



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:00 PM UTC

PDB ID : 3U0S / pdb_00003u0s
Title : Crystal Structure of an Enzyme Redesigned Through Multiplayer Online Gaming: CE6
Authors : Bale, J.B.; Shen, B.W.; Stoddard, B.L.
Deposited on : 2011-09-29
Resolution : 2.60 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

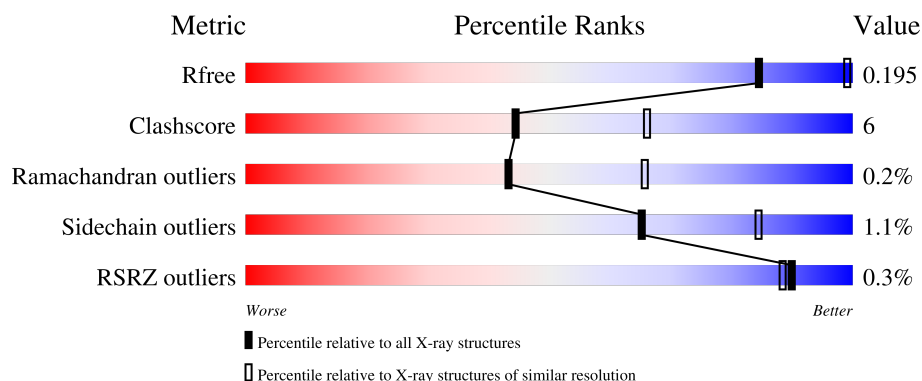
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	337	 85% 12% .
1	B	337	 83% 13% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5614 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 Diisopropyl-fluorophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	9	0
			2627	1674	453	484	16			
1	B	327	Total	C	N	O	S	0	13	0
			2649	1684	453	496	16			

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	THR	GLU	engineered mutation	UNP Q7SIG4
A	36	SER	-	SEE REMARK 999	UNP Q7SIG4
A	38	LEU	GLU	SEE REMARK 999	UNP Q7SIG4
A	39	SER	VAL	SEE REMARK 999	UNP Q7SIG4
A	41	ALA	VAL	SEE REMARK 999	UNP Q7SIG4
A	42	LEU	ASN	SEE REMARK 999	UNP Q7SIG4
A	43	THR	GLY	SEE REMARK 999	UNP Q7SIG4
A	45	ALA	-	SEE REMARK 999	UNP Q7SIG4
A	46	ASN	-	SEE REMARK 999	UNP Q7SIG4
A	47	SER	-	SEE REMARK 999	UNP Q7SIG4
A	49	ALA	-	SEE REMARK 999	UNP Q7SIG4
A	50	GLU	-	SEE REMARK 999	UNP Q7SIG4
A	51	ALA	-	SEE REMARK 999	UNP Q7SIG4
A	52	TYR	-	SEE REMARK 999	UNP Q7SIG4
A	53	LYS	-	SEE REMARK 999	UNP Q7SIG4
A	54	ALA	-	SEE REMARK 999	UNP Q7SIG4
A	55	SER	-	SEE REMARK 999	UNP Q7SIG4
A	56	ARG	-	SEE REMARK 999	UNP Q7SIG4
A	57	GLY	-	SEE REMARK 999	UNP Q7SIG4
A	85	SER	ILE	engineered mutation	UNP Q7SIG4
A	87	ILE	ALA	engineered mutation	UNP Q7SIG4
A	133	ALA	ASN	engineered mutation	UNP Q7SIG4
A	134	TYR	ASP	engineered mutation	UNP Q7SIG4
A	157	PHE	TYR	engineered mutation	UNP Q7SIG4
A	159	ILE	ARG	engineered mutation	UNP Q7SIG4

Continued on next page...

Continued from previous page...

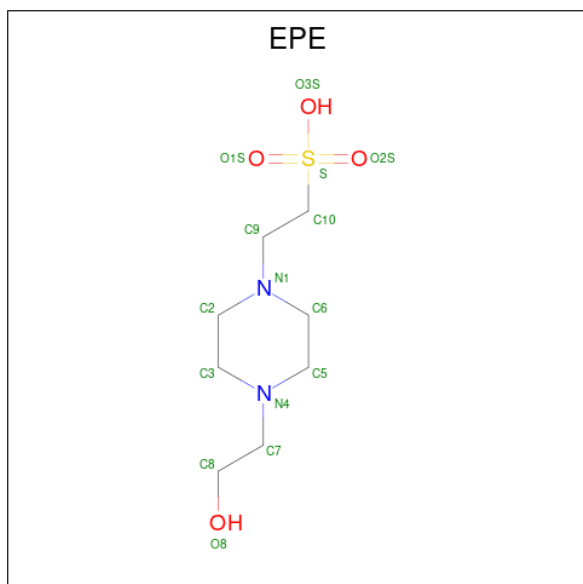
Chain	Residue	Modelled	Actual	Comment	Reference
A	161	LEU	MET	engineered mutation	UNP Q7SIG4
A	162	ARG	GLN	engineered mutation	UNP Q7SIG4
A	186	CYS	PHE	engineered mutation	UNP Q7SIG4
A	188	ALA	ASN	engineered mutation	UNP Q7SIG4
A	208	GLN	THR	engineered mutation	UNP Q7SIG4
A	238	LYS	GLU	engineered mutation	UNP Q7SIG4
A	242	ALA	ASP	engineered mutation	UNP Q7SIG4
A	284	ALA	SER	engineered mutation	UNP Q7SIG4
A	328	GLY	-	expression tag	UNP Q7SIG4
A	329	SER	-	expression tag	UNP Q7SIG4
A	330	LEU	-	expression tag	UNP Q7SIG4
A	331	GLU	-	expression tag	UNP Q7SIG4
A	332	HIS	-	expression tag	UNP Q7SIG4
A	333	HIS	-	expression tag	UNP Q7SIG4
A	334	HIS	-	expression tag	UNP Q7SIG4
A	335	HIS	-	expression tag	UNP Q7SIG4
A	336	HIS	-	expression tag	UNP Q7SIG4
A	337	HIS	-	expression tag	UNP Q7SIG4
B	21	THR	GLU	engineered mutation	UNP Q7SIG4
B	36	SER	-	SEE REMARK 999	UNP Q7SIG4
B	38	LEU	GLU	SEE REMARK 999	UNP Q7SIG4
B	39	SER	VAL	SEE REMARK 999	UNP Q7SIG4
B	41	ALA	VAL	SEE REMARK 999	UNP Q7SIG4
B	42	LEU	ASN	SEE REMARK 999	UNP Q7SIG4
B	43	THR	GLY	SEE REMARK 999	UNP Q7SIG4
B	45	ALA	-	SEE REMARK 999	UNP Q7SIG4
B	46	ASN	-	SEE REMARK 999	UNP Q7SIG4
B	47	SER	-	SEE REMARK 999	UNP Q7SIG4
B	49	ALA	-	SEE REMARK 999	UNP Q7SIG4
B	50	GLU	-	SEE REMARK 999	UNP Q7SIG4
B	51	ALA	-	SEE REMARK 999	UNP Q7SIG4
B	52	TYR	-	SEE REMARK 999	UNP Q7SIG4
B	53	LYS	-	SEE REMARK 999	UNP Q7SIG4
B	54	ALA	-	SEE REMARK 999	UNP Q7SIG4
B	55	SER	-	SEE REMARK 999	UNP Q7SIG4
B	56	ARG	-	SEE REMARK 999	UNP Q7SIG4
B	57	GLY	-	SEE REMARK 999	UNP Q7SIG4
B	85	SER	ILE	engineered mutation	UNP Q7SIG4
B	87	ILE	ALA	engineered mutation	UNP Q7SIG4
B	133	ALA	ASN	engineered mutation	UNP Q7SIG4
B	134	TYR	ASP	engineered mutation	UNP Q7SIG4
B	157	PHE	TYR	engineered mutation	UNP Q7SIG4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	159	ILE	ARG	engineered mutation	UNP Q7SIG4
B	161	LEU	MET	engineered mutation	UNP Q7SIG4
B	162	ARG	GLN	engineered mutation	UNP Q7SIG4
B	186	CYS	PHE	engineered mutation	UNP Q7SIG4
B	188	ALA	ASN	engineered mutation	UNP Q7SIG4
B	208	GLN	THR	engineered mutation	UNP Q7SIG4
B	238	LYS	GLU	engineered mutation	UNP Q7SIG4
B	242	ALA	ASP	engineered mutation	UNP Q7SIG4
B	284	ALA	SER	engineered mutation	UNP Q7SIG4
B	328	GLY	-	expression tag	UNP Q7SIG4
B	329	SER	-	expression tag	UNP Q7SIG4
B	330	LEU	-	expression tag	UNP Q7SIG4
B	331	GLU	-	expression tag	UNP Q7SIG4
B	332	HIS	-	expression tag	UNP Q7SIG4
B	333	HIS	-	expression tag	UNP Q7SIG4
B	334	HIS	-	expression tag	UNP Q7SIG4
B	335	HIS	-	expression tag	UNP Q7SIG4
B	336	HIS	-	expression tag	UNP Q7SIG4
B	337	HIS	-	expression tag	UNP Q7SIG4

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Na	0	0
			2	2		

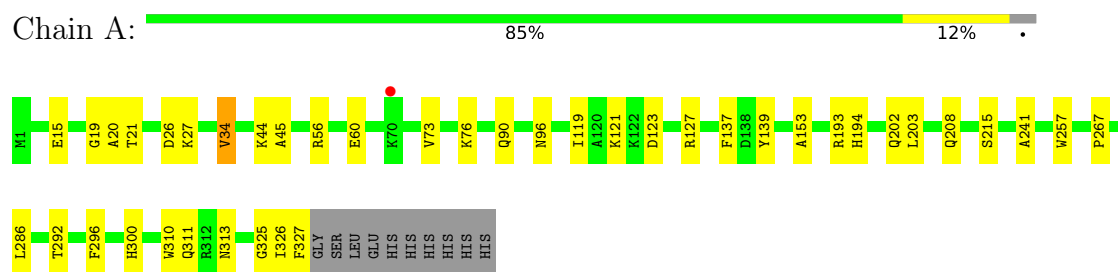
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	118	Total	O	0	0
			118	118		
6	B	122	Total	O	0	0
			122	122		

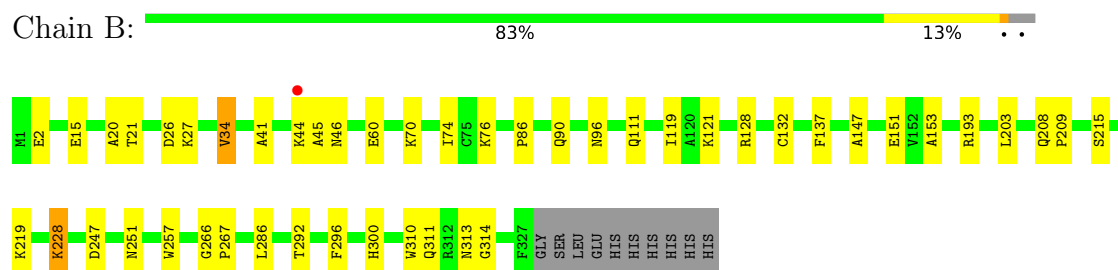
3 Residue-property plots

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: Diisopropyl-fluorophosphatase



• Molecule 1: Diisopropyl-fluorophosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	87.00Å 87.00Å 163.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.15 – 2.60 46.15 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (46.15-2.60) 100.0 (46.15-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.23 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.171 , 0.198 0.167 , 0.195	Depositor DCC
R_{free} test set	1870 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 24.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5614	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% 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, NA, EPE, GOL

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	0.65	0/2703	0.83	1/3649 (0.0%)
1	B	0.66	0/2725	0.83	1/3681 (0.0%)
All	All	0.66	0/5428	0.83	2/7330 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	ILE	N-CA-C	6.22	117.78	111.00
1	A	119	ILE	N-CA-C	6.05	117.60	111.00

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	2627	0	2608	30	0
1	B	2649	0	2604	34	0
2	A	15	0	17	0	0
2	B	15	0	17	0	0
3	A	18	0	24	1	0
3	B	18	0	24	0	0
4	A	15	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	15	0	0	0	0
5	B	2	0	0	0	0
6	A	118	0	0	0	0
6	B	122	0	0	3	0
All	All	5614	0	5294	64	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 6.

All (64) 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:B:111[B]:GLN:HG2	6:B:440:HOH:O	1.69	0.90
1:B:128:ARG:HH21	1:B:151[A]:GLU:HG2	1.46	0.81
1:A:139:TYR:H	1:A:194:HIS:HE1	1.32	0.77
1:A:139:TYR:H	1:A:194:HIS:CE1	2.07	0.73
1:B:26:ASP:HB2	1:B:96:ASN:HD21	1.55	0.71
1:A:26:ASP:HB2	1:A:96:ASN:HD21	1.56	0.70
1:A:193:ARG:NH2	1:A:267:PRO:HA	2.06	0.70
1:A:27:LYS:H	1:A:96:ASN:HD21	1.44	0.66
1:A:325:GLY:HA3	3:A:339:GOL:H2	1.78	0.64
1:A:27:LYS:H	1:A:96:ASN:ND2	1.96	0.63
1:B:257:TRP:HE1	1:B:300:HIS:CD2	2.18	0.62
1:A:257:TRP:HE1	1:A:300:HIS:CD2	2.18	0.61
1:B:21:THR:HG23	1:B:34:VAL:HG22	1.83	0.60
1:B:60:GLU:HG2	1:B:76:LYS:HG2	1.84	0.60
1:B:151[B]:GLU:HA	1:B:151[B]:GLU:OE1	2.01	0.59
1:B:128:ARG:HH21	1:B:151[B]:GLU:HG3	1.66	0.58
1:A:310:TRP:CG	1:A:311:GLN:H	2.22	0.57
1:B:121[B]:LYS:NZ	1:B:153:ALA:O	2.38	0.56
1:B:310:TRP:CG	1:B:311:GLN:H	2.24	0.55
1:A:121[B]:LYS:NZ	1:A:153:ALA:O	2.39	0.55
1:B:193:ARG:NH2	1:B:267:PRO:HA	2.22	0.54
1:B:27:LYS:H	1:B:96:ASN:ND2	2.06	0.54
1:A:60:GLU:HG2	1:A:76:LYS:HG2	1.90	0.53
1:A:21:THR:HG23	1:A:34:VAL:HG22	1.90	0.53
1:B:86:PRO:HD2	6:B:432:HOH:O	2.08	0.53
1:B:128:ARG:NH2	1:B:151[A]:GLU:HG2	2.21	0.52
1:B:228:LYS:HG2	6:B:349:HOH:O	2.08	0.51
1:A:73:VAL:HG11	1:A:76:LYS:HE3	1.93	0.50
1:A:20:ALA:O	1:A:300:HIS:HE1	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:THR:O	1:A:313:ASN:HA	2.12	0.49
1:A:310:TRP:CG	1:A:311:GLN:N	2.80	0.49
1:B:310:TRP:CG	1:B:311:GLN:N	2.80	0.49
1:A:208:GLN:HG3	1:A:241:ALA:O	2.11	0.49
1:B:44[A]:LYS:HG3	1:B:45:ALA:N	2.28	0.49
1:B:2[A]:GLU:HA	1:B:2[A]:GLU:OE1	2.13	0.49
1:A:90:GLN:HE21	1:A:137:PHE:H	1.61	0.48
1:A:56[A]:ARG:NH2	4:A:344:SO4:O4	2.41	0.48
1:B:27:LYS:H	1:B:96:ASN:HD21	1.61	0.48
1:A:123:ASP:OD2	1:A:127:ARG:HB2	2.15	0.47
1:B:21:THR:CG2	1:B:34:VAL:HG22	2.46	0.46
1:B:90:GLN:HE21	1:B:137:PHE:H	1.64	0.46
1:B:41:ALA:HA	1:B:44[B]:LYS:HE2	1.98	0.45
1:B:26:ASP:HB2	1:B:96:ASN:ND2	2.28	0.45
1:B:292:THR:O	1:B:313:ASN:HA	2.16	0.45
1:B:247:ASP:HA	1:B:314:GLY:HA2	1.98	0.45
1:B:286:LEU:HA	1:B:296:PHE:O	2.17	0.45
1:A:26:ASP:HB2	1:A:96:ASN:ND2	2.28	0.44
1:B:251:ASN:HD22	1:B:266:GLY:HA2	1.83	0.44
1:B:20:ALA:O	1:B:300:HIS:HE1	2.00	0.43
1:B:203:LEU:O	1:B:215:SER:HA	2.17	0.43
1:A:193:ARG:HB3	1:A:202:GLN:HB3	2.00	0.43
1:B:132:CYS:HA	1:B:147:ALA:HA	2.01	0.43
1:A:326:ILE:HG13	1:A:327:PHE:CD2	2.55	0.42
1:B:70[A]:LYS:HE2	1:B:70[A]:LYS:HB2	1.86	0.42
1:B:219:LYS:HA	1:B:219:LYS:HD3	1.81	0.42
1:A:44[A]:LYS:HG2	1:A:45:ALA:N	2.34	0.42
1:A:44[A]:LYS:HE2	1:A:44[A]:LYS:HB3	1.68	0.42
1:A:19:GLY:O	1:A:20:ALA:C	2.63	0.41
1:A:21:THR:CG2	1:A:34:VAL:HG22	2.50	0.41
1:A:257:TRP:HE1	1:A:300:HIS:HD2	1.66	0.41
1:B:208:GLN:HB3	1:B:209:PRO:HD3	2.03	0.40
1:A:203:LEU:O	1:A:215:SER:HA	2.21	0.40
1:A:286:LEU:HA	1:A:296:PHE:O	2.22	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	335/337 (99%)	321 (96%)	14 (4%)	0	100	100
1	B	338/337 (100%)	322 (95%)	14 (4%)	2 (1%)	21	42
All	All	673/674 (100%)	643 (96%)	28 (4%)	2 (0%)	43	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	46[A]	ASN
1	B	46[B]	ASN

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	278/277 (100%)	276 (99%)	2 (1%)	76	89
1	B	281/277 (101%)	276 (98%)	5 (2%)	51	76
All	All	559/554 (101%)	552 (99%)	7 (1%)	65	82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	34	VAL
1	B	15[A]	GLU
1	B	15[B]	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	34	VAL
1	B	74	ILE
1	B	228	LYS

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

Mol	Chain	Res	Type
1	A	46	ASN
1	A	90	GLN
1	A	96	ASN
1	A	194	HIS
1	A	251	ASN
1	A	300	HIS
1	B	90	GLN
1	B	96	ASN
1	B	179	GLN
1	B	208	GLN
1	B	250	ASN
1	B	251	ASN
1	B	300	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	GOL	B	339	-	5,5,5	0.42	0	5,5,5	0.19	0
4	SO4	B	346	-	4,4,4	0.23	0	6,6,6	0.39	0
3	GOL	A	340	-	5,5,5	0.47	0	5,5,5	0.32	0
3	GOL	A	339	-	5,5,5	0.43	0	5,5,5	0.66	0
4	SO4	A	344	-	4,4,4	0.24	0	6,6,6	0.24	0
4	SO4	B	345	-	4,4,4	0.29	0	6,6,6	0.16	0
4	SO4	A	343	-	4,4,4	0.25	0	6,6,6	0.20	0
2	EPE	B	338	-	15,15,15	1.08	1 (6%)	19,20,20	1.95	5 (26%)
3	GOL	B	341	-	5,5,5	0.40	0	5,5,5	0.19	0
4	SO4	A	342	-	4,4,4	0.31	0	6,6,6	0.21	0
3	GOL	B	340	-	5,5,5	0.46	0	5,5,5	0.28	0
3	GOL	A	341	-	5,5,5	0.47	0	5,5,5	0.38	0
2	EPE	A	338	-	15,15,15	1.12	1 (6%)	19,20,20	2.24	8 (42%)
4	SO4	B	344	5	4,4,4	0.52	0	6,6,6	0.19	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	GOL	B	339	-	-	0/4/4/4	-
3	GOL	A	340	-	-	0/4/4/4	-
3	GOL	A	339	-	-	2/4/4/4	-
2	EPE	B	338	-	-	4/9/19/19	0/1/1/1
3	GOL	B	341	-	-	2/4/4/4	-
3	GOL	B	340	-	-	1/4/4/4	-
3	GOL	A	341	-	-	4/4/4/4	-
2	EPE	A	338	-	-	4/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	338	EPE	C10-S	3.90	1.83	1.77
2	B	338	EPE	C10-S	3.70	1.82	1.77

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	338	EPE	C5-N4-C3	5.02	119.65	108.84
2	A	338	EPE	C5-N4-C3	4.81	119.21	108.84
2	A	338	EPE	C7-N4-C3	3.52	120.63	111.24
2	B	338	EPE	C7-N4-C5	3.43	120.38	111.24
2	A	338	EPE	C7-N4-C5	3.30	120.02	111.24
2	B	338	EPE	C7-N4-C3	3.22	119.81	111.24
2	A	338	EPE	O2S-S-C10	2.84	111.02	106.73
2	A	338	EPE	C2-C3-N4	2.76	116.22	110.65
2	A	338	EPE	C6-N1-C2	2.64	114.54	108.84
2	B	338	EPE	O3S-S-O2S	-2.57	104.97	111.40
2	B	338	EPE	O3S-S-C10	2.56	111.00	106.00
2	A	338	EPE	O1S-S-C10	2.40	110.36	106.73
2	A	338	EPE	C5-C6-N1	2.11	114.90	110.65

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	338	EPE	S-C10-C9-N1
2	B	338	EPE	C10-C9-N1-C6
2	B	338	EPE	S-C10-C9-N1
3	A	341	GOL	O1-C1-C2-C3
3	B	341	GOL	O1-C1-C2-C3
2	A	338	EPE	C8-C7-N4-C5
2	B	338	EPE	C8-C7-N4-C5
3	A	341	GOL	O1-C1-C2-O2
3	A	339	GOL	C1-C2-C3-O3
3	A	341	GOL	C1-C2-C3-O3
3	A	339	GOL	O2-C2-C3-O3
3	A	341	GOL	O2-C2-C3-O3
3	B	341	GOL	O1-C1-C2-O2
2	A	338	EPE	C10-C9-N1-C6
2	B	338	EPE	C10-C9-N1-C2
2	A	338	EPE	C10-C9-N1-C2
3	B	340	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	339	GOL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	344	SO4	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 [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	327/337 (97%)	-1.75	1 (0%) 90 88	19, 41, 56, 76	9 (2%)
1	B	327/337 (97%)	-1.74	1 (0%) 90 88	20, 42, 57, 76	13 (3%)
All	All	654/674 (97%)	-1.75	2 (0%) 90 88	19, 41, 56, 76	22 (3%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70[A]	LYS	5.8
1	B	44[A]	LYS	2.1

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	GOL	A	339	6/6	0.98	0.09	135,138,142,142	0
4	SO4	B	344	5/5	0.98	0.06	130,133,135,137	0
4	SO4	B	345	5/5	0.98	0.06	118,122,124,124	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NA	B	342	1/1	0.98	0.08	137,137,137,137	0
3	GOL	A	341	6/6	0.99	0.06	86,88,89,89	0
3	GOL	B	339	6/6	0.99	0.06	100,101,102,102	0
3	GOL	B	340	6/6	0.99	0.05	103,104,105,106	0
3	GOL	B	341	6/6	0.99	0.07	76,78,79,82	0
4	SO4	A	342	5/5	0.99	0.05	105,105,106,108	0
4	SO4	A	343	5/5	0.99	0.05	92,93,94,95	0
4	SO4	A	344	5/5	0.99	0.04	101,104,105,105	0
2	EPE	B	338	15/15	0.99	0.06	82,101,118,119	0
2	EPE	A	338	15/15	0.99	0.05	83,95,114,115	0
4	SO4	B	346	5/5	0.99	0.06	137,140,145,147	0
3	GOL	A	340	6/6	0.99	0.05	88,88,89,92	0
5	NA	B	343	1/1	0.99	0.05	103,103,103,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.