0.52
1:A:106:GLN:OE1	5:A:348:IOD:I	2.97	0.52
1:C:93:PHE:HB3	1:D:93:PHE:HB3	1.92	0.51
1:A:93:PHE:CZ	1:B:93:PHE:CE1	2.98	0.51
1:C:0:SER:OG	1:C:0:SER:O	2.26	0.51
1:A:183:HIS:HB3	1:A:272:ASP:HB2	1.92	0.51
1:A:93:PHE:CE1	1:B:93:PHE:CE1	2.99	0.50
1:D:284[B]:ARG:CG	1:D:284[B]:ARG:NH1	2.75	0.50
1:D:182:ARG:HG2	5:D:350:IOD:I	2.82	0.50
1:A:92:ILE:HD13	1:B:224:ALA:HB3	1.93	0.49
1:C:183:HIS:HB3	1:C:272:ASP:HB2	1.94	0.49
1:D:179:LEU:HA	5:D:350:IOD:I	2.83	0.48
1:D:215:HIS:O	1:D:245:PRO:HA	2.14	0.48
1:C:19:SER:O	1:C:20:ARG:C	2.53	0.47
1:A:19:SER:HB2	5:A:347:IOD:I	2.84	0.47
1:C:193:MET:SD	1:C:291:VAL:HG12	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:THR:HG23	1:C:23:MET:CE	2.46	0.46
1:D:6:HIS:CD2	1:D:128:TRP:CE3	3.03	0.46
1:A:16:THR:HG22	1:A:89:MET:CE	2.45	0.46
1:A:268:ARG:NE	6:A:520:HOH:O	2.49	0.46
1:D:182:ARG:CG	5:D:350:IOD:I	3.34	0.46
1:B:56:ALA:HB3	1:B:57:PRO:HD3	1.97	0.45
1:D:55:ILE:HG22	6:D:439:HOH:O	2.16	0.45
1:D:19:SER:HB2	5:D:349:IOD:I	2.86	0.45
1:D:12:HIS:CE1	1:D:14:PRO:CG	3.01	0.44
1:D:12:HIS:CE1	1:D:14:PRO:HG3	2.53	0.44
1:D:141:ARG:CG	5:D:350:IOD:I	3.35	0.44
1:B:120:GLU:OE2	1:B:121:HIS:CE1	2.71	0.43
1:D:20:ARG:O	1:D:24:ARG:NH2	2.50	0.43
1:D:284[B]:ARG:NH1	1:D:284[B]:ARG:HG3	2.33	0.43
1:B:16:THR:CG2	1:B:89:MET:SD	3.06	0.43
1:A:56:ALA:HB3	1:A:57:PRO:HD3	2.01	0.43
1:A:83:ASP:HB2	6:A:532:HOH:O	2.18	0.43
1:C:93:PHE:CZ	1:D:93:PHE:CE1	3.07	0.43
1:D:233:GLY:O	1:D:238:LEU:HD13	2.19	0.43
1:C:93:PHE:CE1	1:D:93:PHE:CE1	3.07	0.42
1:A:93:PHE:CE1	1:B:93:PHE:CZ	3.08	0.42
1:C:76:GLU:HG3	5:C:344:IOD:I	2.89	0.42
1:D:182:ARG:HB2	5:D:350:IOD:I	2.89	0.42
1:A:119:GLY:HA3	5:A:343:IOD:I	2.90	0.42
1:B:302:GLY:O	1:B:336:PHE:HA	2.20	0.42
1:C:223:PRO:O	1:C:224:ALA:HB3	2.20	0.42
1:D:222:TYR:HB2	5:D:343:IOD:I	2.90	0.42
1:A:194:HIS:CE1	1:A:288:GLN:OE1	2.72	0.41
1:C:16:THR:HG23	1:C:23:MET:HE3	2.01	0.41
1:C:157:HIS:NE2	3:C:401:SO4:O2	2.53	0.41
1:A:116:CYS:N	1:A:117:PRO:CD	2.83	0.41
1:B:157:HIS:CE1	1:B:222:TYR:HE2	2.38	0.41
1:A:96:GLU:HA	1:A:97:PRO:C	2.41	0.41
1:A:103:VAL:HG23	5:A:348:IOD:I	2.90	0.41
1:A:186:VAL:O	1:A:209:VAL:HA	2.21	0.41
1:B:64:THR:HG23	1:C:261:ASP:OD1	2.20	0.41
1:A:36:LEU:HD23	1:A:36:LEU:HA	1.91	0.40
1:A:99:ALA:HB3	6:B:411:HOH:O	2.21	0.40
1:C:134:LEU:HD21	1:C:174:ILE:CG2	2.51	0.40
1:C:134:LEU:HD21	1:C:174:ILE:HG22	2.03	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	338/362 (93%)	328 (97%)	10 (3%)	0	100	100
1	B	342/362 (94%)	333 (97%)	9 (3%)	0	100	100
1	C	335/362 (92%)	316 (94%)	18 (5%)	1 (0%)	41	46
1	D	339/362 (94%)	330 (97%)	9 (3%)	0	100	100
All	All	1354/1448 (94%)	1307 (96%)	46 (3%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	20	ARG

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	247/272 (91%)	240 (97%)	7 (3%)	43	56
1	B	249/272 (92%)	245 (98%)	4 (2%)	62	76
1	C	234/272 (86%)	230 (98%)	4 (2%)	60	74
1	D	242/272 (89%)	238 (98%)	4 (2%)	60	74
All	All	972/1088 (89%)	953 (98%)	19 (2%)	57	69

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13[A]	HIS
1	A	13[B]	HIS
1	A	27	GLN
1	A	28	GLU
1	A	63	ASP
1	A	156	HIS
1	A	182	ARG
1	B	19	SER
1	B	28	GLU
1	B	92	ILE
1	B	156	HIS
1	C	28	GLU
1	C	64	THR
1	C	91	ASN
1	C	156	HIS
1	D	28	GLU
1	D	61	VAL
1	D	75	ARG
1	D	156	HIS

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

Mol	Chain	Res	Type
1	A	106	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](#)

Of 49 ligands modelled in this entry, 43 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
3	SO4	B	403	-	4,4,4	0.14	0	6,6,6	0.58	0
3	SO4	C	401	2	4,4,4	0.18	0	6,6,6	0.59	0
3	SO4	D	401	2	4,4,4	0.12	0	6,6,6	0.75	0
3	SO4	B	401	2	4,4,4	0.31	0	6,6,6	0.27	0
3	SO4	A	401	2	4,4,4	0.31	0	6,6,6	0.52	0
3	SO4	D	403	-	4,4,4	0.22	0	6,6,6	0.38	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.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	SO4	1	0
3	D	401	SO4	1	0
3	B	401	SO4	1	0
3	A	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	339/362 (93%)	-0.75	0 100 100	9, 18, 33, 39	0
1	B	342/362 (94%)	-0.60	0 100 100	15, 25, 40, 46	0
1	C	337/362 (93%)	-0.29	2 (0%) 89 88	19, 36, 55, 67	0
1	D	339/362 (93%)	-0.41	5 (1%) 73 72	10, 29, 48, 61	0
All	All	1357/1448 (93%)	-0.51	7 (0%) 91 90	9, 27, 49, 67	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	338	ALA	3.8
1	D	17	TYR	3.1
1	D	16	THR	2.6
1	D	44	GLY	2.5
1	D	41	PHE	2.3
1	C	303	HIS	2.3
1	C	83	ASP	2.1

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
3	SO4	D	403	5/5	0.79	0.22	66,69,71,71	0
5	IOD	C	347	1/1	0.90	0.10	57,57,57,57	1
5	IOD	C	346	1/1	0.92	0.07	46,46,46,46	1
3	SO4	B	403	5/5	0.94	0.18	58,59,60,60	0
4	K	C	402	1/1	0.94	0.20	57,57,57,57	0
5	IOD	D	349	1/1	0.94	0.09	38,38,38,38	1
3	SO4	C	401	5/5	0.95	0.17	47,49,52,55	0
5	IOD	B	350	1/1	0.96	0.07	44,44,44,44	1
5	IOD	D	344	1/1	0.96	0.06	45,45,45,45	1
5	IOD	B	346	1/1	0.96	0.07	45,45,45,45	1
5	IOD	D	350	1/1	0.96	0.07	34,34,34,34	1
3	SO4	D	401	5/5	0.97	0.13	33,35,39,40	0
5	IOD	C	348	1/1	0.97	0.13	43,43,43,43	1
5	IOD	D	342	1/1	0.97	0.08	38,38,38,38	0
5	IOD	A	348	1/1	0.97	0.06	39,39,39,39	1
5	IOD	D	345	1/1	0.97	0.06	47,47,47,47	1
5	IOD	C	343	1/1	0.97	0.05	42,42,42,42	1
5	IOD	A	350	1/1	0.97	0.08	41,41,41,41	1
5	IOD	A	346	1/1	0.98	0.06	44,44,44,44	1
5	IOD	B	347	1/1	0.98	0.08	39,39,39,39	1
5	IOD	C	349	1/1	0.98	0.09	40,40,40,40	1
5	IOD	B	348	1/1	0.98	0.11	47,47,47,47	1
5	IOD	D	343	1/1	0.98	0.08	44,44,44,44	1
5	IOD	A	347	1/1	0.98	0.05	36,36,36,36	1
2	ZN	D	400	1/1	0.98	0.07	50,50,50,50	0
5	IOD	D	347	1/1	0.98	0.11	40,40,40,40	1
5	IOD	C	344	1/1	0.98	0.05	46,46,46,46	1
2	ZN	C	400	1/1	0.98	0.05	55,55,55,55	0
5	IOD	B	342	1/1	0.99	0.05	42,42,42,42	0
5	IOD	B	343	1/1	0.99	0.06	38,38,38,38	0
5	IOD	A	345	1/1	0.99	0.04	38,38,38,38	0
3	SO4	B	401	5/5	0.99	0.12	29,35,38,40	0
2	ZN	A	400	1/1	0.99	0.04	36,36,36,36	0
5	IOD	B	349	1/1	0.99	0.07	38,38,38,38	1
4	K	B	402	1/1	0.99	0.11	39,39,39,39	0
5	IOD	C	342	1/1	0.99	0.07	40,40,40,40	0
5	IOD	D	346	1/1	0.99	0.08	46,46,46,46	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	IOD	A	349	1/1	0.99	0.07	36,36,36,36	1
5	IOD	D	348	1/1	0.99	0.05	44,44,44,44	1
3	SO4	A	401	5/5	0.99	0.12	23,28,31,33	0
5	IOD	C	345	1/1	0.99	0.05	47,47,47,47	1
5	IOD	B	344	1/1	1.00	0.04	38,38,38,38	0
5	IOD	B	345	1/1	1.00	0.04	43,43,43,43	1
4	K	D	402	1/1	1.00	0.05	37,37,37,37	0
5	IOD	A	342	1/1	1.00	0.09	23,23,23,23	0
5	IOD	A	343	1/1	1.00	0.04	34,34,34,34	0
5	IOD	A	344	1/1	1.00	0.05	36,36,36,36	0
2	ZN	B	400	1/1	1.00	0.03	43,43,43,43	0
4	K	A	402	1/1	1.00	0.06	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.