



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 11:40 pm BST

PDB ID : 3GEA  
Title : Donor strand complemented FaeG monomer of F4 variant ad  
Authors : Van Molle, I.; Moonens, K.; Garcia-Pino, A.; Buts, L.; Bouckaert, J.; De Greve, H.  
Deposited on : 2009-02-25  
Resolution : 1.70 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

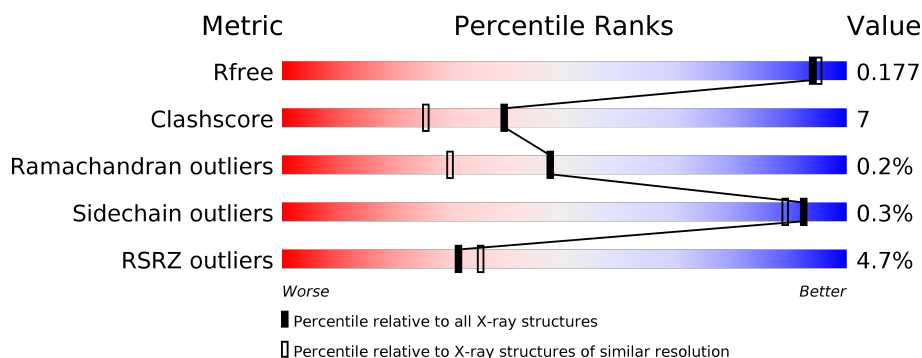
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 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	274	
1	B	274	

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
3	GOL	A	278	-	X	-	-
3	GOL	B	275	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4453 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 K88 fimbrial protein AD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	1	0
			2014	1263	346	400	5			
1	B	261	Total	C	N	O	S	0	0	0
			1873	1179	319	371	4			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	HIS	-	LINKER	UNP P14191
A	6	HIS	-	LINKER	UNP P14191
A	7	HIS	-	LINKER	UNP P14191
A	8	HIS	-	LINKER	UNP P14191
A	9	HIS	-	LINKER	UNP P14191
A	10	HIS	-	LINKER	UNP P14191
A	27	SER	ASN	SEE REMARK 999	UNP P14191
A	254	ASP	-	LINKER	UNP P14191
A	255	ASN	-	LINKER	UNP P14191
A	256	LYS	-	LINKER	UNP P14191
A	257	GLN	-	LINKER	UNP P14191
B	5	HIS	-	LINKER	UNP P14191
B	6	HIS	-	LINKER	UNP P14191
B	7	HIS	-	LINKER	UNP P14191
B	8	HIS	-	LINKER	UNP P14191
B	9	HIS	-	LINKER	UNP P14191
B	10	HIS	-	LINKER	UNP P14191
B	27	SER	ASN	SEE REMARK 999	UNP P14191
B	254	ASP	-	LINKER	UNP P14191
B	255	ASN	-	LINKER	UNP P14191
B	256	LYS	-	LINKER	UNP P14191
B	257	GLN	-	LINKER	UNP P14191

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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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	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

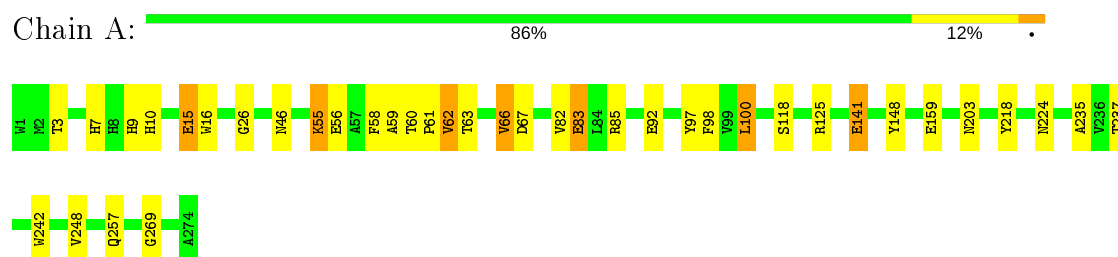
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	314	Total	O	0	0
			314	314		
4	B	207	Total	O	0	0
			207	207		

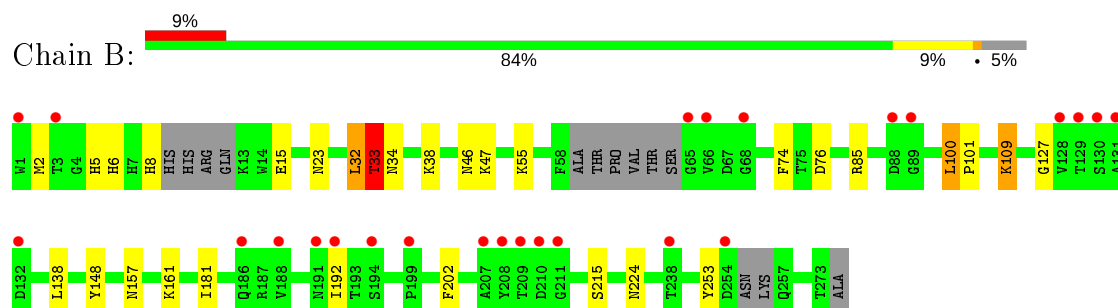
### 3 Residue-property plots [i](#)

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: K88 fimbrial protein AD



- Molecule 1: K88 fimbrial protein AD



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.97Å 123.97Å 95.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.68 – 1.70 28.68 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.68-1.70) 99.9 (28.68-1.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 1.70Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.159 , 0.183 0.154 , 0.177	Depositor DCC
$R_{free}$ test set	4691 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.8	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 54.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4453	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	1.54	16/2057 (0.8%)	1.36	10/2797 (0.4%)
1	B	1.24	7/1906 (0.4%)	1.15	7/2591 (0.3%)
All	All	1.40	23/3963 (0.6%)	1.27	17/5388 (0.3%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	GLU	CB-CG	-9.44	1.34	1.52
1	A	62	VAL	CB-CG2	-8.51	1.34	1.52
1	B	109	LYS	CE-NZ	8.21	1.69	1.49
1	A	56	GLU	CG-CD	6.87	1.62	1.51
1	A	118	SER	CB-OG	6.81	1.51	1.42
1	A	248	VAL	CB-CG2	6.66	1.66	1.52
1	A	83	GLU	CG-CD	6.43	1.61	1.51
1	A	58	PHE	CE1-CZ	6.38	1.49	1.37
1	A	148	TYR	CD2-CE2	6.08	1.48	1.39
1	B	148	TYR	CE2-CZ	5.99	1.46	1.38
1	A	141	GLU	CG-CD	5.72	1.60	1.51
1	A	218	TYR	CD1-CE1	5.72	1.48	1.39
1	A	92	GLU	CD-OE2	-5.71	1.19	1.25
1	B	148	TYR	CD1-CE1	5.68	1.47	1.39
1	B	109	LYS	CD-CE	-5.67	1.37	1.51
1	B	253	TYR	CD2-CE2	5.64	1.47	1.39
1	B	47	LYS	CB-CG	5.36	1.67	1.52
1	A	148	TYR	CD1-CE1	5.35	1.47	1.39
1	A	235	ALA	CA-CB	5.28	1.63	1.52
1	A	97	TYR	CD2-CE2	5.21	1.47	1.39
1	A	15	GLU	CD-OE2	-5.14	1.20	1.25
1	A	16	TRP	CE3-CZ3	5.12	1.47	1.38
1	B	74	PHE	CD1-CE1	5.11	1.49	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ARG	NE-CZ-NH2	-9.49	115.55	120.30
1	A	125	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	B	32	LEU	CB-CG-CD2	-7.37	98.48	111.00
1	B	33	THR	N-CA-CB	-6.25	98.43	110.30
1	A	85	ARG	CG-CD-NE	-6.21	98.76	111.80
1	B	85	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	5	HIS	CA-C-N	-6.10	103.78	117.20
1	B	76	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	A	26	GLY	O-C-N	5.74	131.88	122.70
1	A	98	PHE	CB-CG-CD1	-5.68	116.82	120.80
1	B	100	LEU	CB-CG-CD1	-5.60	101.48	111.00
1	A	83	GLU	N-CA-CB	-5.56	100.60	110.60
1	A	100	LEU	CB-CA-C	-5.38	99.97	110.20
1	A	148	TYR	CG-CD1-CE1	-5.21	117.13	121.30
1	B	148	TYR	CZ-CE2-CD2	-5.11	115.20	119.80
1	A	55	LYS	CD-CE-NZ	-5.09	99.99	111.70
1	A	218	TYR	CD1-CE1-CZ	-5.05	115.26	119.80

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	2014	0	1952	35	0
1	B	1873	0	1773	22	0
2	A	15	0	0	0	0
3	A	18	0	23	1	0
3	B	12	0	15	6	0
4	A	314	0	0	4	3
4	B	207	0	0	1	0
All	All	4453	0	3763	57	3

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 7.

All (57) 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:109:LYS:NZ	1:B:109:LYS:CE	1.69	1.56
1:B:46:ASN:H	3:B:275:GOL:H31	1.26	0.98
1:B:46:ASN:OD1	3:B:275:GOL:H11	1.70	0.89
1:A:15:GLU:CG	1:A:55:LYS:HG2	2.02	0.88
1:A:3:THR:HG21	1:A:55:LYS:NZ	1.89	0.88
1:B:46:ASN:H	3:B:275:GOL:C3	1.98	0.77
1:A:7:HIS:CD2	1:A:9:HIS:H	2.05	0.75
1:B:109:LYS:NZ	1:B:109:LYS:CD	2.47	0.74
1:B:33:THR:HG22	1:B:38:LYS:HB3	1.70	0.74
1:A:3:THR:HG21	1:A:55:LYS:HZ3	1.52	0.73
1:A:7:HIS:HD2	1:A:9:HIS:H	1.35	0.73
1:A:66[B]:VAL:HG12	1:A:67:ASP:H	1.53	0.70
1:A:62:VAL:HB	4:A:612:HOH:O	1.92	0.69
1:A:3:THR:HG21	1:A:55:LYS:HZ2	1.60	0.67
1:A:15:GLU:HG2	1:A:55:LYS:HG2	1.76	0.67
1:A:15:GLU:HG3	1:A:55:LYS:HG2	1.78	0.65
1:B:23:ASN:HB2	4:B:577:HOH:O	1.96	0.64
1:A:62:VAL:HG12	1:A:63:THR:N	2.13	0.64
1:A:46:ASN:ND2	1:A:224:ASN:H	1.96	0.63
1:B:34:ASN:HA	3:B:276:GOL:H32	1.79	0.63
1:A:141:GLU:H	1:A:203:ASN:ND2	1.97	0.63
1:A:7:HIS:CD2	1:A:10:HIS:H	2.18	0.61
1:A:7:HIS:HE1	1:A:257:GLN:NE2	1.98	0.60
1:A:66[B]:VAL:HG12	1:A:67:ASP:N	2.17	0.59
1:B:157:ASN:HD22	1:B:161:LYS:NZ	2.00	0.59
1:B:2:MET:CE	1:B:2:MET:CG	2.80	0.59
1:B:46:ASN:ND2	1:B:224:ASN:H	2.00	0.59
1:A:237:THR:O	4:A:361:HOH:O	2.17	0.58
1:A:7:HIS:HD2	1:A:10:HIS:H	1.50	0.58
1:A:15:GLU:HG2	1:A:55:LYS:CG	2.34	0.56
1:B:6:HIS:CD2	1:B:8:HIS:H	2.24	0.56
1:B:157:ASN:HD22	1:B:161:LYS:HZ3	1.54	0.56
1:B:2:MET:CE	1:B:2:MET:HB3	2.36	0.56
1:A:15:GLU:CG	1:A:55:LYS:CG	2.80	0.55
1:B:181:ILE:HG23	1:B:215:SER:HB3	1.88	0.54
1:A:60:THR:HB	1:A:61:PRO:HA	1.90	0.54
1:A:66[A]:VAL:HG23	1:A:67:ASP:N	2.23	0.54
1:A:66[A]:VAL:HG23	1:A:67:ASP:H	1.73	0.53
1:B:127:GLY:O	1:B:192:ILE:HD11	2.08	0.53
1:B:34:ASN:CA	3:B:276:GOL:H32	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:GLU:CG	1:B:55:LYS:CG	2.89	0.50
1:A:83:GLU:HA	4:A:402:HOH:O	2.13	0.48
1:A:62:VAL:CG1	1:A:63:THR:N	2.76	0.48
1:A:59:ALA:HB1	4:A:364:HOH:O	2.14	0.47
1:A:159:GLU:OE2	3:A:278:GOL:H12	2.14	0.47
1:A:3:THR:CG2	1:A:55:LYS:HZ2	2.29	0.46
1:A:3:THR:HG22	1:A:55:LYS:HD2	1.98	0.45
1:A:7:HIS:HE1	1:A:257:GLN:HE21	1.65	0.45
1:A:7:HIS:CE1	1:A:257:GLN:HE21	2.34	0.45
1:B:100:LEU:HB2	1:B:101:PRO:HD2	1.99	0.45
1:B:46:ASN:N	3:B:275:GOL:H31	2.11	0.42
1:A:7:HIS:CE1	1:A:257:GLN:NE2	2.82	0.42
1:B:138:LEU:HA	1:B:202:PHE:O	2.19	0.42
1:A:3:THR:CG2	1:A:55:LYS:NZ	2.73	0.42
1:A:242:TRP:CZ3	1:A:269:GLY:HA2	2.54	0.41
1:B:32:LEU:HA	1:B:32:LEU:HD23	1.95	0.40
1:A:82:VAL:HG21	1:A:100:LEU:CD2	2.51	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:825:HOH:O	4:A:828:HOH:O[2_655]	1.64	0.56
4:A:826:HOH:O	4:A:830:HOH:O[3_664]	1.76	0.44
4:A:449:HOH:O	4:A:662:HOH:O[3_664]	2.01	0.19

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	273/274 (100%)	268 (98%)	3 (1%)	2 (1%)	22 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	253/274 (92%)	250 (99%)	3 (1%)	0	100	100
All	All	526/548 (96%)	518 (98%)	6 (1%)	2 (0%)	47	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66[A]	VAL
1	A	66[B]	VAL

### 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	209/212 (99%)	209 (100%)	0	100	100
1	B	185/212 (87%)	184 (100%)	1 (0%)	88	83
All	All	394/424 (93%)	393 (100%)	1 (0%)	92	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	33	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	46	ASN
1	A	157	ASN
1	A	203	ASN
1	A	224	ASN
1	A	247	ASN
1	A	257	GLN
1	B	6	HIS

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Mol	Chain	Res	Type
1	B	116	ASN
1	B	157	ASN
1	B	184	GLN
1	B	241	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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	A	278	-	5,5,5	1.62	1 (20%)	5,5,5	2.51	2 (40%)
2	SO4	A	276	-	4,4,4	1.10	0	6,6,6	0.85	0
3	GOL	A	280	-	5,5,5	0.19	0	5,5,5	1.73	2 (40%)
3	GOL	B	275	-	5,5,5	0.55	0	5,5,5	1.25	1 (20%)
3	GOL	B	276	-	5,5,5	1.07	1 (20%)	5,5,5	1.23	0
2	SO4	A	277	-	4,4,4	0.60	0	6,6,6	0.97	0
3	GOL	A	279	-	5,5,5	0.91	0	5,5,5	4.42	1 (20%)
2	SO4	A	275	-	4,4,4	0.49	0	6,6,6	0.87	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	A	278	-	-	3/4/4/4	-
3	GOL	B	276	-	-	3/4/4/4	-
3	GOL	A	280	-	-	2/4/4/4	-
3	GOL	A	279	-	-	3/4/4/4	-
3	GOL	B	275	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	278	GOL	C1-C2	-2.40	1.41	1.51
3	B	276	GOL	O2-C2	-2.29	1.36	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	279	GOL	C3-C2-C1	-9.55	74.57	111.70
3	A	278	GOL	C3-C2-C1	-4.87	92.77	111.70
3	A	280	GOL	O1-C1-C2	-2.55	97.99	110.20
3	A	280	GOL	C3-C2-C1	-2.51	101.93	111.70
3	A	278	GOL	O2-C2-C3	2.38	119.62	109.12
3	B	275	GOL	O2-C2-C3	-2.04	100.16	109.12

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	280	GOL	O1-C1-C2-C3
3	B	275	GOL	C1-C2-C3-O3
3	B	276	GOL	O1-C1-C2-O2
3	A	279	GOL	O1-C1-C2-C3
3	A	278	GOL	O1-C1-C2-C3
3	A	278	GOL	C1-C2-C3-O3
3	B	275	GOL	O1-C1-C2-C3
3	B	276	GOL	O1-C1-C2-C3
3	B	276	GOL	C1-C2-C3-O3
3	A	278	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	280	GOL	O1-C1-C2-O2
3	B	275	GOL	O2-C2-C3-O3
3	A	279	GOL	O1-C1-C2-O2
3	A	279	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	278	GOL	1	0
3	B	275	GOL	4	0
3	B	276	GOL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 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, 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	274/274 (100%)	-0.40	0 100 100	6, 12, 25, 34	0
1	B	261/274 (95%)	0.16	25 (9%) 8 9	10, 23, 55, 76	0
All	All	535/548 (97%)	-0.13	25 (4%) 31 35	6, 16, 46, 76	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	209	THR	5.1
1	B	131	ALA	4.6
1	B	66	VAL	4.6
1	B	129	THR	3.9
1	B	208	TYR	3.8
1	B	89	GLY	3.5
1	B	3	THR	3.5
1	B	207	ALA	3.5
1	B	65	GLY	3.0
1	B	191	ASN	2.6
1	B	128	VAL	2.6
1	B	188	VAL	2.5
1	B	210	ASP	2.5
1	B	254	ASP	2.5
1	B	68	GLY	2.4
1	B	132	ASP	2.4
1	B	211	GLY	2.4
1	B	199	PRO	2.3
1	B	192	ILE	2.3
1	B	194	SER	2.3
1	B	130	SER	2.2
1	B	1	TRP	2.2
1	B	186	GLN	2.1
1	B	238	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	88	ASP	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 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	B	276	6/6	0.82	0.17	45,48,51,54	0
3	GOL	A	280	6/6	0.84	0.18	40,43,44,48	0
3	GOL	B	275	6/6	0.85	0.21	30,38,40,43	0
3	GOL	A	279	6/6	0.90	0.13	17,33,38,41	0
2	SO4	A	275	5/5	0.92	0.23	53,56,56,59	0
2	SO4	A	277	5/5	0.93	0.20	29,31,49,51	0
2	SO4	A	276	5/5	0.93	0.21	16,41,44,44	0
3	GOL	A	278	6/6	0.93	0.14	16,27,28,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.