



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:48 PM UTC

PDB ID : 3OZB / pdb_00003ozb
Title : Crystal Structure of 5'-methylthioinosine phosphorylase from *Pseudomonas 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

<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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

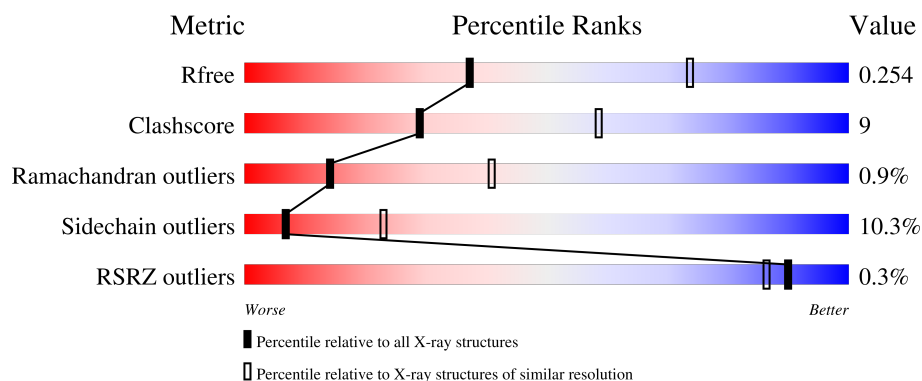
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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	259	
1	B	259	
1	C	259	
1	D	259	
1	E	259	

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Mol	Chain	Length	Quality of chain
1	F	259	% 73% 15% • 8%

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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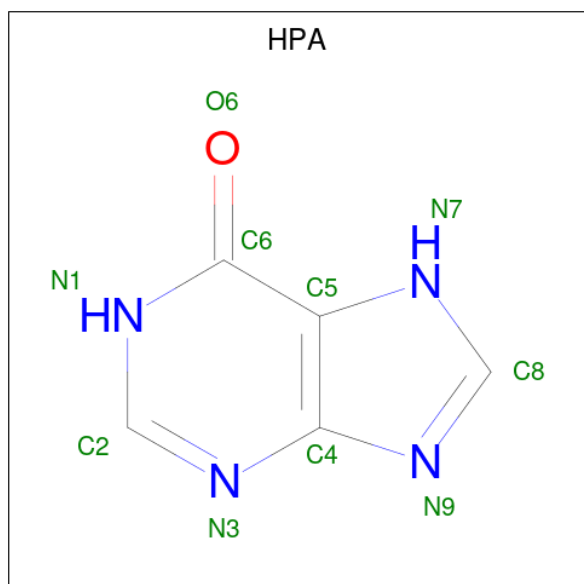
Chain	Residue	Modelled	Actual	Comment	Reference
B	4	HIS	-	expression tag	UNP Q02PG8
B	5	HIS	-	expression tag	UNP Q02PG8
B	6	HIS	-	expression tag	UNP Q02PG8
B	7	HIS	-	expression tag	UNP Q02PG8
B	8	GLU	-	expression tag	UNP Q02PG8
B	9	ASN	-	expression tag	UNP Q02PG8
B	10	LEU	-	expression tag	UNP Q02PG8
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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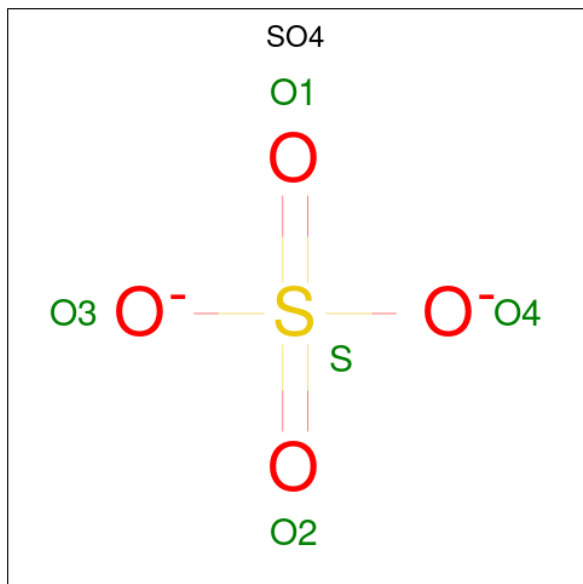
Chain	Residue	Modelled	Actual	Comment	Reference
E	4	HIS	-	expression tag	UNP Q02PG8
E	5	HIS	-	expression tag	UNP Q02PG8
E	6	HIS	-	expression tag	UNP Q02PG8
E	7	HIS	-	expression tag	UNP Q02PG8
E	8	GLU	-	expression tag	UNP Q02PG8
E	9	ASN	-	expression tag	UNP Q02PG8
E	10	LEU	-	expression tag	UNP Q02PG8
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 (CCD ID: HPA) (formula: $C_5H_4N_4O$).



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

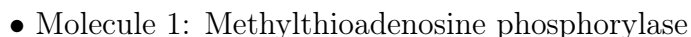
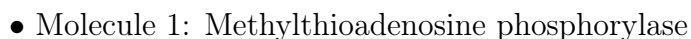
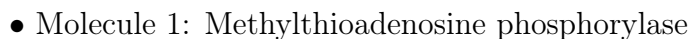


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

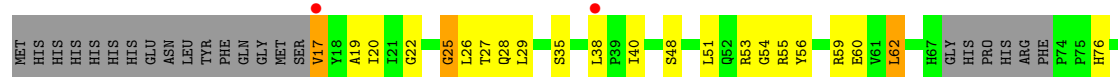
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total 12	O 12	0	0
4	B	11	Total 11	O 11	0	0
4	C	14	Total 14	O 14	0	0
4	D	11	Total 11	O 11	0	0
4	E	6	Total 6	O 6	0	0
4	F	9	Total 9	O 9	0	0

- Molecule 1: Methylthioadenosine phosphorylase

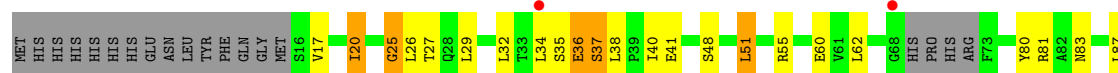
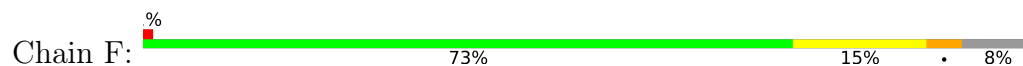




• Molecule 1: Methylthioadenosine phosphorylase



• Molecule 1: Methylthioadenosine phosphorylase



4 Data and refinement statistics

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) 98.8 (19.96-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.202 , 0.262 0.199 , 0.254	Depositor DCC
R_{free} test set	2126 reflections (5.06%)	wwPDB-VP
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 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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

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	0.79	0/1868	0.99	2/2540 (0.1%)
1	B	0.73	0/1825	0.97	0/2482
1	C	0.78	0/1843	1.01	5/2506 (0.2%)
1	D	0.75	0/1837	1.00	2/2499 (0.1%)
1	E	0.75	0/1821	0.99	2/2477 (0.1%)
1	F	0.70	0/1837	1.00	5/2499 (0.2%)
All	All	0.75	0/11031	0.99	16/15003 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	PHE	CA-C-N	-6.42	115.04	119.66
1	C	73	PHE	C-N-CA	-6.42	115.04	119.66
1	D	25	GLY	N-CA-C	-6.26	105.84	114.67
1	F	25	GLY	N-CA-C	-5.80	107.67	115.21
1	E	25	GLY	N-CA-C	-5.77	107.04	113.79
1	F	209	ARG	N-CA-C	5.49	118.02	111.71
1	C	145	HIS	CA-C-N	5.46	126.67	119.84
1	C	145	HIS	C-N-CA	5.46	126.67	119.84
1	C	186	ILE	N-CA-C	-5.38	105.29	110.72
1	A	25	GLY	N-CA-C	-5.20	107.49	114.25
1	E	135	ILE	N-CA-C	5.11	119.97	109.34
1	A	219	ALA	N-CA-C	5.11	116.85	108.52
1	D	17	VAL	N-CA-C	5.08	116.00	108.23
1	F	145	HIS	CA-C-N	5.08	125.15	119.87
1	F	145	HIS	C-N-CA	5.08	125.15	119.87
1	F	246	ILE	N-CA-C	5.06	115.67	110.36

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	30	0
1	B	1788	0	1780	26	0
1	C	1805	0	1796	34	0
1	D	1799	0	1788	42	0
1	E	1781	0	1777	40	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	1	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	188	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 9.

All (188) 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:HE21	1:C:176:GLN:HA	1.21	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:HE21	1:C:176:GLN:CA	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:C:176:GLN:HA	1:C:176:GLN:NE2	1.99	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:27:THR:C	1:B:29:LEU:H	2.00	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:HG23	1:B:118:GLN:NE2	2.08	0.69
1:A:182:THR:HG21	1:B:119:LEU:O	1.92	0.69
1:F:36:GLU:HA	1:F:37:SER:CB	2.12	0.68
1:D:176:GLN:HE21	1:D:176:GLN:HA	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:HA	1:E:176:GLN:HE21	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:ARG:NH2	1:E:168:SER:O	2.29	0.66
1:C:126:ARG:HE	1:C:176:GLN:HE22	1.45	0.65
1:C:182:THR:CG2	1:C:185:GLU:H	1.91	0.65
1:F:37:SER:HB2	1:F:51:LEU:O	1.97	0.65
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
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:C:181:GLU:OE1	2:C:260:HPA:N1	2.32	0.56
1:F:80:TYR:HD1	1:F:204:GLU:HG3	1.70	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:C:119:LEU:C	1:C:119:LEU:HD12	2.32	0.54
1:A:81:ARG:HD2	1:A:127:GLU:HB3	1.89	0.53
1:A:118:GLN:NE2	1:C:182:THR:HG23	2.22	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:B:20:ILE:HD11	1:B:257:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:LEU:HD21	1:F:87:LEU:HD23	1.91	0.53
1:B:27:THR:C	1:B:29:LEU:N	2.68	0.52
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:D:119:LEU:C	1:D:119:LEU:HD12	2.34	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
1:F:96:ILE:HD11	1:F:151:LEU:HD13	1.93	0.50
1:F:126:ARG:HE	1:F:176:GLN:NE2	2.08	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:D:255:ARG:HH21	1:D:255:ARG:HG2	1.75	0.50
1:E:56:TYR:OH	1:E:254:ALA:HB1	2.11	0.50
1:E:119:LEU:C	1:E:119:LEU:HD12	2.37	0.50
1:F:119:LEU:HD12	1:F:119:LEU:C	2.37	0.50
1:D:173:ALA:HB2	1:D:194:ASN:CG	2.38	0.49
1:B:19:ALA:HA	1:B:62:LEU:O	2.12	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:C:25:GLY:O	1:C:250:ARG:HD3	2.13	0.48
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: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:188:ARG:HG3	1:A:189:LEU:N	2.26	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:A:148:ASP:OD1	1:A:150:PRO:HD2	2.14	0.47
1:B:59:ARG:HG2	1:B:61:VAL:HG23	1.95	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:B:176:GLN:OE1	1:B:176:GLN:HA	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:E:202:MET:HE1	1:E:206:ALA:HB2	1.96	0.47
1:A:140:HIS:HB3	1:C:180:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:THR:OG1	1:E:146:PRO:HG3	2.15	0.47
1:E:126:ARG:NE	1:E:176:GLN:HE22	2.08	0.46
1:A:27:THR:HG22	1:A:34:LEU:HD11	1.98	0.46
1:A:51:LEU:HD12	1:A:62:LEU:HD22	1.97	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:D:126:ARG:NE	1:D:176:GLN:HE22	2.05	0.46
1:F:36:GLU:CA	1:F:37:SER:CB	2.81	0.46
1:A:255:ARG:NH1	4:A:266:HOH:O	2.49	0.46
1:F:17:VAL:HG22	1:F:60:GLU:HB3	1.98	0.46
1:D:240:GLN:HE21	1:D:240:GLN:HA	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
1:F:26:LEU:O	1:F:29:LEU:HD13	2.16	0.45
1:F:20:ILE:HD11	1:F:257:LEU:HD21	1.99	0.45
1:C:209:ARG:HH11	1:C:209:ARG:CG	2.29	0.45
1:B:203:PRO:O	1:B:204:GLU:C	2.60	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:A:113:LEU:O	1:A:166:HIS:HA	2.18	0.44
1:E:22:GLY:HA3	1:E:26:LEU:CD1	2.48	0.44
1:B:119:LEU:HD12	1:B:119:LEU:C	2.42	0.44
1:C:41:GLU:OE2	1:C:41:GLU:HA	2.18	0.44
1:A:172:TYR:CE1	1:A:174:CYS:HB2	2.53	0.43
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:B:84:LEU:HD13	1:B:84:LEU:HA	1.87	0.43
1:B:17:VAL:HG13	1:B:93:GLU:HG3	2.00	0.43
1:B:174:CYS:HA	1:B:198:GLY:O	2.19	0.43
1:D:148:ASP:O	1:D:152:ARG:HG3	2.18	0.43
1:C:148:ASP:O	1:C:152:ARG:HG3	2.18	0.43
1:D:209:ARG:CG	1:D:209:ARG:HH11	2.32	0.43
1:A:173:ALA:HB2	1:A:194:ASN:CG	2.44	0.43
1:A:224:PRO:HG2	1:A:229:SER:HB3	1.99	0.43
1:D:172:TYR:CD1	1:D:172:TYR:C	2.97	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:D:225:ALA:O	1:D:226:ALA:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ARG:CD	1:A:127:GLU:HB3	2.50	0.42
1:C:35:SER:C	1:C:36:GLU:HG2	2.45	0.41
1:D:66:ARG:HH21	1:D:204:GLU:CD	2.27	0.41
1:B:182:THR:H	1:B:185:GLU:HB2	1.84	0.41
1:D:119:LEU:O	1:D:119:LEU:HD12	2.20	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:D:122:TYR:CZ	1:D:189:LEU:HD12	2.56	0.41
1:F:182:THR:HG22	1:F:185:GLU:N	2.22	0.41
1:D:28:GLN:HG3	1:D:250:ARG:NH1	2.36	0.40
1:D:66:ARG:CZ	1:D:99:ASN:HD21	2.34	0.40
1:E:81:ARG:HD2	1:E:127:GLU:CB	2.45	0.40
1:A:56:TYR:CD1	1:A:56:TYR:C	2.98	0.40
1:A:117:HIS:HB3	1:A:152:ARG:NH2	2.37	0.40
1:D:62:LEU:HD23	1:D:92:ALA:HB2	2.04	0.40
1:B:151:LEU:HA	1:B:151:LEU:HD13	1.82	0.40
1:D:66:ARG:HH12	1:D:99:ASN:ND2	2.20	0.40
1:D:171:VAL:HB	1:D:194:ASN:HA	2.03	0.40
1:D:172:TYR:C	1:D:172:TYR:HD1	2.29	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%)	30	60
1	B	234/259 (90%)	219 (94%)	13 (6%)	2 (1%)	14	41
1	C	235/259 (91%)	225 (96%)	9 (4%)	1 (0%)	30	60
1	D	235/259 (91%)	224 (95%)	9 (4%)	2 (1%)	14	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	233/259 (90%)	221 (95%)	8 (3%)	4 (2%)	7	25
1	F	235/259 (91%)	223 (95%)	10 (4%)	2 (1%)	14	41
All	All	1410/1554 (91%)	1339 (95%)	59 (4%)	12 (1%)	14	41

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
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%)	161 (88%)	23 (12%)	4	15
1	B	180/199 (90%)	164 (91%)	16 (9%)	9	29
1	C	182/199 (92%)	164 (90%)	18 (10%)	7	24
1	D	181/199 (91%)	160 (88%)	21 (12%)	5	18
1	E	180/199 (90%)	163 (91%)	17 (9%)	8	27
1	F	181/199 (91%)	164 (91%)	17 (9%)	8	27
All	All	1088/1194 (91%)	976 (90%)	112 (10%)	7	23

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	20	ILE
1	A	40	ILE
1	A	42	THR
1	A	51	LEU
1	A	69	HIS
1	A	81	ARG
1	A	110	THR
1	A	113	LEU
1	A	136	GLU
1	A	138	VAL
1	A	139	THR
1	A	151	LEU
1	A	160	ARG
1	A	180	LEU
1	A	182	THR
1	A	188	ARG
1	A	189	LEU
1	A	209	ARG
1	A	212	ASP
1	A	213	LEU
1	A	233	ILE
1	A	242	LEU
1	B	17	VAL
1	B	33	THR
1	B	51	LEU
1	B	52	GLN
1	B	59	ARG
1	B	61	VAL
1	B	62	LEU
1	B	84	LEU
1	B	113	LEU
1	B	151	LEU
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	17	VAL
1	C	36	GLU
1	C	37	SER
1	C	48	SER

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Mol	Chain	Res	Type
1	C	52	GLN
1	C	62	LEU
1	C	64	LEU
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	257	LEU
1	D	28	GLN
1	D	33	THR
1	D	50	PRO
1	D	59	ARG
1	D	61	VAL
1	D	62	LEU
1	D	64	LEU
1	D	113	LEU
1	D	119	LEU
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	197	VAL
1	D	209	ARG
1	D	217	CYS
1	D	240	GLN
1	D	255	ARG
1	E	17	VAL
1	E	20	ILE
1	E	27	THR
1	E	38	LEU
1	E	40	ILE
1	E	51	LEU
1	E	62	LEU

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Mol	Chain	Res	Type
1	E	134	ASP
1	E	138	VAL
1	E	148	ASP
1	E	176	GLN
1	E	182	THR
1	E	188	ARG
1	E	209	ARG
1	E	217	CYS
1	E	218	LEU
1	E	246	ILE
1	F	20	ILE
1	F	38	LEU
1	F	40	ILE
1	F	51	LEU
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	189	LEU
1	F	213	LEU
1	F	248	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	83	ASN
1	A	99	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	145	HIS
1	B	240	GLN

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Mol	Chain	Res	Type
1	C	76	HIS
1	C	83	ASN
1	C	99	ASN
1	C	118	GLN
1	C	145	HIS
1	C	176	GLN
1	D	52	GLN
1	D	83	ASN
1	D	99	ASN
1	D	118	GLN
1	D	145	HIS
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	145	HIS
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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	SO4	A	262	-	4,4,4	0.28	0	6,6,6	0.28	0
2	HPA	C	260	-	10,11,11	1.79	1 (10%)	11,15,15	2.48	6 (54%)
3	SO4	C	261	-	4,4,4	0.32	0	6,6,6	0.39	0
2	HPA	E	260	-	10,11,11	1.75	1 (10%)	11,15,15	2.92	8 (72%)
2	HPA	D	260	-	10,11,11	2.02	2 (20%)	11,15,15	2.94	7 (63%)
2	HPA	A	260	-	10,11,11	1.61	2 (20%)	11,15,15	2.90	8 (72%)
3	SO4	B	261	-	4,4,4	0.36	0	6,6,6	0.25	0
2	HPA	B	260	-	10,11,11	1.76	2 (20%)	11,15,15	2.78	7 (63%)
3	SO4	A	261	-	4,4,4	0.29	0	6,6,6	0.39	0
2	HPA	F	260	-	10,11,11	1.81	2 (20%)	11,15,15	2.46	6 (54%)

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	C	260	-	-	-	0/2/2/2
2	HPA	E	260	-	-	-	0/2/2/2
2	HPA	D	260	-	-	-	0/2/2/2
2	HPA	A	260	-	-	-	0/2/2/2
2	HPA	B	260	-	-	-	0/2/2/2
2	HPA	F	260	-	-	-	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	260	HPA	C2-N3	4.95	1.39	1.30
2	D	260	HPA	C2-N3	4.84	1.39	1.30
2	C	260	HPA	C2-N3	4.59	1.38	1.30
2	B	260	HPA	C2-N3	4.39	1.38	1.30
2	F	260	HPA	C2-N3	4.38	1.38	1.30
2	A	260	HPA	C2-N3	3.71	1.37	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	260	HPA	C5-N7	-3.24	1.33	1.38
2	B	260	HPA	C5-N7	-2.74	1.34	1.38
2	F	260	HPA	C2-N1	2.55	1.40	1.35
2	A	260	HPA	C5-N7	-2.35	1.34	1.38

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	260	HPA	N1-C2-N3	-5.67	118.97	125.50
2	B	260	HPA	N1-C2-N3	-4.74	120.04	125.50
2	D	260	HPA	C5-C6-N1	4.56	120.27	110.26
2	D	260	HPA	N1-C2-N3	-4.48	120.34	125.50
2	E	260	HPA	C5-C6-N1	4.45	120.01	110.26
2	E	260	HPA	C2-N1-C6	-4.40	119.06	125.09
2	D	260	HPA	C2-N1-C6	-4.34	119.14	125.09
2	B	260	HPA	C5-C6-N1	3.92	118.86	110.26
2	F	260	HPA	N1-C2-N3	-3.90	121.00	125.50
2	C	260	HPA	C5-C6-N1	3.80	118.59	110.26
2	C	260	HPA	N1-C2-N3	-3.70	121.24	125.50
2	C	260	HPA	C2-N1-C6	-3.69	120.03	125.09
2	A	260	HPA	C5-C6-N1	3.67	118.32	110.26
2	E	260	HPA	N1-C2-N3	-3.53	121.43	125.50
2	B	260	HPA	C2-N1-C6	-3.48	120.32	125.09
2	D	260	HPA	O6-C6-C5	-3.40	119.07	127.26
2	B	260	HPA	O6-C6-C5	-3.25	119.43	127.26
2	F	260	HPA	C5-C6-N1	3.21	117.30	110.26
2	F	260	HPA	C2-N1-C6	-3.20	120.70	125.09
2	F	260	HPA	N7-C8-N9	-3.17	109.30	112.98
2	A	260	HPA	O6-C6-C5	-3.07	119.85	127.26
2	A	260	HPA	C6-C5-C4	-3.07	119.51	121.61
2	E	260	HPA	C2-N3-C4	3.02	120.81	113.34
2	A	260	HPA	C2-N3-C4	2.95	120.63	113.34
2	B	260	HPA	C2-N3-C4	2.94	120.59	113.34
2	D	260	HPA	C2-N3-C4	2.92	120.55	113.34
2	E	260	HPA	C6-C5-C4	-2.80	119.70	121.61
2	E	260	HPA	N7-C8-N9	-2.77	109.77	112.98
2	C	260	HPA	O6-C6-C5	-2.74	120.66	127.26
2	E	260	HPA	O6-C6-C5	-2.71	120.71	127.26
2	A	260	HPA	C2-N1-C6	-2.63	121.48	125.09
2	C	260	HPA	C2-N3-C4	2.57	119.67	113.34
2	A	260	HPA	C8-N9-C4	2.52	107.24	102.89
2	B	260	HPA	N7-C8-N9	-2.51	110.07	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	260	HPA	C2-N3-C4	2.50	119.51	113.34
2	D	260	HPA	C6-C5-C4	-2.44	119.94	121.61
2	E	260	HPA	C8-N9-C4	2.40	107.04	102.89
2	F	260	HPA	C8-N9-C4	2.32	106.89	102.89
2	A	260	HPA	N7-C8-N9	-2.31	110.30	112.98
2	D	260	HPA	N7-C8-N9	-2.20	110.43	112.98
2	B	260	HPA	C8-N9-C4	2.07	106.46	102.89
2	C	260	HPA	C8-N9-C4	2.04	106.41	102.89

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 [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	241/259 (93%)	-0.55	0	100 100	26, 48, 72, 81	1 (0%)
1	B	238/259 (91%)	-0.52	0	100 100	36, 54, 81, 90	0
1	C	239/259 (92%)	-0.51	0	100 100	33, 48, 76, 93	0
1	D	239/259 (92%)	-0.44	1 (0%)	88 84	34, 51, 80, 91	0
1	E	236/259 (91%)	-0.38	2 (0%)	82 75	31, 55, 88, 103	1 (0%)
1	F	239/259 (92%)	-0.43	2 (0%)	82 75	37, 56, 93, 110	0
All	All	1432/1554 (92%)	-0.47	5 (0%)	90 86	26, 51, 83, 110	2 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	68	GLY	4.1
1	F	34	LEU	3.5
1	D	67	HIS	2.5
1	E	38	LEU	2.4
1	E	17	VAL	2.2

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 oligosaccharides 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	B	261	5/5	0.83	0.11	101,102,102,103	0
3	SO4	C	261	5/5	0.89	0.09	94,94,95,95	0
3	SO4	A	262	5/5	0.92	0.09	88,89,90,90	0
3	SO4	A	261	5/5	0.93	0.11	90,90,90,90	0
2	HPA	E	260	10/10	0.93	0.08	45,48,50,50	0
2	HPA	B	260	10/10	0.94	0.06	45,46,47,48	0
2	HPA	F	260	10/10	0.94	0.07	45,48,49,49	0
2	HPA	D	260	10/10	0.94	0.06	41,43,44,44	0
2	HPA	C	260	10/10	0.95	0.06	39,40,42,42	0
2	HPA	A	260	10/10	0.96	0.05	44,46,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.