Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2024 – 12:36 pm GMT

PDB ID	:	5NST
Title	:	Human monoclonal antibody with a LAIR1 insertion
Authors	:	Hsieh, F.-L.; Higgins, M.K.
Deposited on	:	2017-04-26
Resolution	:	2.52 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 (1)) were used in the production of this report:

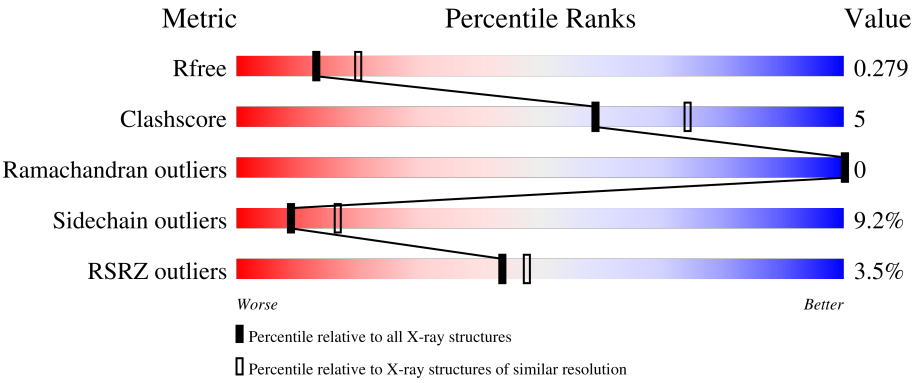
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.52 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	214	79% 18%
1	C	214	2% 76% 20%
2	B	360	3% 78% 15% 7%
2	D	360	6% 75% 12% 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
3	GOL	B	402	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8361 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.

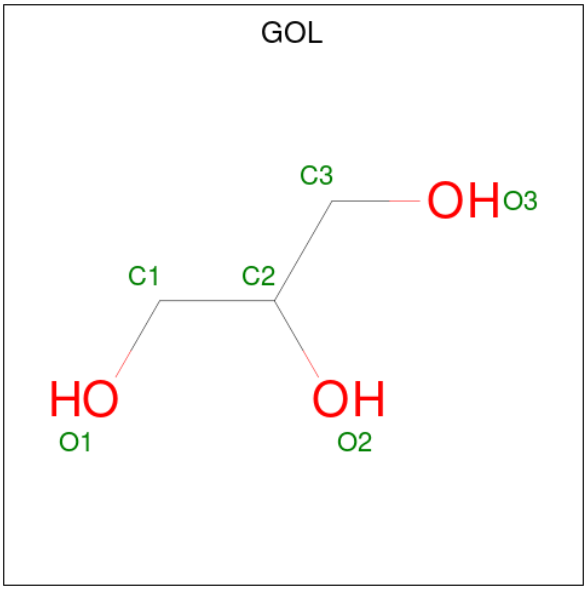
- Molecule 1 is a protein called Light Chain of antibody MGD21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1618	1005	280	325	8			
1	C	208	Total	C	N	O	S	0	0	0
			1593	989	274	322	8			

- Molecule 2 is a protein called Heavy Chain of antibody MGD21.

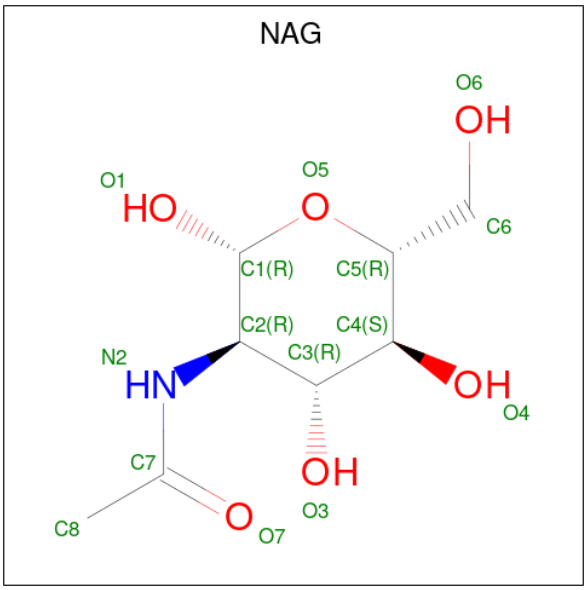
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	336	Total	C	N	O	S	0	0	0
			2578	1620	439	510	9			
2	D	322	Total	C	N	O	S	0	0	0
			2475	1554	424	489	8			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total O 5 5	0	0
5	B	10	Total O 10 10	0	0
5	C	14	Total O 14 14	0	0

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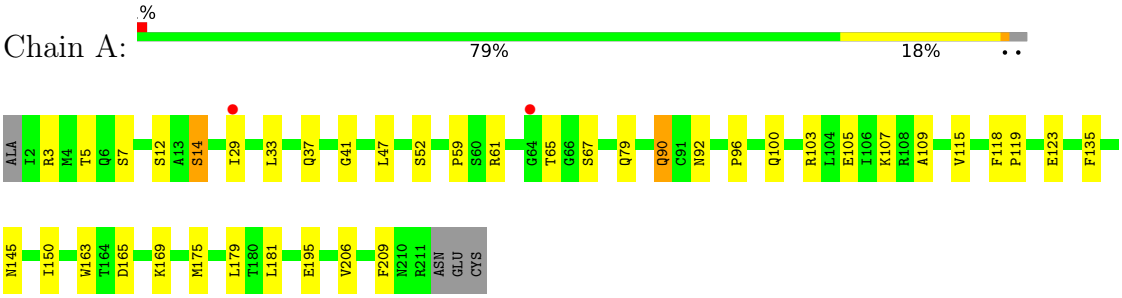
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	16	Total O 16 16	0	0

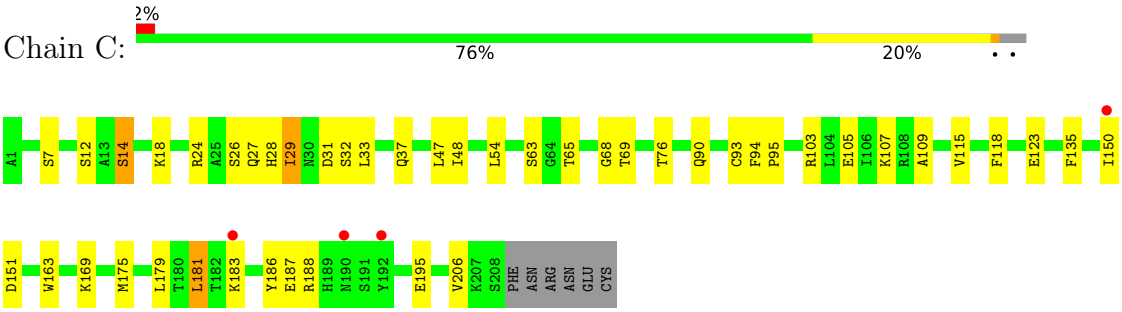
3 Residue-property plots (i)

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.

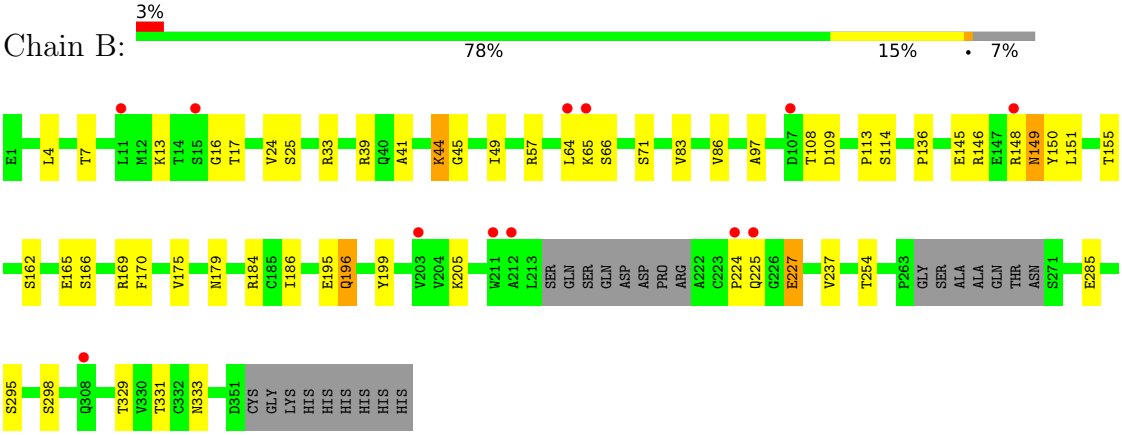
• Molecule 1: Light Chain of antibody MGD21



• Molecule 1: Light Chain of antibody MGD21

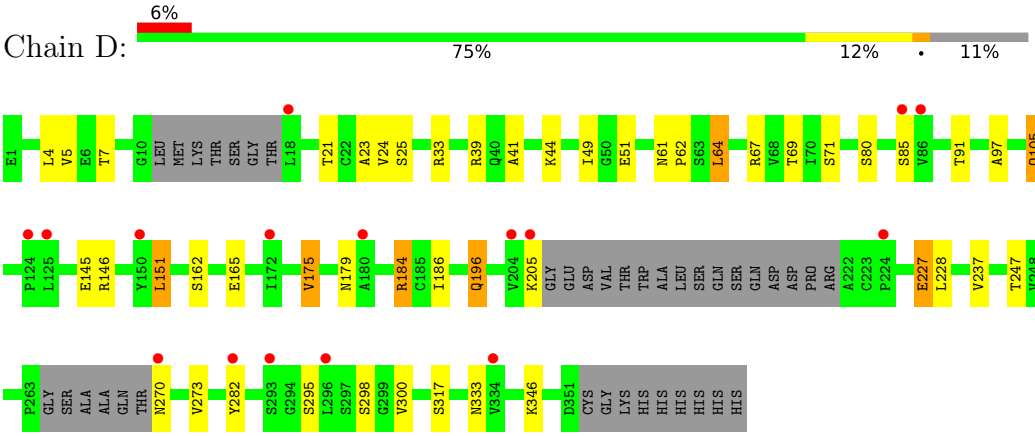


• Molecule 2: Heavy Chain of antibody MGD21



• Molecule 2: Heavy Chain of antibody MGD21

Chain D:


6%
75%
12%
11%
E1 L4 V5 E6 T7 G10 LEU MET LYS THR SER GLY THR L18 T21 C22 A23 V24 S25 R33 R39 Q40 A41 K44 I49 G50 E51 N61 P62 S63 L64 R67 V68 T69 I70 S71 S80 S85 V86 T91 A97 Q105 R106 D107 T108 D109
P124 L125 E145 R146 Y150 L151 S162 E165 I172 V175 N179 A180 R184 C185 I186 Q196 V204 K205 GLY GLU ASP VAL THR TRP ALA LEU SER GLN SER GLN ASP ASP PRO ARG A222 C223 P224 E227 L228 V237 T247 V248 S249 S250 P256
P263 GLY SER ALA ALA GLN THR N270 V273 Y282 S293 G294 S295 L296 S297 S298 G299 V300 S317 N333 V334 K346 D351 CYS GLY LYS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	169.82Å 86.46Å 104.00Å 90.00° 126.65° 90.00°	Depositor
Resolution (Å)	81.90 – 2.52 73.00 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.7 (81.90-2.52) 99.7 (73.00-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.219 , 0.267 0.228 , 0.279	Depositor DCC
R_{free} test set	1968 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	51.9	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 56.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8361	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: NAG, 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	0.52	0/1656	0.71	0/2247
1	C	0.52	0/1630	0.73	0/2213
2	B	0.53	0/2639	0.76	0/3606
2	D	0.53	0/2533	0.76	0/3460
All	All	0.53	0/8458	0.74	0/11526

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	1618	0	1547	18	0
1	C	1593	0	1527	20	0
2	B	2578	0	2525	26	0
2	D	2475	0	2420	20	0
3	A	12	0	16	1	0
3	B	6	0	8	3	0
3	C	6	0	8	0	0
4	B	14	0	13	0	0
4	D	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	5	0	0	0	0
5	B	10	0	0	0	0
5	C	14	0	0	0	0
5	D	16	0	0	0	0
All	All	8361	0	8077	77	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 5.

All (77) 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:B:224:PRO:HG2	2:B:227:GLU:HB2	1.43	1.01
2:B:169:ARG:HH22	3:B:402:GOL:H12	1.39	0.86
2:D:105:GLN:HG2	2:D:106:ARG:O	1.80	0.81
2:B:224:PRO:HG2	2:B:227:GLU:CB	2.11	0.79
1:C:29:ILE:HG13	1:C:68:GLY:O	1.88	0.74
1:A:59:PRO:HG2	1:A:61:ARG:HH21	1.55	0.72
1:C:48:ILE:HD13	1:C:54:LEU:HD23	1.71	0.70
1:C:48:ILE:CD1	1:C:54:LEU:HD23	2.22	0.68
2:D:105:GLN:HG2	2:D:106:ARG:N	2.09	0.67
2:B:41:ALA:HB3	2:B:44:LYS:HB3	1.79	0.64
2:D:41:ALA:HB3	2:D:44:LYS:HB2	1.80	0.63
1:C:150:ILE:HD11	1:C:179:LEU:HD21	1.82	0.61
2:B:169:ARG:HH22	3:B:402:GOL:C1	2.15	0.59
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.85	0.58
2:D:67:ARG:HD2	2:D:85:SER:HB2	1.85	0.58
1:A:90:GLN:NE2	1:A:96:PRO:HA	2.19	0.57
1:A:195:GLU:HG2	1:A:206:VAL:HG12	1.86	0.57
1:C:195:GLU:HG2	1:C:206:VAL:HG12	1.86	0.57
1:A:61:ARG:HH12	1:A:79:GLN:HB2	1.70	0.57
2:B:44:LYS:HG3	2:B:45:GLY:N	2.19	0.57
2:B:184:ARG:HG3	2:B:199:TYR:CD1	2.40	0.57
1:C:94:PHE:O	2:D:227:GLU:HB3	2.08	0.53
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.89	0.53
2:B:136:PRO:O	2:B:166:SER:HB3	2.08	0.53
2:B:146:ARG:O	2:B:150:TYR:HA	2.09	0.53
1:C:181:LEU:HD13	1:C:186:TYR:HB2	1.89	0.52
2:D:175:VAL:HA	2:D:179:ASN:HD22	1.73	0.52
2:B:149:ASN:HB3	2:B:151:LEU:HG	1.92	0.52
2:B:146:ARG:HD3	2:B:151:LEU:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:ARG:HB3	2:D:49:ILE:HD11	1.92	0.51
1:A:12:SER:HB3	1:A:107:LYS:HB2	1.91	0.51
1:A:109:ALA:HA	2:D:298:SER:HB3	1.92	0.51
2:D:146:ARG:HD2	2:D:151:LEU:HD12	1.91	0.51
1:A:29:ILE:HD11	1:A:92:ASN:HB3	1.93	0.51
1:C:12:SER:HB3	1:C:107:LYS:HB2	1.92	0.51
1:A:90:GLN:HE22	1:A:96:PRO:HA	1.77	0.50
1:C:118:PHE:HE1	1:C:135:PHE:CD2	2.29	0.50
1:C:163:TRP:CD1	1:C:175:MET:HG3	2.46	0.50
2:B:64:LEU:HD23	2:B:64:LEU:N	2.27	0.49
2:B:39:ARG:HB3	2:B:49:ILE:HD11	1.94	0.49
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.93	0.49
2:B:298:SER:HB3	1:C:109:ALA:HA	1.95	0.48
1:A:14:SER:HB3	1:C:169:LYS:HD3	1.96	0.48
2:B:169:ARG:NH2	3:B:402:GOL:H12	2.18	0.47
1:C:18:LYS:HG3	1:C:76:THR:HG22	1.97	0.47
1:A:163:TRP:CD1	1:A:175:MET:HG3	2.49	0.47
2:B:44:LYS:CG	2:B:45:GLY:N	2.78	0.47
2:D:300:VAL:HA	2:D:317:SER:O	2.15	0.47
2:B:175:VAL:HA	2:B:179:ASN:HD22	1.81	0.46
1:A:169:LYS:HD3	1:C:14:SER:HB3	1.98	0.46
2:D:61:ASN:HB3	2:D:64:LEU:HD12	1.97	0.46
1:C:28:HIS:HA	1:C:69:THR:HG23	1.97	0.45
1:A:119:PRO:HB3	1:A:209:PHE:CE1	2.51	0.45
1:A:118:PHE:HE2	1:A:135:PHE:CD2	2.35	0.45
1:C:93:CYS:HB3	2:D:227:GLU:HB2	1.99	0.45
2:D:5:VAL:HG22	2:D:23:ALA:HB3	1.98	0.45
1:C:95:PRO:HG3	2:D:62:PRO:HD2	1.99	0.45
1:A:118:PHE:HE2	1:A:135:PHE:CE2	2.35	0.44
2:B:17:THR:HA	2:B:83:VAL:O	2.17	0.44
2:B:64:LEU:HD23	2:B:64:LEU:H	1.82	0.43
2:B:4:LEU:HD22	2:B:24:VAL:HG22	2.00	0.43
2:D:4:LEU:HD22	2:D:24:VAL:HG22	2.01	0.42
2:B:97:ALA:HB1	2:B:237:VAL:HG13	2.00	0.42
2:D:256:PRO:HB3	2:D:282:TYR:HB3	2.02	0.42
2:D:91:THR:HG23	2:D:247:THR:HA	2.00	0.42
2:D:97:ALA:HB1	2:D:237:VAL:HG13	2.01	0.42
2:B:16:GLY:O	2:B:86:VAL:HG22	2.20	0.42
2:D:186:ILE:HB	2:D:196:GLN:HG3	2.02	0.41
1:A:41:GLY:H	3:A:301:GOL:H2	1.85	0.41
2:B:225:GLN:C	2:B:227:GLU:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:ILE:HB	2:B:196:GLN:HG3	2.01	0.41
1:C:27:GLN:HG2	1:C:28:HIS:H	1.85	0.41
2:B:155:THR:HG22	2:B:170:PHE:CZ	2.56	0.40
2:B:113:PRO:HD2	2:B:195:GLU:O	2.21	0.40
2:D:145:GLU:HB2	2:D:184:ARG:HG3	2.04	0.40
1:A:115:VAL:HA	1:A:135:PHE:O	2.21	0.40
1:C:115:VAL:HA	1:C:135:PHE:O	2.21	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	208/214 (97%)	199 (96%)	9 (4%)	0	100	100
1	C	206/214 (96%)	194 (94%)	12 (6%)	0	100	100
2	B	330/360 (92%)	313 (95%)	17 (5%)	0	100	100
2	D	314/360 (87%)	301 (96%)	13 (4%)	0	100	100
All	All	1058/1148 (92%)	1007 (95%)	51 (5%)	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	185/188 (98%)	169 (91%)	16 (9%)	10 19
1	C	182/188 (97%)	163 (90%)	19 (10%)	7 12
2	B	296/316 (94%)	270 (91%)	26 (9%)	10 18
2	D	285/316 (90%)	259 (91%)	26 (9%)	9 17
All	All	948/1008 (94%)	861 (91%)	87 (9%)	9 17

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	5	THR
1	A	7	SER
1	A	14	SER
1	A	33	LEU
1	A	52	SER
1	A	65	THR
1	A	67	SER
1	A	90	GLN
1	A	100	GLN
1	A	103	ARG
1	A	105	GLU
1	A	123	GLU
1	A	145	ASN
1	A	165	ASP
1	A	181	LEU
2	B	7	THR
2	B	13	LYS
2	B	25	SER
2	B	33	ARG
2	B	44	LYS
2	B	57	ARG
2	B	65	LYS
2	B	66	SER
2	B	71	SER
2	B	108	THR
2	B	109	ASP
2	B	114	SER
2	B	145	GLU
2	B	148	ARG
2	B	149	ASN
2	B	162	SER
2	B	165	GLU

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Mol	Chain	Res	Type
2	B	196	GLN
2	B	205	LYS
2	B	227	GLU
2	B	254	THR
2	B	285	GLU
2	B	295	SER
2	B	329	THR
2	B	331	THR
2	B	333	ASN
1	C	7	SER
1	C	14	SER
1	C	24	ARG
1	C	26	SER
1	C	29	ILE
1	C	31	ASP
1	C	32	SER
1	C	33	LEU
1	C	63	SER
1	C	65	THR
1	C	90	GLN
1	C	103	ARG
1	C	105	GLU
1	C	123	GLU
1	C	151	ASP
1	C	181	LEU
1	C	183	LYS
1	C	187	GLU
1	C	188	ARG
2	D	7	THR
2	D	21	THR
2	D	25	SER
2	D	33	ARG
2	D	51	GLU
2	D	64	LEU
2	D	69	THR
2	D	71	SER
2	D	80	SER
2	D	105	GLN
2	D	108	THR
2	D	109	ASP
2	D	151	LEU
2	D	162	SER

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Mol	Chain	Res	Type
2	D	165	GLU
2	D	175	VAL
2	D	184	ARG
2	D	196	GLN
2	D	205	LYS
2	D	227	GLU
2	D	228	LEU
2	D	270	ASN
2	D	273	VAL
2	D	295	SER
2	D	333	ASN
2	D	346	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	92	ASN
1	A	138	ASN
1	A	198	HIS
2	B	32	ASN
2	B	105	GLN
2	B	179	ASN
2	B	308	GLN
1	C	28	HIS
1	C	53	ASN
1	C	92	ASN
1	C	145	ASN
1	C	198	HIS
2	D	32	ASN
2	D	179	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	B	402	-	5,5,5	0.06	0	5,5,5	0.28	0
3	GOL	A	302	-	5,5,5	0.06	0	5,5,5	0.26	0
4	NAG	D	401	2	14,14,15	0.34	0	17,19,21	0.37	0
4	NAG	B	401	2	14,14,15	0.40	0	17,19,21	1.56	4 (23%)
3	GOL	A	301	-	5,5,5	0.07	0	5,5,5	0.32	0
3	GOL	C	301	-	5,5,5	0.12	0	5,5,5	0.39	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	B	402	-	-	2/4/4/4	-
3	GOL	A	302	-	-	3/4/4/4	-
4	NAG	D	401	2	-	0/6/23/26	0/1/1/1
4	NAG	B	401	2	-	3/6/23/26	0/1/1/1
3	GOL	A	301	-	-	1/4/4/4	-
3	GOL	C	301	-	-	0/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	401	NAG	C1-C2-N2	4.06	117.43	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	401	NAG	C2-N2-C7	3.25	127.53	122.90
4	B	401	NAG	C1-O5-C5	2.51	115.59	112.19
4	B	401	NAG	O5-C1-C2	-2.41	107.49	111.29

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	GOL	O1-C1-C2-C3
4	B	401	NAG	O5-C5-C6-O6
4	B	401	NAG	C4-C5-C6-O6
3	A	301	GOL	O1-C1-C2-C3
3	A	302	GOL	O1-C1-C2-C3
3	A	302	GOL	C1-C2-C3-O3
3	B	402	GOL	O1-C1-C2-O2
4	B	401	NAG	C1-C2-N2-C7
3	A	302	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	GOL	3	0
3	A	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	210/214 (98%)	0.03	2 (0%)	82	84	42, 66, 98, 118	0
1	C	208/214 (97%)	0.13	4 (1%)	66	70	40, 65, 111, 129	0
2	B	336/360 (93%)	0.11	12 (3%)	42	46	40, 64, 103, 136	0
2	D	322/360 (89%)	0.38	20 (6%)	20	22	43, 74, 111, 142	0
All	All	1076/1148 (93%)	0.18	38 (3%)	44	48	40, 67, 107, 142	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	107	ASP	4.9
2	B	107	ASP	4.7
2	B	225	GLN	4.6
2	D	205	LYS	4.2
2	D	85	SER	4.2
2	B	212	ALA	4.2
2	B	308	GLN	4.0
2	D	249	SER	3.9
2	B	211	TRP	3.8
2	D	172	ILE	3.8
1	C	190	ASN	3.6
2	D	296	LEU	3.5
2	D	125	LEU	3.4
2	D	270	ASN	3.3
1	A	29	ILE	3.2
2	B	148	ARG	3.0
2	B	65	LYS	3.0
1	C	150	ILE	2.9
2	B	64	LEU	2.7
2	D	86	VAL	2.7
2	D	204	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	192	TYR	2.7
2	D	124	PRO	2.6
1	A	64	GLY	2.6
2	D	250	SER	2.4
2	D	150	TYR	2.4
2	D	293	SER	2.4
2	D	180	ALA	2.3
2	D	108	THR	2.3
2	B	15	SER	2.2
1	C	183	LYS	2.1
2	D	282	TYR	2.1
2	D	18	LEU	2.1
2	D	334	VAL	2.1
2	B	203	VAL	2.0
2	B	224	PRO	2.0
2	D	224	PRO	2.0
2	B	11	LEU	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
3	GOL	B	402	6/6	0.72	0.52	99,100,100,102	0
4	NAG	D	401	14/15	0.76	0.28	126,129,133,134	0
4	NAG	B	401	14/15	0.82	0.14	118,122,125,126	0
3	GOL	C	301	6/6	0.86	0.30	76,77,77,78	0
3	GOL	A	301	6/6	0.88	0.19	78,79,81,81	0
3	GOL	A	302	6/6	0.89	0.25	75,79,81,83	0

6.5 Other polymers (i)

There are no such residues in this entry.