



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:08 AM GMT

PDB ID : 3QPQ  
Title : Crystal structure of ANTI-TLR3 antibody C1068 FAB  
Authors : Luo, J.; Obmolova, G.; Teplyakov, A.; Gilliland, G.L.  
Deposited on : 2011-02-14  
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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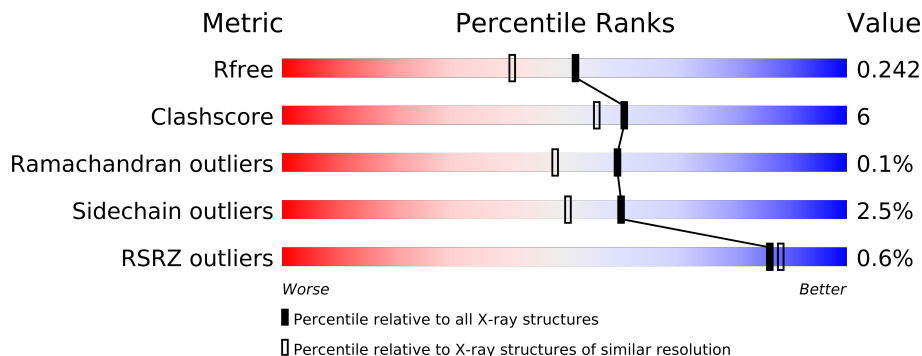
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	C	215	
1	E	215	
1	I	215	
1	L	215	
2	D	223	
2	F	223	
2	H	223	
2	J	223	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	C	218	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	C	219	-	X
3	GOL	C	220	-	X
3	GOL	C	221	-	X
3	GOL	D	224	-	X
3	GOL	E	216	-	X
3	GOL	I	216	-	X
3	GOL	I	217	-	X
3	GOL	J	225	-	X
3	GOL	L	216	-	X
3	GOL	L	217	-	X
4	SO4	L	219	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15233 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

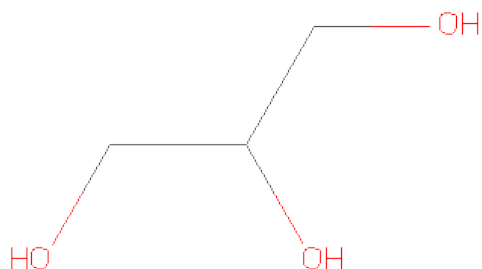
- Molecule 1 is a protein called C1068 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	6	0
			1691	1059	282	343	7			
1	E	215	Total	C	N	O	S	0	5	0
			1682	1054	280	341	7			
1	C	215	Total	C	N	O	S	0	4	0
			1677	1052	279	339	7			
1	I	215	Total	C	N	O	S	0	3	0
			1672	1049	279	337	7			

- Molecule 2 is a protein called C1068 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	2	0
			1652	1049	275	321	7			
2	F	221	Total	C	N	O	S	0	4	0
			1710	1085	289	329	7			
2	D	219	Total	C	N	O	S	0	2	0
			1682	1067	284	324	7			
2	J	217	Total	C	N	O	S	0	1	0
			1659	1053	278	321	7			

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



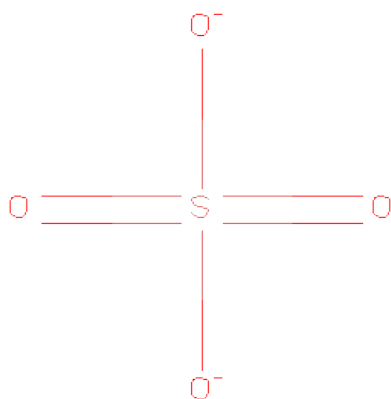
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	L	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		

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

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	228	Total	O	0	0
			228	228		
5	H	222	Total	O	0	0
			222	222		
5	E	229	Total	O	0	0
			229	229		
5	F	189	Total	O	0	0
			189	189		
5	C	229	Total	O	0	0
			229	229		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	223	Total 223	O 223	0	0
5	I	184	Total 184	O 184	0	0
5	J	197	Total 197	O 197	0	0

### 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 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 ( $RSRZ > 2$ ). 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.

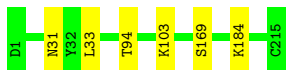
- Molecule 1: C1068 light chain

Chain L: 



- Molecule 1: C1068 light chain

Chain E: 



- Molecule 1: C1068 light chain

Chain C: 



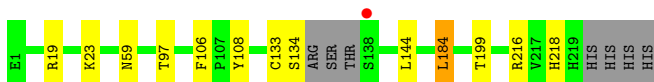
- Molecule 1: C1068 light chain

Chain I: 



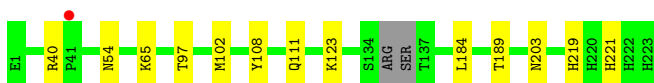
- Molecule 2: C1068 heavy chain

Chain H: 



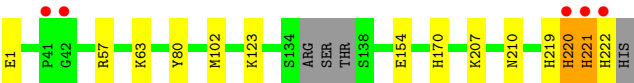
- Molecule 2: C1068 heavy chain

Chain F: 



- Molecule 2: C1068 heavy chain

Chain D: 



● Molecule 2: C1068 heavy chain

Chain J: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.48Å 136.94Å 83.25Å 90.00° 114.95° 90.00°	Depositor
Resolution (Å)	44.55 – 1.90 44.55 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.2 (44.55-1.90) 89.2 (44.55-1.90)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 1.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_601)	Depositor
R, $R_{free}$	0.201 , 0.256 0.187 , 0.242	Depositor DCC
$R_{free}$ test set	5910 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 49.3	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	2 of 117330 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15233	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.31 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.9489e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PCA, 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	C	0.39	0/1727	0.55	0/2342
1	E	0.38	0/1735	0.56	0/2352
1	I	0.38	0/1719	0.54	0/2331
1	L	0.41	0/1744	0.56	0/2365
2	D	0.35	0/1726	0.53	0/2359
2	F	0.34	0/1761	0.53	0/2406
2	H	0.35	0/1693	0.56	1/2314 (0.0%)
2	J	0.33	0/1698	0.55	0/2321
All	All	0.37	0/13803	0.55	1/18790 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	184	LEU	CA-CB-CG	6.23	129.64	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1677	0	0	9	0
1	E	1682	0	0	1	0
1	I	1672	0	0	5	0
1	L	1691	0	0	7	0
2	D	1682	0	34	14	0
2	F	1710	0	41	9	0
2	H	1652	0	13	11	0
2	J	1659	0	20	17	0
3	C	36	0	48	3	0
3	D	6	0	8	1	0
3	E	6	0	8	2	0
3	F	6	0	8	0	0
3	I	12	0	16	3	0
3	J	18	0	24	5	0
3	L	18	0	24	5	0
4	L	5	0	0	1	0
5	C	229	0	0	5	1
5	D	223	0	0	5	0
5	E	229	0	0	3	0
5	F	189	0	0	4	0
5	H	222	0	0	5	1
5	I	184	0	0	3	0
5	J	197	0	0	9	1
5	L	228	0	0	10	1
All	All	15233	0	244	81	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (81) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:216:GOL:H31	5:I:484:HOH:O	1.46	1.15
3:L:216:GOL:H2	5:L:526:HOH:O	0.95	1.12
2:D:221:HIS:O	2:D:222:HIS:HB2	1.68	0.93
2:J:46:GLU:OE1	5:J:417:HOH:O	1.93	0.86
2:D:219:HIS:O	2:D:220:HIS:HB2	1.73	0.85
1:L:92:TRP:O	5:L:312:HOH:O	1.93	0.85
2:D:221:HIS:O	2:D:222:HIS:CB	2.29	0.80
1:L:200[A]:GLN:OE1	5:L:442:HOH:O	1.99	0.80
2:D:219:HIS:HD2	2:D:220:HIS:HD2	1.26	0.80
2:D:219:HIS:HD2	2:D:220:HIS:CD2	2.00	0.79
1:L:94:THR:OG1	5:L:451:HOH:O	2.00	0.78
3:E:216:GOL:O3	5:E:512:HOH:O	2.02	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:216:GOL:C2	5:L:526:HOH:O	1.70	0.76
2:F:219:HIS:HD2	2:F:221:HIS:H	1.34	0.76
2:H:59:ASN:ND2	5:H:500:HOH:O	2.18	0.76
2:F:189:THR:OG1	5:F:424:HOH:O	2.03	0.76
2:D:219:HIS:CD2	2:D:220:HIS:HD2	2.06	0.73
2:F:123:LYS:NZ	5:F:427:HOH:O	2.20	0.73
1:C:166:GLU:N	3:C:221:GOL:HO2	1.87	0.71
1:C:66:GLU:O	3:C:219:GOL:H32	1.90	0.71
2:J:218:HIS:ND1	5:J:497:HOH:O	2.22	0.70
1:C:123:ASP:OD1	5:C:409:HOH:O	2.10	0.69
2:J:220:HIS:H	3:J:226:GOL:H11	1.59	0.68
1:I:74:LYS:NZ	5:I:363:HOH:O	2.26	0.67
2:D:207:LYS:N	5:D:357:HOH:O	2.26	0.67
2:J:57:ARG:NH2	5:J:308:HOH:O	2.28	0.67
2:J:31:THR:OG1	5:J:486:HOH:O	2.15	0.64
1:C:60:SER:O	5:C:393:HOH:O	2.14	0.63
1:I:213:GLY:N	3:I:217:GOL:HO3	1.97	0.63
1:L:148:GLN:NE2	5:L:436:HOH:O	2.32	0.61
1:C:215:CYS:O	3:C:217:GOL:H32	2.01	0.61
2:J:57:ARG:NH2	2:J:57:ARG:CG	2.64	0.60
1:E:184:LYS:NZ	5:E:468:HOH:O	2.34	0.60
2:F:219:HIS:CD2	2:F:221:HIS:HB2	2.38	0.59
1:C:120:PRO:O	2:D:222:HIS:CE1	2.56	0.58
3:L:217:GOL:H32	5:L:343:HOH:O	2.04	0.58
2:H:216:ARG:CZ	2:H:218:HIS:HD2	2.18	0.57
2:D:1:PCA:N	5:D:504:HOH:O	2.37	0.56
2:H:199:THR:CG2	5:H:514:HOH:O	2.53	0.56
2:J:219:HIS:CD2	2:J:219:HIS:H	2.25	0.54
3:L:216:GOL:C1	5:L:526:HOH:O	2.27	0.54
2:J:3:GLN:NE2	5:J:364:HOH:O	2.41	0.53
2:F:65:LYS:O	5:F:468:HOH:O	2.19	0.53
2:D:207:LYS:O	2:D:210:ASN:N	2.42	0.53
3:E:216:GOL:C3	5:E:512:HOH:O	2.55	0.53
2:H:216:ARG:CZ	2:H:218:HIS:CD2	2.91	0.53
2:D:170:HIS:CD2	3:D:224:GOL:H11	2.44	0.53
3:I:216:GOL:C3	5:I:484:HOH:O	2.27	0.52
2:H:133:CYS:O	2:H:134:SER:C	2.47	0.52
2:D:80:TYR:OH	5:D:421:HOH:O	2.19	0.51
1:L:79[B]:GLN:NE2	5:L:405:HOH:O	2.44	0.51
2:F:97[A]:THR:CG2	2:F:108:TYR:O	2.59	0.50
2:J:43:GLN:NE2	5:J:445:HOH:O	2.45	0.49
2:F:219:HIS:HD2	2:F:221:HIS:N	2.07	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:218:HIS:HB3	3:J:226:GOL:H2	1.95	0.48
2:J:43:GLN:NE2	5:J:436:HOH:O	2.45	0.48
2:D:123:LYS:NZ	5:D:445:HOH:O	2.48	0.47
2:J:219:HIS:CD2	2:J:219:HIS:N	2.80	0.47
2:J:171:THR:O	3:J:224:GOL:H12	2.16	0.46
2:F:219:HIS:CD2	2:F:221:HIS:H	2.23	0.46
1:C:76:ASN:ND2	5:C:466:HOH:O	2.49	0.45
2:J:97[B]:THR:CG2	2:J:108:TYR:O	2.64	0.45
1:L:98:PHE:CD2	4:L:219:SO4:O4	2.70	0.45
2:D:154:GLU:OE1	5:D:393:HOH:O	2.20	0.45
1:I:39:LYS:NZ	1:I:81:GLU:O	2.50	0.45
1:I:49:TYR:CE1	3:J:225:GOL:H31	2.53	0.44
2:J:40:ARG:N	5:J:332:HOH:O	2.51	0.44
2:J:220:HIS:HB3	3:J:226:GOL:O1	2.18	0.43
1:C:40:GLN:NE2	5:C:493:HOH:O	2.51	0.43
3:L:216:GOL:H11	5:L:526:HOH:O	2.04	0.43
1:C:150:LYS:NZ	5:C:431:HOH:O	2.51	0.43
2:H:23:LYS:NZ	5:H:444:HOH:O	2.51	0.43
2:F:54:ASN:ND2	5:F:383:HOH:O	2.51	0.42
2:H:216:ARG:NH2	2:H:218:HIS:HD2	2.18	0.42
1:I:125:GLN:O	1:I:128:SER:OG	2.38	0.42
2:H:19:ARG:NH1	5:H:309:HOH:O	2.54	0.41
2:H:19:ARG:NH1	5:H:356:HOH:O	2.53	0.41
2:H:97[B]:THR:CG2	2:H:106:PHE:CB	2.99	0.41
2:H:97[B]:THR:CG2	2:H:108:TYR:O	2.69	0.41
1:L:199:HIS:CD2	1:L:201:GLY:N	2.89	0.41
2:J:38:LYS:NZ	5:J:304:HOH:O	2.53	0.41

All (2) 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	Distance(Å)	Clash(Å)
5:C:510:HOH:O	5:J:483:HOH:O[2_646]	2.06	0.14
5:L:505:HOH:O	5:H:459:HOH:O[2_846]	2.13	0.07

## 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	C	217/215 (101%)	211 (97%)	6 (3%)	0	100	100
1	E	218/215 (101%)	214 (98%)	4 (2%)	0	100	100
1	I	216/215 (100%)	211 (98%)	5 (2%)	0	100	100
1	L	219/215 (102%)	214 (98%)	5 (2%)	0	100	100
2	D	217/223 (97%)	207 (95%)	8 (4%)	2 (1%)	25	10
2	F	221/223 (99%)	214 (97%)	7 (3%)	0	100	100
2	H	214/223 (96%)	208 (97%)	6 (3%)	0	100	100
2	J	214/223 (96%)	209 (98%)	5 (2%)	0	100	100
All	All	1736/1752 (99%)	1688 (97%)	46 (3%)	2 (0%)	59	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	221	HIS
2	D	220	HIS

### 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	C	192/188 (102%)	186 (97%)	6 (3%)	52	41
1	E	193/188 (103%)	188 (97%)	5 (3%)	59	49
1	I	191/188 (102%)	185 (97%)	6 (3%)	52	41
1	L	194/188 (103%)	190 (98%)	4 (2%)	66	59
2	D	192/194 (99%)	189 (98%)	3 (2%)	75	70
2	F	196/194 (101%)	191 (97%)	5 (3%)	59	49
2	H	189/194 (97%)	187 (99%)	2 (1%)	84	82
2	J	189/194 (97%)	183 (97%)	6 (3%)	51	39
All	All	1536/1528 (100%)	1499 (98%)	37 (2%)	60	53

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	31	ASN
1	L	40	GLN
1	L	105	GLU
1	L	106	LEU
2	H	144	LEU
2	H	184	LEU
1	E	31	ASN
1	E	33	LEU
1	E	94	THR
1	E	103	LYS
1	E	169	SER
2	F	40	ARG
2	F	102	MET
2	F	111	GLN
2	F	184	LEU
2	F	203	ASN
1	C	1	ASP
1	C	31	ASN
1	C	103	LYS
1	C	105	GLU
1	C	155	LEU
1	C	157	SER
2	D	57	ARG
2	D	63	LYS
2	D	102	MET
1	I	39	LYS
1	I	45	GLN
1	I	70	GLN
1	I	76	ASN
1	I	105	GLU
1	I	157	SER
2	J	102	MET
2	J	111	GLN
2	J	139	GLU
2	J	156	VAL
2	J	184	LEU
2	J	195	LEU

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

Mol	Chain	Res	Type
2	H	218	HIS
2	H	219	HIS

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Mol	Chain	Res	Type
2	F	219	HIS
2	F	221	HIS
2	D	219	HIS
2	D	220	HIS
2	J	219	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	PCA	D	1	2	8,8,9	6.90	2 (25%)	8,10,12	5.57	4 (50%)
2	PCA	F	1	2	8,8,9	6.55	3 (37%)	8,10,12	5.60	4 (50%)
2	PCA	H	1	2	8,8,9	6.61	3 (37%)	8,10,12	6.38	4 (50%)
2	PCA	J	1	2	8,8,9	6.54	3 (37%)	8,10,12	5.08	3 (37%)

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	PCA	D	1	2	-	0/0/11/13	0/1/1/1
2	PCA	F	1	2	-	0/0/11/13	0/1/1/1
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1
2	PCA	J	1	2	-	0/0/11/13	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	PCA	O-C	18.55	1.24	1.11
2	H	1	PCA	O-C	17.59	1.23	1.11
2	J	1	PCA	O-C	17.45	1.23	1.11
2	F	1	PCA	O-C	17.40	1.23	1.11
2	F	1	PCA	CD-N	5.92	1.47	1.34
2	H	1	PCA	CD-N	5.83	1.46	1.34
2	D	1	PCA	CD-N	5.66	1.46	1.34
2	J	1	PCA	CD-N	5.55	1.46	1.34
2	J	1	PCA	CA-C	2.43	1.52	1.48
2	H	1	PCA	CA-C	2.28	1.52	1.48
2	F	1	PCA	CA-C	2.15	1.52	1.48

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	PCA	CA-N-CD	-14.36	103.14	114.37
2	F	1	PCA	CA-N-CD	-13.98	103.44	114.37
2	H	1	PCA	CA-N-CD	-12.72	104.43	114.37
2	J	1	PCA	CA-N-CD	-12.29	104.76	114.37
2	H	1	PCA	C-CA-N	-11.93	108.02	110.71
2	J	1	PCA	C-CA-N	5.85	112.03	110.71
2	F	1	PCA	C-CA-N	5.47	111.95	110.71
2	D	1	PCA	C-CA-N	-4.22	109.76	110.71
2	F	1	PCA	OE-CD-CG	-3.51	121.19	126.70
2	D	1	PCA	OE-CD-CG	-3.38	121.39	126.70
2	J	1	PCA	OE-CD-CG	-3.20	121.68	126.70
2	H	1	PCA	OE-CD-CG	-2.92	122.11	126.70
2	F	1	PCA	CB-CA-N	2.60	111.20	103.72
2	D	1	PCA	CB-CA-N	2.37	110.53	103.72
2	H	1	PCA	CB-CA-N	2.14	109.89	103.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

18 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	C	216	-	5,5,5	0.34	0	5,5,5	0.33	0
3	GOL	C	217	-	5,5,5	0.37	0	5,5,5	0.39	0
3	GOL	C	218	-	5,5,5	0.38	0	5,5,5	0.22	0
3	GOL	C	219	-	5,5,5	0.30	0	5,5,5	0.47	0
3	GOL	C	220	-	5,5,5	0.39	0	5,5,5	0.24	0
3	GOL	C	221	-	5,5,5	0.38	0	5,5,5	0.55	0
3	GOL	D	224	-	5,5,5	0.33	0	5,5,5	0.36	0
3	GOL	E	216	-	5,5,5	0.41	0	5,5,5	0.13	0
3	GOL	F	224	-	5,5,5	0.37	0	5,5,5	0.26	0
3	GOL	I	216	-	5,5,5	0.41	0	5,5,5	0.35	0
3	GOL	I	217	-	5,5,5	0.39	0	5,5,5	0.21	0
3	GOL	J	224	-	5,5,5	0.36	0	5,5,5	0.33	0
3	GOL	J	225	-	5,5,5	0.31	0	5,5,5	0.45	0
3	GOL	J	226	-	5,5,5	0.39	0	5,5,5	0.41	0
3	GOL	L	216	-	5,5,5	0.33	0	5,5,5	0.34	0
3	GOL	L	217	-	5,5,5	0.29	0	5,5,5	0.40	0
3	GOL	L	218	-	5,5,5	0.35	0	5,5,5	0.27	0
4	SO4	L	219	-	4,4,4	0.20	0	6,6,6	0.18	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	C	216	-	-	0/4/4/4	0/0/0/0
3	GOL	C	217	-	-	0/4/4/4	0/0/0/0
3	GOL	C	218	-	-	0/4/4/4	0/0/0/0
3	GOL	C	219	-	-	0/4/4/4	0/0/0/0
3	GOL	C	220	-	-	0/4/4/4	0/0/0/0
3	GOL	C	221	-	-	0/4/4/4	0/0/0/0
3	GOL	D	224	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	E	216	-	-	0/4/4/4	0/0/0/0
3	GOL	F	224	-	-	0/4/4/4	0/0/0/0
3	GOL	I	216	-	-	0/4/4/4	0/0/0/0
3	GOL	I	217	-	-	0/4/4/4	0/0/0/0
3	GOL	J	224	-	-	0/4/4/4	0/0/0/0
3	GOL	J	225	-	-	0/4/4/4	0/0/0/0
3	GOL	J	226	-	-	0/4/4/4	0/0/0/0
3	GOL	L	216	-	-	0/4/4/4	0/0/0/0
3	GOL	L	217	-	-	0/4/4/4	0/0/0/0
3	GOL	L	218	-	-	0/4/4/4	0/0/0/0
4	SO4	L	219	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	C	215/215 (100%)	-0.47	0 100 100	17, 26, 41, 63	0
1	E	215/215 (100%)	-0.48	0 100 100	15, 25, 41, 56	0
1	I	215/215 (100%)	-0.42	0 100 100	18, 29, 46, 64	0
1	L	215/215 (100%)	-0.49	0 100 100	15, 23, 41, 56	0
2	D	219/223 (98%)	-0.32	5 (2%) 57 59	18, 28, 53, 86	0
2	F	221/223 (99%)	-0.21	1 (0%) 88 90	18, 32, 52, 91	0
2	H	216/223 (96%)	-0.36	1 (0%) 88 90	16, 26, 46, 85	0
2	J	217/223 (97%)	-0.20	3 (1%) 72 74	19, 31, 58, 82	0
All	All	1733/1752 (98%)	-0.37	10 (0%) 86 88	15, 27, 48, 91	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	222	HIS	3.8
2	D	41	PRO	3.5
2	J	220	HIS	3.4
2	D	220	HIS	3.3
2	J	41	PRO	2.7
2	F	41	PRO	2.5
2	D	221	HIS	2.4
2	D	42	GLY	2.4
2	H	138	SER	2.3
2	J	42	GLY	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PCA	J	1	8/9	0.10	1.88	34,35,37,38	0
2	PCA	D	1	8/9	0.09	0.82	21,32,46,50	0
2	PCA	F	1	8/9	0.09	-0.11	32,42,48,49	0
2	PCA	H	1	8/9	0.08	-0.84	27,36,45,51	0

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	C	219	6/6	0.30	15.81	51,61,67,71	0
3	GOL	C	221	6/6	0.28	14.37	30,44,56,56	0
4	SO4	L	219	5/5	0.25	12.85	11,32,37,37	5
3	GOL	E	216	6/6	0.22	11.15	39,45,50,50	0
3	GOL	D	224	6/6	0.18	7.69	40,51,61,72	0
3	GOL	C	220	6/6	0.16	7.36	47,49,52,55	0
3	GOL	C	218	6/6	0.27	7.18	24,38,42,54	0
3	GOL	L	216	6/6	0.17	5.68	34,42,45,49	0
3	GOL	I	216	6/6	0.22	3.99	30,40,45,47	0
3	GOL	L	217	6/6	0.17	3.66	35,48,49,58	0
3	GOL	I	217	6/6	0.15	3.05	36,42,49,53	0
3	GOL	J	225	6/6	0.13	2.14	27,43,45,45	0
3	GOL	J	224	6/6	0.15	1.88	34,48,49,56	0
3	GOL	L	218	6/6	0.12	1.46	37,43,50,55	0
3	GOL	J	226	6/6	0.19	0.80	42,51,53,57	0
3	GOL	F	224	6/6	0.08	0.27	30,35,40,44	0
3	GOL	C	216	6/6	0.09	0.19	31,35,41,42	0
3	GOL	C	217	6/6	0.10	-0.14	33,41,42,48	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.