



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2021 – 04:23 PM EDT

PDB ID : 4RFE  
Title : Crystal structure of ADCC-potent ANTI-HIV-1 Rhesus macaque antibody JR4 Fab  
Authors : Wu, X.; Gohain, N.; Tolbert, W.D.; Pazgier, M.  
Deposited on : 2014-09-25  
Resolution : 1.91 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 : 2.18  
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) : 2.18

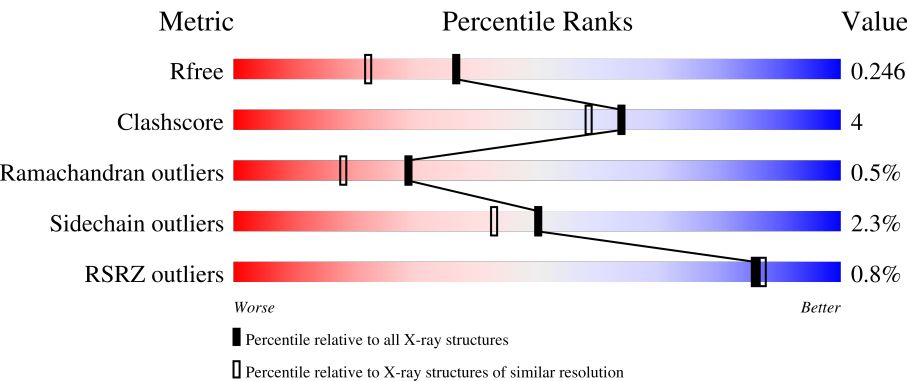
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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 <sub>free</sub>	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 of 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	233	<div><div></div><div>83%9%8%</div></div>
1	C	233	<div><div>2%</div><div>79%11%8%</div></div>
1	E	233	<div><div>2%</div><div>82%9%8%</div></div>
1	H	233	<div><div>2%</div><div>80%11%8%</div></div>
2	B	216	<div><div></div><div>88%8%</div></div>

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Mol	Chain	Length	Quality of chain
2	D	216	89% 9% .
2	F	216	96% ..
2	L	216	86% 11% .

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
5	GOL	E	301	-	X	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14217 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 Fab heavy chain of ADCC-potent anti-HIV-1 antibody JR4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	215	Total	C	N	O	S	0	0	0
			1625	1033	271	317	4			
1	A	215	Total	C	N	O	S	0	0	0
			1625	1033	271	317	4			
1	C	214	Total	C	N	O	S	0	0	0
			1619	1030	270	315	4			
1	E	215	Total	C	N	O	S	0	0	0
			1625	1033	271	317	4			

- Molecule 2 is a protein called Fab light chain of ADCC-potent anti-HIV-1 antibody JR4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	210	Total	C	N	O	S	0	0	0
			1553	972	261	316	4			
2	B	210	Total	C	N	O	S	0	0	0
			1553	972	261	316	4			
2	D	212	Total	C	N	O	S	0	0	0
			1568	980	264	320	4			
2	F	212	Total	C	N	O	S	0	0	0
			1568	980	264	320	4			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	3	Total	Cl	0	0
			3	3		
4	B	3	Total	Cl	0	0
			3	3		
4	D	1	Total	Cl	0	0
			1	1		
4	F	2	Total	Cl	0	0
			2	2		

- Molecule 5 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
5	E	1	Total	C	O	0	0
			6	3	3		

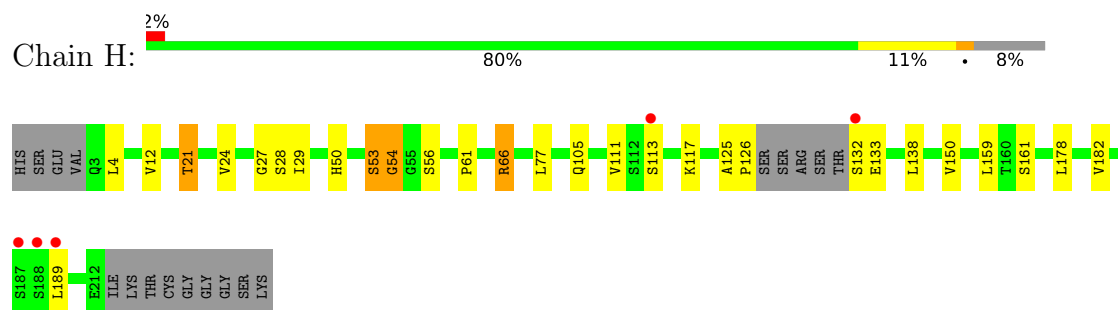
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	177	Total	O	0	0
			177	177		
6	L	191	Total	O	0	0
			191	191		
6	A	169	Total	O	0	0
			169	169		
6	B	195	Total	O	0	0
			195	195		
6	C	140	Total	O	0	0
			140	140		
6	D	210	Total	O	0	0
			210	210		
6	E	154	Total	O	0	0
			154	154		
6	F	220	Total	O	0	0
			220	220		

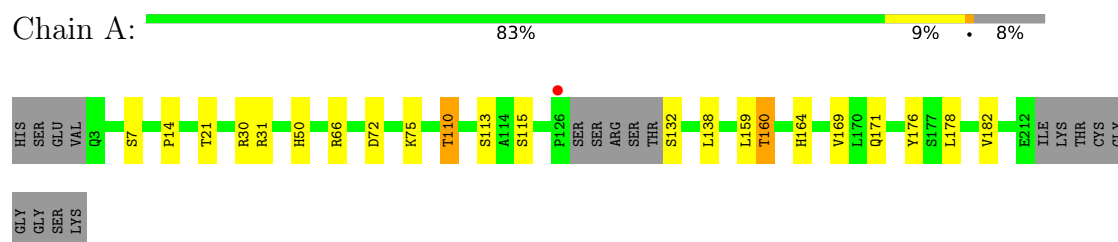
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

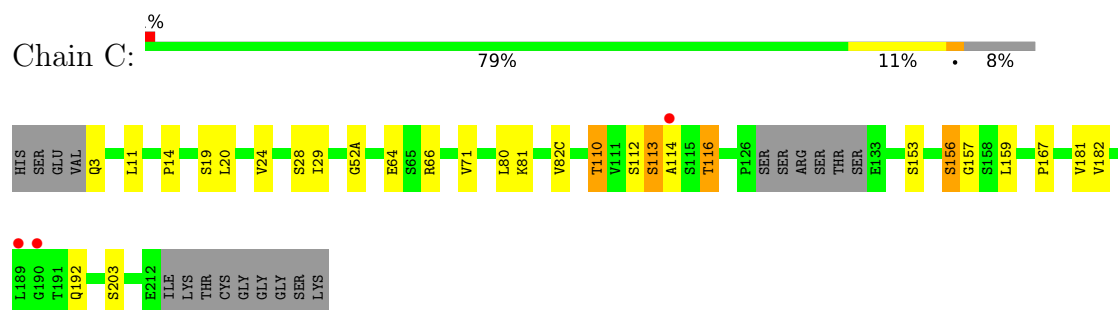
- Molecule 1: Fab heavy chain of ADCC-potent anti-HIV-1 antibody JR4



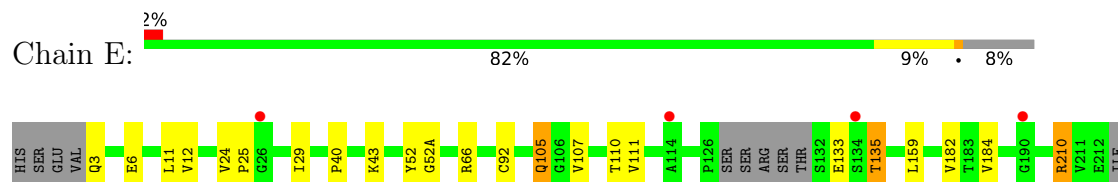
- Molecule 1: Fab heavy chain of ADCC-potent anti-HIV-1 antibody JR4



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- Molecule 1: Fab heavy chain of ADCC-potent anti-HIV-1 antibody JR4



LYS  
THR  
CYS  
GLY  
GLY  
SER  
LYS

- Molecule 2: Fab light chain of ADCC-potent anti-HIV-1 antibody JR4

Chain L:  86% 11% .


GLN SER V3 L4 S9 K18 S27 R30 P40 G41 A74 T75 T76 S77 L78 V95B G99 L104 L106A P120 A130 T131 L132 D151 E160 W185 H188 Q194 E203 A207 P208 THR GLU CYS SER

- Molecule 2: Fab light chain of ADCC-potent anti-HIV-1 antibody JR4

Chain B:  88% 8% ..

GLN SER V3 L4 S27A R30 V39 P40 G41 K66 S67 G68 A71 G99 L106A G107 Q108 S121 S122 E123 L132 L135 Y140 P141 S175 P208 THR GLU CYS SER

- Molecule 2: Fab light chain of ADCC-potent anti-HIV-1 antibody JR4

Chain D:  89% 9% .

Q1 L4 S27 L28 G29 Y32 D50 D60 K66 A71 G77 L78 G99 L106A L135 S165 S190 V206 A207 P208 THR GLU CYS SER

- Molecule 2: Fab light chain of ADCC-potent anti-HIV-1 antibody JR4

Chain F:  96% ..

Q1 S9 D60 L106A P208 THR GLU CYS SER



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.42Å 79.58Å 82.04Å 78.79° 82.89° 65.17°	Depositor
Resolution (Å)	40.20 – 1.91 40.19 – 1.88	Depositor EDS
% Data completeness (in resolution range)	93.8 (40.20-1.91) 93.5 (40.19-1.88)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.192 , 0.246 0.192 , 0.246	Depositor DCC
$R_{free}$ test set	6780 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.0	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14217	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 5.51% 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: CL, 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	0.88	0/1670	0.89	3/2287 (0.1%)
1	C	0.81	0/1664	0.81	2/2279 (0.1%)
1	E	0.83	1/1670 (0.1%)	0.84	2/2287 (0.1%)
1	H	0.84	2/1670 (0.1%)	0.86	2/2287 (0.1%)
2	B	0.92	1/1589 (0.1%)	0.87	6/2167 (0.3%)
2	D	0.90	0/1604	0.86	4/2187 (0.2%)
2	F	0.92	0/1604	0.87	4/2187 (0.2%)
2	L	0.91	1/1589 (0.1%)	0.86	2/2167 (0.1%)
All	All	0.88	5/13060 (0.0%)	0.86	25/17848 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
2	F	0	1
2	L	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	9	SER	C-N	9.37	1.55	1.34
1	H	117	LYS	CE-NZ	6.53	1.65	1.49
1	E	92	CYS	CB-SG	-6.20	1.71	1.82
1	H	117	LYS	CD-CE	5.65	1.65	1.51
2	B	107	GLY	N-CA	-5.41	1.38	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	66	ARG	NE-CZ-NH2	-11.98	114.31	120.30
1	H	66	ARG	NE-CZ-NH1	10.97	125.78	120.30
1	E	66	ARG	NE-CZ-NH2	-10.54	115.03	120.30
1	A	66	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	C	66	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	E	66	ARG	NE-CZ-NH1	8.40	124.50	120.30
2	D	106(A)	LEU	C-N-CA	8.23	139.58	122.30
2	L	106(A)	LEU	C-N-CA	7.42	137.89	122.30
2	F	106(A)	LEU	C-N-CA	6.75	136.48	122.30
2	D	106(A)	LEU	CA-C-N	6.58	129.36	116.20
2	F	106(A)	LEU	CA-C-N	6.40	129.00	116.20
1	A	66	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	C	66	ARG	NE-CZ-NH1	6.05	123.32	120.30
2	B	68	GLY	N-CA-C	-6.04	97.99	113.10
2	L	106(A)	LEU	CA-C-N	5.86	127.92	116.20
2	B	41	GLY	N-CA-C	-5.57	99.18	113.10
2	B	108	GLN	N-CA-C	-5.48	96.21	111.00
2	D	60	ASP	CB-CA-C	-5.37	99.65	110.40
2	D	106(A)	LEU	O-C-N	-5.35	114.10	123.20
2	F	106(A)	LEU	O-C-N	-5.30	114.20	123.20
1	A	160	THR	N-CA-C	5.24	125.16	111.00
2	B	106(A)	LEU	C-N-CA	5.22	133.26	122.30
2	B	106(A)	LEU	CA-C-N	5.21	126.62	116.20
2	F	60	ASP	CB-CA-C	-5.07	100.27	110.40
2	B	106(A)	LEU	O-C-N	-5.06	114.60	123.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	106(A)	LEU	Peptide
2	B	67	SER	Peptide
2	F	9	SER	Mainchain
2	L	9	SER	Mainchain

## 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	1625	0	1584	12	0
1	C	1619	0	1579	18	0
1	E	1625	0	1584	13	0
1	H	1625	0	1584	19	0
2	B	1553	0	1517	12	0
2	D	1568	0	1533	17	0
2	F	1568	0	1533	4	0
2	L	1553	0	1517	22	0
3	E	5	0	0	1	0
3	H	5	0	0	0	0
4	B	3	0	0	0	0
4	D	1	0	0	0	0
4	F	2	0	0	0	0
4	L	3	0	0	0	0
5	E	6	0	8	0	0
6	A	169	0	0	3	0
6	B	195	0	0	0	0
6	C	140	0	0	2	1
6	D	210	0	0	2	0
6	E	154	0	0	1	0
6	F	220	0	0	0	1
6	H	177	0	0	1	2
6	L	191	0	0	3	0
All	All	14217	0	12439	105	2

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 4.

All (105) 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)
2:L:188:HIS:CD2	2:D:1:GLN:HG3	1.90	1.05
2:B:121:SER:HB2	2:B:123:GLU:OE2	1.59	1.01
1:H:54:GLY:HA3	1:H:56:SER:H	1.38	0.88
2:L:188:HIS:NE2	2:D:1:GLN:HG3	1.88	0.87
2:F:1:GLN:N	2:F:1:GLN:OE1	2.09	0.85
1:H:66:ARG:HD3	6:D:595:HOH:O	1.78	0.83
2:L:151:ASP:OD2	2:D:1:GLN:HB3	1.81	0.81
1:C:156:SER:OG	1:C:157:GLY:N	2.09	0.77
1:E:105:GLN:H	1:E:105:GLN:CD	1.88	0.77
1:C:14:PRO:HG2	1:C:113:SER:HB3	1.68	0.75
2:L:18:LYS:HG3	2:L:76:THR:HG22	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:SER:CB	2:B:123:GLU:OE2	2.36	0.74
2:B:27(A):SER:O	2:B:30:ARG:HD2	1.89	0.73
2:L:120:PRO:HD3	2:L:132:LEU:CD2	2.19	0.71
1:C:11:LEU:HD11	1:C:112:SER:HB3	1.73	0.68
1:H:61:PRO:HD2	2:L:95(B):VAL:HG11	1.74	0.68
2:B:123:GLU:H	2:B:123:GLU:CD	1.98	0.67
2:D:4:LEU:HB2	2:D:99:GLY:HA2	1.78	0.66
1:H:159:LEU:HD21	1:H:182:VAL:HG21	1.77	0.66
2:L:160:GLU:CG	6:L:590:HOH:O	2.44	0.64
1:H:150:VAL:CG2	1:H:178:LEU:HD21	2.27	0.64
1:C:24:VAL:HG12	1:C:24:VAL:O	1.98	0.62
2:D:4:LEU:HD13	2:D:28:ILE:HD11	1.81	0.62
1:C:19:SER:OG	1:C:81:LYS:HD3	2.00	0.61
1:C:181:VAL:HG21	2:D:135:LEU:HD12	1.81	0.61
2:L:120:PRO:HD3	2:L:132:LEU:HD23	1.82	0.59
1:A:138:LEU:HD12	1:A:182:VAL:HG12	1.85	0.59
2:L:27:SER:O	2:L:30:ARG:HG2	2.03	0.58
2:L:185:TRP:CZ2	2:L:208:PRO:HA	2.39	0.58
2:F:1:GLN:N	2:F:1:GLN:CD	2.57	0.58
1:C:181:VAL:HG21	2:D:135:LEU:CD1	2.34	0.57
2:L:74:ALA:HB2	1:A:132:SER:HA	1.87	0.57
1:A:110:THR:CG2	6:A:468:HOH:O	2.53	0.57
1:A:110:THR:HG23	6:A:468:HOH:O	2.03	0.56
2:L:4:LEU:HB2	2:L:99:GLY:HA2	1.88	0.56
1:C:110:THR:CG2	6:C:440:HOH:O	2.54	0.55
2:B:39:VAL:HG12	2:B:40:PRO:O	2.06	0.55
2:B:4:LEU:HB2	2:B:99:GLY:HA2	1.89	0.55
1:E:6:GLU:HB2	1:E:107:VAL:HG13	1.90	0.54
1:C:20:LEU:HD12	1:C:80:LEU:HD23	1.89	0.54
1:H:178:LEU:C	1:H:178:LEU:HD12	2.28	0.54
1:E:40:PRO:HB2	1:E:43:LYS:HD2	1.89	0.53
1:H:54:GLY:HA3	1:H:56:SER:N	2.15	0.53
1:A:30:ARG:O	1:A:31:ARG:HB2	2.08	0.53
1:H:61:PRO:CD	2:L:95(B):VAL:HG11	2.37	0.53
1:C:110:THR:HG23	6:C:440:HOH:O	2.08	0.53
1:C:116:THR:HG23	1:C:203:SER:HB3	1.91	0.53
1:E:52:TYR:OH	3:E:302:SO4:O2	2.19	0.53
1:A:159:LEU:O	1:A:159:LEU:HD12	2.09	0.52
2:F:1:GLN:CD	2:F:1:GLN:H3	2.08	0.52
1:H:21:THR:HG23	1:H:77:LEU:HD22	1.91	0.52
1:H:53:SER:O	1:H:54:GLY:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLN:HG3	6:A:336:HOH:O	2.10	0.51
2:L:120:PRO:HG3	2:L:130:ALA:HB1	1.94	0.50
1:E:210:ARG:NH1	6:E:494:HOH:O	2.45	0.50
2:F:1:GLN:OE1	2:F:1:GLN:CA	2.58	0.50
1:H:66:ARG:CD	6:D:595:HOH:O	2.49	0.49
1:C:159:LEU:HD21	1:C:182:VAL:HG11	1.95	0.47
2:L:160:GLU:HG3	6:L:590:HOH:O	2.13	0.47
2:B:132:LEU:HD12	2:B:132:LEU:N	2.30	0.46
1:H:12:VAL:CG1	1:H:111:VAL:HG22	2.45	0.46
2:L:194:GLN:HG2	2:L:203:GLU:HB2	1.98	0.46
2:L:188:HIS:NE2	2:D:1:GLN:CG	2.71	0.46
1:C:167:PRO:HG2	2:D:165:SER:OG	2.15	0.46
1:E:105:GLN:CD	1:E:105:GLN:N	2.66	0.45
1:A:159:LEU:O	1:A:159:LEU:HG	2.15	0.45
1:E:29:ILE:O	1:E:52(A):GLY:HA3	2.16	0.45
1:E:105:GLN:H	1:E:105:GLN:NE2	2.13	0.45
1:A:159:LEU:O	1:A:159:LEU:CG	2.65	0.45
1:H:125:ALA:HA	1:H:126:PRO:HD2	1.64	0.44
1:E:3:GLN:O	1:E:25:PRO:HD2	2.17	0.44
1:E:12:VAL:O	1:E:111:VAL:HA	2.18	0.44
1:C:181:VAL:CG2	2:D:135:LEU:CD1	2.96	0.44
2:D:190:SER:HB2	2:D:206:VAL:O	2.17	0.44
1:H:189:LEU:HD23	1:H:189:LEU:HA	1.90	0.43
1:H:105:GLN:HG2	6:H:444:HOH:O	2.17	0.43
2:B:140:TYR:HA	2:B:141:PRO:C	2.38	0.43
1:C:19:SER:OG	1:C:81:LYS:CD	2.65	0.43
1:E:135:THR:HA	1:E:184:VAL:O	2.19	0.43
2:L:160:GLU:HG2	6:L:590:HOH:O	2.13	0.43
1:C:29:ILE:O	1:C:52(A):GLY:HA3	2.19	0.43
1:C:153:SER:CB	1:C:156:SER:O	2.67	0.43
2:D:207:ALA:HA	2:D:208:PRO:HD3	1.91	0.43
2:D:77:GLY:O	2:D:78:LEU:C	2.58	0.42
1:E:11:LEU:HD12	1:E:110:THR:O	2.20	0.42
2:L:40:PRO:HA	2:L:41:GLY:HA2	1.90	0.42
2:B:107:GLY:HA3	2:B:140:TYR:OH	2.20	0.42
2:D:27:SER:HA	2:D:29:GLY:HA3	2.01	0.42
1:H:4:LEU:CD2	1:H:24:VAL:HG22	2.50	0.41
2:L:78:LEU:HD21	2:L:104:LEU:HD21	2.02	0.41
1:A:178:LEU:C	1:A:178:LEU:HD12	2.41	0.41
1:E:159:LEU:HD21	1:E:182:VAL:HG21	2.02	0.41
2:B:66:LYS:HA	2:B:71:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:LEU:HD23	2:B:175:SER:HB3	2.01	0.41
2:D:66:LYS:HA	2:D:71:ALA:HA	2.02	0.41
1:A:169:VAL:O	1:A:176:TYR:HA	2.21	0.41
1:C:153:SER:HB2	1:C:156:SER:O	2.21	0.41
1:H:27:GLY:O	1:H:29:ILE:N	2.54	0.41
2:D:1:GLN:NE2	2:D:1:GLN:HA	2.35	0.41
1:H:61:PRO:HD2	2:L:95(B):VAL:CG1	2.46	0.40
2:B:123:GLU:CD	2:B:123:GLU:N	2.69	0.40
2:L:207:ALA:HA	2:L:208:PRO:HD3	1.93	0.40
2:D:32:TYR:HB3	2:D:50:ASP:HA	2.04	0.40
1:H:12:VAL:HG13	1:H:111:VAL:HG22	2.03	0.40
1:A:72:ASP:OD2	1:A:75:LYS:HG3	2.21	0.40

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	Interatomic distance (Å)	Clash overlap (Å)
6:H:577:HOH:O	6:C:384:HOH:O[1_655]	1.72	0.48
6:H:571:HOH:O	6:F:603:HOH:O[1_564]	2.13	0.07

## 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	211/233 (91%)	204 (97%)	6 (3%)	1 (0%)	29	18
1	C	210/233 (90%)	200 (95%)	8 (4%)	2 (1%)	15	6
1	E	211/233 (91%)	203 (96%)	6 (3%)	2 (1%)	17	7
1	H	211/233 (91%)	205 (97%)	5 (2%)	1 (0%)	29	18
2	B	208/216 (96%)	198 (95%)	10 (5%)	0	100	100
2	D	210/216 (97%)	202 (96%)	7 (3%)	1 (0%)	29	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	210/216 (97%)	202 (96%)	7 (3%)	1 (0%)	29	18
2	L	208/216 (96%)	202 (97%)	6 (3%)	0	100	100
All	All	1679/1796 (94%)	1616 (96%)	55 (3%)	8 (0%)	29	18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	THR
1	H	54	GLY
1	C	113	SER
2	D	60	ASP
2	F	60	ASP
1	E	133	GLU
1	E	135	THR
1	C	114	ALA

### 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	186/201 (92%)	178 (96%)	8 (4%)	29	18
1	C	185/201 (92%)	176 (95%)	9 (5%)	25	14
1	E	186/201 (92%)	183 (98%)	3 (2%)	62	58
1	H	186/201 (92%)	177 (95%)	9 (5%)	25	15
2	B	176/182 (97%)	175 (99%)	1 (1%)	86	86
2	D	178/182 (98%)	177 (99%)	1 (1%)	86	86
2	F	178/182 (98%)	176 (99%)	2 (1%)	73	72
2	L	176/182 (97%)	176 (100%)	0	100	100
All	All	1451/1532 (95%)	1418 (98%)	33 (2%)	50	43

All (33) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	H	21	THR
1	H	28	SER
1	H	50	HIS
1	H	53	SER
1	H	113	SER
1	H	132	SER
1	H	133	GLU
1	H	138	LEU
1	H	161	SER
1	A	7	SER
1	A	14	PRO
1	A	21	THR
1	A	50	HIS
1	A	110	THR
1	A	113	SER
1	A	115	SER
1	A	164	HIS
2	B	30	ARG
1	C	3	GLN
1	C	28	SER
1	C	64	GLU
1	C	71	VAL
1	C	82(C)	VAL
1	C	110	THR
1	C	116	THR
1	C	156	SER
1	C	192	GLN
2	D	60	ASP
1	E	24	VAL
1	E	105	GLN
1	E	210	ARG
2	F	1	GLN
2	F	60	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	$\# Z  > 2$
5	GOL	E	301	-	5,5,5	1.11	1 (20%)	5,5,5	1.21	1 (20%)
3	SO4	E	302	-	4,4,4	0.17	0	6,6,6	0.38	0
3	SO4	H	301	-	4,4,4	0.18	0	6,6,6	0.58	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
5	GOL	E	301	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	301	GOL	O2-C2	-2.18	1.36	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	301	GOL	O2-C2-C1	-2.24	99.28	109.12

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	301	GOL	O1-C1-C2-O2
5	E	301	GOL	O1-C1-C2-C3
5	E	301	GOL	C1-C2-C3-O3
5	E	301	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	302	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

### 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	215/233 (92%)	-0.31	1 (0%) 91 92	11, 21, 35, 41	0
1	C	214/233 (91%)	-0.21	3 (1%) 75 77	13, 24, 39, 46	0
1	E	215/233 (92%)	-0.23	4 (1%) 66 69	11, 24, 38, 49	0
1	H	215/233 (92%)	-0.27	5 (2%) 60 63	12, 21, 38, 47	0
2	B	210/216 (97%)	-0.48	0 100 100	12, 19, 29, 33	0
2	D	212/216 (98%)	-0.41	0 100 100	10, 17, 28, 35	0
2	F	212/216 (98%)	-0.46	0 100 100	10, 16, 26, 32	0
2	L	210/216 (97%)	-0.48	0 100 100	10, 18, 29, 39	0
All	All	1703/1796 (94%)	-0.35	13 (0%) 86 87	10, 20, 35, 49	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	113	SER	3.4
1	C	114	ALA	3.2
1	C	189	LEU	3.1
1	A	126	PRO	2.8
1	E	134	SER	2.7
1	H	132	SER	2.6
1	E	26	GLY	2.5
1	E	190	GLY	2.4
1	C	190	GLY	2.4
1	H	189	LEU	2.3
1	E	114	ALA	2.3
1	H	187	SER	2.2
1	H	188	SER	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 monosaccharides 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
4	CL	L	301	1/1	0.86	0.19	52,52,52,52	0
5	GOL	E	301	6/6	0.90	0.14	18,23,25,26	0
4	CL	B	302	1/1	0.91	0.08	57,57,57,57	0
4	CL	B	301	1/1	0.91	0.13	55,55,55,55	0
4	CL	L	303	1/1	0.92	0.10	54,54,54,54	0
3	SO4	H	301	5/5	0.94	0.13	38,42,44,45	0
4	CL	F	302	1/1	0.94	0.09	49,49,49,49	0
4	CL	L	302	1/1	0.94	0.08	48,48,48,48	0
4	CL	F	301	1/1	0.95	0.18	51,51,51,51	0
4	CL	B	303	1/1	0.96	0.04	47,47,47,47	0
4	CL	D	301	1/1	0.97	0.14	51,51,51,51	0
3	SO4	E	302	5/5	0.98	0.09	38,38,40,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.