



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2017 – 03:49 AM EDT

PDB ID : 3U0S  
Title : Crystal Structure of an Enzyme Redesigned Through Multiplayer Online Gaming: CE6  
Authors : Bale, J.B.; Shen, B.W.; Stoddard, B.L.  
Deposited on : unknown  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

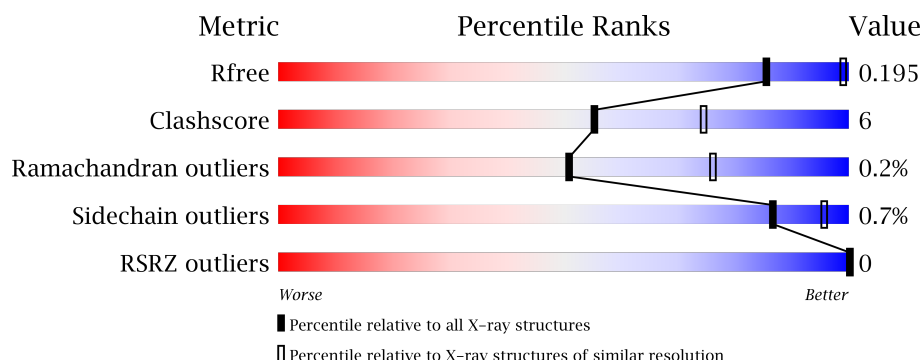
# 1 Overall quality at a glance

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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	
1	B	337	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EPE	A	338	-	-	-	X
2	EPE	B	338	-	-	-	X
3	GOL	A	339	-	-	-	X
3	GOL	A	340	-	-	-	X
3	GOL	A	341	-	-	-	X
3	GOL	B	339	-	-	-	X
3	GOL	B	340	-	-	-	X
3	GOL	B	341	-	-	-	X
4	SO4	B	344	-	-	-	X

## 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

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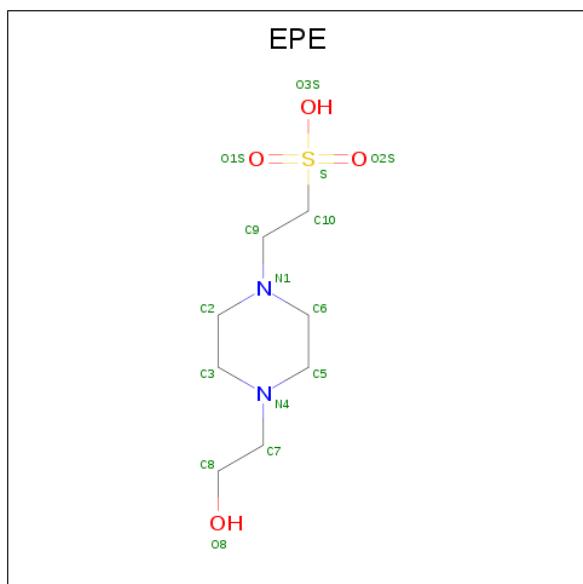
Chain	Residue	Modelled	Actual	Comment	Reference
A	161	LEU	MET	ENGINEERED MUTATION	UNP Q7SIG4
A	162	ARG	GLN	ENGINEERED MUTATION	UNP Q7SIG4
A	186	CYS	PHE	ENGINEERED MUTATION	UNP Q7SIG4
A	188	ALA	ASN	ENGINEERED MUTATION	UNP Q7SIG4
A	208	GLN	THR	ENGINEERED MUTATION	UNP Q7SIG4
A	238	LYS	GLU	ENGINEERED MUTATION	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

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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 (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



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

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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 (three-letter code: 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 (three-letter code: 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 (three-letter code: NA) (formula: Na).

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

- Molecule 6 is water.

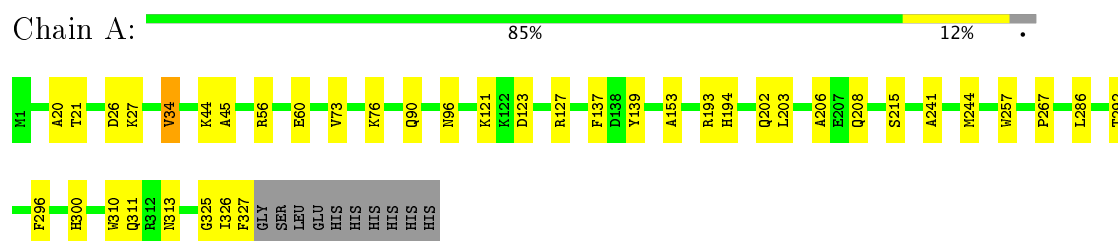
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	118	Total	O	0	0
			118	118		
6	B	122	Total	O	0	0
			122	122		



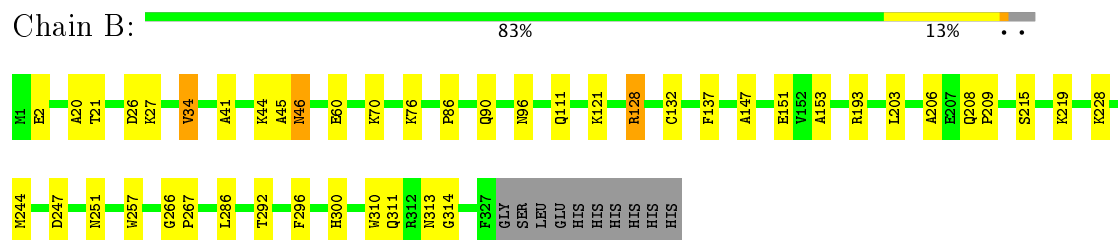
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.6	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 19.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5614	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, EPE, SO4, NA

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	0.60	0/2703	0.64	0/3649
1	B	0.59	0/2725	0.64	0/3681
All	All	0.59	0/5428	0.64	0/7330

There are no bond length outliers.

There are no bond angle outliers.

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	2627	0	2608	29	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
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	63	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 (63) 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:193:ARG:NH2	1:A:267:PRO:HA	2.06	0.70
1:A:26:ASP:HB2	1:A:96:ASN:HD21	1.56	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:B:121[B]:LYS:NZ	1:B:153:ALA:O	2.38	0.56
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:310:TRP:CG	1:A:311:GLN:N	2.80	0.50
1:A:20:ALA:O	1:A:300:HIS:HE1	1.95	0.49
1:A:292:THR:O	1:A:313:ASN:HA	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:THR:CG2	1:B:34:VAL:HG22	2.46	0.46
1:B:206:ALA:HB2	1:B:244:MET:HE1	1.98	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:A:206:ALA:HB2	1:A:244:MET:HE1	1.99	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:HB2	1:B:70[A]:LYS:HE2	1.86	0.42
1:B:219:LYS:HD3	1:B:219:LYS:HA	1.81	0.42
1:A:44[A]:LYS:HG2	1:A:45:ALA:N	2.34	0.42
1:A:44[A]:LYS:HB3	1:A:44[A]:LYS:HE2	1.68	0.42
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	338/337 (100%)	322 (95%)	14 (4%)	2 (1%)	28	53
All	All	673/674 (100%)	643 (96%)	28 (4%)	2 (0%)	51	70

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%)	277 (100%)	1 (0%)	93	98
1	B	281/277 (101%)	277 (99%)	4 (1%)	71	89
All	All	559/554 (101%)	554 (99%)	5 (1%)	87	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	VAL
1	B	34	VAL
1	B	46[A]	ASN
1	B	46[B]	ASN
1	B	128	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	96	ASN
1	A	111	GLN
1	A	194	HIS

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Mol	Chain	Res	Type
1	A	251	ASN
1	A	300	HIS
1	A	317	GLN
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
1	B	317	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 carbohydrates 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	$\# Z  > 2$
2	EPE	A	338	-	15,15,15	1.08	1 (6%)	18,20,20	2.63	8 (44%)
3	GOL	A	339	-	5,5,5	0.39	0	5,5,5	0.54	0
3	GOL	A	340	-	5,5,5	0.45	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	A	341	-	5,5,5	0.42	0	5,5,5	0.39	0
4	SO4	A	342	-	4,4,4	0.25	0	6,6,6	0.21	0
4	SO4	A	343	-	4,4,4	0.18	0	6,6,6	0.18	0
4	SO4	A	344	-	4,4,4	0.16	0	6,6,6	0.22	0
2	EPE	B	338	-	15,15,15	1.04	1 (6%)	18,20,20	2.21	6 (33%)
3	GOL	B	339	-	5,5,5	0.39	0	5,5,5	0.12	0
3	GOL	B	340	-	5,5,5	0.41	0	5,5,5	0.29	0
3	GOL	B	341	-	5,5,5	0.36	0	5,5,5	0.14	0
4	SO4	B	344	5	4,4,4	0.50	0	6,6,6	0.25	0
4	SO4	B	345	-	4,4,4	0.21	0	6,6,6	0.14	0
4	SO4	B	346	-	4,4,4	0.15	0	6,6,6	0.37	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
2	EPE	A	338	-	-	0/9/19/19	0/1/1/1
3	GOL	A	339	-	-	0/4/4/4	0/0/0/0
3	GOL	A	340	-	-	0/4/4/4	0/0/0/0
3	GOL	A	341	-	-	0/4/4/4	0/0/0/0
4	SO4	A	342	-	-	0/0/0/0	0/0/0/0
4	SO4	A	343	-	-	0/0/0/0	0/0/0/0
4	SO4	A	344	-	-	0/0/0/0	0/0/0/0
2	EPE	B	338	-	-	0/9/19/19	0/1/1/1
3	GOL	B	339	-	-	0/4/4/4	0/0/0/0
3	GOL	B	340	-	-	0/4/4/4	0/0/0/0
3	GOL	B	341	-	-	0/4/4/4	0/0/0/0
4	SO4	B	344	5	-	0/0/0/0	0/0/0/0
4	SO4	B	345	-	-	0/0/0/0	0/0/0/0
4	SO4	B	346	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	338	EPE	C10-S	3.56	1.82	1.77
2	A	338	EPE	C10-S	3.75	1.83	1.77

All (14) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	338	EPE	O3S-S-O2S	-2.79	104.97	111.37
2	A	338	EPE	C5-C6-N1	2.11	114.90	110.63
2	B	338	EPE	O2S-S-C10	2.35	108.81	106.79
2	A	338	EPE	C6-N1-C2	2.50	114.54	108.87
2	A	338	EPE	C2-C3-N4	2.76	116.22	110.63
2	B	338	EPE	C7-N4-C3	3.34	119.81	111.26
2	A	338	EPE	C7-N4-C5	3.42	120.02	111.26
2	B	338	EPE	C7-N4-C5	3.56	120.38	111.26
2	A	338	EPE	C7-N4-C3	3.66	120.63	111.26
2	B	338	EPE	O3S-S-C10	4.02	111.00	106.06
2	A	338	EPE	O1S-S-C10	4.15	110.36	106.79
2	A	338	EPE	C5-N4-C3	4.56	119.21	108.87
2	B	338	EPE	C5-N4-C3	4.76	119.65	108.87
2	A	338	EPE	O2S-S-C10	4.92	111.02	106.79

There are no chirality outliers.

There are no torsion outliers.

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
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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	327/337 (97%)	-0.40	0 100 100	29, 42, 57, 76	0
1	B	327/337 (97%)	-0.39	0 100 100	30, 42, 58, 76	0
All	All	654/674 (97%)	-0.39	0 100 100	29, 42, 58, 76	0

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	B	339	6/6	0.83	0.36	13.75	100,101,102,102	0
4	SO4	B	344	5/5	0.85	0.24	11.61	130,133,135,137	0
2	EPE	A	338	15/15	0.69	0.36	9.26	83,95,114,115	0
2	EPE	B	338	15/15	0.62	0.38	6.55	82,101,118,119	0
3	GOL	A	339	6/6	0.86	0.28	4.79	135,138,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	B	341	6/6	0.78	0.22	4.53	76,78,79,82	0
3	GOL	A	340	6/6	0.84	0.29	4.39	88,88,89,92	0
3	GOL	A	341	6/6	0.77	0.23	3.81	86,88,89,89	0
3	GOL	B	340	6/6	0.69	0.28	2.22	103,104,105,106	0
4	SO4	A	342	5/5	0.90	0.15	1.29	105,105,106,108	0
4	SO4	B	345	5/5	0.93	0.17	-	118,122,124,124	0
4	SO4	A	343	5/5	0.96	0.14	-	92,93,94,95	0
4	SO4	B	346	5/5	0.88	0.17	-	137,140,145,147	0
5	NA	B	342	1/1	0.81	0.34	-	137,137,137,137	0
4	SO4	A	344	5/5	0.91	0.14	-	101,104,105,105	0
5	NA	B	343	1/1	0.87	0.38	-	103,103,103,103	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.