



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:47 AM UTC

PDB ID : 5NYX / pdb_00005nyx
Title : human Fab fragment 5H2 against NHBA from Neisseria meningitidis
Authors : Malito, E.; Maritan, M.
Deposited on : 2017-05-12
Resolution : 1.88 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

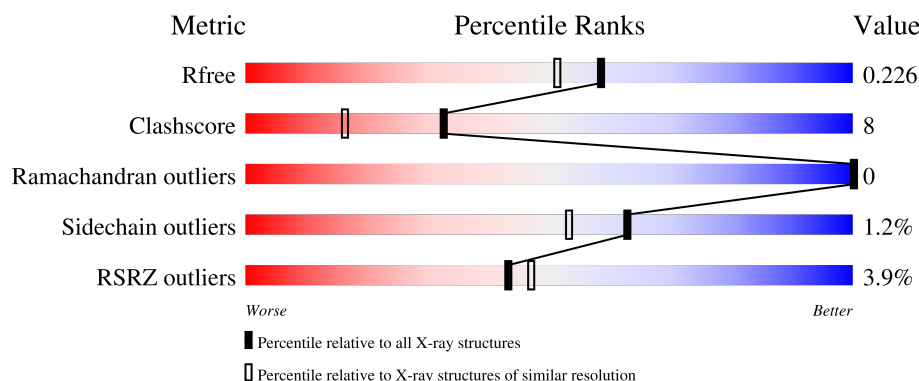
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	H	265	4% 71% 13% 15%
1	M	265	4% 69% 14% 16%
1	O	265	3% 74% 10% 15%
2	L	213	2% 83% 16%
2	N	213	5% 83% 15%

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Mol	Chain	Length	Quality of chain
2	P	213	3% 77% 16% • 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10709 atoms, of which 96 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 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	224	Total	C	N	O	S	0	2	0
			1675	1055	278	335	7			
1	M	223	Total	C	N	O	S	0	6	0
			1687	1062	280	338	7			
1	O	224	Total	C	N	O	S	0	2	0
			1675	1055	278	336	6			

- Molecule 2 is a protein called LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	2	0
			1618	1006	274	331	7			
2	N	210	Total	C	N	O	S	0	1	0
			1608	1001	272	329	6			
2	P	199	Total	C	N	O	S	0	2	0
			1542	959	262	314	7			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	H	O	0	0
			14	3	8	3		
3	L	1	Total	C	H	O	0	0
			14	3	8	3		
3	L	1	Total	C	H	O	0	0
			14	3	8	3		
3	M	1	Total	C	H	O	0	0
			14	3	8	3		
3	M	1	Total	C	H	O	0	0
			14	3	8	3		
3	M	1	Total	C	H	O	0	0
			14	3	8	3		
3	N	1	Total	C	H	O	0	0
			14	3	8	3		
3	N	1	Total	C	H	O	0	0
			14	3	8	3		
3	O	1	Total	C	H	O	0	0
			14	3	8	3		
3	P	1	Total	C	H	O	0	0
			14	3	8	3		
3	P	1	Total	C	H	O	0	0
			14	3	8	3		
3	P	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

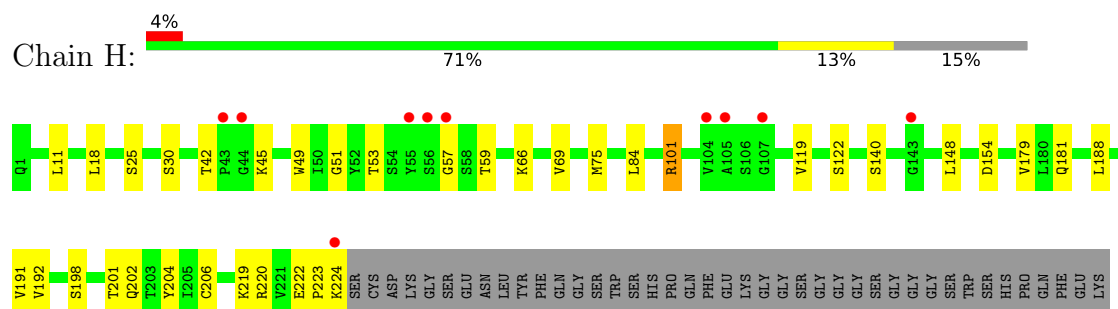
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	136	Total	O	0	0
			136	136		
5	L	123	Total	O	0	0
			123	123		
5	M	106	Total	O	0	0
			106	106		
5	N	108	Total	O	0	0
			108	108		
5	O	138	Total	O	0	0
			138	138		
5	P	115	Total	O	0	0
			115	115		

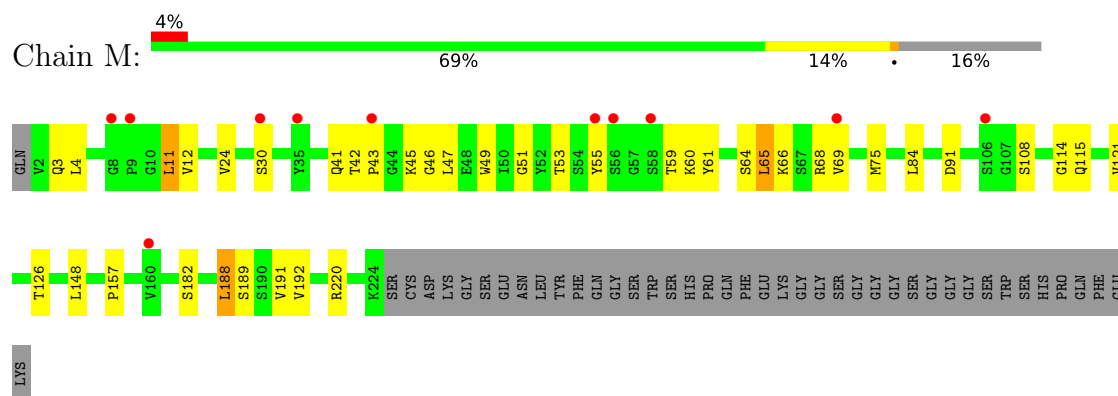
3 Residue-property plots [i](#)

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.

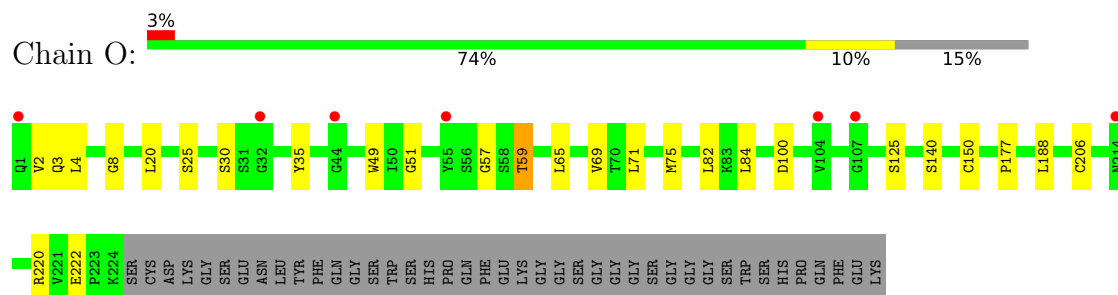
• Molecule 1: HEAVY CHAIN



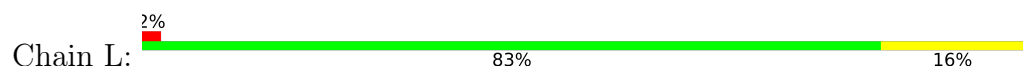
• Molecule 1: HEAVY CHAIN

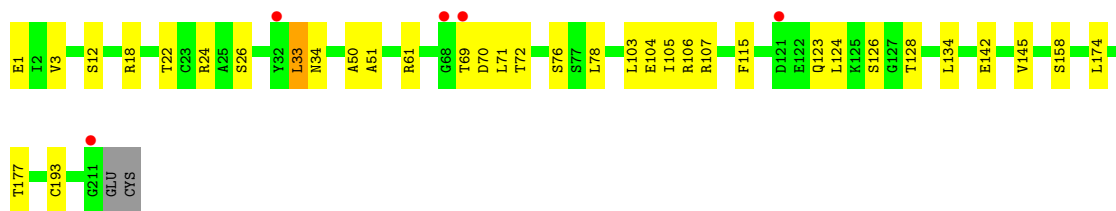


• Molecule 1: HEAVY CHAIN

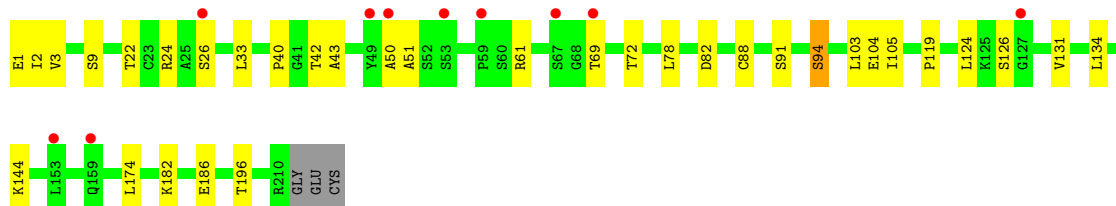
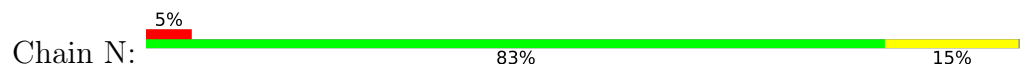


• Molecule 2: LIGHT CHAIN

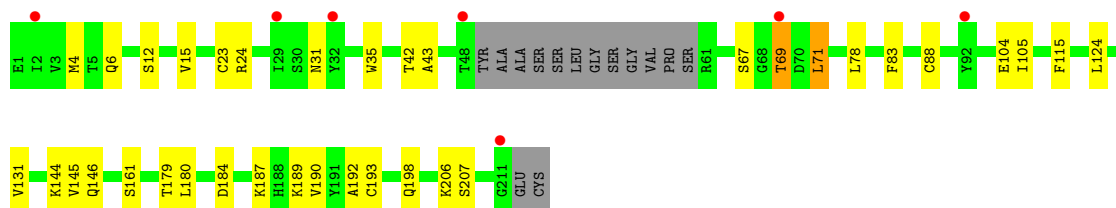
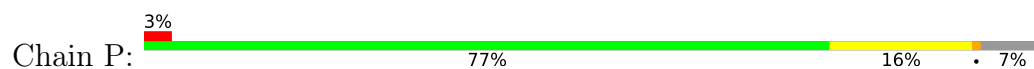




● Molecule 2: LIGHT CHAIN



● Molecule 2: LIGHT CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.03Å 105.75Å 86.26Å 90.00° 112.00° 90.00°	Depositor
Resolution (Å)	47.02 – 1.88 47.02 – 1.88	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.02-1.88) 98.7 (47.02-1.88)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.88Å)	Xtriage
Refinement program	PHENIX (dev_2356: ???)	Depositor
R, R_{free}	0.186 , 0.226 0.188 , 0.226	Depositor DCC
R_{free} test set	5541 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10709	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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, 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	H	0.32	0/1715	0.56	0/2337
1	M	0.27	0/1728	0.51	0/2355
1	O	0.31	0/1715	0.55	0/2337
2	L	0.30	0/1651	0.54	0/2243
2	N	0.28	0/1641	0.51	0/2230
2	P	0.30	0/1572	0.53	0/2133
All	All	0.29	0/10022	0.53	0/13635

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1675	0	1649	30	0
1	M	1687	0	1655	38	0
1	O	1675	0	1651	18	0
2	L	1618	0	1573	27	0
2	N	1608	0	1566	25	0
2	P	1542	0	1499	27	0
3	H	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	12	16	16	0	0
3	M	18	24	24	4	0
3	N	12	16	16	2	0
3	O	6	8	8	0	0
3	P	18	24	24	1	0
4	L	5	0	0	0	0
4	P	5	0	0	0	0
5	H	136	0	0	4	3
5	L	123	0	0	1	0
5	M	106	0	0	2	0
5	N	108	0	0	3	0
5	O	138	0	0	0	1
5	P	115	0	0	1	2
All	All	10613	96	9689	154	3

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 8.

All (154) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:30:SER:HB3	1:H:75:MET:HE1	1.22	1.16
1:H:101:ARG:HG2	1:H:101:ARG:HH11	1.27	0.99
2:P:6:GLN:HG3	2:P:23[B]:CYS:SG	2.09	0.92
1:M:55:TYR:HB2	1:M:75:MET:HE2	1.57	0.85
1:M:42:THR:OG1	1:M:45:LYS:HE3	1.80	0.82
1:H:30:SER:HB3	1:H:75:MET:CE	2.06	0.82
1:H:66:LYS:NZ	5:H:401:HOH:O	2.14	0.79
1:O:69:VAL:HG12	1:O:84:LEU:CD1	2.12	0.78
1:M:55:TYR:HB2	1:M:75:MET:CE	2.18	0.74
2:L:24:ARG:NH1	2:L:70:ASP:OD2	2.21	0.74
2:L:107:ARG:HH22	3:M:302:GOL:C1	2.00	0.74
1:O:69:VAL:HG12	1:O:84:LEU:HD13	1.68	0.74
1:H:30:SER:CB	1:H:75:MET:HE1	2.11	0.73
1:H:57:GLY:O	1:H:59:THR:HG23	1.89	0.72
2:L:107:ARG:HH22	3:M:302:GOL:H11	1.52	0.71
1:H:18:LEU:HD12	1:H:119:VAL:HG11	1.72	0.71
1:H:25:SER:HB3	1:O:25:SER:HB3	1.74	0.70
1:M:11:LEU:HD13	1:M:157:PRO:HG3	1.74	0.69
1:H:154:ASP:OD1	1:H:181:GLN:NE2	2.25	0.69
1:H:101:ARG:HH11	1:H:101:ARG:CG	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:42:THR:OG1	1:H:45:LYS:HE3	1.96	0.66
2:L:22:THR:HG23	5:N:484:HOH:O	1.95	0.64
1:M:12:VAL:HG13	1:M:121:VAL:HG22	1.80	0.64
1:M:114:GLY:O	2:N:43:ALA:HB2	1.98	0.64
1:M:191:VAL:HG11	2:N:134:LEU:HD22	1.80	0.63
2:N:72:THR:HG22	5:N:446:HOH:O	1.99	0.62
2:P:144:LYS:HE2	2:P:146:GLN:CD	2.24	0.62
1:O:8:GLY:HA3	1:O:20:LEU:CD2	2.30	0.62
2:P:4:MET:HE3	2:P:23[A]:CYS:SG	2.40	0.61
2:L:12:SER:HB2	2:L:106:ARG:HE	1.65	0.61
2:L:33:LEU:HD13	2:L:34:ASN:N	2.16	0.60
1:H:179:VAL:HG12	5:H:493:HOH:O	2.01	0.59
1:M:60:LYS:HE3	2:N:94:SER:OG	2.01	0.59
1:M:3:GLN:C	1:M:4:LEU:HD23	2.28	0.59
1:M:53:THR:OG1	1:M:59:THR:HG22	2.03	0.59
1:H:53:THR:OG1	1:H:59:THR:HG22	2.03	0.58
1:H:101:ARG:HG2	1:H:101:ARG:NH1	2.07	0.58
2:N:78:LEU:HD11	2:N:103:LEU:HD21	1.86	0.58
2:P:206:LYS:HE2	3:P:302:GOL:O3	2.03	0.58
1:H:18:LEU:CD1	1:H:119:VAL:HG11	2.34	0.58
1:H:148:LEU:O	1:H:191:VAL:HG13	2.05	0.57
2:P:42:THR:HG22	2:P:43:ALA:N	2.20	0.57
1:H:206[A]:CYS:SG	1:H:219:LYS:HB3	2.45	0.56
1:M:49:TRP:CZ2	1:M:51:GLY:HA2	2.41	0.56
1:O:177:PRO:HD2	2:P:161:SER:OG	2.06	0.56
2:P:15:VAL:HG23	2:P:105:ILE:HD11	1.88	0.55
2:P:189:LYS:HG2	2:P:190:VAL:HG23	1.88	0.55
2:P:31:ASN:OD1	2:P:67:SER:HB2	2.07	0.55
1:O:57:GLY:O	1:O:59:THR:HG23	2.07	0.55
2:N:1:GLU:HB3	5:N:409:HOH:O	2.07	0.54
2:L:72:THR:HG22	5:L:420:HOH:O	2.08	0.54
1:M:55:TYR:HD1	1:M:75:MET:HE1	1.72	0.54
1:M:189:SER:HB2	3:N:301:GOL:H32	1.90	0.54
2:L:3:VAL:HB	2:L:26:SER:OG	2.08	0.54
2:P:179:THR:O	2:P:180:LEU:HD23	2.07	0.54
2:L:61:ARG:HD2	2:L:76:SER:O	2.08	0.53
2:N:24:ARG:HA	2:N:69:THR:O	2.07	0.53
2:P:83:PHE:CE2	2:P:105:ILE:HD12	2.43	0.53
1:M:61:TYR:HD2	1:M:66:LYS:HG3	1.74	0.53
2:N:40:PRO:O	2:N:42:THR:HG23	2.08	0.53
2:N:3:VAL:HB	2:N:26:SER:OG	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:61:ARG:NH1	2:N:82:ASP:OD1	2.42	0.52
1:O:8:GLY:HA3	1:O:20:LEU:HD22	1.91	0.52
1:M:4:LEU:HD22	1:M:24:VAL:HG22	1.92	0.52
2:P:42:THR:HG22	2:P:43:ALA:H	1.75	0.52
1:H:223:PRO:O	1:H:224:LYS:HB3	2.10	0.52
1:M:220:ARG:NH1	5:M:402:HOH:O	2.42	0.52
1:H:69:VAL:HG22	1:H:84:LEU:HD13	1.93	0.51
2:L:33:LEU:HD13	2:L:33:LEU:C	2.36	0.51
1:O:69:VAL:HG12	1:O:84:LEU:HD12	1.93	0.51
1:M:182:SER:H	3:M:301:GOL:H11	1.75	0.50
1:M:108:SER:HB3	2:N:91:SER:HB2	1.94	0.50
1:M:11:LEU:HD13	1:M:157:PRO:CG	2.40	0.50
1:M:115:GLN:HG2	1:M:115:GLN:O	2.10	0.50
2:L:145:VAL:HG13	2:L:193[B]:CYS:SG	2.52	0.49
2:L:124:LEU:O	2:L:126:SER:O	2.29	0.49
2:L:24:ARG:HA	2:L:69:THR:O	2.13	0.49
1:O:71:LEU:HD11	1:O:82:LEU:HD13	1.95	0.49
1:M:188:LEU:HD12	1:M:188:LEU:C	2.38	0.49
1:M:69:VAL:HG12	1:M:84:LEU:HD13	1.94	0.48
1:H:101:ARG:CG	1:H:101:ARG:NH1	2.72	0.48
2:L:78:LEU:HD11	2:L:103:LEU:HD21	1.95	0.48
2:P:192:ALA:HB2	2:P:207:SER:HB3	1.95	0.48
2:N:144:LYS:HB3	2:N:196:THR:HB	1.96	0.48
2:P:145:VAL:HG13	2:P:193[B]:CYS:SG	2.53	0.48
2:P:71:LEU:HD22	2:P:71:LEU:N	2.28	0.48
1:H:49:TRP:CZ2	1:H:51:GLY:HA2	2.49	0.47
1:O:3:GLN:C	1:O:4:LEU:HD12	2.39	0.47
2:N:9:SER:H	3:N:302:GOL:H2	1.78	0.47
2:P:42:THR:HB	5:P:419:HOH:O	2.14	0.47
1:M:12:VAL:CG1	1:M:121:VAL:HG22	2.44	0.47
1:H:220:ARG:HD2	1:H:222:GLU:OE2	2.15	0.47
1:O:2:VAL:HG12	1:O:4:LEU:CD1	2.44	0.47
1:H:18:LEU:C	1:H:18:LEU:HD23	2.40	0.47
1:O:150[A]:CYS:SG	1:O:206:CYS:SG	3.12	0.47
2:L:158:SER:HA	2:L:177:THR:O	2.14	0.47
2:N:33:LEU:HD11	2:N:88:CYS:HB2	1.95	0.47
1:O:30:SER:HB3	1:O:75:MET:SD	2.55	0.47
2:P:198:GLN:O	2:P:198:GLN:HG2	2.14	0.47
2:N:119:PRO:HD3	2:N:131:VAL:HG22	1.96	0.46
1:O:140:SER:HA	2:P:115:PHE:CD2	2.50	0.46
1:M:68:ARG:NH2	1:M:91:ASP:OD2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:49:TRP:CZ2	1:O:51:GLY:HA2	2.51	0.45
1:H:202:GLN:HG2	1:H:204:TYR:CZ	2.51	0.45
1:H:140:SER:HA	2:L:115:PHE:HB3	1.98	0.45
1:M:61:TYR:CD2	1:M:66:LYS:HG3	2.52	0.45
2:N:124:LEU:O	2:N:126:SER:O	2.34	0.45
2:P:12:SER:HA	2:P:104:GLU:O	2.17	0.45
1:M:148:LEU:O	1:M:191:VAL:HG13	2.17	0.45
2:L:107:ARG:HH22	3:M:302:GOL:H12	1.82	0.45
2:L:104:GLU:HG2	2:L:105:ILE:N	2.33	0.45
2:L:18:ARG:NH1	2:L:76:SER:OG	2.50	0.44
1:O:220:ARG:HD2	1:O:222:GLU:OE2	2.16	0.44
1:O:35:TYR:HB2	1:O:100:ASP:HB3	1.99	0.44
1:H:191:VAL:HG12	1:H:192:VAL:N	2.32	0.44
1:M:65:LEU:HD11	5:M:443:HOH:O	2.18	0.44
2:N:69:THR:O	2:N:69:THR:CG2	2.66	0.44
1:M:11:LEU:HD22	1:M:126:THR:HG22	2.00	0.44
2:N:174:LEU:C	2:N:174:LEU:HD23	2.43	0.44
1:H:191:VAL:HG11	2:L:134:LEU:HD22	2.00	0.43
1:M:191:VAL:HG12	1:M:192:VAL:N	2.34	0.43
2:N:24:ARG:CZ	2:N:24:ARG:HB2	2.49	0.43
1:M:191:VAL:HG11	2:N:134:LEU:CD2	2.48	0.43
1:H:201:THR:HG21	5:H:520:HOH:O	2.18	0.42
2:P:4:MET:CE	2:P:23[A]:CYS:SG	3.08	0.42
2:L:123:GLN:HG2	2:L:128:THR:O	2.19	0.42
1:O:65:LEU:HB3	1:O:69:VAL:CG1	2.49	0.42
2:L:50:ALA:O	2:L:51:ALA:HB3	2.18	0.42
1:H:198:SER:HB3	5:H:445:HOH:O	2.20	0.42
2:L:142:GLU:H	2:L:142:GLU:CD	2.27	0.42
2:N:50:ALA:O	2:N:51:ALA:HB3	2.19	0.42
1:M:3:GLN:O	1:M:4:LEU:HD23	2.19	0.42
1:H:11:LEU:HD22	1:H:122:SER:HB3	2.01	0.41
2:L:1:GLU:O	2:L:1:GLU:HG2	2.20	0.41
2:N:104:GLU:HG2	2:N:105:ILE:N	2.35	0.41
2:P:15:VAL:HG13	2:P:78:LEU:O	2.19	0.41
1:M:30:SER:HA	1:M:55:TYR:HB3	2.01	0.41
1:M:64:SER:OG	1:M:65:LEU:HD13	2.20	0.41
2:L:174:LEU:C	2:L:174:LEU:HD23	2.46	0.41
1:M:41:GLN:HB2	1:M:47:LEU:HD23	2.02	0.41
2:N:1:GLU:HB3	2:N:2:ILE:H	1.63	0.41
2:N:182:LYS:HE2	2:N:186:GLU:OE2	2.20	0.41
2:L:71:LEU:N	2:L:71:LEU:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:42:THR:OG1	1:M:45:LYS:HB2	2.21	0.41
1:M:42:THR:O	1:M:43:PRO:C	2.64	0.41
2:P:35:TRP:CZ3	2:P:88:CYS:HB3	2.56	0.41
2:P:124:LEU:HD23	2:P:124:LEU:HA	1.92	0.41
2:P:192:ALA:CB	2:P:207:SER:HB3	2.51	0.40
1:M:45:LYS:HB3	1:M:46:GLY:H	1.75	0.40
1:M:114:GLY:O	2:N:43:ALA:CB	2.67	0.40
2:P:24:ARG:HA	2:P:69:THR:O	2.21	0.40
2:L:33:LEU:C	2:L:33:LEU:CD1	2.95	0.40
2:P:144:LYS:HE2	2:P:146:GLN:CG	2.51	0.40
2:P:184:ASP:HA	2:P:187:LYS:HD2	2.03	0.40

All (3) 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)
5:H:515:HOH:O	5:P:429:HOH:O[2_446]	1.76	0.44
5:H:466:HOH:O	5:P:501:HOH:O[2_446]	2.15	0.05
5:H:501:HOH:O	5:O:465:HOH:O[2_446]	2.19	0.01

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	H	224/265 (84%)	219 (98%)	5 (2%)	0	100	100
1	M	227/265 (86%)	221 (97%)	6 (3%)	0	100	100
1	O	224/265 (84%)	220 (98%)	4 (2%)	0	100	100
2	L	211/213 (99%)	207 (98%)	4 (2%)	0	100	100
2	N	209/213 (98%)	205 (98%)	4 (2%)	0	100	100
2	P	197/213 (92%)	192 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1292/1434 (90%)	1264 (98%)	28 (2%)	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	H	195/224 (87%)	193 (99%)	2 (1%)	68	60
1	M	196/224 (88%)	193 (98%)	3 (2%)	57	46
1	O	195/224 (87%)	192 (98%)	3 (2%)	57	46
2	L	186/186 (100%)	185 (100%)	1 (0%)	81	76
2	N	185/186 (100%)	183 (99%)	2 (1%)	65	56
2	P	178/186 (96%)	175 (98%)	3 (2%)	53	40
All	All	1135/1230 (92%)	1121 (99%)	14 (1%)	63	53

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	101	ARG
1	H	188	LEU
2	L	33	LEU
1	M	11	LEU
1	M	65	LEU
1	M	188	LEU
2	N	22	THR
2	N	94	SER
1	O	59	THR
1	O	125	SER
1	O	188	LEU
2	P	69	THR
2	P	71	LEU
2	P	131	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	1	GLN
1	M	202	GLN
2	N	159	GLN
1	O	5	GLN
1	O	41	GLN
1	O	79	GLN
1	O	115	GLN
1	O	209	ASN
1	O	214	ASN
2	P	38	GLN
2	P	209	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	M	302	-	5,5,5	0.35	0	5,5,5	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	L	302	-	5,5,5	0.39	0	5,5,5	0.52	0
3	GOL	P	303	-	5,5,5	0.31	0	5,5,5	0.38	0
4	SO4	P	304	-	4,4,4	0.31	0	6,6,6	0.24	0
4	SO4	L	303	-	4,4,4	0.25	0	6,6,6	0.12	0
3	GOL	P	301	-	5,5,5	0.30	0	5,5,5	0.36	0
3	GOL	P	302	-	5,5,5	0.36	0	5,5,5	0.26	0
3	GOL	H	301	-	5,5,5	0.40	0	5,5,5	0.45	0
3	GOL	N	301	-	5,5,5	0.41	0	5,5,5	0.48	0
3	GOL	M	301	-	5,5,5	0.41	0	5,5,5	0.18	0
3	GOL	O	301	-	5,5,5	0.58	0	5,5,5	1.00	0
3	GOL	M	303	-	5,5,5	0.37	0	5,5,5	0.27	0
3	GOL	L	301	-	5,5,5	0.38	0	5,5,5	0.19	0
3	GOL	N	302	-	5,5,5	0.32	0	5,5,5	0.33	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	M	302	-	-	4/4/4/4	-
3	GOL	L	302	-	-	3/4/4/4	-
3	GOL	P	303	-	-	2/4/4/4	-
3	GOL	P	301	-	-	2/4/4/4	-
3	GOL	P	302	-	-	2/4/4/4	-
3	GOL	H	301	-	-	2/4/4/4	-
3	GOL	N	301	-	-	4/4/4/4	-
3	GOL	M	301	-	-	3/4/4/4	-
3	GOL	O	301	-	-	2/4/4/4	-
3	GOL	M	303	-	-	2/4/4/4	-
3	GOL	L	301	-	-	2/4/4/4	-
3	GOL	N	302	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	301	GOL	O1-C1-C2-C3
3	L	301	GOL	O1-C1-C2-C3
3	L	302	GOL	C1-C2-C3-O3
3	L	302	GOL	O2-C2-C3-O3
3	M	301	GOL	O1-C1-C2-C3
3	M	302	GOL	C1-C2-C3-O3
3	M	303	GOL	O1-C1-C2-C3
3	N	301	GOL	O1-C1-C2-C3
3	N	301	GOL	C1-C2-C3-O3
3	N	301	GOL	O2-C2-C3-O3
3	O	301	GOL	C1-C2-C3-O3
3	P	302	GOL	C1-C2-C3-O3
3	P	302	GOL	O2-C2-C3-O3
3	P	303	GOL	O1-C1-C2-C3
3	L	301	GOL	O1-C1-C2-O2
3	M	301	GOL	O1-C1-C2-O2
3	L	302	GOL	O1-C1-C2-C3
3	P	301	GOL	C1-C2-C3-O3
3	H	301	GOL	O1-C1-C2-O2
3	M	302	GOL	O2-C2-C3-O3
3	M	303	GOL	O1-C1-C2-O2
3	O	301	GOL	O2-C2-C3-O3
3	P	303	GOL	O1-C1-C2-O2
3	P	301	GOL	O2-C2-C3-O3
3	N	302	GOL	O1-C1-C2-O2
3	M	302	GOL	O1-C1-C2-O2
3	N	301	GOL	O1-C1-C2-O2
3	M	302	GOL	O1-C1-C2-C3
3	M	301	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	302	GOL	3	0
3	P	302	GOL	1	0
3	N	301	GOL	1	0
3	M	301	GOL	1	0
3	N	302	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, 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	H	224/265 (84%)	0.05	10 (4%)	38 41	11, 28, 46, 55	2 (0%)
1	M	223/265 (84%)	0.42	11 (4%)	35 37	12, 34, 50, 69	6 (2%)
1	O	224/265 (84%)	0.06	7 (3%)	51 56	11, 30, 49, 57	2 (0%)
2	L	211/213 (99%)	0.30	5 (2%)	59 66	15, 33, 50, 59	2 (0%)
2	N	210/213 (98%)	0.51	10 (4%)	35 37	16, 38, 55, 60	2 (0%)
2	P	199/213 (93%)	0.25	7 (3%)	47 52	15, 34, 52, 59	2 (1%)
All	All	1291/1434 (90%)	0.26	50 (3%)	43 47	11, 32, 51, 69	16 (1%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	9[A]	PRO	8.7
1	M	69	VAL	4.3
2	L	68	GLY	4.1
1	M	8[A]	GLY	4.1
1	O	44	GLY	3.3
1	M	55	TYR	3.3
1	O	55	TYR	3.2
1	O	104	VAL	3.2
2	N	127	GLY	3.1
2	L	211	GLY	3.1
1	H	43	PRO	2.8
1	M	30	SER	2.8
1	H	107	GLY	2.8
1	O	107	GLY	2.8
2	L	69	THR	2.8
2	N	153	LEU	2.8
1	M	106	SER	2.7
2	L	32	TYR	2.7
2	P	32	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	N	59	PRO	2.7
1	H	104	VAL	2.7
2	P	211	GLY	2.6
2	N	49	TYR	2.6
1	M	43	PRO	2.6
1	M	58	SER	2.6
1	M	35	TYR	2.5
2	N	26	SER	2.5
2	N	53	SER	2.5
1	H	57	GLY	2.4
2	N	159	GLN	2.4
1	M	56	SER	2.4
1	H	224	LYS	2.4
2	P	92	TYR	2.3
1	H	105	ALA	2.3
1	O	1	GLN	2.3
1	M	160	VAL	2.3
1	O	214	ASN	2.3
1	H	56	SER	2.2
2	P	48	THR	2.2
2	P	2	ILE	2.2
1	H	44	GLY	2.2
1	H	143	GLY	2.2
2	N	67	SER	2.2
2	L	121	ASP	2.2
2	N	50	ALA	2.2
1	O	32	GLY	2.1
1	H	55	TYR	2.1
2	N	69	THR	2.1
2	P	69	THR	2.1
2	P	29	ILE	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(Å ²)	Q<0.9
3	GOL	M	301	6/6	0.71	0.14	52,62,72,83	0
3	GOL	L	301	6/6	0.73	0.14	51,62,72,87	0
3	GOL	M	303	6/6	0.74	0.12	60,72,87,87	0
3	GOL	P	303	6/6	0.75	0.13	55,66,78,82	0
3	GOL	P	302	6/6	0.79	0.13	44,55,67,75	0
3	GOL	N	302	6/6	0.80	0.12	50,64,68,77	0
3	GOL	N	301	6/6	0.84	0.13	25,43,52,57	0
3	GOL	O	301	6/6	0.84	0.12	26,33,41,49	0
3	GOL	H	301	6/6	0.86	0.10	25,37,52,63	0
3	GOL	M	302	6/6	0.86	0.11	29,48,57,67	0
4	SO4	L	303	5/5	0.86	0.09	63,72,76,78	0
3	GOL	P	301	6/6	0.88	0.10	49,59,64,70	0
3	GOL	L	302	6/6	0.91	0.08	31,39,49,49	0
4	SO4	P	304	5/5	0.96	0.08	32,33,49,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.