



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 04:50 PM UTC

PDB ID : 4HX9 / pdb_00004hx9
Title : Designed Phosphodeoxyribosyltransferase
Authors : Kaminski, P.A.; Labesse, G.
Deposited on : 2012-11-09
Resolution : 2.68 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

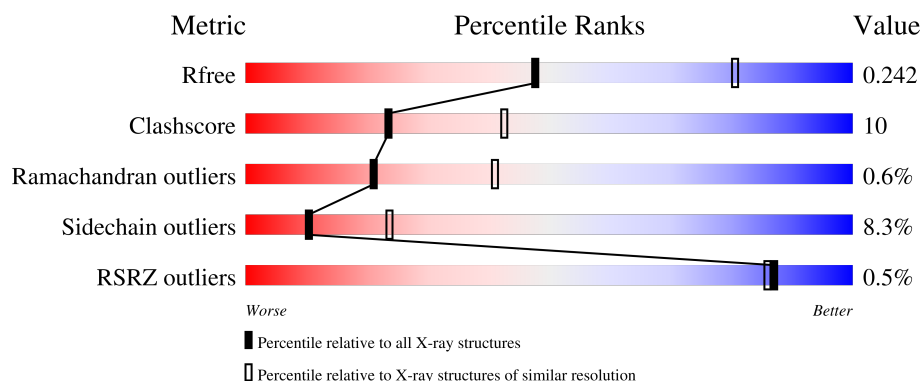
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	157	 80% 17% ..
1	B	157	 76% 20% ...
1	C	157	 2% 76% 22% ..
1	D	157	 78% 19% ..
1	E	157	 75% 22% ..

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Mol	Chain	Length	Quality of chain
1	F	157	75% 20% . .
1	G	157	% 75% 20% . ..
1	H	157	% 68% 27% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10448 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 Nucleoside deoxyribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1261	809	204	243	5			
1	B	154	Total	C	N	O	S	0	2	0
			1256	807	201	242	6			
1	E	156	Total	C	N	O	S	0	0	0
			1261	809	204	243	5			
1	F	156	Total	C	N	O	S	0	1	0
			1266	812	204	245	5			
1	C	156	Total	C	N	O	S	0	0	0
			1261	809	204	243	5			
1	D	155	Total	C	N	O	S	0	2	0
			1255	806	199	245	5			
1	G	156	Total	C	N	O	S	0	0	0
			1261	809	204	243	5			
1	H	156	Total	C	N	O	S	0	2	0
			1270	814	204	247	5			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ARG	PHE	engineered mutation	UNP Q9R5V5
A	91	GLN	GLU	engineered mutation	UNP Q9R5V5
A	92	GLY	ASP	engineered mutation	UNP Q9R5V5
A	93	THR	VAL	engineered mutation	UNP Q9R5V5
A	123	SER	ASN	engineered mutation	UNP Q9R5V5
B	13	ARG	PHE	engineered mutation	UNP Q9R5V5
B	91	GLN	GLU	engineered mutation	UNP Q9R5V5
B	92	GLY	ASP	engineered mutation	UNP Q9R5V5
B	93	THR	VAL	engineered mutation	UNP Q9R5V5
B	123	SER	ASN	engineered mutation	UNP Q9R5V5
E	13	ARG	PHE	engineered mutation	UNP Q9R5V5
E	91	GLN	GLU	engineered mutation	UNP Q9R5V5
E	92	GLY	ASP	engineered mutation	UNP Q9R5V5

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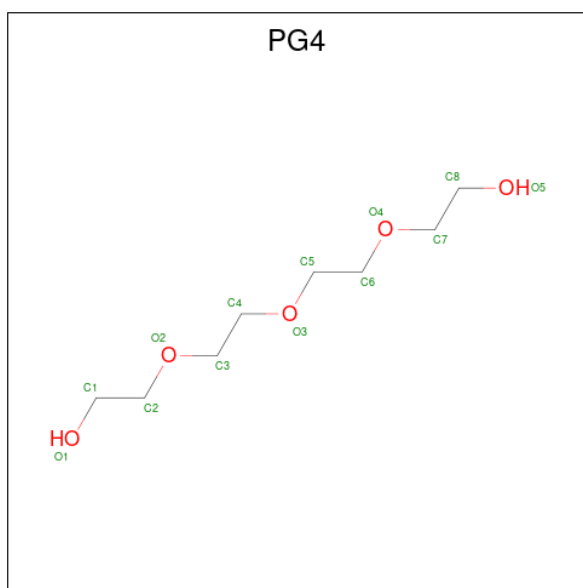
Chain	Residue	Modelled	Actual	Comment	Reference
E	93	THR	VAL	engineered mutation	UNP Q9R5V5
E	123	SER	ASN	engineered mutation	UNP Q9R5V5
F	13	ARG	PHE	engineered mutation	UNP Q9R5V5
F	91	GLN	GLU	engineered mutation	UNP Q9R5V5
F	92	GLY	ASP	engineered mutation	UNP Q9R5V5
F	93	THR	VAL	engineered mutation	UNP Q9R5V5
F	123	SER	ASN	engineered mutation	UNP Q9R5V5
C	13	ARG	PHE	engineered mutation	UNP Q9R5V5
C	91	GLN	GLU	engineered mutation	UNP Q9R5V5
C	92	GLY	ASP	engineered mutation	UNP Q9R5V5
C	93	THR	VAL	engineered mutation	UNP Q9R5V5
C	123	SER	ASN	engineered mutation	UNP Q9R5V5
D	13	ARG	PHE	engineered mutation	UNP Q9R5V5
D	91	GLN	GLU	engineered mutation	UNP Q9R5V5
D	92	GLY	ASP	engineered mutation	UNP Q9R5V5
D	93	THR	VAL	engineered mutation	UNP Q9R5V5
D	123	SER	ASN	engineered mutation	UNP Q9R5V5
G	13	ARG	PHE	engineered mutation	UNP Q9R5V5
G	91	GLN	GLU	engineered mutation	UNP Q9R5V5
G	92	GLY	ASP	engineered mutation	UNP Q9R5V5
G	93	THR	VAL	engineered mutation	UNP Q9R5V5
G	123	SER	ASN	engineered mutation	UNP Q9R5V5
H	13	ARG	PHE	engineered mutation	UNP Q9R5V5
H	91	GLN	GLU	engineered mutation	UNP Q9R5V5
H	92	GLY	ASP	engineered mutation	UNP Q9R5V5
H	93	THR	VAL	engineered mutation	UNP Q9R5V5
H	123	SER	ASN	engineered mutation	UNP Q9R5V5

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	B	1	Total	C	O	0	0
			13	8	5		
3	F	1	Total	C	O	0	0
			13	8	5		
3	F	1	Total	C	O	0	0
			13	8	5		
3	D	1	Total	C	O	0	0
			13	8	5		
3	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total	O	0	0
			36	36		
4	B	45	Total	O	0	0
			45	45		
4	E	23	Total	O	0	0
			23	23		
4	F	30	Total	O	0	0
			30	30		
4	C	8	Total	O	0	0
			8	8		

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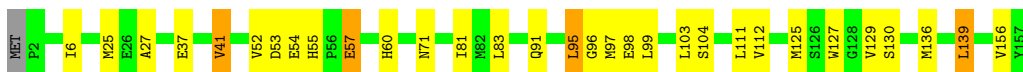
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	30	Total 30	O 30	0	0
4	G	13	Total 13	O 13	0	0
4	H	24	Total 24	O 24	0	0

3 Residue-property plots

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.

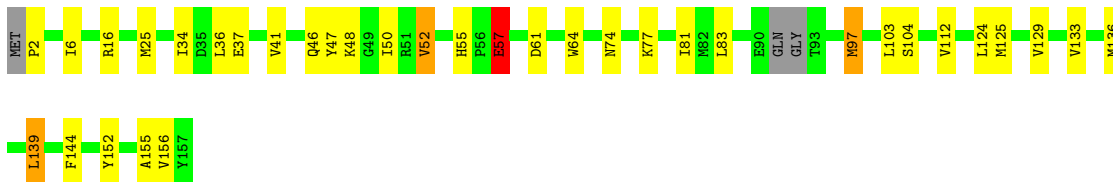
- Molecule 1: Nucleoside deoxyribosyltransferase

Chain A: 



- Molecule 1: Nucleoside deoxyribosyltransferase

Chain B: 



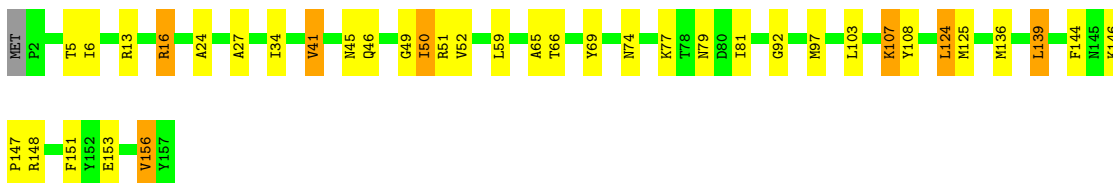
- Molecule 1: Nucleoside deoxyribosyltransferase

Chain E: 

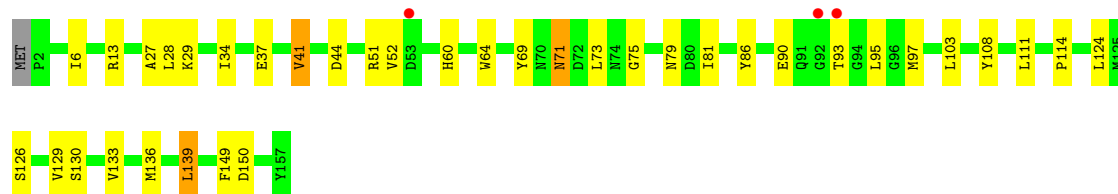
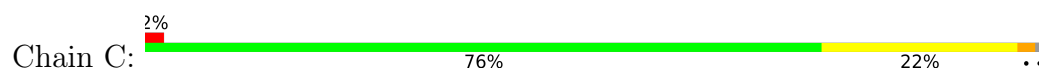


- Molecule 1: Nucleoside deoxyribosyltransferase

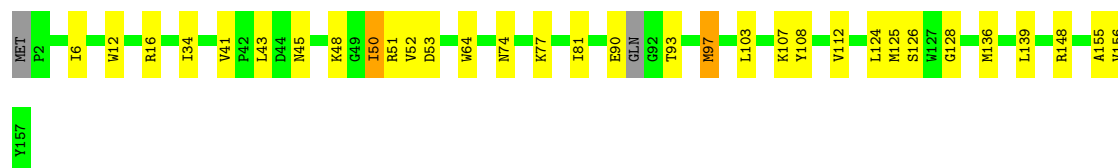
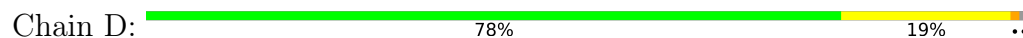
Chain F: 



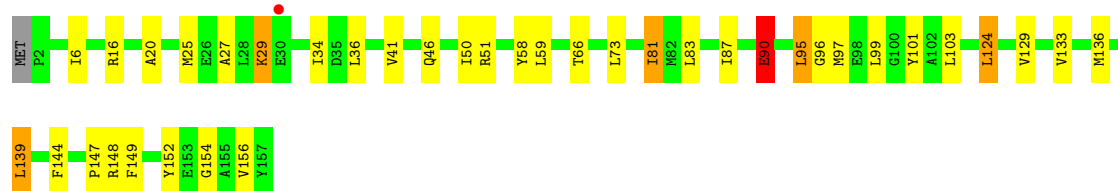
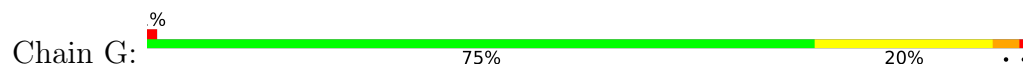
- Molecule 1: Nucleoside deoxyribosyltransferase



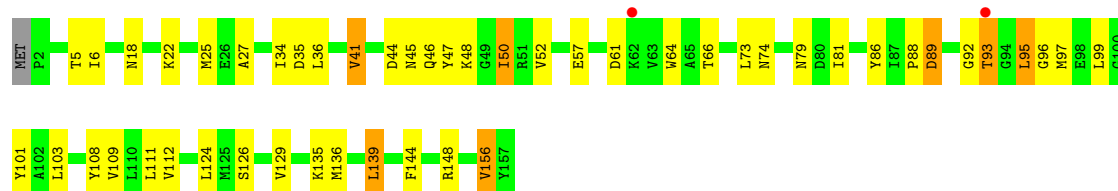
- Molecule 1: Nucleoside deoxyribosyltransferase



- Molecule 1: Nucleoside deoxyribosyltransferase



- Molecule 1: Nucleoside deoxyribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	218.45Å 218.45Å 218.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.62 – 2.68 38.62 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.62-2.68) 99.8 (38.62-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.195 , 0.250 0.192 , 0.242	Depositor DCC
R_{free} test set	2436 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.028 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10448	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PG4

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	0.68	1/1293 (0.1%)	0.84	0/1751
1	B	0.74	0/1295	0.88	0/1752
1	C	0.57	0/1293	0.76	0/1751
1	D	0.63	0/1294	0.76	0/1752
1	E	0.59	0/1293	0.78	0/1751
1	F	0.65	0/1302	0.80	0/1763
1	G	0.54	0/1293	0.81	0/1751
1	H	0.63	0/1310	0.83	0/1774
All	All	0.63	1/10373 (0.0%)	0.81	0/14045

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	VAL	CA-CB	8.78	1.62	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1261	0	1218	22	0
1	B	1256	0	1211	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1261	0	1218	29	0
1	D	1255	0	1200	25	0
1	E	1261	0	1218	33	0
1	F	1266	0	1220	36	0
1	G	1261	0	1218	30	0
1	H	1270	0	1220	37	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
2	G	10	0	0	0	0
2	H	10	0	0	0	0
3	A	13	0	18	0	0
3	B	13	0	18	0	0
3	D	26	0	36	1	0
3	F	26	0	36	0	0
4	A	36	0	0	1	0
4	B	45	0	0	2	0
4	C	8	0	0	0	0
4	D	30	0	0	0	0
4	E	23	0	0	1	0
4	F	30	0	0	1	0
4	G	13	0	0	0	0
4	H	24	0	0	1	0
All	All	10448	0	9831	204	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 10.

All (204) 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:E:125:MET:HE3	1:F:97:MET:SD	1.91	1.10
1:G:6:ILE:HG22	1:G:81:ILE:HB	1.52	0.92
1:G:95:LEU:HD13	1:G:99:LEU:HD11	1.55	0.89
1:F:52:VAL:HG21	1:F:59:LEU:HD21	1.63	0.80
1:A:125:MET:O	1:A:129:VAL:HG12	1.84	0.78
1:E:125:MET:CE	1:F:97:MET:SD	2.73	0.76
1:H:112:VAL:HG11	1:H:136:MET:HE3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:MET:O	1:E:129:VAL:HG12	1.87	0.75
1:G:129:VAL:HB	1:H:97:MET:HE3	1.71	0.72
1:B:6:ILE:HD12	1:B:6:ILE:C	2.14	0.72
1:E:25:MET:HE1	1:E:36:LEU:HD21	1.71	0.71
1:E:6:ILE:HG22	1:E:81:ILE:HB	1.72	0.71
1:A:95:LEU:HD12	1:A:99:LEU:HD11	1.73	0.70
1:F:16:ARG:HG2	1:F:16:ARG:HH11	1.58	0.68
1:B:136:MET:HE3	1:B:136:MET:HA	1.75	0.68
1:B:112:VAL:HG11	1:B:136:MET:HE3	1.76	0.67
1:F:136:MET:HE1	1:F:139:LEU:HD12	1.77	0.67
1:E:52:VAL:HG11	1:E:64:TRP:CZ2	2.30	0.67
1:G:59:LEU:HD22	1:H:156:VAL:O	1.95	0.67
1:C:6:ILE:HG22	1:C:81:ILE:HB	1.77	0.66
1:C:52:VAL:HG11	1:C:64:TRP:CZ2	2.33	0.64
1:G:25:MET:HE1	1:G:36:LEU:HD21	1.80	0.64
1:E:136:MET:CE	1:E:139:LEU:HD12	2.28	0.64
1:E:71:ASN:ND2	1:C:149:PHE:H	1.95	0.63
1:D:112:VAL:HG11	1:D:136:MET:HE3	1.81	0.63
1:G:46:GLN:OE1	1:G:51:ARG:HG3	1.99	0.62
1:E:136:MET:HE1	1:E:139:LEU:HD12	1.82	0.62
1:A:6:ILE:HG22	1:A:81:ILE:HB	1.81	0.61
1:H:6:ILE:HG22	1:H:81:ILE:HB	1.81	0.61
1:E:25:MET:CE	1:E:36:LEU:HD21	2.30	0.61
1:B:136:MET:HE1	1:B:139:LEU:HD12	1.83	0.61
1:E:99:LEU:HD22	1:E:109:VAL:CG1	2.30	0.61
1:D:74:ASN:HD22	1:D:77:LYS:HE2	1.64	0.61
1:B:25:MET:HE1	4:B:337:HOH:O	2.00	0.61
1:F:108:TYR:CE2	1:F:147:PRO:HB2	2.35	0.61
1:F:52:VAL:HG21	1:F:59:LEU:CD2	2.30	0.60
1:G:96:GLY:HA2	1:G:99:LEU:HD12	1.83	0.60
1:F:124:LEU:HD23	1:F:156:VAL:HG21	1.84	0.60
1:B:112:VAL:HG11	1:B:136:MET:CE	2.32	0.60
1:C:60:HIS:CD2	1:D:155:ALA:HB2	2.36	0.60
1:D:6:ILE:HG23	1:D:34:ILE:HD12	1.84	0.60
1:B:25:MET:CE	4:B:337:HOH:O	2.51	0.59
1:B:74:ASN:ND2	1:B:77:LYS:HE2	2.17	0.59
1:H:112:VAL:HG11	1:H:136:MET:CE	2.34	0.58
1:E:97:MET:SD	1:F:125:MET:HE3	2.43	0.57
1:C:86:TYR:HB2	1:C:111:LEU:HD22	1.86	0.57
1:C:41:VAL:HG13	1:C:44:ASP:HB2	1.86	0.57
1:C:129:VAL:HG23	1:D:97:MET:HE2	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:MET:HE1	1:A:139:LEU:HD12	1.86	0.57
1:F:6:ILE:HG22	1:F:81:ILE:HB	1.86	0.57
1:F:24:ALA:HA	1:F:136:MET:CE	2.35	0.57
1:D:108:TYR:HD2	1:H:74:ASN:HD21	1.52	0.56
1:A:6:ILE:HD12	1:A:6:ILE:C	2.30	0.56
1:G:6:ILE:C	1:G:6:ILE:HD12	2.30	0.56
1:H:124:LEU:HD23	1:H:156:VAL:HG11	1.87	0.56
1:A:97:MET:HE3	1:B:129:VAL:HG23	1.87	0.56
1:F:24:ALA:HA	1:F:136:MET:HE1	1.88	0.56
1:H:136:MET:HE3	1:H:136:MET:HA	1.88	0.56
1:H:136:MET:CE	1:H:139:LEU:HD12	2.37	0.55
1:F:34:ILE:HD11	1:F:144:PHE:CD1	2.41	0.55
1:B:136:MET:CE	1:B:139:LEU:HD12	2.36	0.55
1:E:81:ILE:HD12	1:E:108:TYR:HB3	1.89	0.55
1:E:99:LEU:HD22	1:E:109:VAL:HG13	1.88	0.55
1:H:27:ALA:HB3	1:H:139:LEU:HD13	1.89	0.55
1:H:48:LYS:O	1:H:50:ILE:HD13	2.07	0.54
1:C:81:ILE:HD12	1:C:108:TYR:HB3	1.89	0.54
1:B:6:ILE:HG22	1:B:81:ILE:HB	1.89	0.54
1:H:124:LEU:C	1:H:124:LEU:HD13	2.32	0.54
1:G:73:LEU:HD22	1:G:101:TYR:CE1	2.43	0.54
1:F:74:ASN:HD21	1:H:108:TYR:HD2	1.56	0.54
1:H:5:THR:CB	1:H:79:ASN:HD22	2.20	0.54
1:H:47:TYR:CD1	1:H:64:TRP:HA	2.43	0.54
1:A:96:GLY:HA2	1:B:97[B]:MET:HE2	1.90	0.54
1:D:52:VAL:HG13	1:D:64:TRP:CH2	2.43	0.54
1:D:6:ILE:HG22	1:D:81:ILE:HB	1.91	0.53
1:H:95:LEU:HD22	1:H:99:LEU:HG	1.91	0.53
1:F:74:ASN:HD22	1:F:77:LYS:HE2	1.73	0.53
1:E:153:GLU:N	1:E:153:GLU:OE1	2.42	0.52
1:G:25:MET:CE	1:G:36:LEU:HD21	2.39	0.52
1:G:87:ILE:HG22	1:G:90:GLU:HB2	1.91	0.52
1:G:73:LEU:HD22	1:G:101:TYR:CD1	2.45	0.52
1:A:103:LEU:HD22	1:A:129:VAL:HG23	1.92	0.52
1:C:27:ALA:HB3	1:C:139:LEU:HD13	1.91	0.52
1:A:53:ASP:OD2	1:A:54:GLU:N	2.42	0.52
1:A:136:MET:CE	1:A:139:LEU:HD12	2.40	0.51
1:F:52:VAL:CG2	1:F:59:LEU:HD21	2.36	0.51
1:B:25:MET:HE3	1:B:36:LEU:HD21	1.92	0.51
1:B:74:ASN:HD22	1:B:77:LYS:HE2	1.75	0.51
4:A:303:HOH:O	1:F:153:GLU:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:ALA:HB1	1:G:136:MET:HE1	1.92	0.51
1:H:73:LEU:HD22	1:H:101:TYR:CD1	2.46	0.51
1:H:99:LEU:HD11	1:H:111:LEU:HD21	1.93	0.50
3:D:204:PG4:H32	1:H:66:THR:HG23	1.93	0.50
1:F:27:ALA:HB1	1:F:139:LEU:HB3	1.94	0.50
1:E:81:ILE:HG23	1:E:108:TYR:O	2.12	0.50
1:G:152:TYR:CE2	1:G:154:GLY:HA3	2.47	0.50
1:H:73:LEU:HD22	1:H:101:TYR:CE1	2.46	0.50
1:D:6:ILE:C	1:D:6:ILE:HD12	2.37	0.50
1:E:12:TRP:CE2	1:E:43:LEU:HD21	2.48	0.49
1:D:136:MET:HE3	1:D:136:MET:HA	1.94	0.49
1:A:111:LEU:HG	1:A:130:SER:OG	2.11	0.49
1:D:112:VAL:HG11	1:D:136:MET:CE	2.43	0.49
1:H:136:MET:HE2	1:H:139:LEU:HD12	1.93	0.49
1:H:86:TYR:CE1	1:H:88:PRO:HA	2.47	0.49
1:G:29:LYS:HD3	1:G:36:LEU:CD2	2.43	0.49
1:F:13:ARG:NE	4:F:320:HOH:O	2.45	0.48
1:C:111:LEU:HB2	1:C:133:VAL:HG22	1.95	0.48
1:B:112:VAL:CG1	1:B:136:MET:HE3	2.41	0.48
1:F:79:ASN:O	1:F:107:LYS:HE3	2.13	0.48
1:C:97:MET:SD	1:D:125:MET:HE3	2.54	0.48
1:C:129:VAL:CG2	1:D:97:MET:HE2	2.43	0.48
1:D:51:ARG:NE	1:D:53[A]:ASP:OD1	2.47	0.48
1:H:34:ILE:HD11	1:H:144:PHE:CD1	2.49	0.48
1:A:104:SER:HB2	1:B:104:SER:HB2	1.95	0.47
1:A:60:HIS:NE2	1:B:155:ALA:HB2	2.29	0.47
1:H:99:LEU:HD22	1:H:109:VAL:CG1	2.45	0.47
1:H:25:MET:HE2	4:H:319:HOH:O	2.13	0.47
1:B:47:TYR:HB3	1:B:64:TRP:CD1	2.49	0.47
1:A:127:TRP:CD1	1:A:156:VAL:HG21	2.49	0.47
1:E:128:GLY:HA3	1:F:69:TYR:CE1	2.50	0.47
1:F:108:TYR:HD2	1:D:74:ASN:HD21	1.62	0.47
1:C:6:ILE:C	1:C:6:ILE:HD12	2.40	0.47
1:A:55:HIS:HA	1:A:57:GLU:OE1	2.15	0.46
1:D:48:LYS:O	1:D:50:ILE:HD12	2.13	0.46
1:E:83:LEU:C	1:E:83:LEU:HD13	2.40	0.46
1:B:55:HIS:C	1:B:57:GLU:HG3	2.40	0.46
1:E:24:ALA:HA	1:E:136:MET:HE1	1.97	0.46
1:A:27:ALA:HB3	1:A:139:LEU:HD13	1.98	0.46
1:H:93:THR:O	1:H:96:GLY:N	2.49	0.46
1:C:126:SER:O	1:C:130:SER:OG	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:MET:HE1	1:C:139:LEU:HD12	1.98	0.46
1:F:66:THR:HG21	1:G:66:THR:HG21	1.97	0.46
1:C:136:MET:CE	1:C:139:LEU:HD12	2.46	0.46
1:H:92:GLY:O	1:H:93:THR:C	2.59	0.46
1:C:28:LEU:HD23	1:C:34:ILE:HG13	1.98	0.45
1:D:148:ARG:HE	1:H:45:ASN:ND2	2.14	0.45
1:H:35:ASP:OD2	1:H:35:ASP:C	2.59	0.45
1:A:136:MET:HA	1:A:136:MET:HE3	1.98	0.45
1:H:25:MET:HE3	1:H:36:LEU:HD21	1.99	0.45
1:B:6:ILE:C	1:B:6:ILE:CD1	2.84	0.45
1:B:61:ASP:OD2	1:B:61:ASP:C	2.60	0.45
1:D:148:ARG:HE	1:H:45:ASN:HD21	1.65	0.44
1:F:49:GLY:O	1:F:50:ILE:C	2.59	0.44
1:F:136:MET:CE	1:F:139:LEU:HD12	2.47	0.44
1:E:22:LYS:NZ	4:E:306:HOH:O	2.51	0.44
1:F:5:THR:CB	1:F:79:ASN:HD22	2.29	0.44
1:G:34:ILE:HD11	1:G:144:PHE:CD1	2.53	0.44
1:G:73:LEU:HD22	1:G:101:TYR:CZ	2.53	0.44
1:H:41:VAL:HG22	1:H:44:ASP:HB2	1.99	0.44
1:B:34:ILE:HD11	1:B:144:PHE:CD1	2.52	0.44
1:C:71:ASN:ND2	1:G:149:PHE:H	2.16	0.43
1:E:124:LEU:O	1:E:127:TRP:HB3	2.18	0.43
1:F:45:ASN:ND2	1:H:148:ARG:HE	2.17	0.43
1:C:149:PHE:CG	1:C:150:ASP:N	2.86	0.43
1:A:97:MET:HE3	1:B:129:VAL:CG2	2.49	0.43
1:G:133:VAL:HG11	1:G:152:TYR:CD1	2.54	0.43
1:C:69:TYR:CE1	1:D:128:GLY:HA3	2.54	0.43
1:A:112:VAL:HG11	1:A:136:MET:CE	2.49	0.43
1:D:112:VAL:CG1	1:D:136:MET:HE3	2.46	0.43
1:F:148:ARG:HE	1:D:45:ASN:HD21	1.66	0.43
1:D:97:MET:SD	1:D:97:MET:O	2.77	0.43
1:G:147:PRO:C	1:G:148:ARG:HD2	2.44	0.43
1:E:71:ASN:HD22	1:C:149:PHE:H	1.64	0.42
1:G:149:PHE:CD2	1:G:149:PHE:C	2.96	0.42
1:C:114:PRO:HA	1:C:136:MET:HB2	2.01	0.42
1:E:62:LYS:HD3	1:F:151:PHE:CG	2.54	0.42
1:G:148:ARG:HD2	1:G:148:ARG:N	2.33	0.42
1:A:60:HIS:CD2	1:B:155:ALA:HB2	2.55	0.42
1:F:108:TYR:CZ	1:F:147:PRO:HB2	2.54	0.42
1:F:124:LEU:HA	1:F:156:VAL:CG2	2.50	0.42
1:C:69:TYR:CD1	1:D:128:GLY:HA3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:29:LYS:HD3	1:G:36:LEU:HD22	2.01	0.42
1:G:27:ALA:HB1	1:G:139:LEU:HB3	2.02	0.42
1:H:61:ASP:OD2	1:H:61:ASP:C	2.63	0.42
1:C:75:GLY:O	1:C:79:ASN:ND2	2.40	0.42
1:C:126:SER:HA	1:C:129:VAL:HG12	2.01	0.42
1:A:98:GLU:HG3	1:B:125:MET:HE2	2.01	0.41
1:E:71:ASN:HD22	1:C:149:PHE:HB3	1.85	0.41
1:C:90:GLU:CG	1:C:90:GLU:O	2.68	0.41
1:B:48:LYS:CB	1:B:50:ILE:HD12	2.50	0.41
1:E:115:ASP:OD1	1:E:136:MET:HB3	2.21	0.41
1:G:6:ILE:HG22	1:G:81:ILE:CB	2.37	0.41
1:G:50:ILE:HD13	1:G:58:TYR:CZ	2.56	0.41
1:B:133:VAL:HG11	1:B:152:TYR:CD1	2.55	0.41
1:C:60:HIS:NE2	1:D:155:ALA:HB2	2.34	0.41
1:G:95:LEU:CD1	1:G:99:LEU:HD11	2.37	0.41
1:E:86:TYR:HB2	1:E:111:LEU:HD22	2.01	0.41
1:F:41:VAL:O	1:F:41:VAL:CG2	2.69	0.41
1:B:83:LEU:HD11	1:B:112:VAL:HG21	2.02	0.41
1:E:92:GLY:HA2	1:F:92:GLY:HA2	2.03	0.41
1:H:89:ASP:OD1	1:H:89:ASP:N	2.52	0.41
1:A:27:ALA:HB1	1:A:139:LEU:HB3	2.03	0.40
1:C:111:LEU:HD23	1:C:111:LEU:HA	1.98	0.40
1:E:108:TYR:CD2	1:E:147:PRO:HB2	2.55	0.40
1:E:113:ILE:HG22	1:E:114:PRO:O	2.21	0.40
1:E:127:TRP:CH2	1:F:65:ALA:HB3	2.57	0.40
1:F:108:TYR:CD2	1:F:147:PRO:HB2	2.57	0.40
1:G:97:MET:HE3	1:H:129:VAL:HB	2.03	0.40
1:E:99:LEU:HD22	1:E:109:VAL:HG11	2.00	0.40
1:D:12:TRP:CE2	1:D:43:LEU:HD21	2.56	0.40
1:E:24:ALA:HA	1:E:136:MET:CE	2.52	0.40
1:F:6:ILE:HD12	1:F:6:ILE:C	2.46	0.40
1:G:124:LEU:HD22	1:G:124:LEU:O	2.21	0.40
1:H:103:LEU:C	1:H:103:LEU:HD13	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	154/157 (98%)	147 (96%)	6 (4%)	1 (1%)	21	41
1	B	152/157 (97%)	148 (97%)	2 (1%)	2 (1%)	9	22
1	C	154/157 (98%)	146 (95%)	7 (4%)	1 (1%)	21	41
1	D	153/157 (98%)	146 (95%)	7 (5%)	0	100	100
1	E	154/157 (98%)	149 (97%)	5 (3%)	0	100	100
1	F	155/157 (99%)	145 (94%)	9 (6%)	1 (1%)	21	41
1	G	154/157 (98%)	146 (95%)	7 (4%)	1 (1%)	21	41
1	H	156/157 (99%)	149 (96%)	6 (4%)	1 (1%)	21	41
All	All	1232/1256 (98%)	1176 (96%)	49 (4%)	7 (1%)	21	41

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	50	ILE
1	C	93	THR
1	B	52	VAL
1	B	57	GLU
1	G	90	GLU
1	H	93	THR
1	A	91	GLN

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	135/136 (99%)	126 (93%)	9 (7%)	15	32
1	B	136/136 (100%)	123 (90%)	13 (10%)	8	18
1	C	135/136 (99%)	124 (92%)	11 (8%)	11	25
1	D	135/136 (99%)	123 (91%)	12 (9%)	9	21
1	E	135/136 (99%)	124 (92%)	11 (8%)	11	25
1	F	136/136 (100%)	126 (93%)	10 (7%)	13	28
1	G	135/136 (99%)	124 (92%)	11 (8%)	11	25
1	H	137/136 (101%)	124 (90%)	13 (10%)	8	18
All	All	1084/1088 (100%)	994 (92%)	90 (8%)	10	24

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	MET
1	A	37	GLU
1	A	41	VAL
1	A	52	VAL
1	A	57	GLU
1	A	71	ASN
1	A	83	LEU
1	A	95	LEU
1	A	139	LEU
1	B	2	PRO
1	B	16	ARG
1	B	37	GLU
1	B	41	VAL
1	B	46	GLN
1	B	52	VAL
1	B	57	GLU
1	B	97[A]	MET
1	B	97[B]	MET
1	B	103	LEU
1	B	124	LEU
1	B	139	LEU
1	B	156	VAL
1	E	13	ARG
1	E	30	GLU
1	E	37	GLU
1	E	41	VAL
1	E	48	LYS

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Mol	Chain	Res	Type
1	E	52	VAL
1	E	73	LEU
1	E	83	LEU
1	E	103	LEU
1	E	124	LEU
1	E	139	LEU
1	F	16	ARG
1	F	41	VAL
1	F	46	GLN
1	F	51	ARG
1	F	103	LEU
1	F	107	LYS
1	F	124	LEU
1	F	139	LEU
1	F	146	LYS
1	F	156	VAL
1	C	13	ARG
1	C	29	LYS
1	C	37	GLU
1	C	41	VAL
1	C	51	ARG
1	C	71	ASN
1	C	73	LEU
1	C	95	LEU
1	C	103	LEU
1	C	124	LEU
1	C	139	LEU
1	D	16	ARG
1	D	41	VAL
1	D	50	ILE
1	D	90	GLU
1	D	93	THR
1	D	97	MET
1	D	103	LEU
1	D	107	LYS
1	D	124	LEU
1	D	126	SER
1	D	139	LEU
1	D	156	VAL
1	G	16	ARG
1	G	29	LYS
1	G	41	VAL

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Mol	Chain	Res	Type
1	G	81	ILE
1	G	83	LEU
1	G	90	GLU
1	G	95	LEU
1	G	103	LEU
1	G	124	LEU
1	G	139	LEU
1	G	156	VAL
1	H	18	ASN
1	H	22	LYS
1	H	41	VAL
1	H	46	GLN
1	H	50	ILE
1	H	52	VAL
1	H	57	GLU
1	H	89	ASP
1	H	95	LEU
1	H	126	SER
1	H	135	LYS
1	H	139	LEU
1	H	156	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	18	ASN
1	B	45	ASN
1	B	46	GLN
1	B	74	ASN
1	B	79	ASN
1	E	45	ASN
1	E	55	HIS
1	E	71	ASN
1	F	45	ASN
1	F	74	ASN
1	F	79	ASN
1	C	38	ASN
1	C	60	HIS
1	C	71	ASN
1	C	91	GLN
1	D	38	ASN

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Mol	Chain	Res	Type
1	D	45	ASN
1	D	60	HIS
1	D	74	ASN
1	D	79	ASN
1	G	18	ASN
1	G	74	ASN
1	G	145	ASN
1	H	45	ASN
1	H	46	GLN
1	H	74	ASN
1	H	79	ASN
1	H	105	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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	H	202	-	4,4,4	0.18	0	6,6,6	0.28	0
3	PG4	F	204	-	12,12,12	0.55	0	11,11,11	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	G	201	-	4,4,4	0.18	0	6,6,6	0.25	0
2	SO4	E	202	-	4,4,4	0.30	0	6,6,6	0.25	0
2	SO4	F	201	-	4,4,4	0.19	0	6,6,6	0.22	0
2	SO4	B	201	-	4,4,4	0.22	0	6,6,6	0.17	0
3	PG4	F	203	-	12,12,12	0.62	0	11,11,11	0.46	0
3	PG4	A	203	-	12,12,12	0.53	0	11,11,11	0.42	0
3	PG4	D	204	-	12,12,12	0.52	0	11,11,11	0.56	0
2	SO4	D	202	-	4,4,4	0.30	0	6,6,6	0.13	0
2	SO4	C	201	-	4,4,4	0.23	0	6,6,6	0.31	0
2	SO4	A	201	-	4,4,4	0.28	0	6,6,6	0.33	0
2	SO4	G	202	-	4,4,4	0.21	0	6,6,6	0.14	0
2	SO4	F	202	-	4,4,4	0.26	0	6,6,6	0.32	0
3	PG4	B	202	-	12,12,12	0.52	0	11,11,11	0.26	0
3	PG4	D	203	-	12,12,12	0.62	0	11,11,11	0.36	0
2	SO4	H	201	-	4,4,4	0.28	0	6,6,6	0.23	0
2	SO4	A	202	-	4,4,4	0.28	0	6,6,6	0.34	0
2	SO4	D	201	-	4,4,4	0.22	0	6,6,6	0.11	0
2	SO4	E	201	-	4,4,4	0.24	0	6,6,6	0.17	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	PG4	D	203	-	-	5/10/10/10	-
3	PG4	F	204	-	-	7/10/10/10	-
3	PG4	F	203	-	-	7/10/10/10	-
3	PG4	A	203	-	-	8/10/10/10	-
3	PG4	B	202	-	-	5/10/10/10	-
3	PG4	D	204	-	-	3/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	204	PG4	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
3	D	204	PG4	O3-C5-C6-O4
3	F	203	PG4	O2-C3-C4-O3
3	B	202	PG4	O3-C5-C6-O4
3	A	203	PG4	O1-C1-C2-O2
3	F	203	PG4	O4-C7-C8-O5
3	F	204	PG4	O1-C1-C2-O2
3	D	203	PG4	O1-C1-C2-O2
3	A	203	PG4	O2-C3-C4-O3
3	D	203	PG4	O2-C3-C4-O3
3	B	202	PG4	O4-C7-C8-O5
3	F	203	PG4	O1-C1-C2-O2
3	A	203	PG4	O4-C7-C8-O5
3	D	204	PG4	O4-C7-C8-O5
3	F	204	PG4	O3-C5-C6-O4
3	F	204	PG4	O4-C7-C8-O5
3	F	203	PG4	O3-C5-C6-O4
3	B	202	PG4	O2-C3-C4-O3
3	A	203	PG4	C1-C2-O2-C3
3	D	203	PG4	C8-C7-O4-C6
3	F	204	PG4	C4-C3-O2-C2
3	B	202	PG4	C4-C3-O2-C2
3	F	203	PG4	C5-C6-O4-C7
3	F	203	PG4	C3-C4-O3-C5
3	A	203	PG4	C8-C7-O4-C6
3	D	203	PG4	C3-C4-O3-C5
3	F	204	PG4	C6-C5-O3-C4
3	D	204	PG4	O1-C1-C2-O2
3	F	203	PG4	C8-C7-O4-C6
3	B	202	PG4	O1-C1-C2-O2
3	A	203	PG4	C3-C4-O3-C5
3	F	204	PG4	C1-C2-O2-C3
3	D	203	PG4	O3-C5-C6-O4
3	A	203	PG4	C4-C3-O2-C2
3	A	203	PG4	C5-C6-O4-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	204	PG4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	156/157 (99%)	-0.48	0	100 100	26, 42, 65, 83	3 (1%)
1	B	154/157 (98%)	-0.64	0	100 100	21, 31, 51, 57	8 (5%)
1	C	156/157 (99%)	0.14	3 (1%)	66 63	45, 69, 95, 108	3 (1%)
1	D	155/157 (98%)	-0.29	0	100 100	29, 51, 82, 95	5 (3%)
1	E	156/157 (99%)	0.12	0	100 100	33, 63, 79, 85	3 (1%)
1	F	156/157 (99%)	-0.37	0	100 100	27, 40, 79, 93	9 (5%)
1	G	156/157 (99%)	0.32	1 (0%)	85 84	49, 76, 99, 104	2 (1%)
1	H	156/157 (99%)	-0.22	2 (1%)	75 73	32, 48, 78, 94	10 (6%)
All	All	1245/1256 (99%)	-0.18	6 (0%)	87 86	21, 52, 88, 108	43 (3%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	62	LYS	2.9
1	G	30	GLU	2.4
1	C	53	ASP	2.3
1	H	93	THR	2.3
1	C	92	GLY	2.0
1	C	93	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

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	E	202	5/5	0.83	0.13	84,85,88,88	0
2	SO4	D	202	5/5	0.87	0.11	98,99,100,103	0
3	PG4	D	203	13/13	0.89	0.14	76,80,83,83	0
3	PG4	B	202	13/13	0.90	0.13	49,56,57,58	0
2	SO4	F	202	5/5	0.91	0.11	79,79,80,83	0
3	PG4	D	204	13/13	0.91	0.15	70,71,74,74	0
3	PG4	A	203	13/13	0.92	0.12	46,49,52,53	0
3	PG4	F	203	13/13	0.92	0.14	62,64,67,68	0
2	SO4	C	201	5/5	0.93	0.08	65,67,68,71	5
3	PG4	F	204	13/13	0.94	0.11	48,54,57,57	0
2	SO4	F	201	5/5	0.95	0.07	69,70,70,71	0
2	SO4	A	202	5/5	0.95	0.08	56,58,59,60	0
2	SO4	G	202	5/5	0.96	0.06	67,69,72,73	5
2	SO4	G	201	5/5	0.96	0.09	80,80,81,83	0
2	SO4	H	201	5/5	0.96	0.09	51,52,53,56	0
2	SO4	H	202	5/5	0.96	0.06	67,70,71,71	0
2	SO4	D	201	5/5	0.96	0.10	65,65,68,69	0
2	SO4	E	201	5/5	0.97	0.04	57,59,60,61	5
2	SO4	B	201	5/5	0.99	0.08	42,43,44,44	0
2	SO4	A	201	5/5	0.99	0.04	42,42,44,45	5

6.5 Other polymers

There are no such residues in this entry.