Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:28 AM GMT

PDB ID	:	3OZB
Title	:	Crystal Structure of 5'-methylthioinosine phosphorylase from Psedomonas aeruginosa in complex with hypoxanthine
Authors	:	Ho, M.; Guan, R.; Almo, S.C.; Schramm, V.L.
Deposited on	:	2010-09-24
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

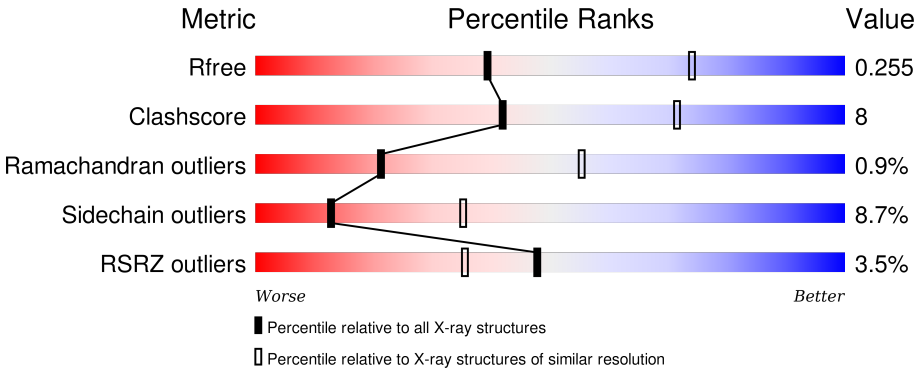
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	259	2% 74% 17% • 7%
1	B	259	% 77% 13% • 8%
1	C	259	3% 75% 14% • 8%
1	D	259	4% 74% 14% • 8%
1	E	259	4% 69% 20% • 9%

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Mol	Chain	Length	Quality of chain
1	F	259	5% 74% 16% 8%

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
3	SO4	B	261	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10943 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 Methylthioadenosine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	1	0
			1828	1155	330	335	8			
1	B	238	Total	C	N	O	S	0	0	0
			1788	1126	324	331	7			
1	C	239	Total	C	N	O	S	0	0	0
			1805	1138	328	332	7			
1	D	239	Total	C	N	O	S	0	0	0
			1799	1135	325	332	7			
1	E	236	Total	C	N	O	S	0	1	0
			1781	1123	322	328	8			
1	F	239	Total	C	N	O	S	0	0	0
			1799	1135	325	332	7			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q02PG8
A	2	HIS	-	EXPRESSION TAG	UNP Q02PG8
A	3	HIS	-	EXPRESSION TAG	UNP Q02PG8
A	4	HIS	-	EXPRESSION TAG	UNP Q02PG8
A	5	HIS	-	EXPRESSION TAG	UNP Q02PG8
A	6	HIS	-	EXPRESSION TAG	UNP Q02PG8
A	7	HIS	-	EXPRESSION TAG	UNP Q02PG8
A	8	GLU	-	EXPRESSION TAG	UNP Q02PG8
A	9	ASN	-	EXPRESSION TAG	UNP Q02PG8
A	10	LEU	-	EXPRESSION TAG	UNP Q02PG8
A	11	TYR	-	EXPRESSION TAG	UNP Q02PG8
A	12	PHE	-	EXPRESSION TAG	UNP Q02PG8
A	13	GLN	-	EXPRESSION TAG	UNP Q02PG8
A	14	GLY	-	EXPRESSION TAG	UNP Q02PG8
B	1	MET	-	EXPRESSION TAG	UNP Q02PG8
B	2	HIS	-	EXPRESSION TAG	UNP Q02PG8
B	3	HIS	-	EXPRESSION TAG	UNP Q02PG8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	HIS	-	EXPRESSION TAG	UNP Q02PG8
B	5	HIS	-	EXPRESSION TAG	UNP Q02PG8
B	6	HIS	-	EXPRESSION TAG	UNP Q02PG8
B	7	HIS	-	EXPRESSION TAG	UNP Q02PG8
B	8	GLU	-	EXPRESSION TAG	UNP Q02PG8
B	9	ASN	-	EXPRESSION TAG	UNP Q02PG8
B	10	LEU	-	EXPRESSION TAG	UNP Q02PG8
B	11	TYR	-	EXPRESSION TAG	UNP Q02PG8
B	12	PHE	-	EXPRESSION TAG	UNP Q02PG8
B	13	GLN	-	EXPRESSION TAG	UNP Q02PG8
B	14	GLY	-	EXPRESSION TAG	UNP Q02PG8
C	1	MET	-	EXPRESSION TAG	UNP Q02PG8
C	2	HIS	-	EXPRESSION TAG	UNP Q02PG8
C	3	HIS	-	EXPRESSION TAG	UNP Q02PG8
C	4	HIS	-	EXPRESSION TAG	UNP Q02PG8
C	5	HIS	-	EXPRESSION TAG	UNP Q02PG8
C	6	HIS	-	EXPRESSION TAG	UNP Q02PG8
C	7	HIS	-	EXPRESSION TAG	UNP Q02PG8
C	8	GLU	-	EXPRESSION TAG	UNP Q02PG8
C	9	ASN	-	EXPRESSION TAG	UNP Q02PG8
C	10	LEU	-	EXPRESSION TAG	UNP Q02PG8
C	11	TYR	-	EXPRESSION TAG	UNP Q02PG8
C	12	PHE	-	EXPRESSION TAG	UNP Q02PG8
C	13	GLN	-	EXPRESSION TAG	UNP Q02PG8
C	14	GLY	-	EXPRESSION TAG	UNP Q02PG8
D	1	MET	-	EXPRESSION TAG	UNP Q02PG8
D	2	HIS	-	EXPRESSION TAG	UNP Q02PG8
D	3	HIS	-	EXPRESSION TAG	UNP Q02PG8
D	4	HIS	-	EXPRESSION TAG	UNP Q02PG8
D	5	HIS	-	EXPRESSION TAG	UNP Q02PG8
D	6	HIS	-	EXPRESSION TAG	UNP Q02PG8
D	7	HIS	-	EXPRESSION TAG	UNP Q02PG8
D	8	GLU	-	EXPRESSION TAG	UNP Q02PG8
D	9	ASN	-	EXPRESSION TAG	UNP Q02PG8
D	10	LEU	-	EXPRESSION TAG	UNP Q02PG8
D	11	TYR	-	EXPRESSION TAG	UNP Q02PG8
D	12	PHE	-	EXPRESSION TAG	UNP Q02PG8
D	13	GLN	-	EXPRESSION TAG	UNP Q02PG8
D	14	GLY	-	EXPRESSION TAG	UNP Q02PG8
E	1	MET	-	EXPRESSION TAG	UNP Q02PG8
E	2	HIS	-	EXPRESSION TAG	UNP Q02PG8
E	3	HIS	-	EXPRESSION TAG	UNP Q02PG8

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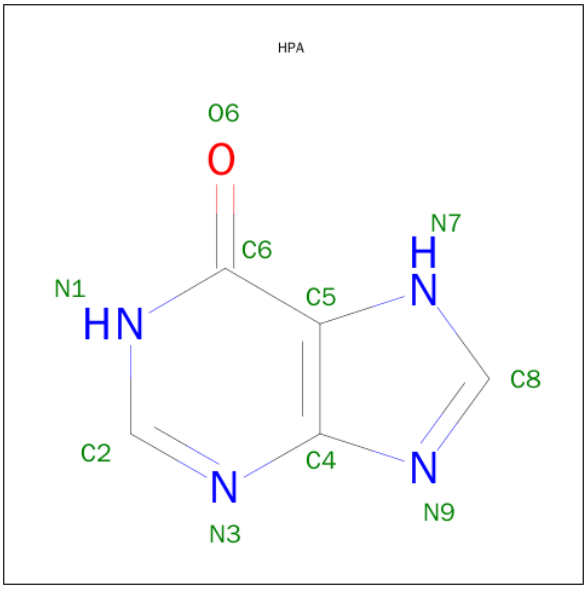
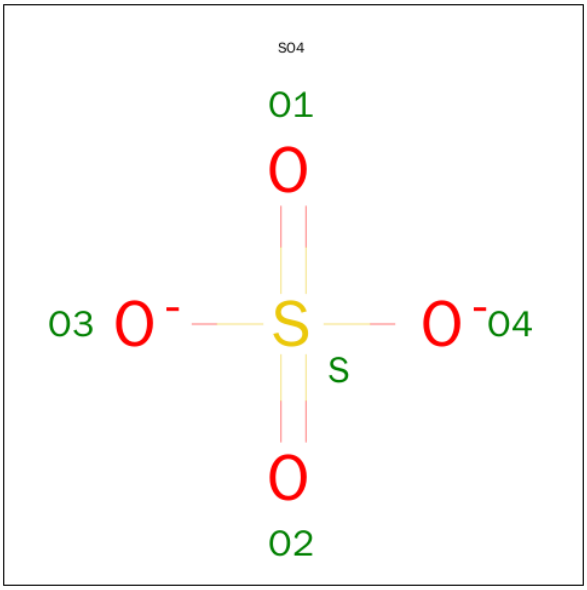
Chain	Residue	Modelled	Actual	Comment	Reference
E	4	HIS	-	EXPRESSION TAG	UNP Q02PG8
E	5	HIS	-	EXPRESSION TAG	UNP Q02PG8
E	6	HIS	-	EXPRESSION TAG	UNP Q02PG8
E	7	HIS	-	EXPRESSION TAG	UNP Q02PG8
E	8	GLU	-	EXPRESSION TAG	UNP Q02PG8
E	9	ASN	-	EXPRESSION TAG	UNP Q02PG8
E	10	LEU	-	EXPRESSION TAG	UNP Q02PG8
E	11	TYR	-	EXPRESSION TAG	UNP Q02PG8
E	12	PHE	-	EXPRESSION TAG	UNP Q02PG8
E	13	GLN	-	EXPRESSION TAG	UNP Q02PG8
E	14	GLY	-	EXPRESSION TAG	UNP Q02PG8
F	1	MET	-	EXPRESSION TAG	UNP Q02PG8
F	2	HIS	-	EXPRESSION TAG	UNP Q02PG8
F	3	HIS	-	EXPRESSION TAG	UNP Q02PG8
F	4	HIS	-	EXPRESSION TAG	UNP Q02PG8
F	5	HIS	-	EXPRESSION TAG	UNP Q02PG8
F	6	HIS	-	EXPRESSION TAG	UNP Q02PG8
F	7	HIS	-	EXPRESSION TAG	UNP Q02PG8
F	8	GLU	-	EXPRESSION TAG	UNP Q02PG8
F	9	ASN	-	EXPRESSION TAG	UNP Q02PG8
F	10	LEU	-	EXPRESSION TAG	UNP Q02PG8
F	11	TYR	-	EXPRESSION TAG	UNP Q02PG8
F	12	PHE	-	EXPRESSION TAG	UNP Q02PG8
F	13	GLN	-	EXPRESSION TAG	UNP Q02PG8
F	14	GLY	-	EXPRESSION TAG	UNP Q02PG8

- Molecule 2 is HYPOXANTHINE (three-letter code: HPA) (formula: $C_5H_4N_4O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 10 5 4 1	0	0
2	B	1	Total C N O 10 5 4 1	0	0
2	C	1	Total C N O 10 5 4 1	0	0
2	D	1	Total C N O 10 5 4 1	0	0
2	E	1	Total C N O 10 5 4 1	0	0
2	F	1	Total C N O 10 5 4 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

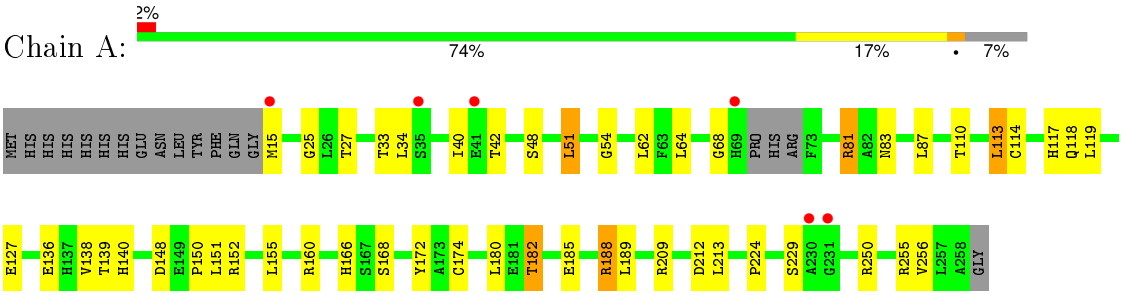
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	B	11	Total O 11 11	0	0
4	C	14	Total O 14 14	0	0
4	D	11	Total O 11 11	0	0
4	E	6	Total O 6 6	0	0
4	F	9	Total O 9 9	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

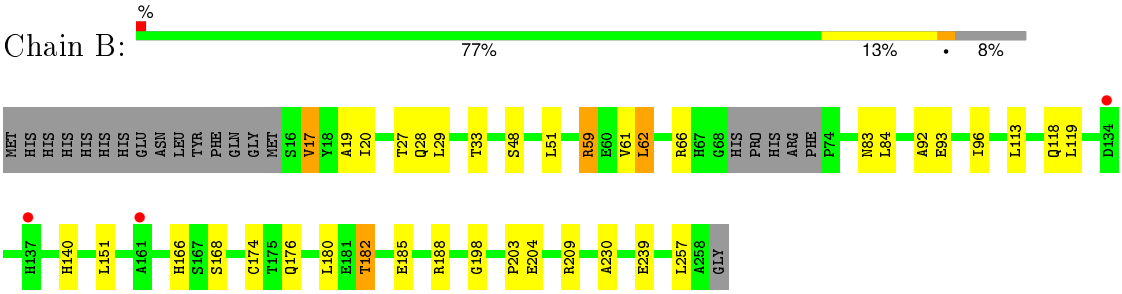
- Molecule 1: Methylthioadenosine phosphorylase

Chain A:



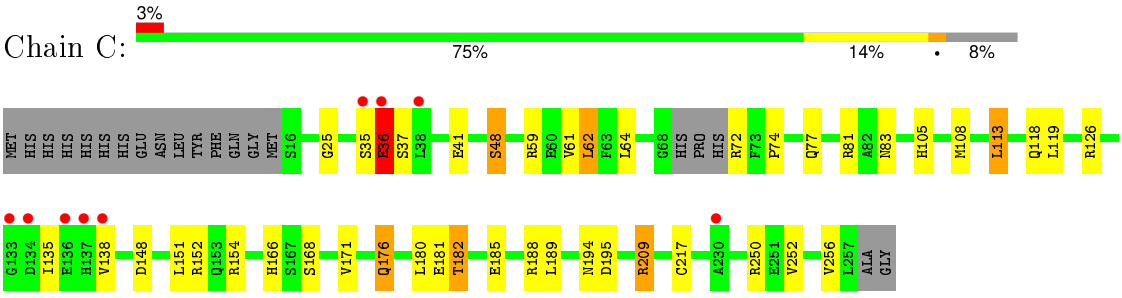
- Molecule 1: Methylthioadenosine phosphorylase

Chain B:



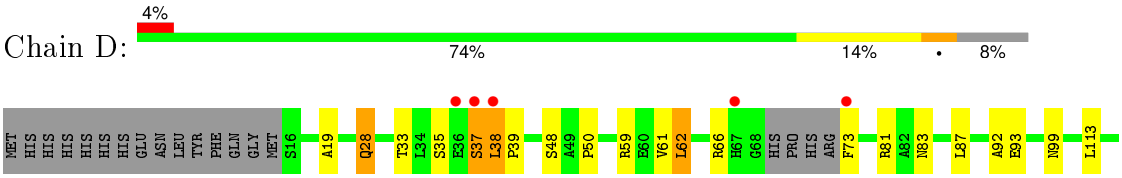
- Molecule 1: Methylthioadenosine phosphorylase

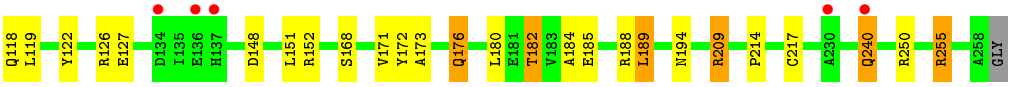
Chain C:



- Molecule 1: Methylthioadenosine phosphorylase

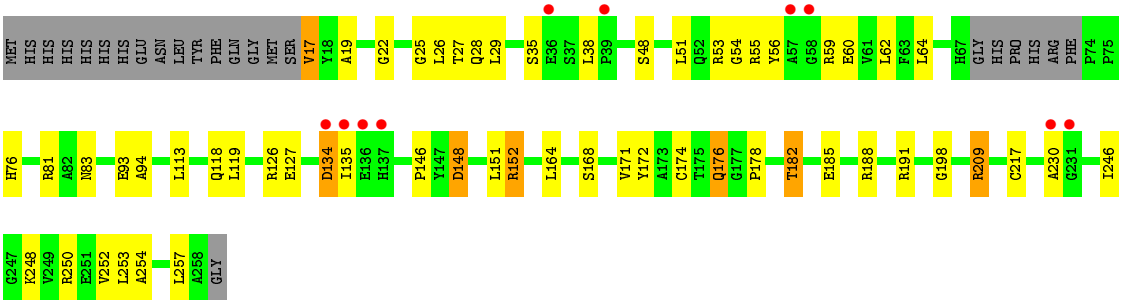
Chain D:





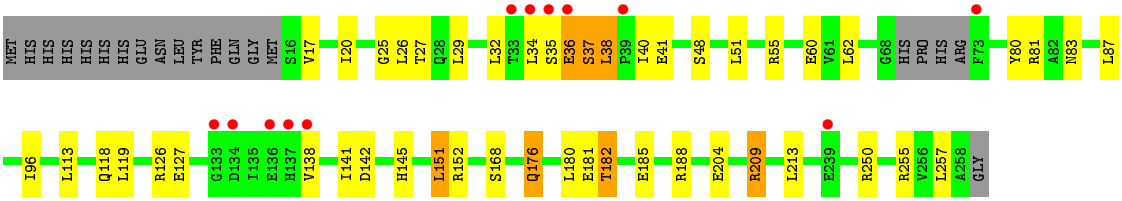
• Molecule 1: Methylthioadenosine phosphorylase

Chain E:



• Molecule 1: Methylthioadenosine phosphorylase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	99.47Å 99.47Å 334.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.80 19.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.96-2.80) 99.1 (19.96-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.202 , 0.262 0.199 , 0.255	Depositor DCC
R_{free} test set	2126 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	56.9	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 42041 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10943	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: HPA, 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	0.64	0/1868	0.73	1/2540 (0.0%)
1	B	0.60	0/1825	0.68	0/2482
1	C	0.62	0/1843	0.75	1/2506 (0.0%)
1	D	0.60	0/1837	0.72	0/2499
1	E	0.59	0/1821	0.76	4/2477 (0.2%)
1	F	0.56	0/1837	0.72	1/2499 (0.0%)
All	All	0.60	0/11031	0.73	7/15003 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	152	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	C	62	LEU	CA-CB-CG	5.64	128.27	115.30
1	E	191	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	E	64	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	64	LEU	CA-CB-CG	5.31	127.51	115.30
1	E	209	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	F	38	LEU	CA-CB-CG	5.10	127.04	115.30

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	1828	0	1812	29	0
1	B	1788	0	1780	26	0
1	C	1805	0	1796	33	0
1	D	1799	0	1788	38	0
1	E	1781	0	1777	39	0
1	F	1799	0	1788	36	0
2	A	10	0	4	0	0
2	B	10	0	4	0	0
2	C	10	0	4	1	0
2	D	10	0	4	0	0
2	E	10	0	4	0	0
2	F	10	0	4	2	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	12	0	0	2	0
4	B	11	0	0	1	0
4	C	14	0	0	0	0
4	D	11	0	0	0	0
4	E	6	0	0	0	0
4	F	9	0	0	1	0
All	All	10943	0	10765	181	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 (181) 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:F:36:GLU:HA	1:F:37:SER:HB3	1.26	1.14
1:C:182:THR:HG22	1:C:185:GLU:H	0.97	1.08
1:C:176:GLN:HA	1:C:176:GLN:HE21	1.21	1.03
1:D:182:THR:HG22	1:D:185:GLU:H	1.25	0.97
1:E:182:THR:HG21	1:F:119:LEU:O	1.64	0.95
1:C:182:THR:HG22	1:C:185:GLU:N	1.82	0.93
1:E:182:THR:HG22	1:E:185:GLU:H	1.36	0.90
1:F:36:GLU:CA	1:F:37:SER:HB3	2.03	0.88
1:F:48:SER:H	1:F:83:ASN:HD21	1.25	0.85
1:F:182:THR:HG22	1:F:185:GLU:H	1.41	0.85
1:D:126:ARG:HE	1:D:176:GLN:HE22	1.26	0.83
1:D:81:ARG:HD2	1:D:127:GLU:HB3	1.60	0.83
1:D:152:ARG:NH2	1:D:168:SER:O	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:LEU:HD11	1:E:254:ALA:HB2	1.63	0.81
1:B:182:THR:HG21	1:C:119:LEU:O	1.81	0.81
1:D:37:SER:HB3	1:D:50:PRO:HB3	1.63	0.80
1:B:182:THR:HG22	1:B:185:GLU:H	1.45	0.80
1:E:182:THR:HG23	1:F:118:GLN:NE2	1.97	0.79
1:A:182:THR:HG22	1:A:185:GLU:H	1.47	0.79
1:D:48:SER:H	1:D:83:ASN:HD21	1.33	0.76
1:C:176:GLN:HA	1:C:176:GLN:NE2	1.99	0.76
1:B:140:HIS:NE2	4:B:267:HOH:O	2.12	0.76
1:E:126:ARG:HE	1:E:176:GLN:HE22	1.31	0.75
1:D:182:THR:HG21	1:E:119:LEU:O	1.86	0.75
1:E:81:ARG:HD2	1:E:127:GLU:HB3	1.69	0.72
1:E:48:SER:H	1:E:83:ASN:HD21	1.36	0.72
1:E:94:ALA:HB1	1:E:151:LEU:HD11	1.71	0.72
1:C:176:GLN:CA	1:C:176:GLN:HE21	2.01	0.72
1:C:209:ARG:NH1	1:C:209:ARG:HG3	2.05	0.71
1:F:152:ARG:NH2	1:F:168:SER:O	2.24	0.71
1:D:119:LEU:O	1:F:182:THR:HG21	1.90	0.70
1:A:119:LEU:O	1:C:182:THR:HG21	1.91	0.70
1:D:126:ARG:HE	1:D:176:GLN:NE2	1.89	0.70
1:B:48:SER:H	1:B:83:ASN:HD21	1.40	0.69
1:A:48:SER:H	1:A:83:ASN:HD21	1.38	0.69
1:A:182:THR:HG21	1:B:119:LEU:O	1.92	0.69
1:A:182:THR:HG23	1:B:118:GLN:NE2	2.08	0.69
1:F:36:GLU:HA	1:F:37:SER:CB	2.12	0.68
1:D:176:GLN:HA	1:D:176:GLN:HE21	1.58	0.68
1:E:182:THR:HG23	1:F:118:GLN:HE22	1.55	0.68
1:D:182:THR:HG23	1:E:118:GLN:NE2	2.09	0.68
1:E:126:ARG:HE	1:E:176:GLN:NE2	1.93	0.67
1:E:176:GLN:HE21	1:E:176:GLN:HA	1.59	0.67
1:E:152:ARG:NH2	1:E:168:SER:O	2.29	0.66
1:C:182:THR:CG2	1:C:185:GLU:H	1.91	0.65
1:C:126:ARG:HE	1:C:176:GLN:HE22	1.45	0.65
1:B:27:THR:C	1:B:29:LEU:H	2.00	0.65
1:F:37:SER:HB2	1:F:51:LEU:O	1.97	0.65
1:A:140:HIS:NE2	4:A:273:HOH:O	2.29	0.64
1:A:152:ARG:NH2	1:A:168:SER:O	2.31	0.64
1:E:25:GLY:O	1:E:250:ARG:HD3	1.98	0.64
1:B:182:THR:HG22	1:B:185:GLU:N	2.14	0.63
1:C:152:ARG:NH2	1:C:168:SER:O	2.33	0.62
1:F:81:ARG:HD2	1:F:127:GLU:HB3	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:THR:HG23	1:E:118:GLN:HE22	1.66	0.61
1:F:176:GLN:HE21	1:F:176:GLN:HA	1.65	0.61
1:E:17:VAL:HG13	1:E:93:GLU:HG3	1.81	0.61
1:E:25:GLY:HA2	1:E:28:GLN:HG2	1.82	0.61
1:E:19:ALA:HA	1:E:62:LEU:O	2.02	0.60
1:C:252:VAL:O	1:C:256:VAL:HG23	2.02	0.59
1:D:118:GLN:NE2	1:F:182:THR:HG23	2.17	0.59
1:A:182:THR:HG23	1:B:118:GLN:HE22	1.65	0.59
1:C:59:ARG:O	1:C:61:VAL:HG23	2.04	0.58
1:E:113:LEU:HD21	1:E:248:LYS:HE3	1.86	0.58
1:D:37:SER:CB	1:D:50:PRO:HB3	2.31	0.58
1:E:17:VAL:HB	1:E:60:GLU:HB3	1.86	0.58
1:F:27:THR:HB	1:F:34:LEU:HD21	1.86	0.58
1:C:209:ARG:HG3	1:C:209:ARG:HH11	1.69	0.57
1:F:126:ARG:HE	1:F:176:GLN:HE22	1.50	0.57
1:A:182:THR:HG22	1:A:185:GLU:N	2.18	0.57
1:A:51:LEU:HD11	1:A:87:LEU:HD23	1.86	0.57
1:F:80:TYR:HD1	1:F:204:GLU:HG3	1.70	0.56
1:C:181:GLU:OE1	2:C:260:HPA:N1	2.32	0.56
1:B:17:VAL:HG22	1:B:92:ALA:HA	1.88	0.56
1:C:105:HIS:HB3	1:C:108:MET:HG3	1.88	0.56
1:C:105:HIS:HB2	1:C:195:ASP:HB3	1.88	0.56
1:C:171:VAL:HB	1:C:194:ASN:HA	1.88	0.55
1:C:35:SER:O	1:C:36:GLU:HG2	2.06	0.55
1:A:48:SER:H	1:A:83:ASN:ND2	2.05	0.55
1:C:48:SER:H	1:C:83:ASN:HD21	1.54	0.54
1:A:118:GLN:NE2	1:C:182:THR:HG23	2.22	0.53
1:A:81:ARG:HD2	1:A:127:GLU:HB3	1.89	0.53
1:F:81:ARG:CD	1:F:127:GLU:HB3	2.39	0.53
1:F:181:GLU:OE2	2:F:260:HPA:H2	2.09	0.53
1:F:51:LEU:HD21	1:F:87:LEU:HD23	1.91	0.53
1:B:20:ILE:HD11	1:B:257:LEU:HD21	1.91	0.53
1:F:145:HIS:O	1:F:209:ARG:NH2	2.38	0.52
1:D:182:THR:HG22	1:D:185:GLU:N	2.09	0.52
1:E:148:ASP:O	1:E:152:ARG:HG3	2.09	0.52
1:A:33:THR:O	1:A:54:GLY:HA3	2.09	0.51
1:C:126:ARG:NE	1:C:176:GLN:HE22	2.09	0.51
1:B:113:LEU:O	1:B:166:HIS:HA	2.10	0.51
1:F:141:ILE:HD13	1:F:209:ARG:HB3	1.93	0.51
1:E:248:LYS:O	1:E:252:VAL:HG23	2.11	0.51
1:D:48:SER:H	1:D:83:ASN:ND2	2.05	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126:ARG:HE	1:F:176:GLN:NE2	2.08	0.50
1:F:96:ILE:HD11	1:F:151:LEU:HD13	1.93	0.50
1:A:155:LEU:HD23	1:A:256:VAL:HG21	1.92	0.50
1:F:25:GLY:O	1:F:250:ARG:NH1	2.42	0.50
1:E:56:TYR:OH	1:E:254:ALA:HB1	2.11	0.50
1:D:255:ARG:HG2	1:D:255:ARG:HH21	1.75	0.50
1:C:119:LEU:C	1:C:119:LEU:HD12	2.32	0.49
1:B:19:ALA:HA	1:B:62:LEU:O	2.12	0.49
1:A:188:ARG:HG3	1:A:189:LEU:N	2.26	0.49
1:B:182:THR:HG23	1:C:118:GLN:NE2	2.27	0.49
1:B:182:THR:HG23	1:C:118:GLN:HE22	1.77	0.49
1:E:182:THR:HG22	1:E:185:GLU:N	2.16	0.48
1:E:253:LEU:O	1:E:257:LEU:HG	2.13	0.48
1:C:25:GLY:O	1:C:250:ARG:HD3	2.13	0.48
1:E:48:SER:N	1:E:83:ASN:HD21	2.06	0.48
1:A:172:TYR:HE1	1:A:174:CYS:HB2	1.78	0.48
1:A:25:GLY:O	1:A:250:ARG:NH1	2.40	0.48
1:D:66:ARG:NH1	1:D:99:ASN:ND2	2.62	0.48
1:B:59:ARG:HG2	1:B:61:VAL:HG23	1.95	0.47
1:A:148:ASP:OD1	1:A:150:PRO:HD2	2.14	0.47
1:B:96:ILE:HD11	1:B:151:LEU:HD12	1.96	0.47
1:E:55:ARG:HA	1:E:59:ARG:O	2.14	0.47
1:D:19:ALA:HB1	1:D:87:LEU:HD22	1.95	0.47
1:E:53:ARG:CG	1:E:54:GLY:N	2.77	0.47
1:B:176:GLN:OE1	1:B:176:GLN:HA	2.14	0.47
1:D:119:LEU:HD12	1:D:119:LEU:C	2.34	0.47
1:D:182:THR:OG1	1:E:146:PRO:HG3	2.15	0.47
1:A:140:HIS:HB3	1:C:180:LEU:HD13	1.96	0.47
1:E:126:ARG:NE	1:E:176:GLN:HE22	2.08	0.46
1:A:51:LEU:HD12	1:A:62:LEU:HD22	1.97	0.46
1:A:27:THR:HG22	1:A:34:LEU:HD11	1.98	0.46
1:C:113:LEU:O	1:C:166:HIS:HA	2.15	0.46
1:E:118:GLN:HB2	1:E:171:VAL:HG22	1.97	0.46
1:E:174[A]:CYS:HA	1:E:198:GLY:O	2.15	0.46
1:F:36:GLU:CA	1:F:37:SER:CB	2.81	0.46
1:D:126:ARG:NE	1:D:176:GLN:HE22	2.05	0.46
1:F:17:VAL:HG22	1:F:60:GLU:HB3	1.98	0.46
1:A:255:ARG:NH1	4:A:266:HOH:O	2.49	0.46
1:D:240:GLN:HA	1:D:240:GLN:HE21	1.81	0.46
1:C:74:PRO:HG2	1:C:77:GLN:HG3	1.98	0.45
1:E:164:LEU:HD22	1:E:248:LYS:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:LEU:C	1:F:119:LEU:HD12	2.37	0.45
1:F:26:LEU:O	1:F:29:LEU:HD13	2.16	0.45
1:E:119:LEU:HD12	1:E:119:LEU:C	2.37	0.45
1:F:20:ILE:HD11	1:F:257:LEU:HD21	1.99	0.45
1:C:209:ARG:CG	1:C:209:ARG:HH11	2.29	0.45
1:D:173:ALA:HB2	1:D:194:ASN:CG	2.38	0.45
1:D:209:ARG:NH1	1:D:209:ARG:CG	2.80	0.44
1:E:76:HIS:CE1	1:E:178:PRO:HD3	2.52	0.44
1:A:48:SER:N	1:A:83:ASN:HD21	2.11	0.44
1:E:22:GLY:HA3	1:E:26:LEU:CD1	2.48	0.44
1:A:113:LEU:O	1:A:166:HIS:HA	2.18	0.44
1:C:41:GLU:OE2	1:C:41:GLU:HA	2.18	0.44
1:F:35:SER:O	1:F:36:GLU:O	2.36	0.43
1:F:181:GLU:OE1	2:F:260:HPA:N1	2.32	0.43
1:A:172:TYR:CE1	1:A:174:CYS:HB2	2.53	0.43
1:B:84:LEU:HA	1:B:84:LEU:HD13	1.87	0.43
1:B:27:THR:C	1:B:29:LEU:N	2.68	0.43
1:B:17:VAL:HG13	1:B:93:GLU:HG3	2.00	0.43
1:D:148:ASP:O	1:D:152:ARG:HG3	2.18	0.43
1:B:174:CYS:HA	1:B:198:GLY:O	2.19	0.43
1:C:148:ASP:O	1:C:152:ARG:HG3	2.18	0.43
1:D:209:ARG:HH11	1:D:209:ARG:CG	2.32	0.43
1:A:224:PRO:HG2	1:A:229:SER:HB3	1.99	0.43
1:D:38:LEU:HA	1:D:39:PRO:HD3	1.93	0.42
1:D:184:ALA:H	1:E:118:GLN:NE2	2.18	0.42
1:F:41:GLU:HG3	4:F:262:HOH:O	2.19	0.42
1:A:81:ARG:CD	1:A:127:GLU:HB3	2.50	0.42
1:D:119:LEU:HD12	1:D:119:LEU:O	2.20	0.41
1:B:182:THR:H	1:B:185:GLU:HB2	1.84	0.41
1:C:154:ARG:HD3	1:C:256:VAL:HG13	2.01	0.41
1:D:93:GLU:O	1:D:214:PRO:HD2	2.20	0.41
1:D:118:GLN:HE22	1:F:182:THR:HG23	1.85	0.41
1:F:27:THR:O	1:F:32:LEU:HD23	2.20	0.41
1:F:182:THR:HG22	1:F:185:GLU:N	2.22	0.41
1:D:122:TYR:CZ	1:D:189:LEU:HD12	2.56	0.41
1:E:81:ARG:HD2	1:E:127:GLU:CB	2.45	0.40
1:D:66:ARG:CZ	1:D:99:ASN:HD21	2.34	0.40
1:D:28:GLN:HG3	1:D:250:ARG:NH1	2.36	0.40
1:B:119:LEU:HD12	1:B:119:LEU:C	2.42	0.40
1:B:203:PRO:O	1:B:204:GLU:C	2.60	0.40
1:A:117:HIS:HB3	1:A:152:ARG:NH2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:LEU:HD23	1:D:92:ALA:HB2	2.04	0.40
1:D:66:ARG:HH12	1:D:99:ASN:ND2	2.20	0.40
1:B:151:LEU:HD13	1:B:151:LEU:HA	1.82	0.40
1:D:171:VAL:HB	1:D:194:ASN:HA	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	238/259 (92%)	227 (95%)	10 (4%)	1 (0%)	39	74
1	B	234/259 (90%)	219 (94%)	13 (6%)	2 (1%)	21	55
1	C	235/259 (91%)	225 (96%)	9 (4%)	1 (0%)	39	74
1	D	235/259 (91%)	224 (95%)	9 (4%)	2 (1%)	21	55
1	E	233/259 (90%)	221 (95%)	8 (3%)	4 (2%)	11	36
1	F	235/259 (91%)	223 (95%)	10 (4%)	2 (1%)	21	55
All	All	1410/1554 (91%)	1339 (95%)	59 (4%)	12 (1%)	21	55

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	230	ALA
1	E	134	ASP
1	E	135	ILE
1	F	36	GLU
1	F	37	SER
1	B	28	GLN
1	D	37	SER
1	A	68	GLY

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Mol	Chain	Res	Type
1	C	36	GLU
1	D	38	LEU
1	E	35	SER
1	E	230	ALA

5.3.2 Protein sidechains

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	184/199 (92%)	165 (90%)	19 (10%)	9 26
1	B	180/199 (90%)	168 (93%)	12 (7%)	20 50
1	C	182/199 (92%)	165 (91%)	17 (9%)	11 32
1	D	181/199 (91%)	162 (90%)	19 (10%)	8 24
1	E	180/199 (90%)	167 (93%)	13 (7%)	18 45
1	F	181/199 (91%)	166 (92%)	15 (8%)	14 38
All	All	1088/1194 (91%)	993 (91%)	95 (9%)	13 35

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	40	ILE
1	A	42	THR
1	A	51	LEU
1	A	81	ARG
1	A	110	THR
1	A	113	LEU
1	A	114	CYS
1	A	136	GLU
1	A	138	VAL
1	A	139	THR
1	A	151	LEU
1	A	160	ARG
1	A	180	LEU

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Mol	Chain	Res	Type
1	A	182	THR
1	A	188	ARG
1	A	209	ARG
1	A	212	ASP
1	A	213	LEU
1	B	17	VAL
1	B	33	THR
1	B	51	LEU
1	B	59	ARG
1	B	62	LEU
1	B	66	ARG
1	B	168	SER
1	B	180	LEU
1	B	182	THR
1	B	188	ARG
1	B	209	ARG
1	B	239	GLU
1	C	36	GLU
1	C	37	SER
1	C	48	SER
1	C	62	LEU
1	C	64	LEU
1	C	72	ARG
1	C	81	ARG
1	C	113	LEU
1	C	135	ILE
1	C	138	VAL
1	C	151	LEU
1	C	176	GLN
1	C	182	THR
1	C	188	ARG
1	C	189	LEU
1	C	209	ARG
1	C	217	CYS
1	D	28	GLN
1	D	33	THR
1	D	35	SER
1	D	59	ARG
1	D	61	VAL
1	D	62	LEU
1	D	73	PHE
1	D	113	LEU

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Mol	Chain	Res	Type
1	D	151	LEU
1	D	172	TYR
1	D	176	GLN
1	D	180	LEU
1	D	182	THR
1	D	188	ARG
1	D	189	LEU
1	D	209	ARG
1	D	217	CYS
1	D	240	GLN
1	D	255	ARG
1	E	17	VAL
1	E	27	THR
1	E	38	LEU
1	E	51	LEU
1	E	134	ASP
1	E	148	ASP
1	E	172	TYR
1	E	176	GLN
1	E	182	THR
1	E	188	ARG
1	E	209	ARG
1	E	217	CYS
1	E	246	ILE
1	F	38	LEU
1	F	40	ILE
1	F	55	ARG
1	F	62	LEU
1	F	113	LEU
1	F	138	VAL
1	F	142	ASP
1	F	151	LEU
1	F	176	GLN
1	F	180	LEU
1	F	182	THR
1	F	188	ARG
1	F	209	ARG
1	F	213	LEU
1	F	255	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	118	GLN
1	A	194	ASN
1	B	28	GLN
1	B	83	ASN
1	B	99	ASN
1	B	118	GLN
1	B	194	ASN
1	C	83	ASN
1	C	118	GLN
1	C	176	GLN
1	C	194	ASN
1	D	83	ASN
1	D	99	ASN
1	D	118	GLN
1	D	176	GLN
1	D	194	ASN
1	D	240	GLN
1	E	83	ASN
1	E	118	GLN
1	E	176	GLN
1	E	194	ASN
1	F	83	ASN
1	F	118	GLN
1	F	176	GLN
1	F	194	ASN
1	F	240	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

10 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	HPA	A	260	-	8,11,11	1.91	3 (37%)	4,15,15	6.76	2 (50%)
3	SO4	A	261	-	4,4,4	0.11	0	6,6,6	0.47	0
3	SO4	A	262	-	4,4,4	0.15	0	6,6,6	0.22	0
2	HPA	B	260	-	8,11,11	1.88	2 (25%)	4,15,15	6.06	3 (75%)
3	SO4	B	261	-	4,4,4	0.19	0	6,6,6	0.24	0
2	HPA	C	260	-	8,11,11	1.93	3 (37%)	4,15,15	5.30	3 (75%)
3	SO4	C	261	-	4,4,4	0.11	0	6,6,6	0.37	0
2	HPA	D	260	-	8,11,11	2.08	3 (37%)	4,15,15	5.77	2 (50%)
2	HPA	E	260	-	8,11,11	1.92	2 (25%)	4,15,15	5.22	2 (50%)
2	HPA	F	260	-	8,11,11	1.99	3 (37%)	4,15,15	5.70	3 (75%)

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
2	HPA	A	260	-	-	0/0/0/0	0/2/2/2
3	SO4	A	261	-	-	0/0/0/0	0/0/0/0
3	SO4	A	262	-	-	0/0/0/0	0/0/0/0
2	HPA	B	260	-	-	0/0/0/0	0/2/2/2
3	SO4	B	261	-	-	0/0/0/0	0/0/0/0
2	HPA	C	260	-	-	0/0/0/0	0/2/2/2
3	SO4	C	261	-	-	0/0/0/0	0/0/0/0
2	HPA	D	260	-	-	0/0/0/0	0/2/2/2
2	HPA	E	260	-	-	0/0/0/0	0/2/2/2
2	HPA	F	260	-	-	0/0/0/0	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	260	HPA	C2-N1	2.69	1.39	1.33
2	C	260	HPA	C2-N1	2.71	1.39	1.33
2	D	260	HPA	C2-N1	2.73	1.39	1.33
2	A	260	HPA	C2-N3	2.75	1.37	1.32
2	C	260	HPA	C6-N1	2.82	1.38	1.33
2	F	260	HPA	C6-N1	2.83	1.38	1.33
2	E	260	HPA	C6-N1	3.04	1.38	1.33
2	D	260	HPA	C6-N1	3.13	1.38	1.33
2	B	260	HPA	C6-N1	3.14	1.38	1.33
2	F	260	HPA	C2-N1	3.26	1.40	1.33
2	F	260	HPA	C2-N3	3.40	1.38	1.32
2	B	260	HPA	C2-N3	3.41	1.38	1.32
2	A	260	HPA	C6-N1	3.49	1.39	1.33
2	C	260	HPA	C2-N3	3.60	1.38	1.32
2	D	260	HPA	C2-N3	3.84	1.39	1.32
2	E	260	HPA	C2-N3	3.95	1.39	1.32

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	260	HPA	N3-C2-N1	-12.96	118.97	128.89
2	B	260	HPA	N3-C2-N1	-11.56	120.04	128.89
2	D	260	HPA	N3-C2-N1	-11.17	120.34	128.89
2	F	260	HPA	N3-C2-N1	-10.31	121.00	128.89
2	C	260	HPA	N3-C2-N1	-10.00	121.24	128.89
2	E	260	HPA	N3-C2-N1	-9.75	121.43	128.89
2	F	260	HPA	C4-C5-N7	-3.79	105.99	109.48
2	E	260	HPA	C4-C5-N7	-2.98	106.74	109.48
2	C	260	HPA	C4-C5-N7	-2.32	107.34	109.48
2	B	260	HPA	C4-C5-N7	-2.27	107.39	109.48
2	D	260	HPA	C2-N1-C6	2.05	119.14	116.04
2	C	260	HPA	C2-N1-C6	2.64	120.03	116.04
2	B	260	HPA	C2-N1-C6	2.83	120.32	116.04
2	F	260	HPA	C2-N1-C6	3.08	120.70	116.04
2	A	260	HPA	C2-N1-C6	3.59	121.48	116.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	260	HPA	1	0
2	F	260	HPA	2	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, 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	241/259 (93%)	-0.34	6 (2%)	61	48	33, 48, 72, 81	0
1	B	238/259 (91%)	-0.35	3 (1%)	79	71	36, 54, 81, 90	0
1	C	239/259 (92%)	-0.27	9 (3%)	44	32	33, 48, 76, 93	0
1	D	239/259 (92%)	-0.23	10 (4%)	40	28	34, 51, 80, 91	0
1	E	236/259 (91%)	-0.13	10 (4%)	40	28	39, 55, 88, 103	0
1	F	239/259 (92%)	-0.19	12 (5%)	32	21	37, 56, 93, 110	0
All	All	1432/1554 (92%)	-0.25	50 (3%)	48	35	33, 51, 83, 110	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	34	LEU	6.2
1	A	230	ALA	5.2
1	C	134	ASP	4.9
1	D	67	HIS	4.1
1	D	137	HIS	4.1
1	C	136	GLU	4.1
1	F	133	GLY	4.0
1	D	134	ASP	4.0
1	F	134	ASP	4.0
1	E	137	HIS	3.9
1	C	137	HIS	3.9
1	D	230	ALA	3.9
1	F	137	HIS	3.6
1	C	36	GLU	3.5
1	E	230	ALA	3.4
1	A	69	HIS	3.4
1	E	134	ASP	3.3
1	A	35	SER	3.2
1	F	136	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	134	ASP	3.2
1	A	15	MET	3.2
1	E	231	GLY	3.1
1	D	36	GLU	3.1
1	C	230	ALA	3.1
1	E	135	ILE	2.9
1	F	35	SER	2.9
1	D	136	GLU	2.9
1	E	36	GLU	2.8
1	A	41	GLU	2.7
1	C	38	LEU	2.6
1	E	136	GLU	2.6
1	F	39	PRO	2.5
1	E	58	GLY	2.5
1	F	33	THR	2.4
1	F	138	VAL	2.3
1	A	231	GLY	2.3
1	D	38	LEU	2.3
1	E	39	PRO	2.3
1	E	57	ALA	2.2
1	D	73	PHE	2.2
1	B	161	ALA	2.2
1	D	37	SER	2.1
1	B	137	HIS	2.1
1	C	35	SER	2.1
1	C	133	GLY	2.1
1	F	239	GLU	2.1
1	D	240	GLN	2.0
1	F	36	GLU	2.0
1	C	138	VAL	2.0
1	F	73	PHE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	B	261	5/5	0.87	0.20	2.13	101,102,102,103	0
3	SO4	C	261	5/5	0.90	0.18	1.71	94,94,95,95	0
3	SO4	A	261	5/5	0.94	0.19	1.70	90,90,90,90	0
2	HPA	A	260	10/10	0.97	0.14	0.50	44,46,47,47	0
2	HPA	F	260	10/10	0.95	0.14	0.35	45,48,49,49	0
2	HPA	B	260	10/10	0.97	0.15	0.34	45,46,47,48	0
2	HPA	E	260	10/10	0.96	0.16	0.25	45,48,50,50	0
3	SO4	A	262	5/5	0.93	0.15	-0.32	88,89,90,90	0
2	HPA	C	260	10/10	0.96	0.14	-0.36	39,40,42,42	0
2	HPA	D	260	10/10	0.98	0.12	-0.66	41,43,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.