Full wwPDB X-ray Structure Validation Report (i)

Jan 9, 2024 – 02:06 AM EST

PDB ID	:	8FHY
Title	:	Crystal structure of the SARS-CoV-2 receptor binding domain in complex with neutralizing antibody WRAIR-5021
Authors	:	Sankhala, R.S.; Jensen, J.L.; Joyce, M.G.
Deposited on	:	2022-12-15
Resolution	:	2.53 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 (i) 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 (i)) were used in the production of this report:

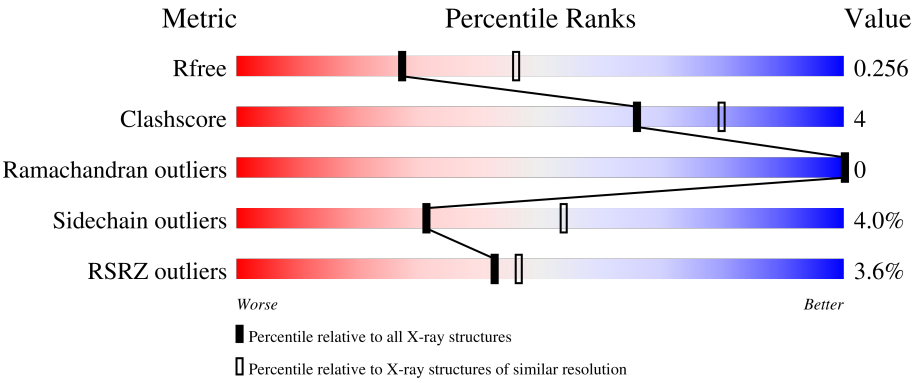
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.53 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 <=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	205	2% 87% 10% ·
1	D	205	87% 8% ·
1	I	205	4% 85% 10% · ·
2	B	214	2% 93% 7%
2	E	214	% 92% 8%

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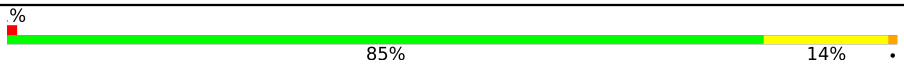
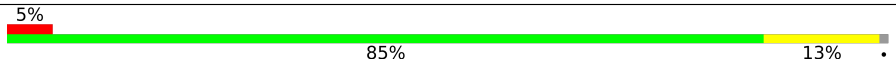
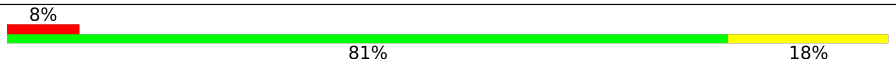
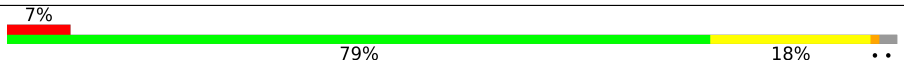
Mol	Chain	Length	Quality of chain
2	L	214	
3	C	220	
3	F	220	
3	H	220	

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	B	301	-	-	-	X
4	GOL	H	301	-	-	-	X
4	GOL	L	301	-	-	-	X
5	NAG	D	606	-	-	-	X
5	NAG	I	603	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 15157 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	196	Total	C	N	O	S	0	0	0
			1546	990	258	290	8			
1	A	199	Total	C	N	O	S	0	0	0
			1569	1004	262	295	8			
1	D	197	Total	C	N	O	S	0	0	0
			1553	994	259	292	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	528	GLY	-	expression tag	UNP P0DTC2
I	529	SER	-	expression tag	UNP P0DTC2
I	530	HIS	-	expression tag	UNP P0DTC2
I	531	HIS	-	expression tag	UNP P0DTC2
I	532	HIS	-	expression tag	UNP P0DTC2
I	533	HIS	-	expression tag	UNP P0DTC2
I	534	HIS	-	expression tag	UNP P0DTC2
I	535	HIS	-	expression tag	UNP P0DTC2
A	528	GLY	-	expression tag	UNP P0DTC2
A	529	SER	-	expression tag	UNP P0DTC2
A	530	HIS	-	expression tag	UNP P0DTC2
A	531	HIS	-	expression tag	UNP P0DTC2
A	532	HIS	-	expression tag	UNP P0DTC2
A	533	HIS	-	expression tag	UNP P0DTC2
A	534	HIS	-	expression tag	UNP P0DTC2
A	535	HIS	-	expression tag	UNP P0DTC2
D	528	GLY	-	expression tag	UNP P0DTC2
D	529	SER	-	expression tag	UNP P0DTC2
D	530	HIS	-	expression tag	UNP P0DTC2
D	531	HIS	-	expression tag	UNP P0DTC2
D	532	HIS	-	expression tag	UNP P0DTC2
D	533	HIS	-	expression tag	UNP P0DTC2
D	534	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	535	HIS	-	expression tag	UNP P0DTC2

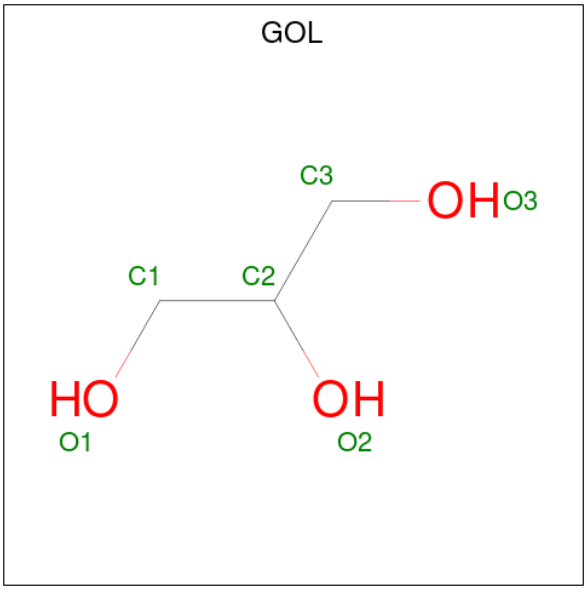
- Molecule 2 is a protein called WRAIR-5021 Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1635	1024	272	334	5			
2	B	214	Total	C	N	O	S	0	0	0
			1641	1027	273	335	6			
2	E	214	Total	C	N	O	S	0	0	0
			1641	1027	273	335	6			

- Molecule 3 is a protein called WRAIR-5021 Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	216	Total	C	N	O	S	0	0	0
			1627	1034	269	320	4			
3	C	217	Total	C	N	O	S	0	0	0
			1634	1038	270	322	4			
3	F	220	Total	C	N	O	S	0	0	0
			1653	1048	273	327	5			

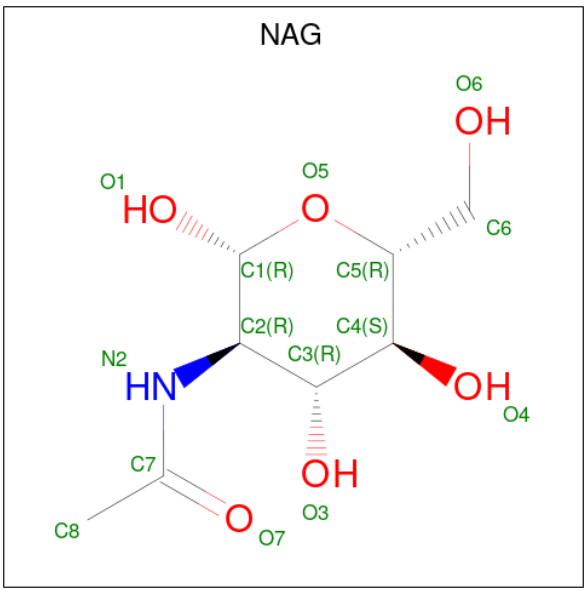
- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

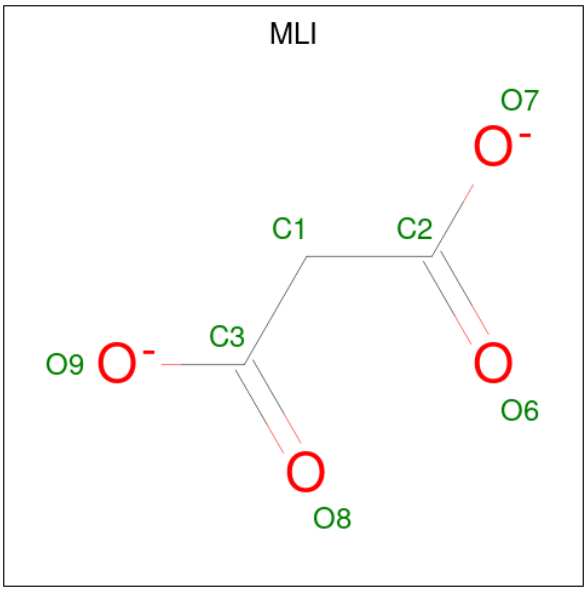
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C O 7 3 4	0	0

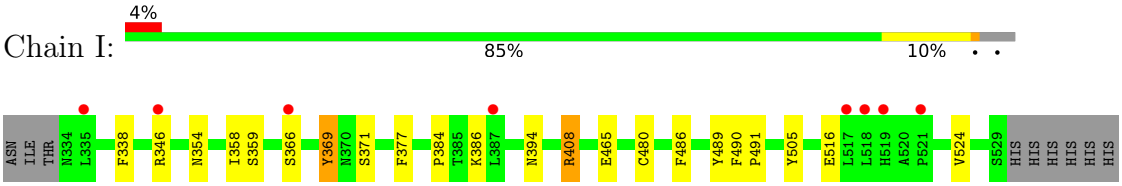
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	48	Total O 48 48	0	0
7	L	44	Total O 44 44	0	0
7	H	42	Total O 42 42	0	0
7	A	57	Total O 57 57	0	0
7	B	78	Total O 78 78	0	0
7	C	47	Total O 47 47	0	0
7	D	50	Total O 50 50	0	0
7	E	69	Total O 69 69	0	0
7	F	48	Total O 48 48	0	0

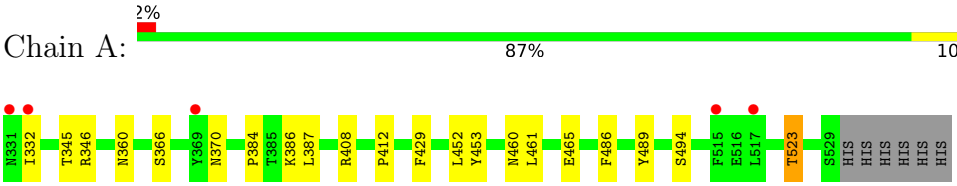
3 Residue-property plots (i)

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.

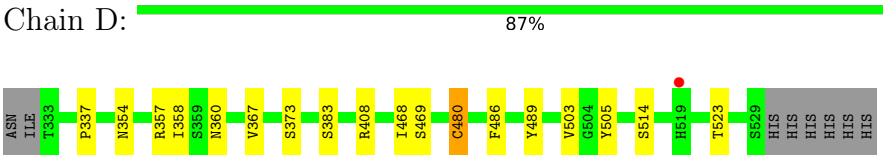
• Molecule 1: Spike protein S1



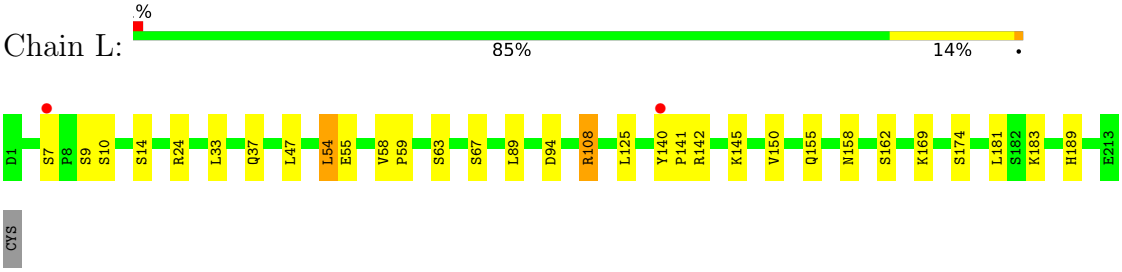
• Molecule 1: Spike protein S1



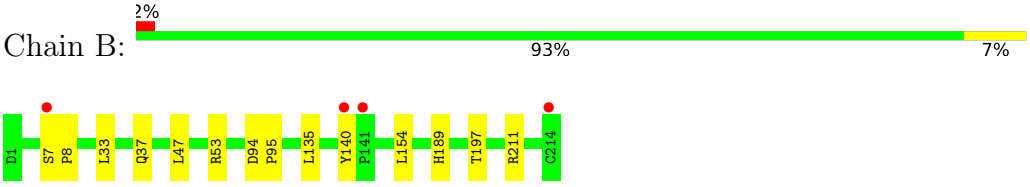
• Molecule 1: Spike protein S1



• Molecule 2: WRAIR-5021 Fab Light chain

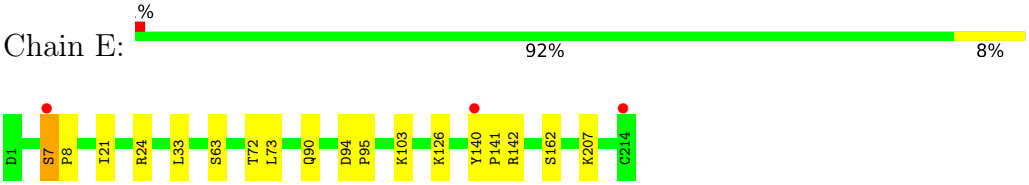


• Molecule 2: WRAIR-5021 Fab Light chain



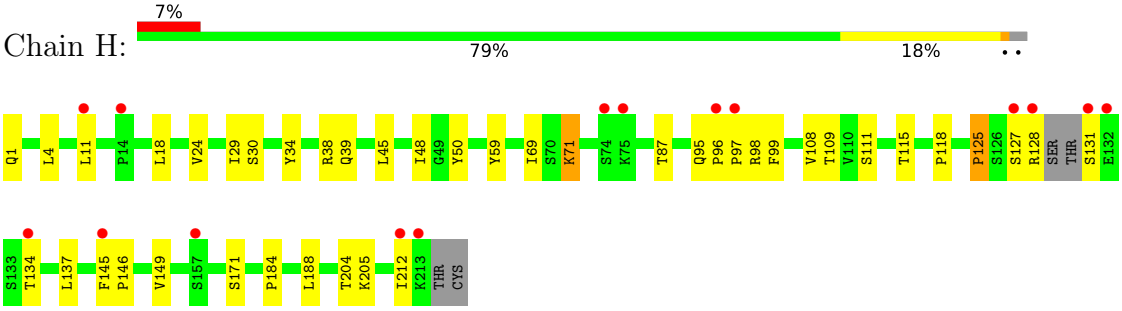
• Molecule 2: WRAIR-5021 Fab Light chain

Chain E:



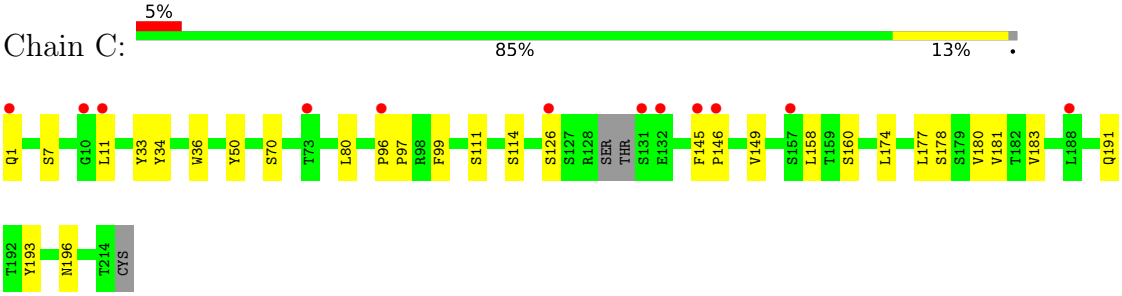
• Molecule 3: WRAIR-5021 Fab Heavy chain

Chain H:



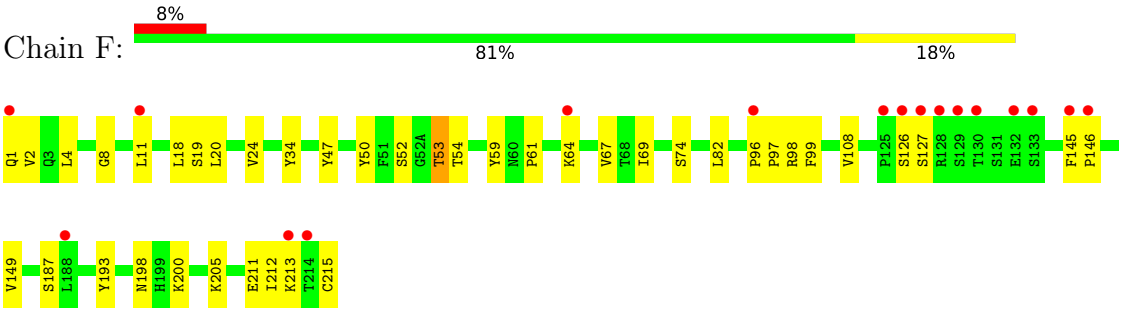
• Molecule 3: WRAIR-5021 Fab Heavy chain

Chain C:



• Molecule 3: WRAIR-5021 Fab Heavy chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	118.92Å 84.13Å 119.86Å 90.00° 113.68° 90.00°	Depositor
Resolution (Å)	99.94 – 2.53 109.77 – 2.53	Depositor EDS
% Data completeness (in resolution range)	97.0 (99.94-2.53) 92.3 (109.77-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.25 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.195 , 0.256 0.200 , 0.256	Depositor DCC
R_{free} test set	1991 reflections (2.82%)	wwPDB-VP
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15157	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MLI, GOL, NAG

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	0.28	0/1613	0.51	0/2196
1	D	0.28	0/1597	0.51	0/2174
1	I	0.28	0/1590	0.51	0/2164
2	B	0.28	0/1677	0.50	0/2277
2	E	0.28	0/1677	0.50	0/2277
2	L	0.27	0/1671	0.49	0/2269
3	C	0.29	0/1676	0.54	0/2290
3	F	0.29	0/1696	0.52	0/2319
3	H	0.28	0/1669	0.53	0/2280
All	All	0.28	0/14866	0.51	0/20246

There are no bond length outliers.

There are no bond angle outliers.

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	1569	0	1484	15	0
1	D	1553	0	1467	8	0
1	I	1546	0	1460	13	0
2	B	1641	0	1588	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1641	0	1588	9	0
2	L	1635	0	1583	14	0
3	C	1634	0	1616	15	0
3	F	1653	0	1634	25	0
3	H	1627	0	1609	24	0
4	A	24	0	32	0	0
4	B	12	0	16	0	0
4	C	6	0	8	0	0
4	D	24	0	32	0	0
4	E	18	0	24	0	0
4	F	12	0	16	1	0
4	H	6	0	8	0	0
4	I	12	0	16	0	0
4	L	12	0	16	1	0
5	A	14	0	13	0	0
5	D	14	0	13	0	0
5	I	14	0	13	0	0
6	D	7	0	2	0	0
7	A	57	0	0	1	0
7	B	78	0	0	0	0
7	C	47	0	0	0	0
7	D	50	0	0	2	0
7	E	69	0	0	0	0
7	F	48	0	0	0	0
7	H	42	0	0	0	0
7	I	48	0	0	0	0
7	L	44	0	0	0	0
All	All	15157	0	14238	116	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 4.

All (116) 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)
3:H:188:LEU:HB3	3:H:212:ILE:HD11	1.57	0.84
2:B:135:LEU:HD22	3:C:180:VAL:HG11	1.69	0.75
1:A:366:SER:HB3	1:A:370:ASN:ND2	2.03	0.73
3:F:53:THR:HG22	3:F:54:THR:HG23	1.75	0.67
3:F:187:SER:HG	3:F:193:TYR:HH	1.45	0.62
3:H:118:PRO:HD2	3:H:204:THR:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:ASN:H	1:D:523:THR:HG22	1.66	0.60
2:L:158:ASN:HB3	1:D:468:ILE:HD11	1.84	0.60
1:A:360:ASN:H	1:A:523:THR:HG23	1.68	0.58
3:H:18:LEU:HD13	3:H:108:VAL:HG11	1.84	0.58
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.84	0.58
1:A:366:SER:HB3	1:A:370:ASN:HD21	1.66	0.58
3:F:145:PHE:HB3	3:F:146:PRO:HD3	1.85	0.58
3:H:96:PRO:HA	3:H:99:PHE:CE1	2.40	0.56
3:F:4:LEU:HD22	3:F:24:VAL:HG22	1.88	0.56
1:A:345:THR:HG22	1:A:346:ARG:HG2	1.87	0.55
3:F:96:PRO:HA	3:F:99:PHE:CE1	2.41	0.55
1:A:332:ILE:HG22	1:A:332:ILE:O	2.06	0.55
3:H:125:PRO:HG3	3:H:137:LEU:HB3	1.89	0.54
1:D:486:PHE:CE2	2:E:94:ASP:HA	2.41	0.54
1:I:338:PHE:HE2	1:I:358:ILE:HD13	1.73	0.54
3:C:34:TYR:HB2	3:C:96:PRO:HD2	1.89	0.54
3:F:59:TYR:HB2	3:F:64:LYS:HG3	1.90	0.52
1:I:486:PHE:CE2	2:L:94:ASP:HA	2.44	0.52
1:A:412:PRO:HG3	1:A:429:PHE:HB3	1.91	0.52
1:A:486:PHE:CE2	2:B:94:ASP:HA	2.44	0.52
3:C:11:LEU:C	3:C:11:LEU:HD23	2.31	0.51
3:H:11:LEU:HD12	3:H:145:PHE:CE2	2.45	0.51
3:H:29:ILE:HG21	3:H:71:LYS:HD3	1.92	0.51
1:D:408:ARG:HH11	1:D:408:ARG:HG3	1.75	0.51
2:E:103:LYS:NZ	2:E:142:ARG:HD2	2.26	0.50
3:F:59:TYR:HE1	3:F:69:ILE:HG13	1.76	0.50
3:F:8:GLY:HA3	3:F:20:LEU:HD23	1.93	0.50
3:F:61:PRO:HA	3:F:64:LYS:HB2	1.93	0.50
1:D:505:TYR:CG	3:F:1:GLN:HG2	2.46	0.49
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.95	0.49
1:A:386:LYS:HG2	1:A:386:LYS:O	2.12	0.49
3:F:198:ASN:OD1	3:F:205:LYS:HG3	2.13	0.49
3:C:145:PHE:HB2	3:C:174:LEU:HD23	1.95	0.48
3:F:34:TYR:HB2	3:F:96:PRO:HD2	1.96	0.48
1:I:338:PHE:CE2	1:I:358:ILE:HD13	2.49	0.48
3:C:96:PRO:HA	3:C:99:PHE:CE2	2.49	0.48
2:L:55:GLU:OE2	3:H:98:ARG:NH2	2.46	0.48
1:A:452:LEU:HD23	1:A:494:SER:HB3	1.95	0.48
2:L:54:LEU:HD21	2:L:58:VAL:O	2.14	0.48
3:F:126:SER:O	3:F:127:SER:HB3	2.14	0.48
1:I:489:TYR:CZ	3:H:97:PRO:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:38:ARG:HB3	3:H:48:ILE:HD11	1.96	0.47
3:F:211:GLU:HG3	3:F:213:LYS:HE2	1.95	0.47
1:D:337:PRO:HD2	1:D:358:ILE:HD12	1.97	0.47
3:F:212:ILE:N	3:F:212:ILE:HD13	2.30	0.47
1:I:366:SER:HA	1:I:369:TYR:CE1	2.50	0.46
1:I:369:TYR:CE2	1:I:384:PRO:HB3	2.50	0.46
3:C:149:VAL:HG11	3:C:177:LEU:CD2	2.45	0.46
2:B:7:SER:OG	2:B:8:PRO:HD3	2.15	0.46
3:C:36:TRP:CE2	3:C:80:LEU:HB2	2.51	0.46
1:A:408:ARG:NH1	7:A:704:HOH:O	2.48	0.46
1:A:460:ASN:OD1	2:B:53:ARG:NH2	2.45	0.45
1:I:465:GLU:HA	2:B:154:LEU:HB2	1.98	0.45
3:H:29:ILE:CG2	3:H:71:LYS:HD3	2.45	0.45
1:D:480:CYS:HA	7:D:707:HOH:O	2.15	0.45
2:L:140:TYR:HB3	2:L:141:PRO:HD3	1.99	0.45
3:H:4:LEU:HD22	3:H:24:VAL:HG22	1.99	0.45
3:H:134:THR:HG22	3:H:184:PRO:HA	2.00	0.44
2:L:7:SER:HB2	2:L:24:ARG:HH12	1.80	0.44
1:A:461:LEU:HD22	1:A:465:GLU:HG2	1.98	0.44
3:F:211:GLU:HB2	3:F:213:LYS:HE2	2.00	0.44
3:C:191:GLN:HG2	3:C:193:TYR:CZ	2.53	0.44
2:L:189:HIS:HE1	7:D:716:HOH:O	2.00	0.44
1:D:489:TYR:CZ	3:F:97:PRO:HD3	2.54	0.43
2:E:21:ILE:HD11	2:E:73:LEU:HD23	1.99	0.43
2:L:125:LEU:O	2:L:183:LYS:HE3	2.19	0.43
3:H:145:PHE:HB3	3:H:146:PRO:HD3	2.01	0.43
3:C:145:PHE:HB3	3:C:146:PRO:HD3	2.00	0.43
3:C:158:LEU:HD21	3:C:181:VAL:HG21	2.01	0.43
1:I:408:ARG:HG2	1:I:408:ARG:HH11	1.84	0.43
2:B:189:HIS:O	2:B:211:ARG:NH1	2.40	0.43
1:I:505:TYR:HB2	3:H:1:GLN:HG2	1.99	0.42
2:L:108:ARG:HD3	2:L:140:TYR:HB2	2.01	0.42
3:H:39:GLN:HB2	3:H:45:LEU:HD23	2.01	0.42
3:C:177:LEU:HD12	3:C:178:SER:N	2.35	0.42
3:H:96:PRO:O	3:H:99:PHE:CE2	2.72	0.42
2:E:140:TYR:HB3	2:E:141:PRO:HD3	2.01	0.42
3:F:149:VAL:O	3:F:149:VAL:HG13	2.19	0.42
2:L:33:LEU:HD22	2:L:89:LEU:O	2.18	0.42
2:L:59:PRO:HD2	4:L:301:GOL:O1	2.20	0.42
3:H:34:TYR:HB2	3:H:96:PRO:HD2	2.02	0.42
3:F:2:VAL:HG12	4:F:302:GOL:H11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:59:TYR:CE1	3:F:69:ILE:HG13	2.54	0.42
3:H:96:PRO:N	3:H:97:PRO:HD2	2.35	0.42
3:C:183:VAL:HG11	3:C:193:TYR:CE1	2.55	0.42
3:H:59:TYR:CE1	3:H:69:ILE:HD12	2.55	0.42
3:H:127:SER:HG	3:H:131:SER:N	2.17	0.42
2:E:7:SER:HB2	2:E:24:ARG:HH12	1.84	0.42
3:F:50:TYR:CD2	3:F:96:PRO:HG2	2.55	0.41
2:E:207:LYS:HA	2:E:207:LYS:HD3	1.95	0.41
1:A:384:PRO:HA	1:A:387:LEU:HD12	2.02	0.41
3:C:50:TYR:CD2	3:C:96:PRO:HG3	2.56	0.41
3:F:18:LEU:HD13	3:F:108:VAL:HG11	2.01	0.41
2:E:126:LYS:HE2	2:E:126:LYS:HB3	1.82	0.41
1:I:359:SER:HA	1:I:524:VAL:HG22	2.02	0.41
1:I:386:LYS:HD3	1:I:386:LYS:HA	1.91	0.41
2:L:150:VAL:CG2	2:L:155:GLN:HG3	2.50	0.41
1:A:489:TYR:CZ	3:C:97:PRO:HD3	2.56	0.41
2:B:94:ASP:HB3	2:B:95:PRO:HD3	2.01	0.41
3:F:11:LEU:HB2	3:F:145:PHE:HE2	1.85	0.41
3:H:115:THR:HG23	3:H:146:PRO:HG2	2.03	0.41
3:F:67:VAL:HG22	3:F:82:LEU:HD13	2.03	0.41
3:H:50:TYR:CD2	3:H:96:PRO:HG2	2.56	0.40
2:E:7:SER:HB3	2:E:8:PRO:HD3	2.02	0.40
3:H:87:THR:HG23	3:H:109:THR:HA	2.03	0.40
1:A:453:TYR:OH	3:C:33:TYR:OH	2.38	0.40
1:I:490:PHE:CD1	1:I:491:PRO:HD2	2.57	0.40
3:F:34:TYR:CE2	3:F:52:SER:HB2	2.56	0.40
1:I:486:PHE:CZ	2:L:94:ASP:HA	2.56	0.40
2:E:94:ASP:HB3	2:E:95:PRO:HD3	2.03	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	197/205 (96%)	191 (97%)	6 (3%)	0	100	100
1	D	195/205 (95%)	187 (96%)	8 (4%)	0	100	100
1	I	194/205 (95%)	188 (97%)	6 (3%)	0	100	100
2	B	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
2	E	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
2	L	211/214 (99%)	201 (95%)	10 (5%)	0	100	100
3	C	213/220 (97%)	205 (96%)	8 (4%)	0	100	100
3	F	218/220 (99%)	208 (95%)	10 (5%)	0	100	100
3	H	212/220 (96%)	204 (96%)	8 (4%)	0	100	100
All	All	1864/1917 (97%)	1792 (96%)	72 (4%)	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	171/177 (97%)	170 (99%)	1 (1%)	86	94
1	D	169/177 (96%)	160 (95%)	9 (5%)	22	40
1	I	168/177 (95%)	159 (95%)	9 (5%)	22	40
2	B	189/189 (100%)	186 (98%)	3 (2%)	62	82
2	E	189/189 (100%)	183 (97%)	6 (3%)	39	63
2	L	188/189 (100%)	175 (93%)	13 (7%)	15	28
3	C	189/192 (98%)	181 (96%)	8 (4%)	30	51
3	F	192/192 (100%)	185 (96%)	7 (4%)	35	59
3	H	188/192 (98%)	179 (95%)	9 (5%)	25	45
All	All	1643/1674 (98%)	1578 (96%)	65 (4%)	31	54

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	346	ARG
1	I	354	ASN
1	I	369	TYR
1	I	371	SER
1	I	377	PHE
1	I	394	ASN
1	I	408	ARG
1	I	480	CYS
1	I	516	GLU
2	L	9	SER
2	L	10	SER
2	L	14	SER
2	L	54	LEU
2	L	63	SER
2	L	67	SER
2	L	108	ARG
2	L	142	ARG
2	L	145	LYS
2	L	162	SER
2	L	169	LYS
2	L	174	SER
2	L	181	LEU
3	H	30	SER
3	H	71	LYS
3	H	95	GLN
3	H	111	SER
3	H	125	PRO
3	H	128	ARG
3	H	149	VAL
3	H	171	SER
3	H	205	LYS
1	A	523	THR
2	B	33	LEU
2	B	140	TYR
2	B	197	THR
3	C	1	GLN
3	C	7	SER
3	C	70	SER
3	C	111	SER
3	C	114	SER
3	C	126	SER
3	C	160	SER
3	C	196	ASN

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Mol	Chain	Res	Type
1	D	354	ASN
1	D	357	ARG
1	D	367	VAL
1	D	373	SER
1	D	383	SER
1	D	469	SER
1	D	480	CYS
1	D	503	VAL
1	D	514	SER
2	E	7	SER
2	E	33	LEU
2	E	63	SER
2	E	72	THR
2	E	90	GLN
2	E	162	SER
3	F	19	SER
3	F	47	TYR
3	F	53	THR
3	F	74	SER
3	F	98	ARG
3	F	200	LYS
3	F	215	CYS

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

25 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	I	601	-	5,5,5	0.90	0	5,5,5	1.01	0
5	NAG	A	605	1	14,14,15	0.26	0	17,19,21	0.40	0
4	GOL	B	301	-	5,5,5	0.09	0	5,5,5	0.23	0
4	GOL	D	601	-	5,5,5	0.93	0	5,5,5	0.84	0
4	GOL	C	301	-	5,5,5	0.93	0	5,5,5	0.99	0
5	NAG	D	606	1	14,14,15	0.30	0	17,19,21	0.51	0
4	GOL	E	303	-	5,5,5	0.91	0	5,5,5	0.93	0
4	GOL	D	605	-	5,5,5	0.88	0	5,5,5	1.00	0
4	GOL	H	301	-	5,5,5	0.09	0	5,5,5	0.31	0
4	GOL	D	603	-	5,5,5	0.84	0	5,5,5	0.95	0
4	GOL	E	302	-	5,5,5	0.95	0	5,5,5	0.90	0
4	GOL	F	301	-	5,5,5	0.95	0	5,5,5	1.01	0
4	GOL	L	302	-	5,5,5	0.92	0	5,5,5	0.92	0
4	GOL	A	604	-	5,5,5	0.90	0	5,5,5	1.00	0
6	MLI	D	602	-	6,6,6	1.30	0	7,7,7	0.97	0
4	GOL	B	302	-	5,5,5	0.93	0	5,5,5	0.95	0
4	GOL	A	601	-	5,5,5	0.91	0	5,5,5	0.97	0
4	GOL	E	301	-	5,5,5	0.85	0	5,5,5	0.98	0
4	GOL	F	302	-	5,5,5	0.93	0	5,5,5	1.00	0
4	GOL	I	602	-	5,5,5	0.91	0	5,5,5	0.95	0
4	GOL	A	603	-	5,5,5	0.96	0	5,5,5	0.91	0
4	GOL	D	604	-	5,5,5	1.02	0	5,5,5	0.94	0
4	GOL	L	301	-	5,5,5	0.07	0	5,5,5	0.25	0
5	NAG	I	603	1	14,14,15	0.18	0	17,19,21	0.45	0
4	GOL	A	602	-	5,5,5	0.92	0	5,5,5	0.98	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	I	601	-	-	0/4/4/4	-
5	NAG	A	605	1	-	2/6/23/26	0/1/1/1
4	GOL	B	301	-	-	2/4/4/4	-
4	GOL	D	601	-	-	0/4/4/4	-
4	GOL	C	301	-	-	2/4/4/4	-
5	NAG	D	606	1	-	0/6/23/26	0/1/1/1
4	GOL	E	303	-	-	0/4/4/4	-
4	GOL	D	605	-	-	2/4/4/4	-
4	GOL	H	301	-	-	4/4/4/4	-
4	GOL	D	603	-	-	0/4/4/4	-
4	GOL	E	302	-	-	2/4/4/4	-
4	GOL	F	301	-	-	1/4/4/4	-
4	GOL	L	302	-	-	4/4/4/4	-
4	GOL	A	604	-	-	2/4/4/4	-
6	MLI	D	602	-	-	4/4/4/4	-
4	GOL	B	302	-	-	0/4/4/4	-
4	GOL	A	601	-	-	0/4/4/4	-
4	GOL	E	301	-	-	1/4/4/4	-
4	GOL	F	302	-	-	2/4/4/4	-
4	GOL	I	602	-	-	2/4/4/4	-
4	GOL	A	603	-	-	4/4/4/4	-
4	GOL	D	604	-	-	0/4/4/4	-
4	GOL	L	301	-	-	2/4/4/4	-
5	NAG	I	603	1	-	2/6/23/26	0/1/1/1
4	GOL	A	602	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	602	GOL	C1-C2-C3-O3
4	L	301	GOL	C1-C2-C3-O3
4	H	301	GOL	O1-C1-C2-C3
4	H	301	GOL	C1-C2-C3-O3
4	A	603	GOL	O1-C1-C2-C3
4	A	603	GOL	C1-C2-C3-O3
4	B	301	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	301	GOL	O1-C1-C2-C3
4	E	302	GOL	O1-C1-C2-C3
4	L	301	GOL	O2-C2-C3-O3
4	C	301	GOL	O1-C1-C2-O2
5	I	603	NAG	C4-C5-C6-O6
4	L	302	GOL	C1-C2-C3-O3
4	A	604	GOL	O1-C1-C2-C3
4	C	301	GOL	O1-C1-C2-C3
4	D	605	GOL	O1-C1-C2-C3
5	I	603	NAG	O5-C5-C6-O6
4	I	602	GOL	O2-C2-C3-O3
4	H	301	GOL	O2-C2-C3-O3
4	A	603	GOL	O2-C2-C3-O3
5	A	605	NAG	C4-C5-C6-O6
4	L	302	GOL	O2-C2-C3-O3
4	A	603	GOL	O1-C1-C2-O2
6	D	602	MLI	C2-C1-C3-O8
4	F	302	GOL	O2-C2-C3-O3
5	A	605	NAG	O5-C5-C6-O6
4	H	301	GOL	O1-C1-C2-O2
6	D	602	MLI	C2-C1-C3-O9
4	L	302	GOL	O1-C1-C2-C3
4	D	605	GOL	O1-C1-C2-O2
4	E	302	GOL	O1-C1-C2-O2
6	D	602	MLI	C3-C1-C2-O6
4	E	301	GOL	C1-C2-C3-O3
6	D	602	MLI	C3-C1-C2-O7
4	L	302	GOL	O1-C1-C2-O2
4	A	604	GOL	O1-C1-C2-O2
4	F	301	GOL	O1-C1-C2-C3
4	F	302	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	302	GOL	1	0
4	L	301	GOL	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^{th} 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	199/205 (97%)	0.15	5 (2%)	57	61	33, 49, 77, 114	0
1	D	197/205 (96%)	0.11	1 (0%)	91	92	39, 55, 82, 124	0
1	I	196/205 (95%)	0.18	8 (4%)	37	41	39, 53, 88, 124	0
2	B	214/214 (100%)	0.00	4 (1%)	66	70	36, 47, 67, 105	0
2	E	214/214 (100%)	0.11	3 (1%)	75	78	37, 46, 64, 115	0
2	L	213/214 (99%)	0.11	2 (0%)	84	86	38, 57, 77, 109	0
3	C	217/220 (98%)	0.22	12 (5%)	25	27	38, 50, 84, 134	0
3	F	220/220 (100%)	0.35	17 (7%)	13	14	38, 51, 96, 172	0
3	H	216/220 (98%)	0.29	15 (6%)	16	17	38, 53, 86, 149	0
All	All	1886/1917 (98%)	0.17	67 (3%)	42	46	33, 51, 81, 172	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	129	SER	8.4
3	H	131	SER	7.8
3	F	128	ARG	7.4
3	C	145	PHE	6.7
2	E	214	CYS	6.5
1	A	332	ILE	6.4
3	H	145	PHE	6.2
2	B	140	TYR	5.7
3	F	130	THR	5.5
3	H	132	GLU	5.1
2	L	140	TYR	4.9
2	E	7	SER	4.5
3	F	145	PHE	4.2
2	B	214	CYS	4.1
3	H	128	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
3	F	214	THR	4.1
3	H	74	SER	3.9
2	L	7	SER	3.8
3	H	127	SER	3.8
3	C	11	LEU	3.6
1	I	518	LEU	3.5
2	E	140	TYR	3.3
3	C	96	PRO	3.2
3	F	126	SER	3.0
3	C	10	GLY	3.0
3	F	213	LYS	2.9
3	F	188	LEU	2.8
3	C	1	GLN	2.7
3	F	96	PRO	2.7
2	B	7	SER	2.7
1	I	521	PRO	2.7
3	F	1	GLN	2.7
1	I	335	LEU	2.7
3	C	126	SER	2.7
3	F	132	GLU	2.6
3	H	75	LYS	2.6
3	F	127	SER	2.5
1	I	519	HIS	2.5
3	C	73	THR	2.5
3	F	11	LEU	2.4
3	C	188	LEU	2.4
3	H	212	ILE	2.4
1	I	346	ARG	2.4
1	A	515	PHE	2.4
3	C	131	SER	2.3
3	C	157	SER	2.3
2	B	141	PRO	2.3
1	I	517	LEU	2.2
3	H	157	SER	2.2
3	H	96	PRO	2.2
3	F	125	PRO	2.1
3	F	146	PRO	2.1
3	H	14	PRO	2.1
1	I	387	LEU	2.1
1	A	517	LEU	2.1
3	H	213	LYS	2.1
3	C	146	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	519	HIS	2.1
3	F	133	SER	2.1
3	H	97	PRO	2.0
1	I	366	SER	2.0
1	A	331	ASN	2.0
3	C	132	GLU	2.0
3	H	134	THR	2.0
3	F	64	LYS	2.0
3	H	11	LEU	2.0
1	A	369	TYR	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^{th} 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(Å^2)	Q<0.9
4	GOL	B	301	6/6	0.57	0.54	66,69,72,82	0
5	NAG	I	603	14/15	0.60	0.43	106,118,129,131	0
5	NAG	D	606	14/15	0.61	0.48	68,97,109,113	0
4	GOL	H	301	6/6	0.68	0.65	70,73,77,79	0
4	GOL	E	303	6/6	0.74	0.38	77,90,92,95	0
6	MLI	D	602	7/7	0.74	0.32	48,56,60,70	0
4	GOL	A	604	6/6	0.76	0.20	75,88,93,96	0
4	GOL	L	301	6/6	0.76	0.41	58,65,70,73	0
4	GOL	I	602	6/6	0.80	0.26	55,75,78,80	0
4	GOL	F	302	6/6	0.81	0.20	56,61,66,71	0
4	GOL	L	302	6/6	0.81	0.25	53,59,61,66	0
4	GOL	C	301	6/6	0.82	0.20	58,69,74,76	0
5	NAG	A	605	14/15	0.83	0.38	74,104,116,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	E	301	6/6	0.83	0.27	56,61,66,72	0
4	GOL	D	604	6/6	0.83	0.28	66,75,78,80	0
4	GOL	D	601	6/6	0.85	0.22	61,64,71,80	0
4	GOL	F	301	6/6	0.86	0.22	42,49,51,52	0
4	GOL	D	603	6/6	0.86	0.26	55,61,68,72	0
4	GOL	A	603	6/6	0.86	0.39	61,66,70,71	0
4	GOL	A	601	6/6	0.87	0.18	59,64,69,76	0
4	GOL	B	302	6/6	0.87	0.22	36,54,55,63	0
4	GOL	A	602	6/6	0.89	0.26	61,64,66,68	0
4	GOL	D	605	6/6	0.89	0.19	74,78,82,84	0
4	GOL	E	302	6/6	0.90	0.34	50,56,62,69	0
4	GOL	I	601	6/6	0.90	0.38	70,72,79,87	0

6.5 Other polymers (i)

There are no such residues in this entry.