Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2025 – 02:28 PM EDT

PDB ID	:	9MYL
Title	:	Fertilization IZUMO1 Protein Ectodomain in Complex with Anti-sperm Antibody OBF13
Authors	:	Tang, S.
Deposited on	:	2025-01-22
Resolution	:	3.18 Å(reported)

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

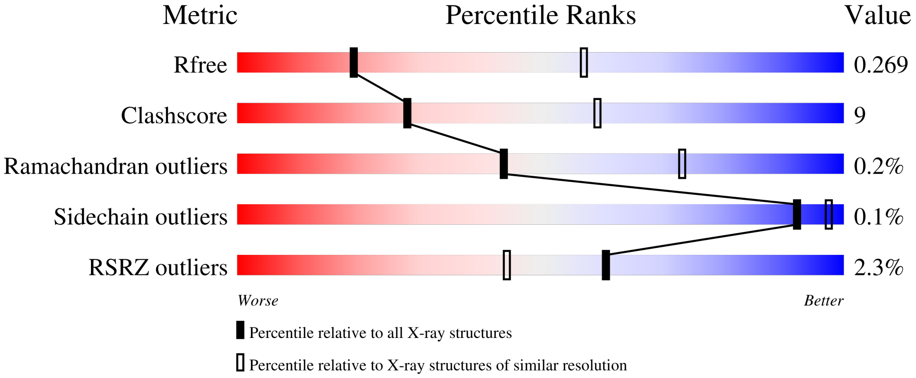
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

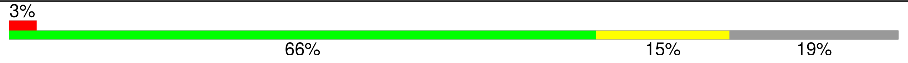
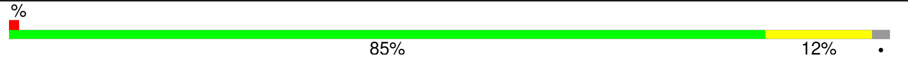
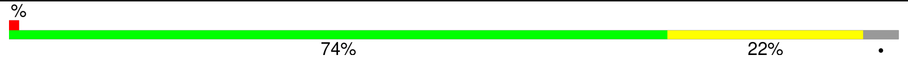
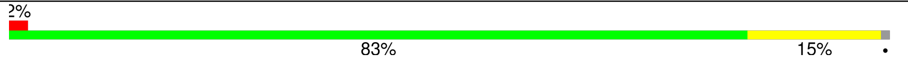
The reported resolution of this entry is 3.18 Å.

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}	164625	1851 (3.20-3.16)
Clashscore	180529	1999 (3.20-3.16)
Ramachandran outliers	177936	1961 (3.20-3.16)
Sidechain outliers	177891	1960 (3.20-3.16)
RSRZ outliers	164620	1852 (3.20-3.16)

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	C	238	
1	D	238	
2	A	217	
2	H	217	
3	B	213	

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Mol	**Chain**	**Length**	**Quality of chain**
3	L	213	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9194 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 Izumo sperm-egg fusion protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	224	1654	1042	279	319	14	0	0	0
1	D	193	1441	914	248	267	12	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	THR	deletion	UNP Q9D9J7
C	256	GLU	-	expression tag	UNP Q9D9J7
C	257	PRO	-	expression tag	UNP Q9D9J7
C	258	GLU	-	expression tag	UNP Q9D9J7
C	259	ALA	-	expression tag	UNP Q9D9J7
D	?	-	THR	deletion	UNP Q9D9J7
D	256	GLU	-	expression tag	UNP Q9D9J7
D	257	PRO	-	expression tag	UNP Q9D9J7
D	258	GLU	-	expression tag	UNP Q9D9J7
D	259	ALA	-	expression tag	UNP Q9D9J7

- Molecule 2 is a protein called Anti-sperm antibody OBF13 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	208	1522	965	248	303	6	0	0	0
2	A	212	1562	986	257	314	5	0	0	0

- Molecule 3 is a protein called Anti-sperm antibody OBF13 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	209	1458	911	239	302	6	0	0	0

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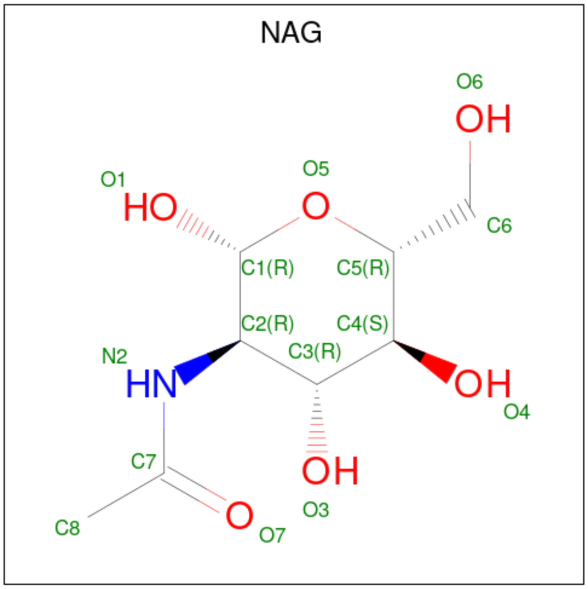
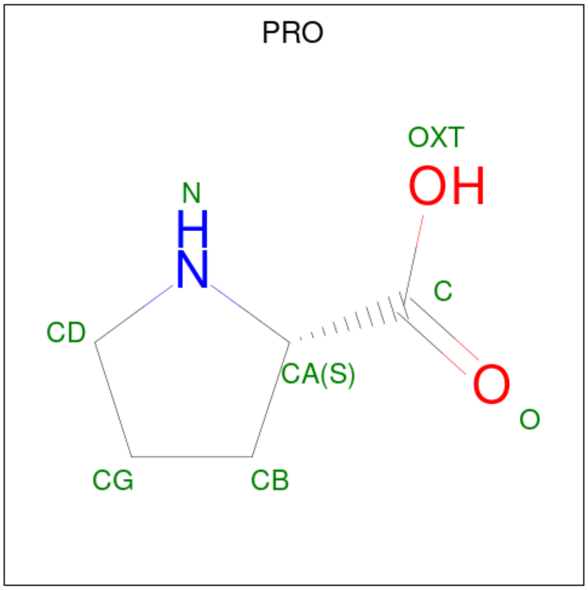
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	210	1513	934	253	320	6	0	0	0

- 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
			Total	C	N	O		
4	C	1	14	8	1	5	0	0
4	D	1	14	8	1	5	0	0

- Molecule 5 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 7 5 1 1	0	0
5	D	1	Total C N O 7 5 1 1	0	0

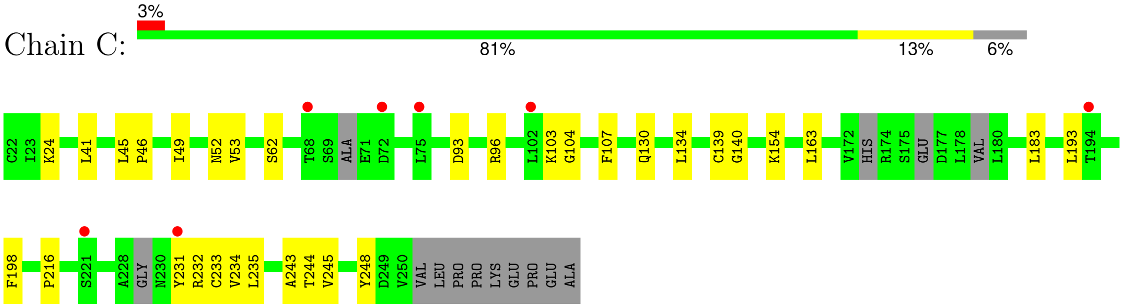
- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total Cl 1 1	0	0
6	A	1	Total Cl 1 1	0	0

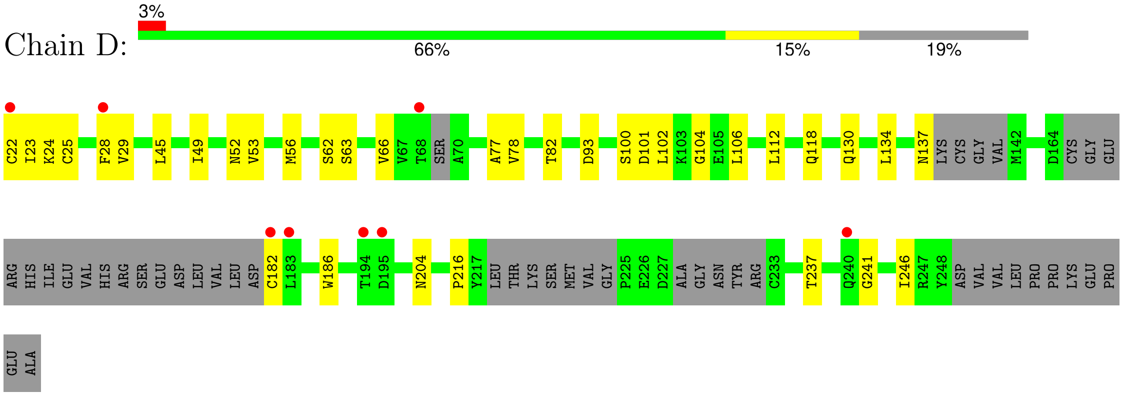
3 Residue-property plots

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.

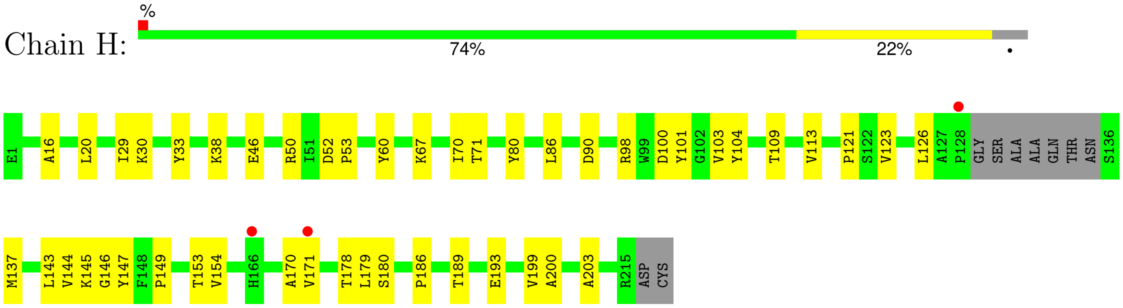
- Molecule 1: Izumo sperm-egg fusion protein 1



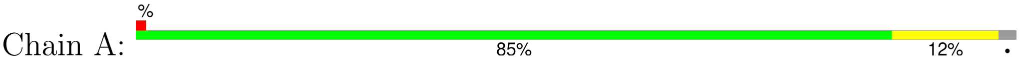
- Molecule 1: Izumo sperm-egg fusion protein 1

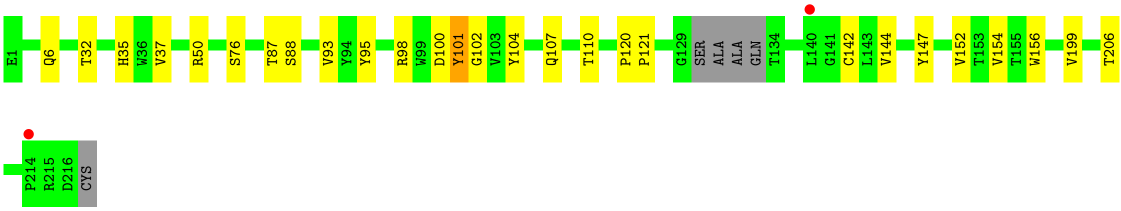


- Molecule 2: Anti-sperm antibody OBF13 heavy chain



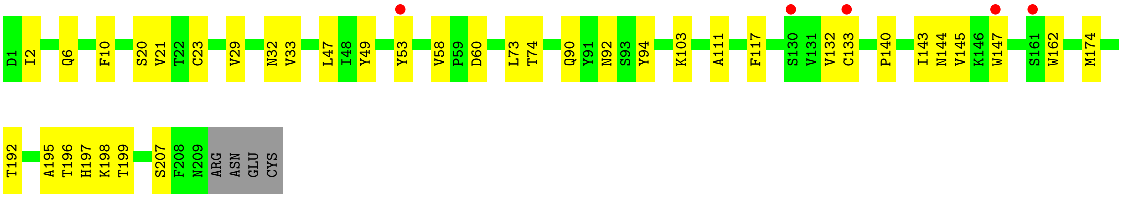
- Molecule 2: Anti-sperm antibody OBF13 heavy chain





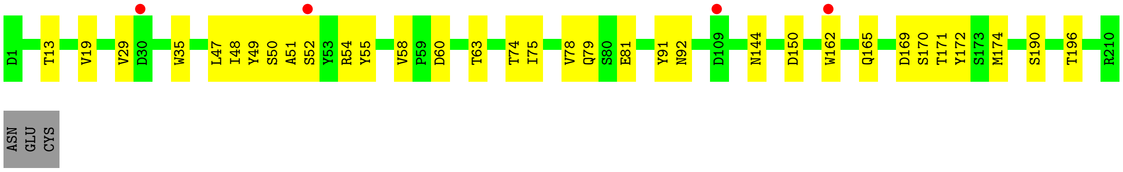
- Molecule 3: Anti-sperm antibody OBF13 light chain

Chain L:



- Molecule 3: Anti-sperm antibody OBF13 light chain

Chain B:



4 Data and refinement statistics

Property	**Value**	**Source**
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	81.07Å 83.21Å 92.61Å 82.85° 89.72° 71.40°	Depositor
Resolution (Å)	40.06 – 3.18 40.06 – 3.18	Depositor EDS
% Data completeness (in resolution range)	90.7 (40.06-3.18) 86.9 (40.06-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.212 , 0.263 0.220 , 0.269	Depositor DCC
R_{free} test set	1849 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	88.7	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 89.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9194	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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, CL

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	C	0.23	0/1683	0.41	0/2289
1	D	0.24	0/1470	0.46	0/1998
2	A	0.27	0/1604	0.51	0/2203
2	H	0.29	0/1564	0.51	0/2154
3	B	0.27	0/1550	0.49	0/2125
3	L	0.26	0/1495	0.47	0/2054
All	All	0.26	0/9366	0.47	0/12823

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	C	1654	0	1455	31	0
1	D	1441	0	1246	32	0
2	A	1562	0	1462	18	0
2	H	1522	0	1417	35	0
3	B	1513	0	1254	27	0
3	L	1458	0	1174	27	0
4	C	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	14	0	13	2	0
5	C	7	0	7	0	0
5	D	7	0	7	0	0
6	A	1	0	0	0	0
6	L	1	0	0	0	0
All	All	9194	0	8048	152	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 9.

All (152) 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:B:29:VAL:HG13	3:B:92:ASN:CB	1.67	1.20
3:B:169:ASP:OD2	3:B:171:THR:OG1	1.70	1.05
3:B:29:VAL:HG13	3:B:92:ASN:HB2	1.04	1.03
3:B:29:VAL:CG1	3:B:92:ASN:HB2	1.91	0.99
2:H:100:ASP:O	2:H:100:ASP:OD1	1.81	0.98
3:L:133:CYS:SG	3:L:147:TRP:CH2	2.60	0.94
1:C:154:LYS:HG2	1:D:28:PHE:CE1	2.07	0.89
2:A:32:THR:HG21	2:A:100:ASP:OD2	1.77	0.84
1:C:49:ILE:HG22	1:C:49:ILE:O	1.79	0.81
1:C:49:ILE:HG21	2:H:101:TYR:CD2	2.18	0.79
1:D:22:CYS:N	1:D:25:CYS:SG	2.59	0.76
3:B:169:ASP:CG	3:B:171:THR:HG1	1.89	0.74
1:C:183:LEU:HB3	1:C:216:PRO:HB2	1.70	0.73
1:D:49:ILE:HG22	1:D:49:ILE:O	1.88	0.72
3:B:169:ASP:OD2	3:B:171:THR:CG2	2.38	0.71
1:D:182:CYS:HA	1:D:246:ILE:HD11	1.73	0.71
3:B:169:ASP:OD2	3:B:171:THR:CB	2.38	0.71
1:C:154:LYS:HG2	1:D:28:PHE:CZ	2.25	0.71
1:C:231:TYR:HB2	1:C:248:TYR:HB2	1.72	0.70
1:D:23:ILE:HG23	1:D:29:VAL:HG21	1.73	0.69
1:D:49:ILE:HD11	2:A:104:TYR:OH	1.92	0.69
3:B:29:VAL:HG13	3:B:92:ASN:HB3	1.69	0.68
3:B:169:ASP:OD2	3:B:171:THR:HG23	1.94	0.68
1:C:49:ILE:HG23	1:C:52:ASN:HB2	1.77	0.67
1:C:49:ILE:HD11	2:H:104:TYR:OH	1.95	0.66
3:B:144:ASN:HB3	3:B:196:THR:HB	1.77	0.66
1:D:49:ILE:HG23	1:D:52:ASN:HB2	1.78	0.65
3:L:133:CYS:SG	3:L:147:TRP:CZ2	2.90	0.64

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:D:78:VAL:CG1	1:D:82:THR:HB	2.27	0.64
3:B:13:THR:HG21	3:B:19:VAL:HG22	1.80	0.62
1:C:49:ILE:HG22	1:C:53:VAL:HG23	1.81	0.62
1:C:49:ILE:O	1:C:49:ILE:CG2	2.46	0.62
3:B:54:ARG:NH2	3:B:60:ASP:OD1	2.33	0.62
2:H:29:ILE:HG12	2:H:53:PRO:HG3	1.82	0.61
3:B:47:LEU:HA	3:B:58:VAL:HG21	1.83	0.61
1:C:103:LYS:HA	1:C:107:PHE:HB2	1.83	0.60
2:H:170:ALA:HB2	2:H:179:LEU:HD23	1.84	0.60
2:A:93:VAL:HG22	2:A:110:THR:HG22	1.83	0.59
1:C:49:ILE:HG21	2:H:101:TYR:HD2	1.63	0.59
1:C:49:ILE:CG2	2:H:101:TYR:CD2	2.87	0.58
3:B:49:TYR:HB3	3:B:55:TYR:CZ	2.38	0.58
3:B:35:TRP:CD1	3:B:48:ILE:HD11	2.38	0.58
1:C:193:LEU:HD13	1:C:235:LEU:HD21	1.87	0.57
3:L:143:ILE:HD12	3:L:197:HIS:HD2	1.69	0.57
2:A:32:THR:CG2	2:A:100:ASP:OD2	2.50	0.57
1:D:237:THR:OG1	1:D:241:GLY:N	2.36	0.56
1:D:49:ILE:O	1:D:49:ILE:CG2	2.52	0.56
3:B:150:ASP:HA	3:B:190:SER:HB2	1.87	0.56
1:C:235:LEU:O	1:C:243:ALA:N	2.35	0.56
3:L:162:TRP:CE2	3:L:174:MET:HG3	2.41	0.55
1:D:24:LYS:HD2	1:D:62:SER:HA	1.87	0.54
2:H:20:LEU:HD22	2:H:109:THR:HG21	1.89	0.54
1:C:24:LYS:HD3	1:C:62:SER:HA	1.89	0.54
1:C:46:PRO:CD	2:H:100:ASP:OD2	2.56	0.54
1:D:130:GLN:HG3	1:D:134:LEU:HD23	1.89	0.53
3:L:29:VAL:HG11	3:L:33:VAL:HG23	1.90	0.53
3:B:75:ILE:HG12	3:B:78:VAL:HG12	1.91	0.53
1:C:163:LEU:HB3	1:C:245:VAL:HG22	1.89	0.53
2:H:145:LYS:HA	2:H:178:THR:HG22	1.91	0.53
3:L:143:ILE:HD12	3:L:197:HIS:CD2	2.43	0.53
1:D:49:ILE:HG22	1:D:53:VAL:HG23	1.91	0.53
2:A:154:VAL:HG22	2:A:199:VAL:HG22	1.91	0.53
2:H:146:GLY:H	2:H:178:THR:HG22	1.73	0.53
1:D:56:MET:SD	3:B:49:TYR:OH	2.66	0.52
3:B:63:THR:OG1	3:B:74:THR:OG1	2.27	0.52
3:B:162:TRP:CD1	3:B:174:MET:HG3	2.45	0.52
1:D:182:CYS:N	1:D:216:PRO:O	2.43	0.52
3:L:197:HIS:ND1	3:L:198:LYS:N	2.57	0.51
2:H:171:VAL:O	2:H:171:VAL:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:ILE:HG21	2:A:101:TYR:CD2	2.45	0.51
3:L:144:ASN:O	3:L:196:THR:N	2.42	0.51
2:H:126:LEU:HD13	3:L:132:VAL:HG21	1.92	0.51
1:C:49:ILE:HD13	2:H:101:TYR:O	2.10	0.50
3:L:197:HIS:ND1	3:L:199:THR:N	2.55	0.50
1:C:198:PHE:CB	1:C:233:CYS:HA	2.42	0.49
2:H:149:PRO:HD2	2:H:203:ALA:HB1	1.95	0.49
2:H:50:ARG:NH1	3:L:94:TYR:OH	2.44	0.48
1:C:198:PHE:HB2	1:C:233:CYS:HA	1.96	0.48
1:D:56:MET:SD	1:D:112:LEU:HD11	2.53	0.48
2:A:87:THR:OG1	2:A:88:SER:N	2.47	0.48
3:L:111:ALA:HA	3:L:199:THR:HG21	1.95	0.48
1:D:100:SER:OG	1:D:101:ASP:N	2.46	0.47
2:H:121:PRO:HB3	2:H:147:TYR:HB3	1.94	0.47
2:A:142:CYS:HB2	2:A:156:TRP:CH2	2.49	0.47
1:D:49:ILE:HD12	2:A:98:ARG:NH2	2.30	0.47
2:H:71:THR:HG23	2:H:80:TYR:HB2	1.95	0.47
1:C:139:CYS:SG	1:C:140:GLY:N	2.88	0.47
1:C:104:GLY:HA2	2:H:100:ASP:HB3	1.97	0.47
2:H:30:LYS:HA	2:H:53:PRO:HG2	1.97	0.47
3:B:79:GLN:HB2	3:B:81:GLU:HG2	1.97	0.46
2:H:143:LEU:HA	2:H:180:SER:HB3	1.97	0.46
3:L:49:TYR:CZ	3:L:53:TYR:HB3	2.51	0.46
2:H:16:ALA:O	2:H:86:LEU:HB2	2.15	0.46
2:A:6:GLN:H	2:A:107:GLN:HE22	1.62	0.46
2:H:101:TYR:CD2	2:H:101:TYR:O	2.69	0.46
3:L:10:PHE:HB2	3:L:103:LYS:O	2.15	0.46
3:L:140:PRO:HG2	3:L:197:HIS:HE1	1.81	0.45
2:A:35:HIS:CE1	2:A:50:ARG:HB2	2.52	0.45
3:B:50:SER:C	3:B:52:SER:H	2.19	0.45
3:B:165:GLN:NE2	3:B:170:SER:O	2.44	0.45
1:C:198:PHE:HB2	1:C:232:ARG:O	2.17	0.44
3:L:117:PHE:HB2	3:L:132:VAL:HG22	1.99	0.44
2:H:67:LYS:HE2	2:H:90:ASP:OD1	2.17	0.44
2:H:154:VAL:HG22	2:H:199:VAL:HG22	1.99	0.44
1:D:49:ILE:CG2	2:A:101:TYR:CD2	3.00	0.44
2:H:33:TYR:CD1	2:H:52:ASP:HB3	2.52	0.44
2:H:137:MET:HG2	2:H:186:PRO:HA	2.00	0.44
3:B:49:TYR:O	3:B:91:TYR:OH	2.22	0.44
2:H:189:THR:O	2:H:193:GLU:N	2.39	0.44
1:C:130:GLN:HA	1:C:134:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:197:HIS:CG	3:L:198:LYS:H	2.37	0.43
3:B:78:VAL:O	3:B:79:GLN:NE2	2.50	0.43
1:D:102:LEU:HD22	1:D:106:LEU:HD13	2.01	0.43
2:A:121:PRO:HB3	2:A:147:TYR:HB3	2.01	0.43
2:A:37:VAL:HG22	2:A:95:TYR:HB2	2.00	0.43
1:D:130:GLN:HA	1:D:134:LEU:HB3	2.01	0.42
2:H:38:LYS:HG2	2:H:46:GLU:HB2	2.01	0.42
2:H:153:THR:HB	2:H:200:ALA:HB3	2.01	0.42
1:D:137:ASN:HB3	1:D:186:TRP:CD1	2.55	0.42
3:L:6:GLN:HG2	3:L:23:CYS:HB2	2.01	0.42
3:L:60:ASP:N	3:L:60:ASP:OD1	2.53	0.42
1:C:46:PRO:HD2	2:H:100:ASP:OD2	2.19	0.42
1:C:140:GLY:HA3	1:C:244:THR:HG22	2.02	0.42
1:D:77:ALA:C	1:D:78:VAL:HG23	2.41	0.41
1:C:93:ASP:OD1	1:C:96:ARG:NH2	2.52	0.41
1:D:93:ASP:OD2	1:D:118:GLN:NE2	2.53	0.41
2:H:123:VAL:HG22	2:H:144:VAL:HG12	2.01	0.41
3:L:20:SER:HA	3:L:74:THR:HA	2.03	0.41
3:L:145:VAL:HA	3:L:195:ALA:HA	2.02	0.41
3:L:197:HIS:CG	3:L:198:LYS:N	2.89	0.41
4:D:301:NAG:O7	4:D:301:NAG:O4	2.18	0.41
3:L:32:ASN:HB2	3:L:92:ASN:HB2	2.03	0.41
1:D:45:LEU:HD13	1:D:53:VAL:HG21	2.02	0.41
1:C:234:VAL:HG22	1:C:245:VAL:HG12	2.03	0.41
1:D:104:GLY:HA2	2:A:100:ASP:HB3	2.03	0.41
1:D:204:ASN:OD1	4:D:301:NAG:H2	2.21	0.41
3:L:47:LEU:HA	3:L:58:VAL:HG21	2.03	0.41
2:A:120:PRO:HB3	2:A:206:THR:HG21	2.02	0.41
1:C:45:LEU:HD13	1:C:53:VAL:HG21	2.02	0.41
1:D:100:SER:OG	1:D:102:LEU:HG	2.21	0.41
2:H:60:TYR:HE1	2:H:70:ILE:HG13	1.85	0.41
2:H:98:ARG:O	2:H:103:VAL:HA	2.20	0.41
3:B:165:GLN:HB2	3:B:172:TYR:CZ	2.55	0.41
1:C:41:LEU:HD22	1:C:45:LEU:HD12	2.03	0.40
2:H:86:LEU:HG	2:H:113:VAL:HG21	2.03	0.40
3:L:21:VAL:N	3:L:73:LEU:O	2.52	0.40
3:L:192:THR:HG22	3:L:207:SER:HB2	2.03	0.40
2:A:102:GLY:HA2	3:B:55:TYR:CZ	2.55	0.40
1:D:78:VAL:HG12	1:D:82:THR:HB	2.04	0.40
2:A:144:VAL:HG11	2:A:152:VAL:HG11	2.03	0.40
1:D:63:SER:O	1:D:66:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2:ILE:HD12	3:L:90:GLN:NE2	2.37	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	C	212/238 (89%)	200 (94%)	12 (6%)	0	100	100
1	D	181/238 (76%)	174 (96%)	7 (4%)	0	100	100
2	A	208/217 (96%)	200 (96%)	7 (3%)	1 (0%)	25	58
2	H	204/217 (94%)	197 (97%)	7 (3%)	0	100	100
3	B	208/213 (98%)	200 (96%)	7 (3%)	1 (0%)	25	58
3	L	207/213 (97%)	199 (96%)	8 (4%)	0	100	100
All	All	1220/1336 (91%)	1170 (96%)	48 (4%)	2 (0%)	44	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	51	ALA
2	A	101	TYR

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	C	165/218 (76%)	165 (100%)	0	100	100
1	D	137/218 (63%)	137 (100%)	0	100	100
2	A	169/186 (91%)	168 (99%)	1 (1%)	84	92
2	H	163/186 (88%)	163 (100%)	0	100	100
3	B	148/190 (78%)	148 (100%)	0	100	100
3	L	132/190 (70%)	132 (100%)	0	100	100
All	All	914/1188 (77%)	913 (100%)	1 (0%)	92	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	76	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	166	HIS
3	B	197	HIS

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 ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PRO	C	302	-	6,7,8	0.64	0	7,8,10	1.33	1 (14%)
4	NAG	C	301	-	14,14,15	0.18	0	17,19,21	0.43	0
5	PRO	D	302	-	6,7,8	0.64	0	7,8,10	1.31	1 (14%)
4	NAG	D	301	1	14,14,15	0.86	1 (7%)	17,19,21	1.07	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PRO	C	302	-	-	0/0/9/11	0/1/1/1
4	NAG	C	301	-	-	2/6/23/26	0/1/1/1
5	PRO	D	302	-	-	0/0/9/11	0/1/1/1
4	NAG	D	301	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	NAG	O5-C1	-2.82	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	302	PRO	O-C-CA	-2.49	118.37	124.77
5	D	302	PRO	O-C-CA	-2.41	118.57	124.77
4	D	301	NAG	C2-N2-C7	2.23	125.89	122.90
4	D	301	NAG	C4-C3-C2	2.22	114.27	111.02
4	D	301	NAG	C3-C4-C5	2.20	114.22	110.23

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	301	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	D	301	NAG	O5-C5-C6-O6
4	C	301	NAG	O5-C5-C6-O6
4	C	301	NAG	C4-C5-C6-O6
4	D	301	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	301	NAG	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	C	224/238 (94%)	0.19	7 (3%)	51	35	66, 114, 204, 281	0
1	D	193/238 (81%)	0.21	8 (4%)	42	27	72, 113, 198, 246	0
2	A	212/217 (97%)	-0.21	2 (0%)	81	67	53, 80, 137, 199	0
2	H	208/217 (95%)	-0.11	3 (1%)	73	58	55, 79, 125, 175	0
3	B	210/213 (98%)	0.14	4 (1%)	66	50	63, 99, 153, 172	0
3	L	209/213 (98%)	0.21	5 (2%)	59	43	44, 100, 147, 189	0
All	All	1256/1336 (94%)	0.07	29 (2%)	61	44	44, 96, 180, 281	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	147	TRP	3.6
3	L	161	SER	3.5
1	D	240	GLN	3.5
1	D	195	ASP	3.3
1	C	102	LEU	3.0
2	H	166	HIS	2.9
3	B	109	ASP	2.9
2	A	214	PRO	2.8
1	C	194	THR	2.6
1	D	68	THR	2.6
2	H	128	PRO	2.5
3	B	52	SER	2.5
3	L	133	CYS	2.5
1	D	28	PHE	2.3
3	L	130	SER	2.3
1	C	72	ASP	2.3
1	D	22	CYS	2.2
2	A	140	LEU	2.2
3	L	53	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	231	TYR	2.2
1	C	75	LEU	2.1
1	D	182	CYS	2.1
2	H	171	VAL	2.1
1	D	183	LEU	2.1
1	C	68	THR	2.0
1	C	221	SER	2.0
1	D	194	THR	2.0
3	B	30	ASP	2.0
3	B	162	TRP	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	NAG	D	301	14/15	0.40	0.13	172,199,205,211	0
4	NAG	C	301	14/15	0.83	0.13	145,171,180,184	0
5	PRO	D	302	7/8	0.85	0.19	128,132,144,147	0
5	PRO	C	302	7/8	0.87	0.11	76,91,116,116	0
6	CL	L	301	1/1	0.87	0.13	90,90,90,90	0
6	CL	A	301	1/1	0.88	0.17	84,84,84,84	0

6.5 Other polymers (i)

There are no such residues in this entry.