



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:39 PM UTC

PDB ID : 4R7O / pdb_00004r7o
Title : Crystal Structure of Putative Glycerophosphoryl Diester Phosphodiesterase from *Bacillus anthracis*
Authors : Kim, Y.; Zhou, M.; Shatsman, S.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2014-08-28
Resolution : 2.53 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

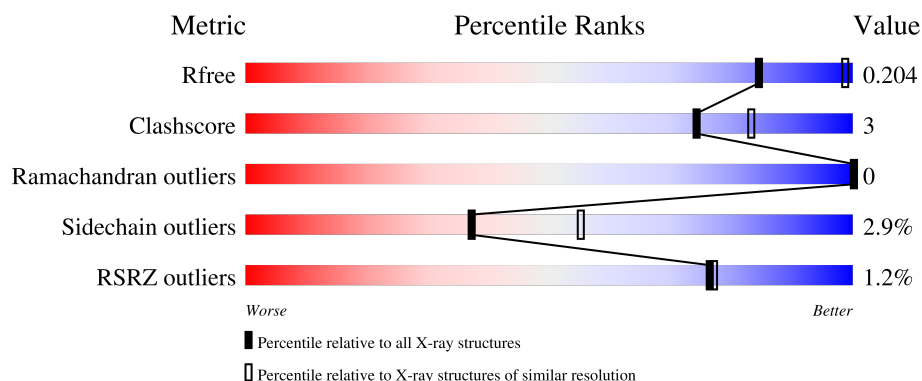
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	292	88% 7% • •
1	B	292	87% 8% • •
1	C	292	85% 10% • •
1	D	292	3% 85% 9% • •
1	E	292	86% 8% • 6%

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Mol	Chain	Length	Quality of chain
1	F	292	87% 5%8%
1	G	292	% 81% 11%7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16503 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 Glycerophosphoryl diester phosphodiesterase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2260	1437	386	426	11			
1	B	279	Total	C	N	O	S	0	1	0
			2268	1442	387	427	12			
1	C	280	Total	C	N	O	S	0	2	0
			2286	1452	391	432	11			
1	D	279	Total	C	N	O	S	0	2	0
			2280	1449	392	428	11			
1	E	275	Total	C	N	O	S	0	0	0
			2231	1421	381	419	10			
1	F	270	Total	C	N	O	S	0	1	0
			2205	1407	374	414	10			
1	G	272	Total	C	N	O	S	0	0	0
			2213	1412	377	414	10			

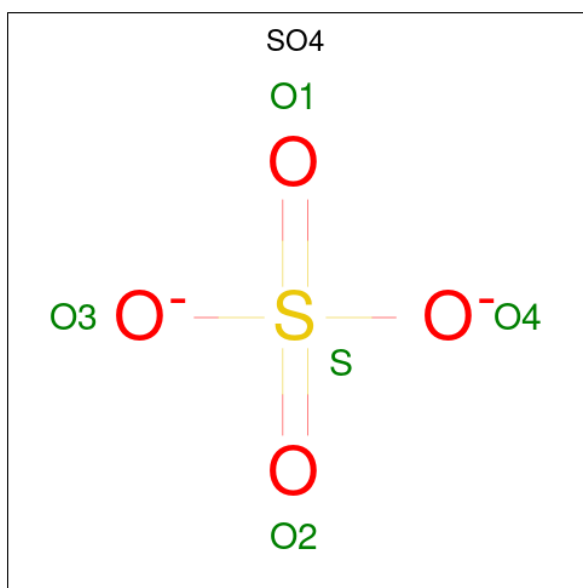
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	SER	-	expression tag	UNP Q81YI6
A	24	ASN	-	expression tag	UNP Q81YI6
B	23	SER	-	expression tag	UNP Q81YI6
B	24	ASN	-	expression tag	UNP Q81YI6
C	23	SER	-	expression tag	UNP Q81YI6
C	24	ASN	-	expression tag	UNP Q81YI6
D	23	SER	-	expression tag	UNP Q81YI6
D	24	ASN	-	expression tag	UNP Q81YI6
E	23	SER	-	expression tag	UNP Q81YI6
E	24	ASN	-	expression tag	UNP Q81YI6
F	23	SER	-	expression tag	UNP Q81YI6
F	24	ASN	-	expression tag	UNP Q81YI6
G	23	SER	-	expression tag	UNP Q81YI6
G	24	ASN	-	expression tag	UNP Q81YI6

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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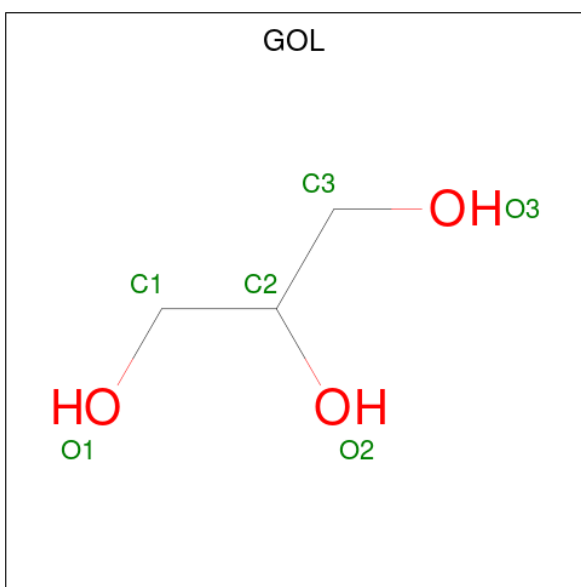
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



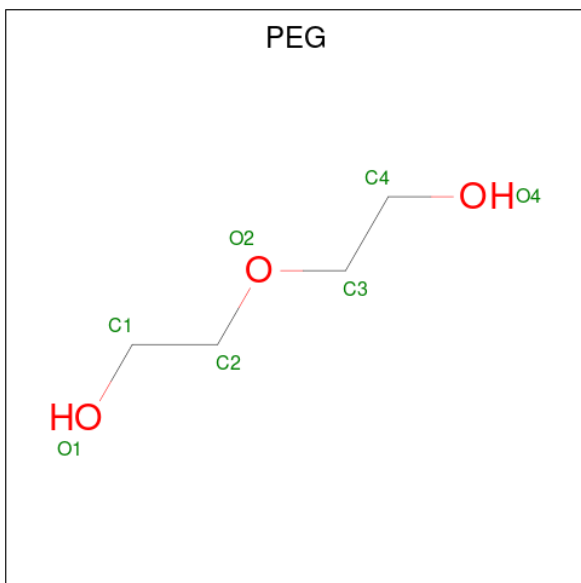
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			7	4	3		
6	E	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is water.

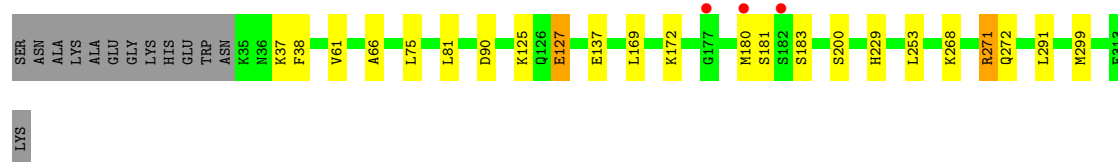
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	108	Total	O	0	0
			108	108		
7	B	102	Total	O	0	0
			102	102		
7	C	124	Total	O	0	0
			124	124		
7	D	92	Total	O	0	0
			92	92		
7	E	116	Total	O	0	0
			116	116		
7	F	85	Total	O	0	0
			85	85		
7	G	23	Total	O	0	0
			23	23		

3 Residue-property plots [i](#)

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

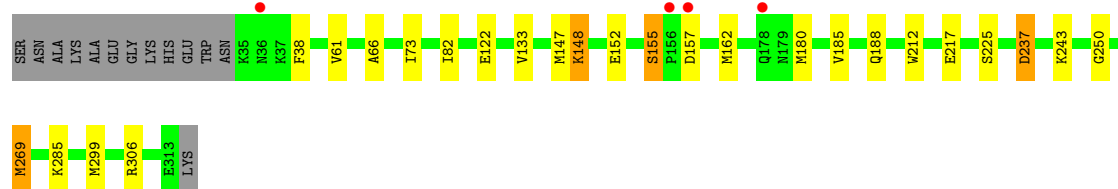
- Molecule 1: Glycerophosphoryl diester phosphodiesterase, putative

Chain A: 



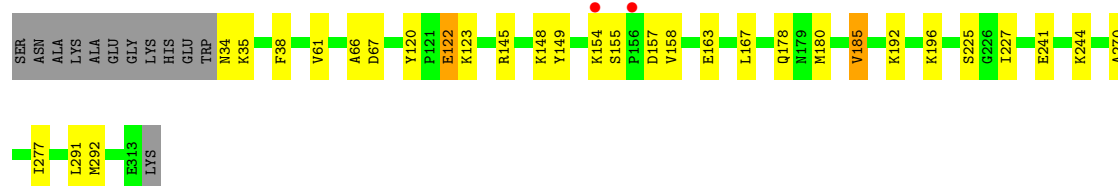
- Molecule 1: Glycerophosphoryl diester phosphodiesterase, putative

Chain B: 



- Molecule 1: Glycerophosphoryl diester phosphodiesterase, putative

Chain C: 



- Molecule 1: Glycerophosphoryl diester phosphodiesterase, putative

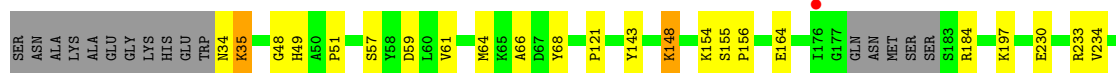
Chain D: 





- Molecule 1: Glycerophosphoryl diester phosphodiesterase, putative

Chain E: 86% 8% 6%



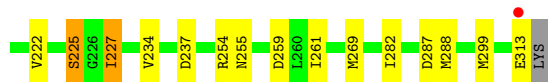
- Molecule 1: Glycerophosphoryl diester phosphodiesterase, putative

Chain F: 87% 5% 8%



- Molecule 1: Glycerophosphoryl diester phosphodiesterase, putative

Chain G: 81% 11% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	209.64Å 85.89Å 191.54Å 90.00° 121.33° 90.00°	Depositor
Resolution (Å)	37.70 – 2.53 37.70 – 2.53	Depositor EDS
% Data completeness (in resolution range)	96.9 (37.70-2.53) 96.5 (37.70-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1745)	Depositor
R, R_{free}	0.154 , 0.204 0.156 , 0.204	Depositor DCC
R_{free} test set	2000 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16503	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: PEG, GOL, MG, EDO, 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	0.51	0/2309	0.81	1/3114 (0.0%)
1	B	0.53	0/2317	0.82	3/3124 (0.1%)
1	C	0.50	0/2335	0.80	0/3148
1	D	0.51	0/2329	0.78	0/3139
1	E	0.51	0/2279	0.78	0/3073
1	F	0.48	0/2253	0.80	0/3040
1	G	0.38	0/2261	0.77	1/3049 (0.0%)
All	All	0.49	0/16083	0.79	5/21687 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	90	ASP	N-CA-C	5.70	117.18	110.97
1	B	250	GLY	CA-C-N	5.68	125.88	120.31
1	B	250	GLY	C-N-CA	5.68	125.88	120.31
1	A	90	ASP	N-CA-C	5.51	116.96	111.07
1	B	185	VAL	N-CA-C	5.01	115.86	108.45

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	2260	0	2257	14	0
1	B	2268	0	2265	13	0
1	C	2286	0	2280	15	0
1	D	2280	0	2281	15	0
1	E	2231	0	2229	16	0
1	F	2205	0	2202	8	0
1	G	2213	0	2215	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
3	A	20	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	1	0
3	E	5	0	0	0	0
3	G	5	0	0	1	0
4	A	4	0	6	0	0
5	A	6	0	7	0	0
5	B	6	0	8	0	0
5	D	6	0	8	0	0
5	E	6	0	8	1	0
6	C	7	0	10	0	0
6	E	7	0	10	0	0
7	A	108	0	0	1	0
7	B	102	0	0	1	0
7	C	124	0	0	0	0
7	D	92	0	0	0	0
7	E	116	0	0	1	0
7	F	85	0	0	1	0
7	G	23	0	0	1	0
All	All	16503	0	15786	98	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 3.

All (98) 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:G:288:MET:HG2	1:G:299:MET:HE1	1.50	0.93
1:A:229:HIS:HD2	1:E:121:PRO:HG3	1.53	0.74
1:D:233[A]:ARG:NH2	3:D:404:SO4:O3	2.21	0.73
1:G:137:GLU:OE2	1:G:172:LYS:NZ	2.27	0.68
1:F:230[B]:GLU:OE1	1:F:233:ARG:NH1	2.27	0.67
1:G:254:ARG:NH1	1:G:287:ASP:OD2	2.30	0.65
1:A:61:VAL:HG13	1:A:66:ALA:HB3	1.79	0.65
1:C:154[B]:LYS:HE2	1:C:158:VAL:HG21	1.79	0.63
1:F:225:SER:HB2	1:F:227:ILE:HG13	1.81	0.61
1:A:271:ARG:HD3	7:A:606:HOH:O	2.00	0.61
1:E:48:GLY:HA2	5:E:403:GOL:H32	1.83	0.61
1:G:147:MET:HE3	1:G:148:LYS:H	1.66	0.61
1:E:61:VAL:HG13	1:E:66:ALA:HB3	1.84	0.60
1:B:237:ASP:OD1	1:B:237:ASP:N	2.36	0.59
1:F:61:VAL:HG13	1:F:66:ALA:HB3	1.84	0.59
1:C:61:VAL:HG13	1:C:66:ALA:HB3	1.86	0.58
1:A:37:LYS:HD3	1:A:38:PHE:H	1.68	0.57
1:A:229:HIS:CD2	1:E:121:PRO:HG3	2.39	0.56
1:B:147:MET:HE3	1:B:148:LYS:H	1.70	0.55
1:F:253:LEU:HD13	1:F:291:LEU:HD21	1.87	0.55
1:B:61:VAL:HG13	1:B:66:ALA:HB3	1.89	0.55
1:D:153:THR:HG22	1:D:189:SER:HB2	1.88	0.54
1:F:111:ASP:OD2	1:F:114:SER:OG	2.22	0.52
1:A:75:LEU:HD13	1:A:81:LEU:HD23	1.91	0.52
1:F:100:ARG:NH2	1:F:158:VAL:O	2.42	0.52
1:C:225:SER:HB2	1:C:227:ILE:HG13	1.92	0.51
1:D:179:ASN:OD1	1:D:179:ASN:N	2.38	0.51
1:G:234:VAL:HG13	1:G:269:MET:HE2	1.93	0.50
1:C:122[B]:GLU:HG2	1:C:123:LYS:HG3	1.93	0.50
1:D:58:TYR:CD1	1:D:69:LEU:HD11	2.46	0.50
1:D:253:LEU:HD13	1:D:291:LEU:HD21	1.94	0.50
1:G:282:ILE:HB	1:G:299:MET:HE3	1.93	0.50
1:D:154[A]:LYS:HG3	1:D:155:SER:N	2.27	0.49
1:E:148:LYS:HG3	1:E:184:ARG:HA	1.95	0.49
1:G:127:GLU:HG3	7:G:523:HOH:O	2.11	0.49
1:D:154[A]:LYS:HE2	1:D:158:VAL:HG11	1.95	0.49
1:B:285:LYS:HE3	1:B:306:ARG:HG2	1.95	0.49
1:G:152:GLU:HB2	1:G:188:GLN:NE2	2.27	0.49
1:G:108:LYS:O	1:G:132:LYS:HE2	2.12	0.48
1:C:67:ASP:O	1:C:148:LYS:HE3	2.13	0.48
1:G:255:ASN:HB3	1:G:261:ILE:HD12	1.94	0.48
1:A:38:PHE:HZ	1:A:299:MET:HE3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:PRO:HG3	7:F:576:HOH:O	2.13	0.48
1:B:122:GLU:CD	1:B:122:GLU:H	2.21	0.47
1:E:59:ASP:OD1	1:E:143:TYR:OH	2.31	0.47
1:B:38:PHE:HZ	1:B:299:MET:HE3	1.79	0.47
1:C:270:ALA:HB3	1:C:277:ILE:HD11	1.96	0.47
1:D:152:GLU:HA	1:D:188:GLN:HG3	1.96	0.47
1:D:218:ASN:HB2	1:D:220:GLU:HG2	1.96	0.47
1:A:253:LEU:HD13	1:A:291:LEU:HD21	1.96	0.47
1:D:218:ASN:N	1:D:218:ASN:OD1	2.48	0.46
1:A:37:LYS:HD3	1:A:38:PHE:N	2.30	0.46
1:A:38:PHE:CZ	1:A:299:MET:HE3	2.50	0.46
1:B:269[A]:MET:HE1	1:E:233:ARG:HA	1.96	0.46
1:B:217:GLU:H	1:B:217:GLU:CD	2.22	0.46
1:C:38:PHE:CZ	1:C:292:MET:HE1	2.50	0.46
1:B:73:ILE:HG13	1:B:162:MET:HE2	1.99	0.45
1:A:125:LYS:HB3	1:A:127:GLU:HG3	1.99	0.45
1:F:68:TYR:OH	1:F:186:MET:HE3	2.16	0.45
1:C:34:ASN:HB3	1:C:35:LYS:H	1.53	0.44
1:C:192:LYS:HG2	1:C:196:LYS:HE2	1.99	0.44
1:G:225:SER:HB2	1:G:227:ILE:HG13	1.98	0.44
1:E:49:HIS:CD2	1:E:64:MET:HE1	2.53	0.44
1:G:152:GLU:HA	1:G:188:GLN:HG3	1.98	0.44
1:E:68:TYR:CE2	1:E:148:LYS:HB3	2.52	0.44
1:E:64:MET:HG2	1:E:305:ASP:HB3	1.99	0.44
1:G:126:GLN:O	1:G:129:VAL:HG22	2.17	0.43
1:D:61:VAL:HG21	1:D:69:LEU:HD13	2.00	0.43
1:D:61:VAL:HG13	1:D:66:ALA:HB3	2.00	0.43
1:D:155:SER:HA	1:D:156:PRO:HD3	1.84	0.43
1:E:156:PRO:HB3	1:E:197:LYS:HE3	2.00	0.43
1:G:170:LEU:HD23	1:G:175:LEU:HD12	2.00	0.43
1:G:237:ASP:N	3:G:402:SO4:O4	2.48	0.43
1:G:218:ASN:H	1:G:218:ASN:HD22	1.67	0.43
1:C:241:GLU:OE2	1:C:244:LYS:NZ	2.39	0.42
1:E:51:PRO:O	1:E:57:SER:HB2	2.19	0.42
1:G:234:VAL:O	1:G:269:MET:HE1	2.19	0.42
1:B:212:TRP:NE1	7:B:594:HOH:O	2.36	0.42
1:E:164:GLU:OE1	1:E:164:GLU:N	2.51	0.42
1:C:149:TYR:HB2	1:C:185:VAL:HG22	2.00	0.42
1:A:137:GLU:OE2	1:A:172:LYS:NZ	2.49	0.42
1:B:155:SER:HB3	1:B:157:ASP:OD1	2.20	0.42
1:E:263:ASN:HB2	7:E:615:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LEU:HD12	1:A:169:LEU:HA	1.90	0.41
1:G:218:ASN:H	1:G:218:ASN:ND2	2.18	0.41
1:D:243:LYS:NZ	1:D:274:GLY:O	2.53	0.41
1:E:68:TYR:CD2	1:E:148:LYS:HB3	2.56	0.41
1:C:120:TYR:HB3	1:C:123:LYS:HD2	2.02	0.41
1:C:163:GLU:O	1:C:167:LEU:HG	2.21	0.41
1:D:113:GLY:HA3	1:D:128:TYR:O	2.21	0.41
1:B:82:ILE:HD12	1:B:133:VAL:HG11	2.03	0.40
1:B:152:GLU:HB2	1:B:188:GLN:NE2	2.37	0.40
1:C:157:ASP:OD1	1:C:158:VAL:N	2.54	0.40
1:E:34:ASN:HB3	1:E:35:LYS:H	1.62	0.40
1:G:108:LYS:HD3	1:G:108:LYS:HA	1.94	0.40
1:A:268:LYS:HE2	1:A:268:LYS:HB2	1.83	0.40
1:C:291:LEU:HA	1:C:291:LEU:HD23	1.84	0.40
1:G:49:HIS:CD2	1:G:64:MET:HE1	2.56	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	277/292 (95%)	273 (99%)	4 (1%)	0	100	100
1	B	278/292 (95%)	270 (97%)	8 (3%)	0	100	100
1	C	280/292 (96%)	277 (99%)	3 (1%)	0	100	100
1	D	279/292 (96%)	271 (97%)	8 (3%)	0	100	100
1	E	271/292 (93%)	266 (98%)	5 (2%)	0	100	100
1	F	267/292 (91%)	259 (97%)	8 (3%)	0	100	100
1	G	268/292 (92%)	264 (98%)	4 (2%)	0	100	100
All	All	1920/2044 (94%)	1880 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	248/258 (96%)	241 (97%)	7 (3%)	38	57
1	B	249/258 (96%)	241 (97%)	8 (3%)	34	51
1	C	251/258 (97%)	244 (97%)	7 (3%)	38	57
1	D	250/258 (97%)	239 (96%)	11 (4%)	25	38
1	E	244/258 (95%)	238 (98%)	6 (2%)	42	60
1	F	241/258 (93%)	239 (99%)	2 (1%)	73	84
1	G	242/258 (94%)	232 (96%)	10 (4%)	27	41
All	All	1725/1806 (96%)	1674 (97%)	51 (3%)	37	53

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	GLU
1	A	180	MET
1	A	181	SER
1	A	183	SER
1	A	200	SER
1	A	271	ARG
1	A	272	GLN
1	B	148	LYS
1	B	155	SER
1	B	180	MET
1	B	225	SER
1	B	237	ASP
1	B	243	LYS
1	B	269[A]	MET
1	B	269[B]	MET
1	C	122[A]	GLU
1	C	122[B]	GLU
1	C	145	ARG

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Mol	Chain	Res	Type
1	C	155	SER
1	C	178	GLN
1	C	180	MET
1	C	185	VAL
1	D	37	LYS
1	D	62	LYS
1	D	65	LYS
1	D	100	ARG
1	D	174	ASN
1	D	178	GLN
1	D	179	ASN
1	D	218	ASN
1	D	243	LYS
1	D	265	SER
1	D	269	MET
1	E	35	LYS
1	E	148	LYS
1	E	154	LYS
1	E	155	SER
1	E	230	GLU
1	E	234	VAL
1	F	193	ASP
1	F	225	SER
1	G	61	VAL
1	G	100	ARG
1	G	148	LYS
1	G	176	ILE
1	G	218	ASN
1	G	222	VAL
1	G	225	SER
1	G	227	ILE
1	G	259	ASP
1	G	313	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	199	HIS
1	A	209	GLN
1	A	240	GLN
1	A	273	ASN

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Mol	Chain	Res	Type
1	B	199	HIS
1	B	218	ASN
1	C	199	HIS
1	C	209	GLN
1	C	302	ASN
1	D	36	ASN
1	E	308	HIS
1	F	117	ASN
1	F	209	GLN
1	F	219	ASN
1	F	240	GLN
1	F	273	ASN
1	G	74	GLN
1	G	117	ASN
1	G	218	ASN

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](#)

Of 27 ligands modelled in this entry, 8 are monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	G	402	-	4,4,4	0.28	0	6,6,6	0.12	0
3	SO4	B	404	-	4,4,4	0.26	0	6,6,6	0.12	0
5	GOL	D	402	-	5,5,5	0.45	0	5,5,5	0.54	0
3	SO4	E	405	-	4,4,4	0.26	0	6,6,6	0.12	0
5	GOL	B	402	-	5,5,5	0.37	0	5,5,5	0.47	0
3	SO4	D	404	-	4,4,4	0.26	0	6,6,6	0.10	0
3	SO4	B	403	-	4,4,4	0.25	0	6,6,6	0.12	0
3	SO4	A	407	-	4,4,4	0.26	0	6,6,6	0.17	0
5	GOL	A	405	2	5,5,5	0.34	0	5,5,5	0.54	0
3	SO4	A	403	-	4,4,4	0.28	0	6,6,6	0.08	0
4	EDO	A	404	-	3,3,3	0.45	0	2,2,2	0.29	0
3	SO4	A	402	-	4,4,4	0.27	0	6,6,6	0.13	0
6	PEG	C	402	-	6,6,6	0.63	0	5,5,5	1.52	0
3	SO4	C	403	-	4,4,4	0.25	0	6,6,6	0.29	0
3	SO4	D	403	-	4,4,4	0.23	0	6,6,6	0.21	0
3	SO4	A	406	-	4,4,4	0.23	0	6,6,6	0.21	0
5	GOL	E	403	-	5,5,5	0.27	0	5,5,5	1.11	0
3	SO4	C	404	-	4,4,4	0.25	0	6,6,6	0.15	0
6	PEG	E	404	-	6,6,6	0.61	0	5,5,5	1.40	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
4	EDO	A	404	-	-	0/1/1/1	-
5	GOL	B	402	-	-	2/4/4/4	-
6	PEG	C	402	-	-	1/4/4/4	-
5	GOL	E	403	-	-	2/4/4/4	-
6	PEG	E	404	-	-	3/4/4/4	-
5	GOL	A	405	2	-	2/4/4/4	-
5	GOL	D	402	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	402	GOL	O1-C1-C2-O2
5	E	403	GOL	O1-C1-C2-C3
6	E	404	PEG	C1-C2-O2-C3
6	C	402	PEG	C1-C2-O2-C3
5	A	405	GOL	O1-C1-C2-C3
5	B	402	GOL	O1-C1-C2-C3
5	D	402	GOL	O1-C1-C2-C3
6	E	404	PEG	O1-C1-C2-O2
5	A	405	GOL	O1-C1-C2-O2
5	E	403	GOL	O1-C1-C2-O2
6	E	404	PEG	O2-C3-C4-O4
5	D	402	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	402	SO4	1	0
3	D	404	SO4	1	0
5	E	403	GOL	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	279/292 (95%)	-0.70	3 (1%) 78 79	18, 32, 61, 127	0
1	B	279/292 (95%)	-0.68	4 (1%) 73 74	12, 33, 62, 105	1 (0%)
1	C	280/292 (95%)	-0.71	2 (0%) 84 86	19, 32, 57, 94	2 (0%)
1	D	279/292 (95%)	-0.53	10 (3%) 46 47	19, 36, 75, 129	2 (0%)
1	E	275/292 (94%)	-0.74	1 (0%) 88 90	19, 32, 59, 105	0
1	F	270/292 (92%)	-0.70	0 100 100	20, 35, 61, 98	1 (0%)
1	G	272/292 (93%)	0.00	3 (1%) 78 79	34, 65, 94, 149	0
All	All	1934/2044 (94%)	-0.58	23 (1%) 76 77	12, 36, 80, 149	6 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	177	GLY	5.1
1	A	182	SER	4.2
1	D	154[A]	LYS	4.2
1	C	154[A]	LYS	3.9
1	A	177	GLY	3.7
1	D	35	LYS	3.7
1	B	157	ASP	3.3
1	D	178	GLN	3.1
1	D	156	PRO	3.0
1	D	36	ASN	2.8
1	D	155	SER	2.8
1	G	118	LYS	2.8
1	E	176	ILE	2.6
1	B	156	PRO	2.5
1	D	158	VAL	2.4
1	D	180	MET	2.2
1	G	35	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	313	GLU	2.2
1	C	156	PRO	2.2
1	B	36	ASN	2.2
1	A	180	MET	2.2
1	D	179	ASN	2.1
1	B	178	GLN	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 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	G	402	5/5	0.54	0.10	133,136,137,139	0
3	SO4	C	404	5/5	0.77	0.13	107,107,109,113	0
4	EDO	A	404	4/4	0.78	0.19	57,64,65,66	0
3	SO4	A	403	5/5	0.81	0.12	104,107,107,109	0
3	SO4	A	407	5/5	0.81	0.15	127,127,128,129	0
3	SO4	B	403	5/5	0.81	0.13	105,108,110,111	0
3	SO4	D	403	5/5	0.82	0.10	93,94,97,99	0
3	SO4	D	404	5/5	0.82	0.12	90,94,94,96	0
3	SO4	B	404	5/5	0.83	0.14	116,119,120,122	0
3	SO4	A	402	5/5	0.84	0.14	93,93,98,101	0
6	PEG	C	402	7/7	0.85	0.17	53,58,63,63	0
5	GOL	E	403	6/6	0.86	0.14	45,46,48,49	0
3	SO4	E	405	5/5	0.87	0.17	85,86,90,91	0
5	GOL	D	402	6/6	0.88	0.12	44,53,56,57	0
6	PEG	E	404	7/7	0.90	0.12	50,50,63,69	0
5	GOL	B	402	6/6	0.92	0.10	49,50,52,54	0
3	SO4	A	406	5/5	0.94	0.09	62,70,76,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	405	6/6	0.96	0.09	51,53,55,57	0
2	MG	D	401	1/1	0.97	0.07	34,34,34,34	0
2	MG	B	401	1/1	0.98	0.11	28,28,28,28	0
2	MG	E	401	1/1	0.98	0.05	29,29,29,29	0
2	MG	E	402	1/1	0.98	0.05	51,51,51,51	0
3	SO4	C	403	5/5	0.98	0.05	32,38,44,46	0
2	MG	F	401	1/1	0.99	0.05	36,36,36,36	0
2	MG	G	401	1/1	0.99	0.04	44,44,44,44	0
2	MG	C	401	1/1	0.99	0.03	28,28,28,28	0
2	MG	A	401	1/1	1.00	0.01	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.