



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:35 PM UTC

PDB ID : 7Z2M / pdb_00007z2m
Title : Crystal Structure of the 11.003 Fab in complex with human IL-17A
Authors : Rondeau, J.M.; Lehmann, S.
Deposited on : 2022-02-28
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

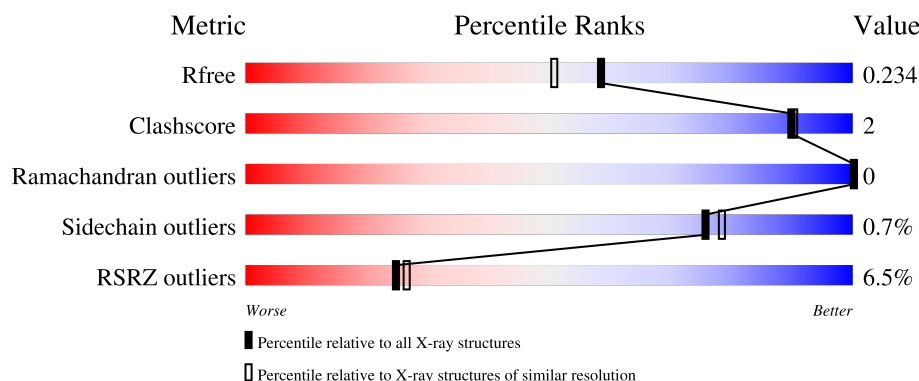
1 Overall quality at a glance

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.



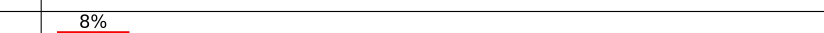
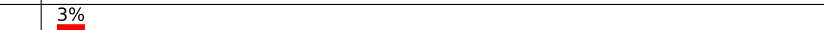
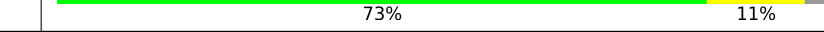
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	214	0% 96% .
1	C	214	6% 91% 8% .
1	E	214	8% 93% 7% .
1	L	214	2% 96% .
2	B	225	4% 95% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	225	
2	F	225	
2	H	225	
3	G	122	
3	I	122	
3	J	122	
3	K	122	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18060 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 11.003 Fab light-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	1	0
			1666	1054	277	331	4			
1	C	213	Total	C	N	O	S	0	2	0
			1678	1062	281	331	4			
1	E	214	Total	C	N	O	S	0	0	0
			1666	1054	277	330	5			
1	L	213	Total	C	N	O	S	0	0	0
			1660	1051	276	329	4			

- Molecule 2 is a protein called 11.003 Fab heavy-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	1	0
			1662	1060	269	325	8			
2	D	220	Total	C	N	O	S	0	2	0
			1674	1066	271	329	8			
2	F	214	Total	C	N	O	S	0	1	0
			1628	1041	263	316	8			
2	H	217	Total	C	N	O	S	0	2	0
			1657	1057	268	323	9			

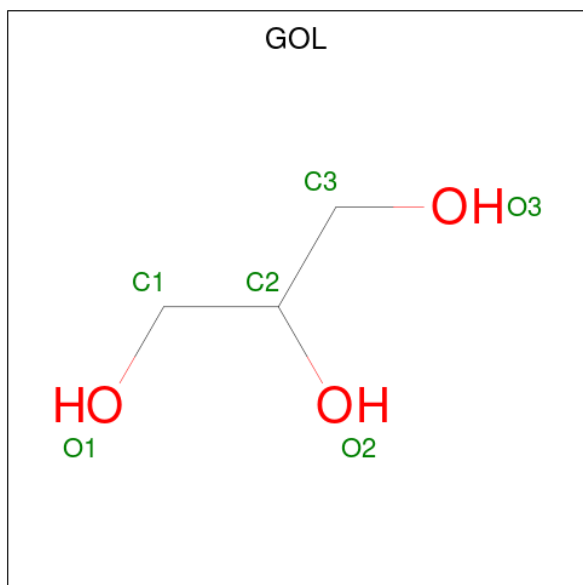
- Molecule 3 is a protein called Interleukin-17A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	103	Total	C	N	O	S	0	0	0
			835	522	156	151	6			
3	I	103	Total	C	N	O	S	0	0	0
			833	516	156	155	6			
3	J	101	Total	C	N	O	S	0	0	0
			819	514	150	149	6			
3	K	94	Total	C	N	O	S	0	0	0
			757	471	138	142	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	106	SER	CYS	engineered mutation	UNP Q16552
I	106	SER	CYS	engineered mutation	UNP Q16552
J	106	SER	CYS	engineered mutation	UNP Q16552
K	106	SER	CYS	engineered mutation	UNP Q16552

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	211	Total O 211 211	0	0
5	B	173	Total O 173 173	0	0
5	C	138	Total O 138 138	0	0
5	D	165	Total O 165 165	0	0

Continued on next page...

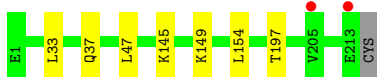
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	92	Total 92	O 92	0	0
5	F	144	Total 144	O 144	0	0
5	G	46	Total 46	O 46	0	0
5	H	180	Total 180	O 180	0	0
5	I	73	Total 73	O 73	0	0
5	J	44	Total 44	O 44	0	0
5	K	53	Total 53	O 53	0	0
5	L	188	Total 188	O 188	0	0

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: 11.003 Fab light-chain



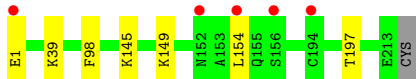
- Molecule 1: 11.003 Fab light-chain



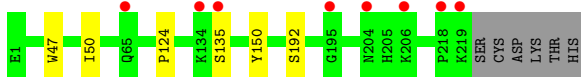
- Molecule 1: 11.003 Fab light-chain



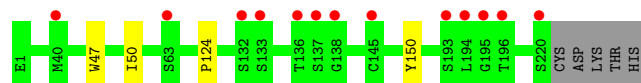
- Molecule 1: 11.003 Fab light-chain



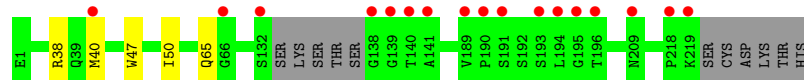
- Molecule 2: 11.003 Fab heavy-chain



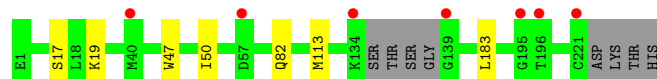
- Molecule 2: 11.003 Fab heavy-chain



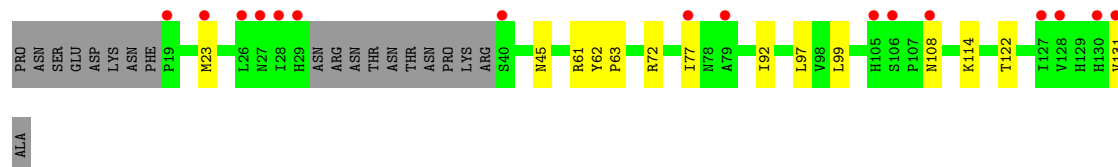
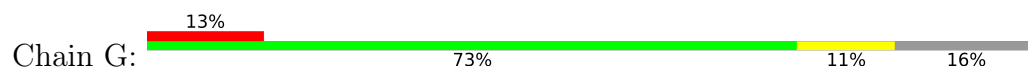
- Molecule 2: 11.003 Fab heavy-chain



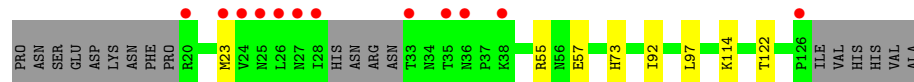
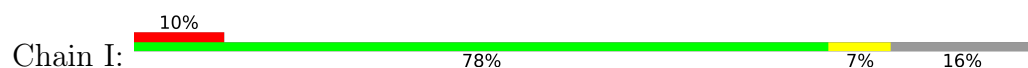
- Molecule 2: 11.003 Fab heavy-chain



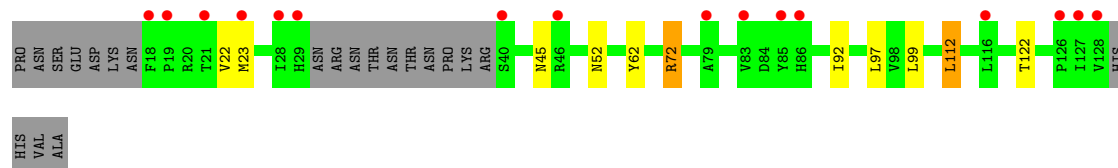
- Molecule 3: Interleukin-17A



- Molecule 3: Interleukin-17A

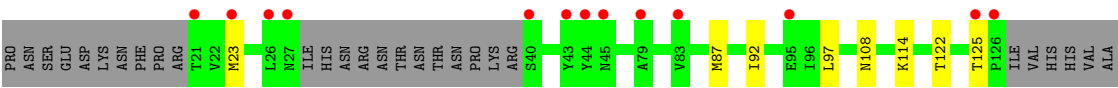


- Molecule 3: Interleukin-17A



- Molecule 3: Interleukin-17A





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.00Å 107.33Å 269.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	134.65 – 1.90 134.65 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (134.65-1.90) 98.0 (134.65-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.90Å)	Xtriage
Refinement program	BUSTER 2.11.7 (20-MAY-2020)	Depositor
R, R_{free}	0.201 , 0.227 0.208 , 0.234	Depositor DCC
R_{free} test set	9498 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18060	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.74	0/1708	0.92	0/2324
1	C	0.69	0/1720	0.94	2/2339 (0.1%)
1	E	0.64	0/1708	0.91	2/2323 (0.1%)
1	L	0.69	0/1702	0.89	1/2315 (0.0%)
2	B	0.72	0/1709	0.88	0/2329
2	D	0.69	0/1721	0.88	0/2345
2	F	0.71	0/1674	0.87	0/2281
2	H	0.68	0/1703	0.88	0/2319
3	G	0.76	1/858 (0.1%)	0.95	0/1170
3	I	0.72	0/853	0.92	0/1162
3	J	0.71	0/841	0.92	0/1147
3	K	0.74	0/776	0.94	0/1058
All	All	0.70	1/16973 (0.0%)	0.90	5/23112 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	77	ILE	CG1-CD1	-5.90	1.28	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	98	PHE	N-CA-C	5.52	119.05	110.17
1	C	32	TYR	N-CA-C	-5.49	101.39	109.62
1	L	98	PHE	N-CA-C	5.47	118.72	109.76
1	C	98	PHE	N-CA-C	5.25	118.63	110.17
1	E	137	ASN	N-CA-C	5.21	117.73	109.24

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	1666	0	1606	3	0
1	C	1678	0	1621	10	0
1	E	1666	0	1606	6	0
1	L	1660	0	1601	4	0
2	B	1662	0	1623	6	0
2	D	1674	0	1632	3	0
2	F	1628	0	1587	5	0
2	H	1657	0	1616	5	0
3	G	835	0	807	8	0
3	I	833	0	808	6	0
3	J	819	0	792	7	0
3	K	757	0	725	7	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	F	6	0	8	0	0
5	A	211	0	0	1	0
5	B	173	0	0	0	0
5	C	138	0	0	0	0
5	D	165	0	0	0	0
5	E	92	0	0	0	0
5	F	144	0	0	0	0
5	G	46	0	0	0	0
5	H	180	0	0	1	0
5	I	73	0	0	0	0
5	J	44	0	0	0	0
5	K	53	0	0	0	0
5	L	188	0	0	2	0
All	All	18060	0	16048	60	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 2.

All (60) 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:D:47[B]:TRP:HE1	2:D:50:ILE:HG23	1.48	0.78
1:C:202:SER:HB3	2:F:65:GLN:HG2	1.68	0.75
3:G:131:VAL:HG21	3:I:73:HIS:CE1	2.22	0.75
2:F:47[A]:TRP:HE1	2:F:50:ILE:HG23	1.51	0.75
2:B:47[B]:TRP:HE1	2:B:50:ILE:HG23	1.52	0.73
2:H:47[B]:TRP:HE1	2:H:50:ILE:HG23	1.54	0.73
1:C:202:SER:CB	2:F:65:GLN:HG2	2.21	0.71
3:K:87:MET:HE1	3:K:125:THR:HG22	1.79	0.65
2:H:113:MET:HE2	5:H:338:HOH:O	2.02	0.58
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.86	0.57
2:H:19:LYS:HG3	2:H:82:GLN:HG2	1.88	0.56
1:C:24:ARG:HG2	1:C:70:ASP:OD1	2.06	0.56
1:L:149:LYS:HG2	1:L:154:LEU:HD23	1.88	0.56
3:G:61:ARG:HD2	3:G:63:PRO:O	2.05	0.55
3:J:23:MET:HE1	3:K:23:MET:HG2	1.88	0.55
1:C:202:SER:HB3	2:F:65:GLN:CG	2.36	0.54
3:I:55:ARG:NH1	3:I:57:GLU:OE2	2.41	0.54
3:K:87:MET:HE1	3:K:125:THR:CG2	2.39	0.53
1:C:105:GLU:HG2	1:C:106:ILE:N	2.22	0.53
3:J:92:ILE:HD11	3:J:122:THR:HB	1.91	0.53
3:G:131:VAL:HG21	3:I:73:HIS:HE1	1.74	0.52
3:I:92:ILE:HD11	3:I:122:THR:HB	1.91	0.52
5:A:396:HOH:O	2:B:135:SER:HB2	2.08	0.52
3:K:92:ILE:HD11	3:K:122:THR:HB	1.93	0.51
3:G:92:ILE:HD11	3:G:122:THR:HB	1.92	0.50
1:E:37:GLN:HB2	1:E:47:LEU:HD11	1.94	0.50
2:B:192:SER:HA	2:H:17:SER:OG	2.12	0.49
3:G:61:ARG:CD	3:G:63:PRO:O	2.60	0.48
3:G:23:MET:SD	3:I:23:MET:HG3	2.53	0.48
2:B:47[B]:TRP:HE1	2:B:50:ILE:CG2	2.25	0.47
1:A:145:LYS:HB3	1:A:197:THR:HB	1.98	0.46
1:E:145:LYS:HB3	1:E:197:THR:HB	1.97	0.46
3:G:62:TYR:HB2	3:G:99:LEU:HB2	1.96	0.46
3:J:92:ILE:HD12	3:K:92:ILE:HD12	1.96	0.46
1:E:11:LEU:HD23	1:E:104:LEU:HD11	1.97	0.46
1:C:145:LYS:HB3	1:C:197:THR:HB	1.98	0.46
1:L:145:LYS:HB3	1:L:197:THR:HB	1.98	0.46
3:J:62:TYR:HB2	3:J:99:LEU:HB2	1.98	0.45
2:D:47[B]:TRP:NE1	2:D:50:ILE:HG23	2.26	0.45
1:E:79:GLU:HG3	1:E:80:PRO:HD2	1.99	0.45
3:K:97:LEU:HD23	3:K:114:LYS:HG2	1.99	0.44
1:L:1:GLU:HG2	5:L:400:HOH:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163[B]:VAL:HG22	1:C:175:LEU:HD12	1.99	0.44
2:H:183:LEU:C	2:H:183:LEU:HD12	2.43	0.44
2:D:124:PRO:HB3	2:D:150:TYR:HB3	2.00	0.43
2:F:38:ARG:CZ	2:F:40:MET:HE3	2.48	0.43
1:A:149:LYS:HD3	1:A:154:LEU:HA	2.01	0.43
1:C:37:GLN:HB2	1:C:47:LEU:HD11	2.02	0.42
1:E:166:GLN:HG3	1:E:173:TYR:CZ	2.54	0.42
3:I:97:LEU:HD23	3:I:114:LYS:HG2	2.01	0.42
3:J:22:VAL:HG12	3:K:108:ASN:HA	2.02	0.42
1:L:39:LYS:NZ	5:L:305:HOH:O	2.50	0.42
2:B:124:PRO:HB3	2:B:150:TYR:HB3	2.01	0.41
3:G:97:LEU:HD23	3:G:114:LYS:HG2	2.02	0.41
1:C:31:SER:O	1:C:50:ASP:HA	2.21	0.41
3:J:97:LEU:HG	3:J:112:LEU:HD21	2.01	0.41
2:B:47[B]:TRP:NE1	2:B:50:ILE:HG23	2.27	0.40
1:C:125:LEU:O	1:C:183:LYS:HD2	2.20	0.40
1:E:105:GLU:HG2	1:E:106:ILE:N	2.37	0.40
3:J:52:ASN:OD1	3:J:72:ARG:HD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
1	C	213/214 (100%)	211 (99%)	2 (1%)	0	100	100
1	E	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
1	L	211/214 (99%)	206 (98%)	5 (2%)	0	100	100
2	B	218/225 (97%)	217 (100%)	1 (0%)	0	100	100
2	D	220/225 (98%)	218 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	211/225 (94%)	209 (99%)	2 (1%)	0	100	100
2	H	215/225 (96%)	214 (100%)	1 (0%)	0	100	100
3	G	99/122 (81%)	98 (99%)	1 (1%)	0	100	100
3	I	99/122 (81%)	98 (99%)	1 (1%)	0	100	100
3	J	97/122 (80%)	97 (100%)	0	0	100	100
3	K	90/122 (74%)	90 (100%)	0	0	100	100
All	All	2097/2244 (93%)	2074 (99%)	23 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	185/185 (100%)	184 (100%)	1 (0%)	81	84
1	C	186/185 (100%)	182 (98%)	4 (2%)	45	42
1	E	185/185 (100%)	183 (99%)	2 (1%)	65	67
1	L	184/185 (100%)	184 (100%)	0	100	100
2	B	187/192 (97%)	187 (100%)	0	100	100
2	D	189/192 (98%)	189 (100%)	0	100	100
2	F	182/192 (95%)	182 (100%)	0	100	100
2	H	187/192 (97%)	187 (100%)	0	100	100
3	G	98/116 (84%)	95 (97%)	3 (3%)	35	29
3	I	98/116 (84%)	98 (100%)	0	100	100
3	J	96/116 (83%)	93 (97%)	3 (3%)	35	29
3	K	89/116 (77%)	89 (100%)	0	100	100
All	All	1866/1972 (95%)	1853 (99%)	13 (1%)	76	78

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	C	22	SER
1	C	50	ASP
1	C	105	GLU
1	C	107	LYS
1	E	70	ASP
1	E	104	LEU
3	G	45	ASN
3	G	72	ARG
3	G	108	ASN
3	J	45	ASN
3	J	72	ARG
3	J	112	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	152	ASN
2	B	65	GLN
2	B	204	ASN
1	C	27	GLN
1	C	38	GLN
1	C	147	GLN
2	D	39	GLN
2	D	204	ASN
1	E	147	GLN
2	F	204	ASN
3	G	45	ASN
3	G	108	ASN
3	G	129	HIS
2	H	204	ASN
3	I	45	ASN
3	J	45	ASN
3	J	108	ASN
3	K	88	ASN
3	K	105	HIS
1	L	27	GLN
1	L	53	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	$\# Z > 2$
4	GOL	B	301	-	5,5,5	0.12	0	5,5,5	0.24	0
4	GOL	C	301	-	5,5,5	0.19	0	5,5,5	0.41	0
4	GOL	F	301	-	5,5,5	0.11	0	5,5,5	0.24	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
4	GOL	B	301	-	-	2/4/4/4	-
4	GOL	C	301	-	-	2/4/4/4	-
4	GOL	F	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	GOL	C1-C2-C3-O3
4	C	301	GOL	O1-C1-C2-C3
4	F	301	GOL	C1-C2-C3-O3
4	F	301	GOL	O1-C1-C2-C3
4	B	301	GOL	O2-C2-C3-O3
4	F	301	GOL	O2-C2-C3-O3
4	C	301	GOL	O1-C1-C2-O2
4	F	301	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th 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 ²)	Q<0.9
1	A	213/214 (99%)	0.30	2 (0%) 81 83	21, 33, 47, 74	1 (0%)
1	C	213/214 (99%)	0.69	13 (6%) 27 29	18, 39, 56, 81	2 (0%)
1	E	214/214 (100%)	0.86	17 (7%) 18 20	30, 49, 64, 85	0
1	L	213/214 (99%)	0.33	5 (2%) 61 65	26, 36, 53, 63	0
2	B	219/225 (97%)	0.38	8 (3%) 45 48	15, 35, 52, 66	1 (0%)
2	D	220/225 (97%)	0.52	13 (5%) 28 30	16, 36, 57, 75	2 (0%)
2	F	214/225 (95%)	0.60	17 (7%) 18 20	16, 41, 67, 76	1 (0%)
2	H	217/225 (96%)	0.33	7 (3%) 50 54	16, 37, 52, 75	2 (0%)
3	G	103/122 (84%)	0.96	16 (15%) 5 5	27, 42, 70, 77	0
3	I	103/122 (84%)	0.74	12 (11%) 9 10	27, 40, 62, 84	0
3	J	101/122 (82%)	1.06	16 (15%) 5 5	29, 47, 73, 93	0
3	K	94/122 (77%)	0.78	13 (13%) 6 6	27, 40, 62, 79	0
All	All	2124/2244 (94%)	0.57	139 (6%) 25 26	15, 39, 61, 93	9 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	28	ILE	6.9
3	J	127	ILE	6.5
3	J	128	VAL	5.6
2	F	138	GLY	5.1
2	F	194	LEU	5.0
3	J	18	PHE	4.9
3	G	130	HIS	4.5
3	G	131	VAL	4.5
3	J	28	ILE	4.2
3	K	126	PRO	4.1
3	G	128	VAL	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	K	79	ALA	4.0
3	J	126	PRO	4.0
3	K	26	LEU	3.8
3	J	19	PRO	3.8
2	D	193[A]	SER	3.7
2	F	140	THR	3.6
3	I	35	THR	3.6
3	G	127	ILE	3.6
1	C	8	PRO	3.6
2	F	139	GLY	3.5
3	G	28	ILE	3.5
2	F	195	GLY	3.5
3	I	33	THR	3.4
1	E	214	CYS	3.3
1	E	11	LEU	3.3
2	F	196	THR	3.3
2	D	63	SER	3.2
3	G	108	ASN	3.2
3	I	26	LEU	3.1
1	E	212	GLY	3.1
2	H	134	LYS	3.1
3	J	40	SER	3.1
3	G	79	ALA	3.1
3	G	27	ASN	3.0
2	D	220	SER	2.9
3	K	43	TYR	2.9
3	G	19	PRO	2.9
2	F	141	ALA	2.9
1	E	10	THR	2.9
1	C	142[A]	ARG	2.9
3	J	29	HIS	2.8
3	I	20	ARG	2.8
2	F	218	PRO	2.8
3	I	27	ASN	2.8
2	F	132	SER	2.7
3	J	79	ALA	2.7
1	C	212	GLY	2.7
1	L	154	LEU	2.7
2	D	132	SER	2.7
1	L	194	CYS	2.6
1	C	163[A]	VAL	2.6
2	D	136	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	15	PRO	2.5
3	I	126	PRO	2.5
1	A	213	GLU	2.5
3	K	27	ASN	2.5
2	F	193	SER	2.5
3	G	105	HIS	2.5
3	I	23	MET	2.5
2	H	221	CYS	2.5
3	I	38	LYS	2.5
2	D	195	GLY	2.5
1	L	1	GLU	2.5
3	J	21	THR	2.5
1	E	56	THR	2.5
3	K	21	THR	2.5
2	B	219	LYS	2.5
2	F	209	ASN	2.4
2	D	133	SER	2.4
1	E	107	LYS	2.4
1	L	152	ASN	2.4
1	C	165	GLU	2.4
2	D	137	SER	2.4
2	D	138	GLY	2.4
1	E	7	SER	2.4
3	J	85	TYR	2.4
3	J	86	HIS	2.4
2	B	195	GLY	2.4
3	K	23	MET	2.4
1	E	78	LEU	2.3
3	K	125	THR	2.3
1	E	40	PRO	2.3
3	G	40	SER	2.3
2	H	196	THR	2.3
2	F	191	SER	2.3
1	C	154	LEU	2.3
1	E	8	PRO	2.3
2	B	135	SER	2.3
3	K	83	VAL	2.3
1	E	80	PRO	2.2
2	H	195	GLY	2.2
3	K	40	SER	2.2
3	G	77	ILE	2.2
3	I	36	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	219	LYS	2.2
3	K	44	TYR	2.2
2	D	40	MET	2.2
3	K	45	ASN	2.2
3	K	95	GLU	2.2
3	G	26	LEU	2.2
1	C	68	GLY	2.2
2	F	66	GLY	2.2
1	E	188	LYS	2.2
2	B	134	LYS	2.2
1	E	163	VAL	2.2
1	C	7	SER	2.2
3	J	46	ARG	2.2
2	F	40	MET	2.1
2	B	65	GLN	2.1
2	D	196	THR	2.1
3	J	116	LEU	2.1
3	G	23	MET	2.1
1	C	184	ALA	2.1
1	C	210	ASN	2.1
1	C	100	GLN	2.1
1	L	156	SER	2.1
2	F	189	VAL	2.1
2	H	139	GLY	2.1
3	J	83	VAL	2.1
2	F	190	PRO	2.1
3	G	106	SER	2.1
2	B	206	LYS	2.1
3	G	29	HIS	2.1
1	A	205	VAL	2.1
1	C	146	VAL	2.1
2	D	145	CYS	2.1
2	H	40	MET	2.0
3	I	25	ASN	2.0
1	E	204	PRO	2.0
1	E	205	VAL	2.0
1	C	181	LEU	2.0
1	E	154	LEU	2.0
2	D	194	LEU	2.0
2	H	57	ASP	2.0
3	J	23	MET	2.0
2	B	204	ASN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	218	PRO	2.0
3	I	24	VAL	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 oligosaccharides 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, 95th 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	GOL	C	301	6/6	0.87	0.15	46,48,49,49	0
4	GOL	F	301	6/6	0.89	0.12	42,45,46,47	0
4	GOL	B	301	6/6	0.93	0.11	41,45,46,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.