



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:20 AM GMT

PDB ID : 2WQR  
Title : THE HIGH RESOLUTION CRYSTAL STRUCTURE OF IGE FC  
Authors : Dhaliwal, B.; Sutton, B.J.; Beavil, A.J.  
Deposited on : 2009-08-26  
Resolution : 1.90 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

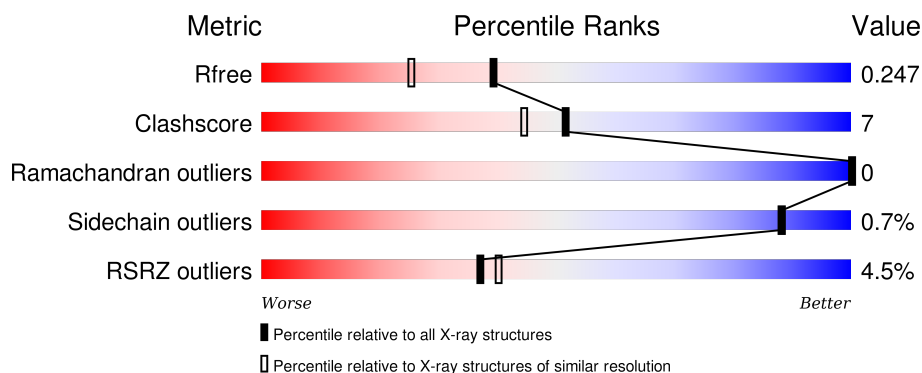
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


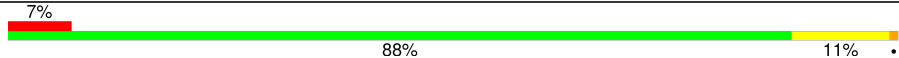
The reported resolution of this entry is 1.90 Å.

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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	323	
1	B	323	

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
4	GOL	A	954	-	-	-	X
5	TRS	A	956	-	-	-	X
6	PG4	A	957	-	-	X	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5725 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 IG EPSILON CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2495	1557	443	484	11			
1	B	323	Total	C	N	O	S	23	0	0
			2522	1571	450	489	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLN	ASN	ENGINEERED MUTATION	UNP P01854
A	371	GLN	ASN	ENGINEERED MUTATION	UNP P01854
B	265	GLN	ASN	ENGINEERED MUTATION	UNP P01854
B	371	GLN	ASN	ENGINEERED MUTATION	UNP P01854

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total	C	N	O	0	0
			61	34	2	25		
2	B	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



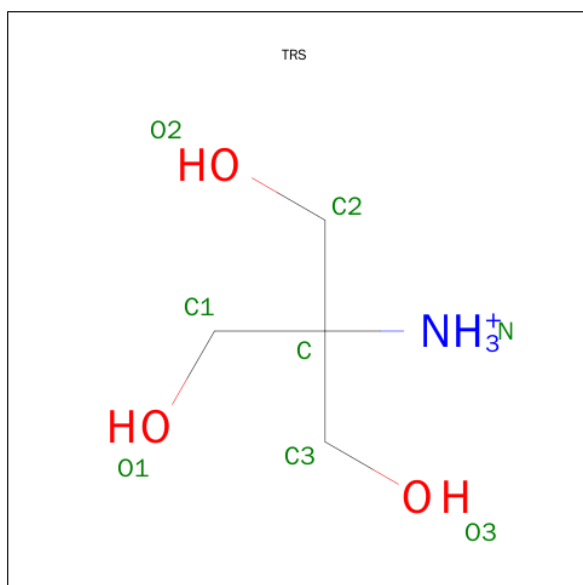
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



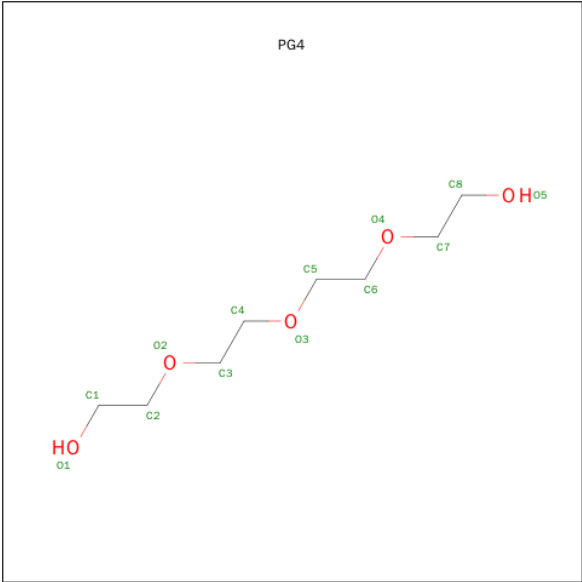
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		

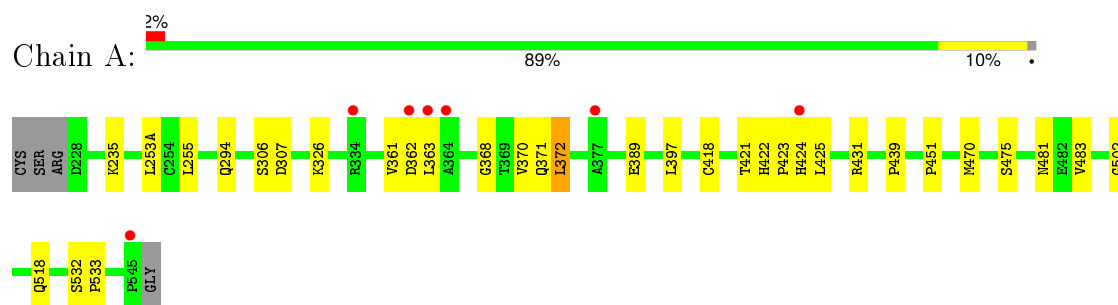
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	258	Total	O	0	0
			258	258		
7	B	274	Total	O	0	0
			274	274		
7	E	1	Total	O	0	0
			1	1		

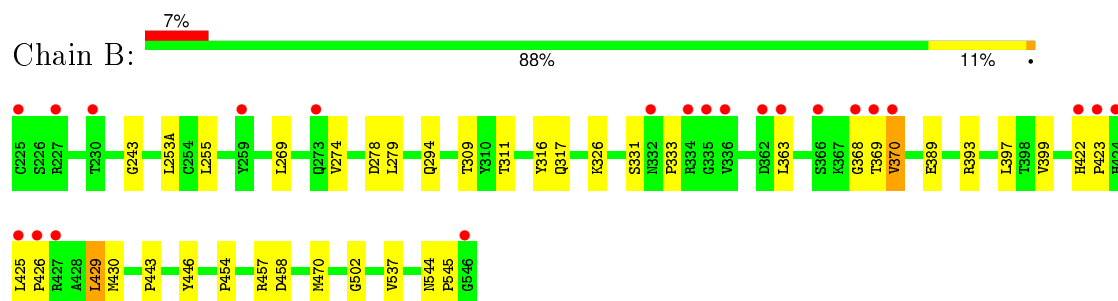
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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: IG EPSILON CHAIN C REGION



#### • Molecule 1: IG EPSILON CHAIN C REGION





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.50Å 75.28Å 79.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.00 – 1.90 49.31 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.00-1.90) 99.1 (49.31-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 1.90Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.193 , 0.234 0.205 , 0.247	Depositor DCC
$R_{free}$ test set	3110 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 48.3	EDS
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 61627 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5725	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, BMA, NAG, PG4, SO4, TRS, MAN

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	0.30	0/2557	0.50	0/3486
1	B	0.30	0/2584	0.53	2/3521 (0.1%)
All	All	0.30	0/5141	0.51	2/7007 (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	370	VAL	CB-CA-C	-6.33	99.38	111.40
1	B	370	VAL	N-CA-C	5.03	124.59	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	2495	0	2434	30	0
1	B	2522	0	2460	42	0
2	A	61	0	52	0	0
2	B	61	0	52	0	0
3	A	15	0	0	0	0
3	B	5	0	0	0	0
4	A	12	0	16	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	8	0	12	1	0
6	A	13	0	18	15	0
7	A	258	0	0	2	0
7	B	274	0	0	1	0
7	E	1	0	0	0	0
All	All	5725	0	5044	69	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 7.

All (69) 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:370:VAL:HG12	1:B:370:VAL:O	1.65	0.95
1:A:372:LEU:HD11	1:A:418:CYS:SG	2.19	0.82
4:A:955:GOL:H11	1:B:393:ARG:HH11	1.43	0.81
6:A:957:PG4:H61	1:B:253(A):LEU:HD21	1.64	0.78
4:A:955:GOL:H11	1:B:393:ARG:NH1	2.04	0.72
6:A:957:PG4:H12	1:B:255:LEU:HD13	1.73	0.70
1:B:389:GLU:HG2	1:B:399:VAL:HG22	1.75	0.68
1:A:370:VAL:HG22	1:A:422:HIS:HD2	1.58	0.68
1:A:294:GLN:OE1	6:A:957:PG4:H42	1.94	0.67
1:A:532:SER:HB2	1:A:533:PRO:HA	1.77	0.66
1:B:370:VAL:O	1:B:370:VAL:CG1	2.36	0.65
1:B:470:MET:HG3	1:B:502:GLY:HA2	1.81	0.63
6:A:957:PG4:H12	1:B:255:LEU:CD1	2.29	0.62
1:A:363:LEU:HD12	1:A:397:LEU:HB3	1.82	0.60
1:A:422:HIS:ND1	1:A:424:HIS:HB3	2.17	0.59
4:A:955:GOL:O3	1:B:393:ARG:HD2	2.03	0.58
6:A:957:PG4:H62	1:B:294:GLN:OE1	2.02	0.57
1:A:294:GLN:OE1	6:A:957:PG4:H32	2.05	0.57
1:B:422:HIS:CG	1:B:423:PRO:HD2	2.39	0.57
1:A:451:PRO:HD2	1:B:446:TYR:CD1	2.40	0.56
1:B:309:THR:HG21	1:B:393:ARG:HH22	1.70	0.55
1:B:317:GLN:HG3	1:B:317:GLN:O	2.07	0.55
1:A:326:LYS:HE2	1:B:243:GLY:O	2.06	0.54
1:B:269:LEU:HB2	1:B:311:THR:HB	1.88	0.54
1:A:253(A):LEU:HD22	6:A:957:PG4:H11	1.89	0.53
1:B:316:TYR:CE2	1:B:317:GLN:HG2	2.44	0.53
6:A:957:PG4:H51	1:B:294:GLN:OE1	2.09	0.53
1:B:309:THR:HG21	1:B:393:ARG:NH2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:GLN:HB2	1:A:421:THR:OG1	2.09	0.52
1:A:294:GLN:OE1	6:A:957:PG4:C4	2.58	0.52
1:A:422:HIS:CE1	1:A:424:HIS:HB3	2.44	0.52
1:A:235:LYS:HE3	1:A:255:LEU:HD12	1.92	0.51
1:A:470:MET:HG3	1:A:502:GLY:HA2	1.94	0.50
1:B:368:GLY:H	1:B:422:HIS:HE2	1.60	0.49
1:A:475:SER:OG	5:A:956:TRS:H32	2.13	0.49
1:B:316:TYR:CD2	1:B:317:GLN:HG2	2.48	0.48
6:A:957:PG4:C6	1:B:253(A):LEU:HD21	2.41	0.48
1:B:363:LEU:CD1	1:B:370:VAL:HG21	2.44	0.47
1:A:389:GLU:HB2	1:A:397:LEU:HD11	1.95	0.47
1:A:370:VAL:HG22	1:A:422:HIS:CD2	2.44	0.47
1:B:363:LEU:HB2	1:B:397:LEU:HB3	1.98	0.46
1:B:369:THR:HG22	1:B:369:THR:O	2.15	0.46
1:A:235:LYS:HZ1	6:A:957:PG4:C8	2.29	0.46
1:A:439:PRO:HG3	1:B:278:ASP:HB3	1.97	0.45
1:B:370:VAL:H	1:B:422:HIS:HD2	1.65	0.45
1:B:269:LEU:HD23	1:B:274:VAL:HA	1.99	0.45
1:B:425:LEU:HA	1:B:426:PRO:HD3	1.85	0.45
1:A:431:ARG:NH2	7:A:2163:HOH:O	2.49	0.44
1:A:235:LYS:NZ	6:A:957:PG4:C8	2.80	0.44
1:B:454:PRO:HA	1:B:457:ARG:HE	1.82	0.44
6:A:957:PG4:H62	1:B:294:GLN:CD	2.39	0.43
1:B:430:MET:HB3	1:B:430:MET:HE2	1.93	0.42
1:A:483:VAL:HG12	7:A:2199:HOH:O	2.19	0.42
1:A:481:ASN:HB2	1:A:518:GLN:HE22	1.83	0.42
1:A:372:LEU:C	1:A:372:LEU:HD12	2.40	0.42
1:A:361:VAL:O	1:A:362:ASP:HB2	2.20	0.42
1:A:306:SER:O	1:A:307:ASP:HB2	2.19	0.42
1:B:363:LEU:HD13	1:B:370:VAL:HG21	2.02	0.42
1:B:370:VAL:N	1:B:422:HIS:HD2	2.18	0.41
1:B:326:LYS:HE2	7:B:2115:HOH:O	2.19	0.41
1:B:544:ASN:HA	1:B:545:PRO:HD3	1.92	0.41
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.91	0.41
1:A:294:GLN:OE1	6:A:957:PG4:C3	2.69	0.41
1:B:443:PRO:HG2	1:B:537:VAL:HG11	2.03	0.41
1:B:425:LEU:HD21	1:B:429:LEU:HD13	2.02	0.41
1:A:368:GLY:HA3	1:A:423:PRO:HG3	2.03	0.40
1:B:368:GLY:H	1:B:422:HIS:CE1	2.39	0.40
6:A:957:PG4:H62	1:B:294:GLN:NE2	2.36	0.40
1:B:331:SER:O	1:B:333:PRO:HD3	2.22	0.40

There are no symmetry-related clashes.

## 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	317/323 (98%)	310 (98%)	7 (2%)	0	100	100
1	B	321/323 (99%)	309 (96%)	12 (4%)	0	100	100
All	All	638/646 (99%)	619 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	283/286 (99%)	282 (100%)	1 (0%)	93	94
1	B	286/286 (100%)	283 (99%)	3 (1%)	82	81
All	All	569/572 (100%)	565 (99%)	4 (1%)	88	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	372	LEU
1	B	279	LEU
1	B	429	LEU
1	B	458	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	HIS
1	A	313	GLN
1	A	383	ASN
1	A	518	GLN
1	B	286	GLN
1	B	317	GLN
1	B	392	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](#)

10 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	946	1,2	14,14,15	0.48	0	15,19,21	1.07	1 (6%)
2	NAG	A	947	2	14,14,15	0.56	0	15,19,21	1.19	3 (20%)
2	BMA	A	948	2	11,11,12	0.69	0	14,15,17	1.81	3 (21%)
2	MAN	A	949	2	11,11,12	0.63	0	14,15,17	0.86	0
2	MAN	A	950	2	11,11,12	0.65	0	14,15,17	0.72	0
2	NAG	B	947	1,2	14,14,15	0.44	0	15,19,21	1.44	2 (13%)
2	NAG	B	948	2	14,14,15	0.46	0	15,19,21	1.04	2 (13%)
2	BMA	B	949	2	11,11,12	0.65	0	14,15,17	1.55	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MAN	B	950	2	11,11,12	0.51	0	14,15,17	1.04	1 (7%)
2	MAN	B	951	2	11,11,12	0.65	0	14,15,17	0.93	1 (7%)

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	NAG	A	946	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	947	2	-	0/6/23/26	0/1/1/1
2	BMA	A	948	2	-	0/2/19/22	0/1/1/1
2	MAN	A	949	2	-	0/2/19/22	0/1/1/1
2	MAN	A	950	2	-	0/2/19/22	0/1/1/1
2	NAG	B	947	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	948	2	-	0/6/23/26	0/1/1/1
2	BMA	B	949	2	-	0/2/19/22	0/1/1/1
2	MAN	B	950	2	-	0/2/19/22	0/1/1/1
2	MAN	B	951	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	948	BMA	O2-C2-C3	-2.75	104.60	110.12
2	B	948	NAG	C2-N2-C7	-2.18	120.23	123.04
2	B	947	NAG	C6-C5-C4	-2.14	107.74	113.02
2	B	951	MAN	C1-O5-C5	-2.13	109.55	112.25
2	A	947	NAG	C2-N2-C7	-2.05	120.41	123.04
2	A	947	NAG	C4-C3-C2	2.24	114.71	111.23
2	B	950	MAN	C1-C2-C3	2.43	112.41	109.54
2	B	948	NAG	C1-O5-C5	2.52	115.44	112.25
2	A	948	BMA	O5-C5-C6	2.65	113.09	107.35
2	A	947	NAG	C1-O5-C5	2.68	115.64	112.25
2	A	946	NAG	C1-O5-C5	3.13	116.22	112.25
2	B	947	NAG	C1-O5-C5	4.34	117.76	112.25
2	B	949	BMA	C1-C2-C3	4.54	114.92	109.54
2	A	948	BMA	C1-C2-C3	4.59	114.97	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

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	SO4	A	951	-	4,4,4	0.21	0	6,6,6	0.08	0
3	SO4	A	952	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	A	953	-	4,4,4	0.14	0	6,6,6	0.12	0
4	GOL	A	954	-	5,5,5	0.35	0	5,5,5	0.28	0
4	GOL	A	955	-	5,5,5	0.31	0	5,5,5	0.23	0
5	TRS	A	956	-	7,7,7	1.00	1 (14%)	9,9,9	0.54	0
6	PG4	A	957	-	12,12,12	0.57	0	11,11,11	1.39	1 (9%)
3	SO4	B	946	-	4,4,4	0.20	0	6,6,6	0.11	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	SO4	A	951	-	-	0/0/0/0	0/0/0/0
3	SO4	A	952	-	-	0/0/0/0	0/0/0/0
3	SO4	A	953	-	-	0/0/0/0	0/0/0/0
4	GOL	A	954	-	-	0/4/4/4	0/0/0/0
4	GOL	A	955	-	-	0/4/4/4	0/0/0/0
5	TRS	A	956	-	-	0/9/9/9	0/0/0/0
6	PG4	A	957	-	-	0/10/10/10	0/0/0/0
3	SO4	B	946	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	956	TRS	C-N	-2.60	1.46	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	957	PG4	O4-C6-C5	2.04	119.43	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	955	GOL	3	0
5	A	956	TRS	1	0
6	A	957	PG4	15	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	319/323 (98%)	-0.03	7 (2%) 65 68	23, 39, 96, 183	0
1	B	320/323 (99%)	0.25	22 (6%) 20 22	21, 39, 90, 148	0
All	All	639/646 (98%)	0.11	29 (4%) 37 40	21, 39, 96, 183	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	427	ARG	7.6
1	B	334	ARG	5.8
1	B	425	LEU	5.5
1	B	225	CYS	5.1
1	B	426	PRO	4.9
1	A	545	PRO	4.7
1	B	363	LEU	4.6
1	B	424	HIS	4.5
1	B	423	PRO	3.9
1	B	422	HIS	3.5
1	B	366	SER	3.1
1	B	370	VAL	3.0
1	B	369	THR	3.0
1	A	363	LEU	2.9
1	B	368	GLY	2.8
1	B	335	GLY	2.7
1	A	334	ARG	2.7
1	B	230	THR	2.6
1	B	336	VAL	2.6
1	B	546	GLY	2.6
1	A	364	ALA	2.4
1	B	273	GLN	2.4
1	B	227	ARG	2.4
1	A	424	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	377	ALA	2.3
1	B	332	ASN	2.3
1	A	362	ASP	2.3
1	B	259	TYR	2.2
1	B	362	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](#)

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( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	946	14/15	0.91	0.17	-0.10	82,88,100,102	0
2	NAG	B	947	14/15	0.95	0.09	-0.63	49,55,64,72	0
2	NAG	B	948	14/15	0.95	0.09	-0.77	41,54,58,64	0
2	MAN	B	951	11/12	0.82	0.23	-	88,94,99,101	0
2	BMA	A	948	11/12	0.85	0.16	-	99,107,114,125	0
2	NAG	A	947	14/15	0.89	0.16	-	79,84,91,92	0
2	MAN	B	950	11/12	0.88	0.14	-	78,85,97,99	0
2	MAN	A	950	11/12	0.29	0.32	-	116,121,128,129	0
2	BMA	B	949	11/12	0.89	0.14	-	52,67,74,80	0
2	MAN	A	949	11/12	0.72	0.26	-	113,116,120,122	0

## 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( $\text{\AA}^2$ )	Q<0.9
6	PG4	A	957	13/13	0.84	0.66	28.03	66,74,83,86	0
5	TRS	A	956	8/8	0.75	0.26	21.94	64,73,96,104	0
4	GOL	A	954	6/6	0.86	0.23	4.68	76,79,93,99	0
4	GOL	A	955	6/6	0.79	0.17	1.56	83,88,90,93	0
3	SO4	A	951	5/5	0.98	0.15	0.73	53,61,71,78	0
3	SO4	A	953	5/5	0.91	0.11	-0.72	103,109,111,111	0
3	SO4	B	946	5/5	0.93	0.12	-	66,67,77,79	0
3	SO4	A	952	5/5	0.89	0.15	-	107,109,114,114	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.