Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 10:20 AM EST

PDB ID	:	1VI9
Title	:	Crystal structure of pyridoxamine kinase
Authors	:	Structural GenomiX
Deposited on	:	2003-12-01
Resolution	:	1.96 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:

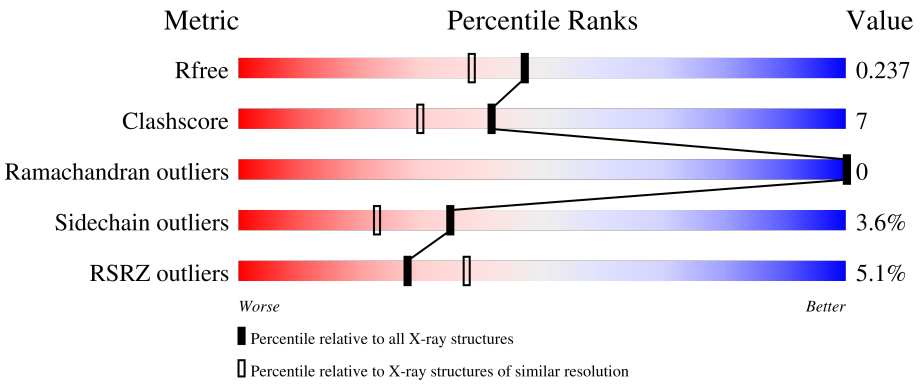
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	299	5% 80% 15% • •
1	B	299	5% 82% 13% • •
1	C	299	7% 76% 17% • •
1	D	299	3% 83% 12% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9760 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 Pyridoxamine kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	288	2200	1401	382	403	5	9	0	1	0
1	B	288	2205	1403	384	405	5	8	0	0	0
1	C	288	2198	1401	381	402	5	9	0	1	0
1	D	288	2203	1403	381	405	5	9	0	1	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	cloning artifact	UNP P77150
A	0	SER	-	cloning artifact	UNP P77150
A	1	LEU	-	cloning artifact	UNP P77150
A	2	MSE	MET	modified residue	UNP P77150
A	26	MSE	MET	modified residue	UNP P77150
A	53	CSD	CYS	modified residue	UNP P77150
A	55	MSE	MET	modified residue	UNP P77150
A	115	MSE	MET	modified residue	UNP P77150
A	196	MSE	MET	modified residue	UNP P77150
A	216	MSE	MET	modified residue	UNP P77150
A	255	MSE	MET	modified residue	UNP P77150
A	261	MSE	MET	modified residue	UNP P77150
A	288	GLU	-	cloning artifact	UNP P77150
A	289	GLY	-	cloning artifact	UNP P77150
A	290	GLY	-	cloning artifact	UNP P77150
A	291	SER	-	cloning artifact	UNP P77150
A	292	HIS	-	cloning artifact	UNP P77150
A	293	HIS	-	cloning artifact	UNP P77150
A	294	HIS	-	cloning artifact	UNP P77150
A	295	HIS	-	cloning artifact	UNP P77150
A	296	HIS	-	cloning artifact	UNP P77150

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Chain	Residue	Modelled	Actual	Comment	Reference
A	297	HIS	-	cloning artifact	UNP P77150
B	-1	MSE	-	cloning artifact	UNP P77150
B	0	SER	-	cloning artifact	UNP P77150
B	1	LEU	-	cloning artifact	UNP P77150
B	2	MSE	MET	modified residue	UNP P77150
B	26	MSE	MET	modified residue	UNP P77150
B	53	CSD	CYS	modified residue	UNP P77150
B	55	MSE	MET	modified residue	UNP P77150
B	115	MSE	MET	modified residue	UNP P77150
B	196	MSE	MET	modified residue	UNP P77150
B	216	MSE	MET	modified residue	UNP P77150
B	255	MSE	MET	modified residue	UNP P77150
B	261	MSE	MET	modified residue	UNP P77150
B	288	GLU	-	cloning artifact	UNP P77150
B	289	GLY	-	cloning artifact	UNP P77150
B	290	GLY	-	cloning artifact	UNP P77150
B	291	SER	-	cloning artifact	UNP P77150
B	292	HIS	-	cloning artifact	UNP P77150
B	293	HIS	-	cloning artifact	UNP P77150
B	294	HIS	-	cloning artifact	UNP P77150
B	295	HIS	-	cloning artifact	UNP P77150
B	296	HIS	-	cloning artifact	UNP P77150
B	297	HIS	-	cloning artifact	UNP P77150
C	-1	MSE	-	cloning artifact	UNP P77150
C	0	SER	-	cloning artifact	UNP P77150
C	1	LEU	-	cloning artifact	UNP P77150
C	2	MSE	MET	modified residue	UNP P77150
C	26	MSE	MET	modified residue	UNP P77150
C	53	CSD	CYS	modified residue	UNP P77150
C	55	MSE	MET	modified residue	UNP P77150
C	115	MSE	MET	modified residue	UNP P77150
C	196	MSE	MET	modified residue	UNP P77150
C	216	MSE	MET	modified residue	UNP P77150
C	255	MSE	MET	modified residue	UNP P77150
C	261	MSE	MET	modified residue	UNP P77150
C	288	GLU	-	cloning artifact	UNP P77150
C	289	GLY	-	cloning artifact	UNP P77150
C	290	GLY	-	cloning artifact	UNP P77150
C	291	SER	-	cloning artifact	UNP P77150
C	292	HIS	-	cloning artifact	UNP P77150
C	293	HIS	-	cloning artifact	UNP P77150
C	294	HIS	-	cloning artifact	UNP P77150

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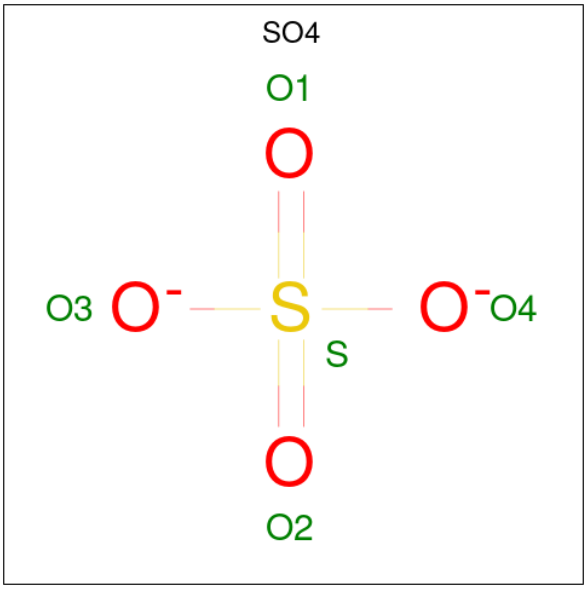
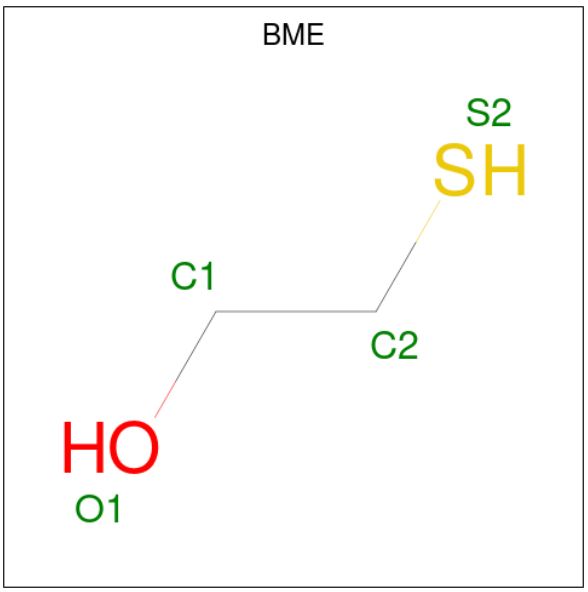
Chain	Residue	Modelled	Actual	Comment	Reference
C	295	HIS	-	cloning artifact	UNP P77150
C	296	HIS	-	cloning artifact	UNP P77150
C	297	HIS	-	cloning artifact	UNP P77150
D	-1	MSE	-	cloning artifact	UNP P77150
D	0	SER	-	cloning artifact	UNP P77150
D	1	LEU	-	cloning artifact	UNP P77150
D	2	MSE	MET	modified residue	UNP P77150
D	26	MSE	MET	modified residue	UNP P77150
D	53	CSD	CYS	modified residue	UNP P77150
D	55	MSE	MET	modified residue	UNP P77150
D	115	MSE	MET	modified residue	UNP P77150
D	196	MSE	MET	modified residue	UNP P77150
D	216	MSE	MET	modified residue	UNP P77150
D	255	MSE	MET	modified residue	UNP P77150
D	261	MSE	MET	modified residue	UNP P77150
D	288	GLU	-	cloning artifact	UNP P77150
D	289	GLY	-	cloning artifact	UNP P77150
D	290	GLY	-	cloning artifact	UNP P77150
D	291	SER	-	cloning artifact	UNP P77150
D	292	HIS	-	cloning artifact	UNP P77150
D	293	HIS	-	cloning artifact	UNP P77150
D	294	HIS	-	cloning artifact	UNP P77150
D	295	HIS	-	cloning artifact	UNP P77150
D	296	HIS	-	cloning artifact	UNP P77150
D	297	HIS	-	cloning artifact	UNP P77150

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
3	B	1	4	2	1	1	0	0
3	D	1	7	4	2	1	0	1

- Molecule 4 is water.

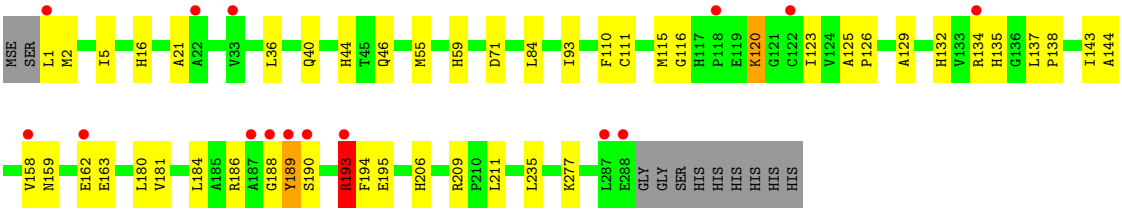
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	235	235	235	0	0
4	B	241	241	241	0	0
4	C	216	216	216	0	0
4	D	231	231	231	0	0

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.

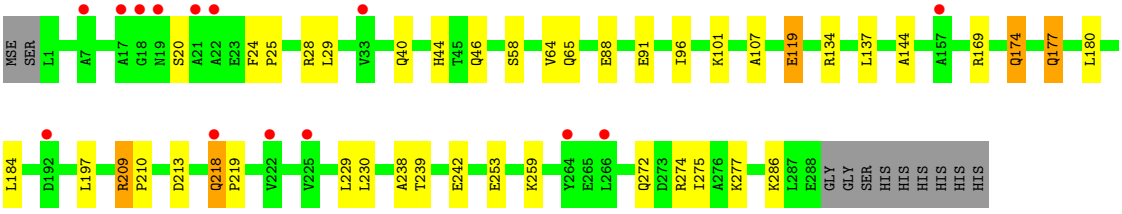
• Molecule 1: Pyridoxamine kinase

Chain A:



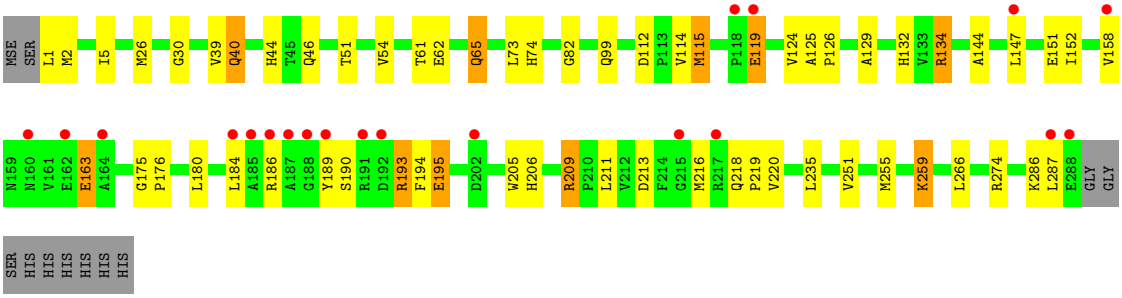
• Molecule 1: Pyridoxamine kinase

Chain B:



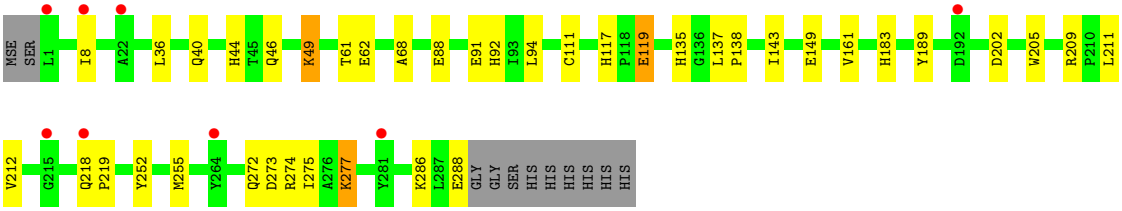
• Molecule 1: Pyridoxamine kinase

Chain C:



• Molecule 1: Pyridoxamine kinase

Chain D:


MSE
SER
L1
I8
A22
L36
Q40
H44
T45
Q46
K49
T61
E62
A68
E88
E91
H92
I93
L94
C111
H117
P118
E119
H135
G136
L137
P138
I143
E149
V161
H183
Y189
D192
D202
W205
R209
P210
L211
V212
G215
Q218
P219
Y252
M255
Y264
Q272
D273
R274
I275
A276
K277
Y281
K286
L287
E288
GLY
GLY
SER
HIS
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.38Å 92.59Å 122.24Å 90.00° 99.42° 90.00°	Depositor
Resolution (Å)	43.03 – 1.96 43.22 – 1.96	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.03-1.96) 98.7 (43.22-1.96)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 1.95Å)	Xtriage
Refinement program	REFMAC 4.0	Depositor
R, R_{free}	0.198 , 0.256 0.189 , 0.237	Depositor DCC
R_{free} test set	4167 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 63.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9760	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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 (i)

5.1 Standard geometry (i)

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

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	0.59	0/2235	1.08	4/3029 (0.1%)
1	B	0.59	0/2237	1.15	7/3032 (0.2%)
1	C	0.57	0/2233	1.09	11/3026 (0.4%)
1	D	0.57	0/2239	1.06	5/3035 (0.2%)
All	All	0.58	0/8944	1.10	27/12122 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	209	ARG	NE-CZ-NH2	16.29	128.45	120.30
1	B	209	ARG	NE-CZ-NH1	-11.32	114.64	120.30
1	B	209	ARG	CD-NE-CZ	10.82	138.75	123.60
1	C	209	ARG	CD-NE-CZ	9.53	136.94	123.60
1	C	163	GLU	CA-CB-CG	8.40	131.88	113.40
1	C	134	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	C	186	ARG	NE-CZ-NH1	-7.81	116.40	120.30
1	D	252	TYR	CB-CG-CD1	-7.53	116.48	121.00
1	C	209	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	B	28	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	209	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	D	252	TYR	CB-CG-CD2	6.71	125.03	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	274	ARG	CD-NE-CZ	6.50	132.71	123.60
1	D	209	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	193	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	B	169	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	B	28	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	C	193	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	115	MSE	CA-CB-CG	5.33	122.36	113.30
1	A	40	GLN	CB-CA-C	5.33	121.06	110.40
1	C	40	GLN	CB-CA-C	5.33	121.06	110.40
1	B	40	GLN	CB-CA-C	5.32	121.05	110.40
1	A	193	ARG	CD-NE-CZ	5.29	131.01	123.60
1	D	274	ARG	CD-NE-CZ	5.23	130.92	123.60
1	C	193	ARG	CD-NE-CZ	5.21	130.89	123.60
1	D	49	LYS	CA-CB-CG	5.13	124.70	113.40
1	C	134	ARG	CD-NE-CZ	5.09	130.73	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	40	GLN	Mainchain

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	2200	0	2203	32	0
1	B	2205	0	2205	22	0
1	C	2198	0	2201	49	0
1	D	2203	0	2199	21	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	B	4	0	5	0	0
3	D	7	0	10	0	0
4	A	235	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	241	0	0	5	1
4	C	216	0	0	5	0
4	D	231	0	0	5	0
All	All	9760	0	8823	123	1

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 (123) 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:115:MSE:HE3	1:C:132:HIS:HB2	1.29	1.08
1:C:115:MSE:CE	1:C:132:HIS:HB2	1.96	0.96
1:A:115:MSE:HE3	1:A:132:HIS:HB2	1.49	0.94
1:A:115:MSE:CE	1:A:132:HIS:HB2	1.98	0.92
1:A:115:MSE:HE2	1:A:129:ALA:HA	1.53	0.89
1:C:115:MSE:HE2	1:C:129:ALA:HA	1.54	0.89
1:C:51:THR:HB	1:D:62:GLU:HG2	1.60	0.81
1:C:115:MSE:HE3	1:C:132:HIS:CB	2.13	0.78
1:A:115:MSE:HE3	1:A:132:HIS:CB	2.24	0.67
1:C:125:ALA:HB1	1:C:126:PRO:HD2	1.77	0.67
1:B:239:THR:OG1	1:B:242:GLU:HG2	1.96	0.66
1:B:218:GLN:HG2	4:B:485:HOH:O	1.94	0.66
1:A:190:SER:HB3	1:A:193:ARG:NH1	2.13	0.64
1:B:286:LYS:HE2	4:B:540:HOH:O	1.97	0.63
1:C:115:MSE:HE2	1:C:129:ALA:CA	2.29	0.62
1:C:193:ARG:NH1	4:C:433:HOH:O	2.32	0.62
1:C:40:GLN:HB2	4:C:452:HOH:O	2.00	0.61
1:C:2:MSE:HE3	1:C:30:GLY:O	2.01	0.61
1:C:61:THR:HG22	1:C:65:GLN:HE22	1.66	0.59
1:A:159:ASN:HA	1:A:186:ARG:HH11	1.68	0.58
1:C:255[A]:MSE:SE	1:C:266:LEU:HD21	2.53	0.58
1:A:194:PHE:HB2	1:A:211:LEU:HD23	1.87	0.57
1:C:115:MSE:SE	4:C:514:HOH:O	2.72	0.57
1:A:116:GLY:HA2	1:A:123:ILE:HG12	1.85	0.57
1:C:251:VAL:O	1:C:255[B]:MSE:HG3	2.05	0.56
1:D:117:HIS:HE1	1:D:149:GLU:OE1	1.89	0.56
1:A:55:MSE:HE3	1:A:59:HIS:NE2	2.21	0.56
1:C:1:LEU:HA	4:C:497:HOH:O	2.06	0.55
1:D:119:GLU:HB3	4:D:461:HOH:O	2.07	0.55
1:D:119:GLU:H	1:D:119:GLU:CD	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:MSE:HE2	1:A:129:ALA:CA	2.32	0.54
1:A:159:ASN:HA	1:A:186:ARG:NH1	2.22	0.54
1:B:29:LEU:HD22	1:B:229:LEU:HD22	1.89	0.53
1:A:189:TYR:HB2	1:A:195:GLU:OE1	2.09	0.53
1:C:5:ILE:HD11	1:C:235:LEU:HD12	1.90	0.53
1:C:39:VAL:HG12	1:C:54:VAL:HA	1.91	0.52
1:C:205:TRP:CH2	1:C:286:LYS:HB2	2.44	0.52
1:D:205:TRP:CZ2	1:D:286:LYS:HE2	2.44	0.52
1:A:158:VAL:HA	1:A:163:GLU:HG3	1.92	0.52
1:C:115:MSE:HE2	1:C:129:ALA:O	2.10	0.51
1:C:184:LEU:HD12	1:C:195:GLU:HB3	1.91	0.51
1:B:137:LEU:HD21	1:B:174:GLN:HG3	1.92	0.51
1:A:144:ALA:HA	1:A:180:LEU:O	2.10	0.50
1:C:46:GLN:HG3	1:C:220:VAL:CG2	2.42	0.49
1:D:94:LEU:HD11	1:D:135:HIS:HB3	1.93	0.49
1:C:193:ARG:NH2	1:C:195:GLU:OE2	2.45	0.49
1:C:46:GLN:HG3	1:C:220:VAL:HG21	1.95	0.49
1:C:73:LEU:CD2	1:C:99:GLN:HG2	2.43	0.49
1:C:147:LEU:O	1:C:151:GLU:HG3	2.11	0.49
1:C:194:PHE:HB2	1:C:211:LEU:HD23	1.93	0.49
1:A:120:LYS:HB3	1:A:120:LYS:NZ	2.29	0.48
1:B:210:PRO:HB2	4:B:451:HOH:O	2.12	0.48
1:D:61:THR:OG1	1:D:92:HIS:HD2	1.96	0.48
1:A:193:ARG:CG	1:A:193:ARG:HH11	2.26	0.48
1:D:92:HIS:HE1	4:D:478:HOH:O	1.97	0.48
1:A:193:ARG:HH11	1:A:193:ARG:HG2	1.80	0.47
1:D:88:GLU:O	1:D:91:GLU:HG2	2.15	0.47
1:C:5:ILE:HG21	1:C:26:MSE:HE1	1.97	0.47
1:D:8:ILE:HA	1:D:36:LEU:O	2.15	0.47
1:C:195:GLU:HG2	1:C:206:HIS:NE2	2.30	0.46
1:B:253:GLU:HG3	1:B:274:ARG:HB3	1.96	0.46
1:B:24:PHE:HB3	1:B:25:PRO:HD3	1.98	0.46
1:B:88:GLU:O	1:B:91:GLU:HG2	2.16	0.45
1:C:195:GLU:HG2	1:C:206:HIS:HE2	1.82	0.45
1:B:238:ALA:HB1	1:B:242:GLU:HG3	1.99	0.45
1:B:44:HIS:CE1	1:B:46:GLN:HB3	2.52	0.45
1:A:162:GLU:H	1:A:162:GLU:CD	2.20	0.44
1:C:115:MSE:HE3	1:C:132:HIS:CG	2.51	0.44
1:B:177:GLN:NE2	4:B:384:HOH:O	2.50	0.44
1:B:272:GLN:HA	1:B:275:ILE:HD12	2.00	0.44
1:A:71:ASP:HB2	4:A:384:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:GLU:H	1:B:119:GLU:CD	2.20	0.44
1:B:213:ASP:O	1:B:259:LYS:NZ	2.31	0.44
1:C:115:MSE:SE	1:C:152:ILE:HG21	2.68	0.44
1:D:218:GLN:HA	1:D:219:PRO:HD3	1.85	0.44
1:B:180:LEU:HD22	1:B:230:LEU:HD22	1.99	0.44
1:D:272:GLN:HA	1:D:275:ILE:HD12	2.00	0.44
1:D:273:ASP:O	1:D:277:LYS:HE2	2.17	0.44
1:D:68:ALA:HA	4:D:450:HOH:O	2.18	0.43
1:B:218:GLN:HA	1:B:219:PRO:HD3	1.93	0.43
1:B:101:LYS:HE2	1:B:107:ALA:O	2.19	0.43
1:C:193:ARG:HE	1:C:193:ARG:HB2	1.58	0.43
1:C:218:GLN:HA	1:C:219:PRO:HD3	1.93	0.43
1:A:5:ILE:HD11	1:A:235:LEU:HD12	2.01	0.43
1:C:119:GLU:H	1:C:119:GLU:HG3	1.56	0.42
1:C:114:VAL:O	1:C:124:VAL:HG11	2.19	0.42
1:C:115:MSE:HE3	1:C:132:HIS:ND1	2.34	0.42
1:D:137:LEU:HB3	1:D:138:PRO:HD3	2.00	0.42
1:B:184:LEU:HD11	1:B:197:LEU:HG	2.00	0.42
1:D:111:CYS:O	1:D:143:ILE:HA	2.19	0.42
1:A:125:ALA:HB1	1:A:126:PRO:HD2	2.02	0.42
1:C:44:HIS:CD2	1:C:46:GLN:HB2	2.55	0.42
1:C:144:ALA:HA	1:C:180:LEU:O	2.20	0.42
1:C:44:HIS:HD2	1:C:46:GLN:H	1.66	0.42
1:C:189:TYR:HB2	1:C:193:ARG:NH2	2.34	0.42
1:B:144:ALA:HA	1:B:180:LEU:O	2.20	0.42
1:A:195:GLU:OE1	1:A:206:HIS:NE2	2.51	0.42
1:A:135:HIS:HD2	4:A:482:HOH:O	2.02	0.42
1:C:74:HIS:HD2	4:C:341:HOH:O	2.02	0.42
1:A:44:HIS:CE1	1:A:46:GLN:HB2	2.55	0.42
1:A:16:HIS:HB3	1:A:21:ALA:HA	2.01	0.41
1:A:111:CYS:O	1:A:143:ILE:HA	2.20	0.41
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.96	0.41
1:A:184:LEU:HD13	1:A:188:GLY:HA2	2.03	0.41
1:B:20:SER:HB3	4:B:337:HOH:O	2.20	0.41
1:B:64:VAL:HG21	1:B:96:ILE:HG12	2.03	0.41
1:C:195:GLU:OE2	1:C:206:HIS:NE2	2.53	0.41
1:D:212:VAL:HG21	1:D:255[B]:MSE:HB3	2.02	0.41
1:C:61:THR:HG22	1:C:65:GLN:NE2	2.34	0.41
1:C:175:GLY:N	1:C:176:PRO:HD2	2.36	0.41
1:A:181:VAL:HG11	1:A:184:LEU:HD23	2.03	0.41
1:C:206:HIS:HB2	1:C:287:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:GLU:HG3	4:D:483:HOH:O	2.20	0.41
1:A:84:LEU:HD21	1:A:93:ILE:HD12	2.03	0.40
1:C:158:VAL:HA	1:C:163:GLU:HG3	2.02	0.40
1:C:213:ASP:O	1:C:259:LYS:HE2	2.20	0.40
1:A:137:LEU:N	1:A:138:PRO:HD2	2.36	0.40
1:C:82:GLY:HA2	1:C:112:ASP:HB3	2.04	0.40
1:D:161:VAL:HG21	1:D:189:TYR:CZ	2.57	0.40
1:A:159:ASN:OD1	1:A:186:ARG:NH1	2.54	0.40
1:C:189:TYR:CD1	1:C:195:GLU:OE2	2.74	0.40
1:D:44:HIS:CE1	1:D:46:GLN:HB3	2.57	0.40
1:D:183:HIS:HE1	4:D:377:HOH:O	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:436:HOH:O	4:B:540:HOH:O[2_655]	2.19	0.01

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	286/299 (96%)	274 (96%)	12 (4%)	0	100	100
1	B	285/299 (95%)	281 (99%)	4 (1%)	0	100	100
1	C	286/299 (96%)	276 (96%)	10 (4%)	0	100	100
1	D	286/299 (96%)	281 (98%)	5 (2%)	0	100	100
All	All	1143/1196 (96%)	1112 (97%)	31 (3%)	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	230/232 (99%)	221 (96%)	9 (4%)	32	19
1	B	231/232 (100%)	222 (96%)	9 (4%)	32	19
1	C	229/232 (99%)	220 (96%)	9 (4%)	32	19
1	D	231/232 (100%)	225 (97%)	6 (3%)	46	36
All	All	921/928 (99%)	888 (96%)	33 (4%)	35	23

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	2	MSE
1	A	36	LEU
1	A	110	PHE
1	A	120	LYS
1	A	134	ARG
1	A	189	TYR
1	A	193	ARG
1	A	277	LYS
1	B	58	SER
1	B	65	GLN
1	B	119	GLU
1	B	134	ARG
1	B	174	GLN
1	B	177	GLN
1	B	209	ARG
1	B	218	GLN
1	B	277	LYS
1	C	62	GLU
1	C	65	GLN
1	C	119	GLU
1	C	134	ARG
1	C	190	SER
1	C	195	GLU

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Mol	Chain	Res	Type
1	C	209	ARG
1	C	216	MSE
1	C	259	LYS
1	D	49	LYS
1	D	119	GLU
1	D	202	ASP
1	D	211	LEU
1	D	277	LYS
1	D	288	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
1	A	183	HIS
1	B	65	GLN
1	B	99	GLN
1	B	174	GLN
1	B	177	GLN
1	B	218	GLN
1	C	44	HIS
1	C	65	GLN
1	C	99	GLN
1	D	92	HIS
1	D	117	HIS
1	D	183	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSD	D	53	1	3,7,8	0.67	0	1,8,10	0.32	0
1	CSD	C	53	1	3,7,8	0.55	0	1,8,10	1.23	0
1	CSD	A	53	1	3,7,8	0.75	0	1,8,10	0.67	0
1	CSD	B	53	1	3,7,8	0.65	0	1,8,10	0.25	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
1	CSD	D	53	1	-	1/2/6/8	-
1	CSD	C	53	1	-	0/2/6/8	-
1	CSD	A	53	1	-	0/2/6/8	-
1	CSD	B	53	1	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	53	CSD	CA-CB-SG-OD1
1	D	53	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	D	298	-	4,4,4	0.63	0	6,6,6	0.25	0
3	BME	D	300[A]	-	3,3,3	0.45	0	1,2,2	0.22	0
2	SO4	B	298	-	4,4,4	0.64	0	6,6,6	0.35	0
2	SO4	C	298	-	4,4,4	0.67	0	6,6,6	0.17	0
2	SO4	A	298	-	4,4,4	0.63	0	6,6,6	0.26	0
3	BME	B	300	1	3,3,3	0.48	0	1,2,2	0.53	0
3	BME	D	300[B]	-	3,3,3	0.50	0	1,2,2	0.16	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	BME	D	300[B]	-	-	0/1/1/1	-
3	BME	D	300[A]	-	-	1/1/1/1	-
3	BME	B	300	1	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	300[A]	BME	O1-C1-C2-S2
3	B	300	BME	O1-C1-C2-S2

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 (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	279/299 (93%)	0.24	15 (5%)	25	34	13, 24, 45, 58	0
1	B	279/299 (93%)	0.28	14 (5%)	28	39	13, 21, 34, 51	0
1	C	279/299 (93%)	0.44	20 (7%)	15	23	16, 25, 49, 65	0
1	D	279/299 (93%)	0.18	8 (2%)	51	60	15, 23, 38, 58	0
All	All	1116/1196 (93%)	0.29	57 (5%)	28	37	13, 23, 42, 65	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	215	GLY	5.2
1	A	288	GLU	5.0
1	D	1	LEU	4.9
1	C	118	PRO	4.6
1	C	191	ARG	4.3
1	C	119	GLU	3.9
1	C	158	VAL	3.8
1	C	189	TYR	3.8
1	D	218	GLN	3.8
1	A	189	TYR	3.7
1	C	288	GLU	3.7
1	C	187	ALA	3.6
1	C	192	ASP	3.6
1	D	264	TYR	3.6
1	A	118	PRO	3.5
1	B	21	ALA	3.4
1	C	188	GLY	3.4
1	D	192	ASP	3.2
1	D	281	TYR	3.1
1	B	33	VAL	3.1
1	A	190	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	188	GLY	3.0
1	C	217	ARG	2.9
1	A	33	VAL	2.9
1	C	215	GLY	2.8
1	A	1	LEU	2.8
1	B	22	ALA	2.7
1	A	187	ALA	2.6
1	A	134	ARG	2.6
1	C	287	LEU	2.6
1	B	192	ASP	2.6
1	A	122	CYS	2.6
1	A	287	LEU	2.5
1	C	160	ASN	2.5
1	C	186	ARG	2.3
1	D	22	ALA	2.3
1	C	147	LEU	2.3
1	A	158	VAL	2.3
1	B	222	VAL	2.3
1	C	162	GLU	2.3
1	B	225	VAL	2.3
1	C	185	ALA	2.3
1	A	193	ARG	2.3
1	A	162	GLU	2.2
1	A	22	ALA	2.2
1	B	7	ALA	2.2
1	D	8	ILE	2.2
1	B	157	ALA	2.2
1	C	184	LEU	2.2
1	C	164	ALA	2.2
1	C	202	ASP	2.1
1	B	264	TYR	2.1
1	B	266	LEU	2.1
1	B	18	GLY	2.1
1	B	17	ALA	2.0
1	B	218	GLN	2.0
1	B	19	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CSD	B	53	8/9	0.90	0.11	20,24,33,37	0
1	CSD	C	53	8/9	0.91	0.11	28,30,36,39	0
1	CSD	A	53	8/9	0.92	0.12	19,24,32,37	0
1	CSD	D	53	8/9	0.93	0.10	25,28,37,39	0

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	C	298	5/5	0.72	0.23	74,74,74,74	0
2	SO4	A	298	5/5	0.83	0.21	65,66,67,67	0
3	BME	D	300[A]	4/4	0.83	0.36	30,30,31,31	3
3	BME	D	300[B]	4/4	0.83	0.36	30,31,31,31	3
2	SO4	D	298	5/5	0.84	0.21	67,67,67,67	0
2	SO4	B	298	5/5	0.92	0.18	49,49,49,50	0
3	BME	B	300	4/4	0.94	0.12	29,32,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.