



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 09:53 AM BST

PDB ID : 5U8R
Title : Structure of the ectodomain of the human Type 1 insulin-like growth factor receptor
Authors : Lawrence, M.; Xu, Y.
Deposited on : 2016-12-14
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

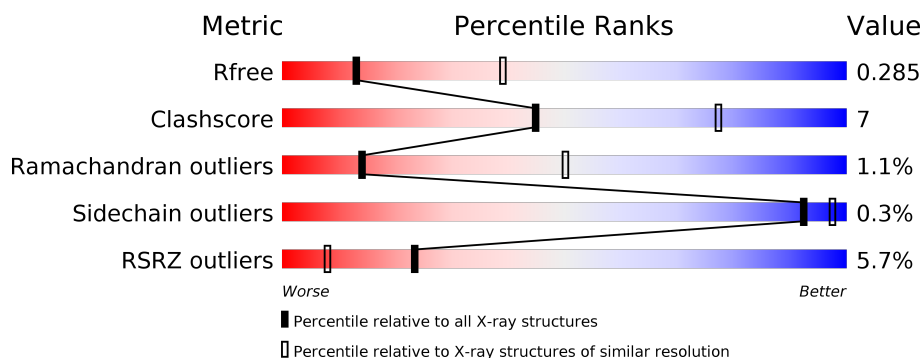
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	885	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>9%</div> </div> </div>
2	H	126	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>6%</div> </div> </div>
3	L	108	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>
4	B	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
4	C	2	<div> <div></div> <div>100%</div> </div>

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
6	MLT	A	1003	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8334 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 Insulin-like growth factor 1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	801	Total	C	N	O	S	0	1	0
			6454	4082	1120	1206	46			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP P08069
A	?	-	THR	deletion	UNP P08069
A	?	-	MET	deletion	UNP P08069
A	?	-	SER	deletion	UNP P08069
A	?	-	SER	deletion	UNP P08069
A	?	-	ARG	deletion	UNP P08069
A	?	-	SER	deletion	UNP P08069
A	?	-	ARG	deletion	UNP P08069
A	?	-	ASN	deletion	UNP P08069
A	?	-	THR	deletion	UNP P08069
A	?	-	THR	deletion	UNP P08069
A	?	-	ALA	deletion	UNP P08069
A	?	-	ALA	deletion	UNP P08069
A	?	-	ASP	deletion	UNP P08069
A	?	-	THR	deletion	UNP P08069
A	?	-	TYR	deletion	UNP P08069
A	?	-	ASN	deletion	UNP P08069
A	?	-	ILE	deletion	UNP P08069
A	?	-	THR	deletion	UNP P08069
A	?	-	ASP	deletion	UNP P08069
A	738	ALA	PRO	conflict	UNP P08069
A	739	GLY	GLU	conflict	UNP P08069
A	740	ASN	GLU	conflict	UNP P08069
A	741	ASN	LEU	conflict	UNP P08069

- Molecule 2 is a protein called Fv 24-60 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	118	Total	C	N	O	S	0	0	0
			916	582	150	181	3			

- Molecule 3 is a protein called Fv 24-60 light chain.

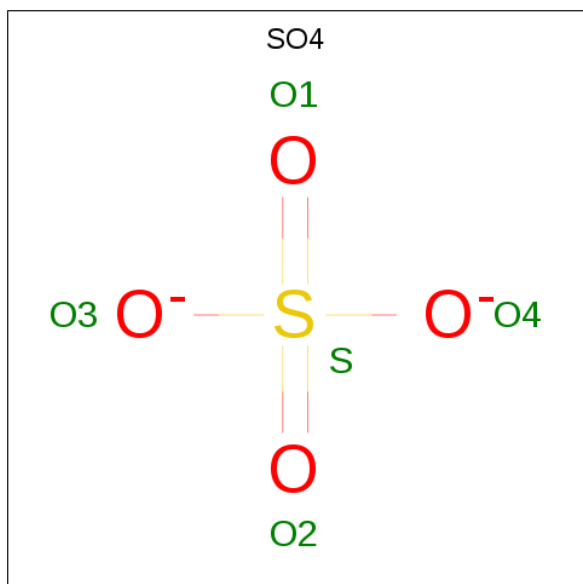
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	108	Total	C	N	O	S	0	0	0
			824	513	141	167	3			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



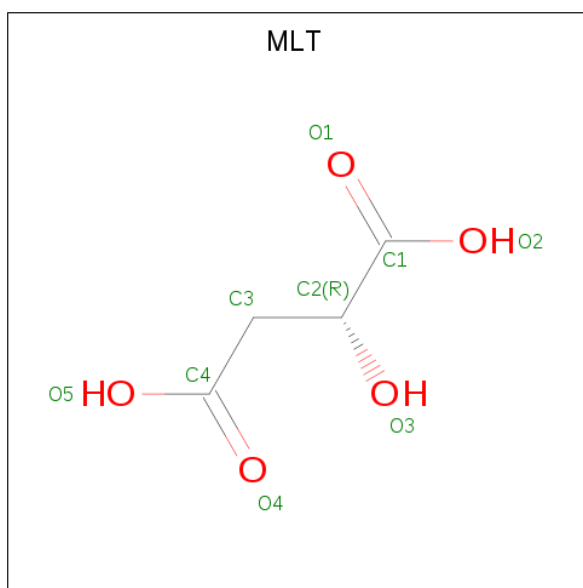
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



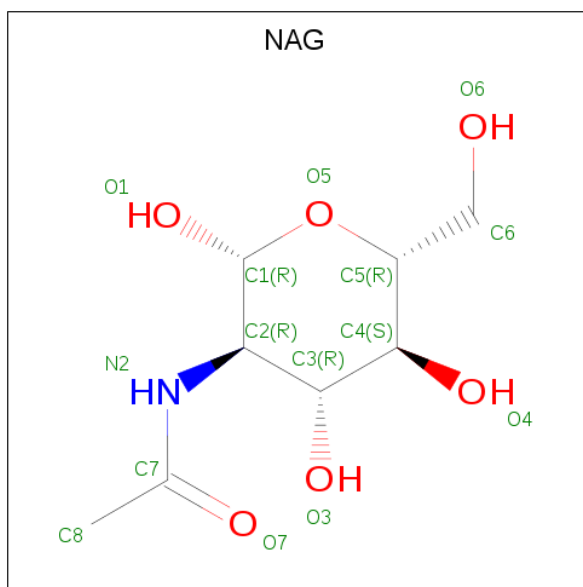
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$).



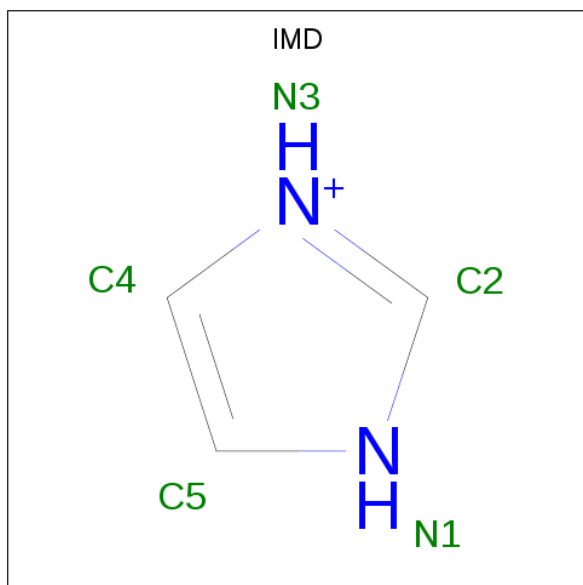
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	4	5		
6	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



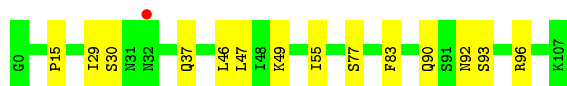
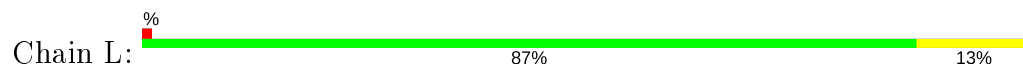
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	H	1	Total	C	N	0	0
			5	3	2		

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.

- [illegible]

- Chain H:
-
- | Position | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |
|---------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Residue | GLY | T | Q | S | A | A | V | N | T | K | Y | A | S | N | L | T | P | E | G | GLN |
| Conservation (bits) | 1.9 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.8 | 0.1 | 0.1 | 0.4 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 1.9 |

- Molecule 3: Fv 24-60 light chain



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.03Å 201.73Å 117.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.36 – 3.00 48.58 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.36-3.00) 99.8 (48.58-3.00)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.01Å)	Xtriage
Refinement program	phenix.refine 1.11.1-2575_1692, PHENIX 1.11.1-2575_1692	Depositor
R, R_{free}	0.256 , 0.285 0.256 , 0.285	Depositor DCC
R_{free} test set	2166 reflections (4.71%)	wwPDB-V
Wilson B-factor (Å ²)	92.4	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 96.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8334	wwPDB-V
Average B, all atoms (Å ²)	133.0	wwPDB-V

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, IMD, MLT, 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	0.24	0/6610	0.44	0/8961
2	H	0.24	0/937	0.44	0/1272
3	L	0.24	0/842	0.44	0/1141
All	All	0.24	0/8389	0.44	0/11374

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	6454	0	6271	93	0
2	H	916	0	890	9	0
3	L	824	0	795	8	0
4	B	28	0	25	2	0
4	C	28	0	25	0	0
5	A	5	0	0	0	0
6	A	18	0	8	0	0
7	A	56	0	52	0	0
8	H	5	0	5	0	0
All	All	8334	0	8071	107	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 7.

All (107) 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:A:874:ARG:HE	1:A:889:PRO:HG3	1.54	0.73
1:A:615:ILE:HD11	1:A:749:GLU:HG2	1.71	0.73
1:A:433:GLU:HA	1:A:436:THR:HB	1.71	0.72
1:A:517:ASN:HB3	1:A:519:TRP:HD1	1.58	0.68
1:A:348:MET:HA	1:A:351:ILE:HD13	1.75	0.68
1:A:626:TYR:O	1:A:628:TYR:N	2.28	0.65
1:A:173:TYR:O	1:A:174:ARG:NH1	2.30	0.65
1:A:700:ILE:HD12	1:A:784:GLY:HA3	1.79	0.64
1:A:126:ASP:HB2	1:A:174:ARG:HD2	1.80	0.64
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.80	0.63
2:H:67:LYS:NZ	2:H:85:ARG:O	2.32	0.62
1:A:503:LYS:O	1:A:573:TYR:OH	2.13	0.62
1:A:256:LEU:O	2:H:55:ASN:ND2	2.33	0.61
1:A:9:ILE:HD13	1:A:16:LEU:HA	1.83	0.61
1:A:308:THR:HG22	1:A:329:ASN:HD22	1.66	0.60
1:A:628:TYR:O	1:A:853:GLN:NE2	2.34	0.60
1:A:222:ARG:NH1	4:B:1:NAG:O6	2.34	0.60
1:A:863:LEU:HB3	1:A:866:LEU:HD11	1.84	0.59
1:A:89:ILE:HG23	1:A:92:MET:HG3	1.84	0.59
1:A:129:LEU:HD11	1:A:182:GLN:HE21	1.68	0.58
3:L:29:ILE:HG23	3:L:92:ASN:HD22	1.69	0.57
2:H:97:ALA:HB1	2:H:105:MET:HB3	1.86	0.56
2:H:6:GLN:H	2:H:110:GLN:HE22	1.52	0.56
1:A:562:ASP:O	1:A:563:HIS:ND1	2.37	0.55
1:A:584:PRO:HG2	1:A:773:ILE:HG22	1.87	0.55
1:A:392:VAL:HG23	1:A:421:ASN:HD21	1.72	0.55
1:A:386:GLY:O	1:A:415:LYS:NZ	2.36	0.54
1:A:595:SER:HA	1:A:763:LEU:HB2	1.90	0.54
1:A:485:PRO:HG3	1:A:565:ARG:HB3	1.89	0.53
1:A:31:ILE:HB	1:A:57:LEU:HD23	1.91	0.53
1:A:8:ASP:HA	1:A:30:HIS:HB2	1.90	0.53
1:A:617:ARG:HG2	1:A:749:GLU:HG3	1.91	0.52
1:A:189:CYS:O	1:A:192:ARG:NH1	2.33	0.52
1:A:48:LEU:HD21	1:A:51:ILE:HD11	1.92	0.52
1:A:64:GLU:HB3	1:A:96:LYS:HE2	1.92	0.51
1:A:831:LEU:HD11	1:A:852:ARG:HE	1.75	0.51
1:A:778:HIS:CD2	1:A:779:GLU:HG2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:THR:HG22	1:A:535:GLY:HA3	1.93	0.50
1:A:561:ASN:O	1:A:563:HIS:N	2.44	0.50
1:A:526:LEU:HD12	1:A:527:PRO:HD2	1.94	0.50
1:A:832:ILE:HD12	1:A:877:ALA:HB1	1.94	0.50
1:A:325:ILE:HG23	1:A:353:VAL:HB	1.95	0.49
1:A:87:LEU:HB3	1:A:111:ILE:HD12	1.94	0.49
1:A:244:TRP:CZ2	1:A:245:ARG:HD3	2.48	0.49
1:A:615:ILE:HG23	1:A:774:HIS:HB2	1.93	0.48
3:L:90:GLN:HE22	3:L:92:ASN:ND2	2.12	0.48
1:A:774:HIS:NE2	1:A:788:SER:HB3	2.28	0.48
1:A:256:LEU:HD21	2:H:59:LYS:HB2	1.96	0.47
1:A:81:LEU:HD11	1:A:108:ARG:HG2	1.96	0.47
1:A:598:ILE:HG22	1:A:759:VAL:HG22	1.96	0.47
1:A:295:GLU:OE1	1:A:295:GLU:N	2.40	0.47
1:A:813:ARG:HB3	1:A:814:PRO:HD2	1.96	0.47
1:A:427:SER:O	1:A:431:ARG:HG2	2.15	0.47
3:L:90:GLN:NE2	3:L:93:SER:H	2.12	0.47
1:A:495:VAL:HG22	1:A:551:VAL:HG12	1.97	0.46
1:A:324:THR:HG23	1:A:325:ILE:HG13	1.96	0.46
3:L:46:LEU:HD21	3:L:49:LYS:HG3	1.97	0.46
1:A:34:ILE:HB	1:A:60:VAL:HG13	1.98	0.46
1:A:72:ASN:HA	1:A:102:ASN:HD22	1.80	0.46
1:A:360:ILE:HB	1:A:392:VAL:HG12	1.98	0.46
1:A:878:THR:HA	1:A:883:ASN:HA	1.98	0.46
1:A:831:LEU:HD11	1:A:852:ARG:NE	2.32	0.45
2:H:40:SER:OG	2:H:42:ALA:O	2.29	0.45
1:A:582:SER:HB3	1:A:604:PRO:HB2	1.97	0.45
1:A:463:LEU:HB2	1:A:569:SER:HB2	1.99	0.44
1:A:126:ASP:OD1	1:A:128:SER:OG	2.29	0.44
1:A:262:ASP:OD1	1:A:262:ASP:N	2.50	0.44
1:A:425:CYS:SG	1:A:456:ALA:HB1	2.58	0.44
1:A:127:TRP:HE3	1:A:130:ILE:HD11	1.82	0.44
1:A:30:HIS:HB3	1:A:32:LEU:HD13	1.99	0.44
1:A:77:ARG:NH2	1:A:221:CYS:O	2.35	0.44
1:A:128:SER:HA	1:A:134:VAL:HG21	1.99	0.43
1:A:352:GLU:HG2	1:A:374:ASN:HB3	2.01	0.43
1:A:438:THR:HG22	1:A:441:ARG:CZ	2.47	0.43
1:A:786:SER:OG	1:A:787:ALA:N	2.51	0.43
1:A:52:THR:HG21	1:A:244:TRP:CD1	2.53	0.43
1:A:544:TRP:N	1:A:577:ASN:O	2.52	0.43
1:A:611:LEU:O	1:A:613:TYR:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:15:PRO:HG3	3:L:83:PHE:HE2	1.84	0.43
1:A:353:VAL:HG22	1:A:377:LEU:HB2	2.01	0.43
1:A:323:CYS:HB2	1:A:351:ILE:HD11	2.00	0.43
1:A:32:LEU:HD11	1:A:56:LEU:HD22	2.01	0.42
1:A:416:MET:HB3	1:A:418:PHE:HE1	1.84	0.42
1:A:507:GLU:HG2	1:A:568:LYS:NZ	2.34	0.42
1:A:436:THR:HG22	1:A:438:THR:HG23	2.01	0.42
1:A:10:ARG:HA	1:A:32:LEU:O	2.19	0.42
1:A:820:LEU:HD12	1:A:837:ILE:HD13	2.00	0.42
1:A:29:LEU:HD23	1:A:55:LEU:HD13	2.01	0.42
1:A:872:THR:HG22	1:A:891:PHE:HD1	1.85	0.42
2:H:47:TRP:HB3	3:L:96:ARG:O	2.20	0.42
1:A:206:LEU:HB2	1:A:222:ARG:HB3	2.02	0.42
1:A:80:LYS:HD3	1:A:80:LYS:HA	1.78	0.42
1:A:329:ASN:OD1	1:A:356:GLY:HA3	2.20	0.41
2:H:101:ASP:OD1	2:H:101:ASP:N	2.52	0.41
2:H:58:THR:HG1	2:H:60:TYR:HE1	1.67	0.41
1:A:193:ALA:HB3	1:A:201:CYS:HB2	2.02	0.41
1:A:504:ASN:N	1:A:504:ASN:OD1	2.54	0.41
1:A:208:SER:OG	1:A:209:CYS:N	2.53	0.41
1:A:327:LYS:HD3	1:A:355:THR:HG21	2.02	0.41
3:L:49:LYS:HG3	3:L:55:ILE:HD11	2.02	0.41
1:A:824:GLU:HB2	1:A:855:TYR:CE2	2.56	0.41
1:A:177:THR:HG23	1:A:180:ARG:H	1.85	0.41
1:A:114:GLU:HA	1:A:140:VAL:O	2.21	0.41
1:A:250:ASP:O	1:A:254:ASN:ND2	2.52	0.41
1:A:618:TRP:HA	1:A:770:ARG:O	2.21	0.41
1:A:378:ILE:O	1:A:411:ILE:HA	2.21	0.41
1:A:107:THR:HG23	4:B:1:NAG:H5	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	790/885 (89%)	727 (92%)	54 (7%)	9 (1%)	14	50
2	H	116/126 (92%)	110 (95%)	6 (5%)	0	100	100
3	L	106/108 (98%)	97 (92%)	7 (7%)	2 (2%)	8	36
All	All	1012/1119 (90%)	934 (92%)	67 (7%)	11 (1%)	14	50

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	451	ASN
1	A	562	ASP
1	A	612	SER
3	L	30	SER
1	A	458	CYS
1	A	539	HIS
1	A	627	LEU
3	L	77	SER
1	A	504	ASN
1	A	380	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	719/787 (91%)	716 (100%)	3 (0%)	91	97
2	H	100/107 (94%)	100 (100%)	0	100	100
3	L	95/95 (100%)	95 (100%)	0	100	100
All	All	914/989 (92%)	911 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ASP
1	A	273	CYS

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Mol	Chain	Res	Type
1	A	294	CYS

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

Mol	Chain	Res	Type
1	A	102	ASN
3	L	92	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](#)

4 monosaccharides 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	NAG	B	1	1,4	14,14,15	0.24	0	17,19,21	0.41	0
4	NAG	B	2	4	14,14,15	0.30	0	17,19,21	0.50	0
4	NAG	C	1	1,4	14,14,15	0.30	0	17,19,21	0.53	0
4	NAG	C	2	4	14,14,15	0.26	0	17,19,21	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
4	NAG	B	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	1/6/23/26	0/1/1/1
4	NAG	C	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2	NAG	O5-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
4	B	1	NAG	O5-C5-C6-O6
4	B	1	NAG	C4-C5-C6-O6
4	B	2	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	NAG	2	0

5.6 Ligand geometry

8 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	$\# Z > 2$
7	NAG	A	1004	1	14,14,15	0.29	0	17,19,21	0.54	0
8	IMD	H	201	-	3,5,5	0.42	0	4,5,5	0.57	0
7	NAG	A	1011	1	14,14,15	0.31	0	17,19,21	0.49	0
7	NAG	A	1010	1	14,14,15	0.24	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MLT	A	1003	-	2,8,8	0.47	0	3,10,10	0.82	0
5	SO4	A	1001	-	4,4,4	0.14	0	6,6,6	0.05	0
7	NAG	A	1007	1	14,14,15	0.21	0	17,19,21	0.41	0
6	MLT	A	1002	-	2,8,8	0.49	0	3,10,10	0.94	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
7	NAG	A	1004	1	-	1/6/23/26	0/1/1/1
8	IMD	H	201	-	-	-	0/1/1/1
7	NAG	A	1011	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1010	1	-	0/6/23/26	0/1/1/1
6	MLT	A	1003	-	-	2/2/8/8	-
7	NAG	A	1007	1	-	2/6/23/26	0/1/1/1
6	MLT	A	1002	-	-	0/2/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1003	MLT	C1-C2-C3-C4
6	A	1003	MLT	O3-C2-C3-C4
7	A	1011	NAG	C4-C5-C6-O6
7	A	1011	NAG	O5-C5-C6-O6
7	A	1007	NAG	O5-C5-C6-O6
7	A	1007	NAG	C4-C5-C6-O6
7	A	1004	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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	A	801/885 (90%)	0.54	56 (6%) 16 5	80, 137, 191, 258	0
2	H	118/126 (93%)	0.27	2 (1%) 70 41	75, 109, 148, 180	0
3	L	108/108 (100%)	0.22	1 (0%) 84 63	77, 111, 137, 170	0
All	All	1027/1119 (91%)	0.48	59 (5%) 23 8	75, 128, 187, 258	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	GLU	5.6
1	A	287	GLN	5.5
1	A	338	ASN	4.3
1	A	198	ASN	4.2
1	A	296	GLY	3.7
1	A	641	ARG	3.5
1	A	620	ARG	3.3
1	A	200	CYS	3.2
1	A	799	GLU	3.1
1	A	808	VAL	3.1
1	A	237	ASN	3.1
1	A	592	ASN	3.0
1	A	880	LEU	3.0
1	A	798	ALA	2.9
1	A	13	TYR	2.9
1	A	189	CYS	2.9
1	A	222	ARG	2.9
1	A	410	THR	2.8
1	A	337	GLY	2.8
1	A	187	SER	2.8
1	A	638	ILE	2.7
1	A	168	ASN	2.7
1	A	197	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	416	MET	2.7
1	A	746	PRO	2.7
1	A	208	SER	2.6
1	A	831	LEU	2.6
1	A	173	TYR	2.6
1	A	639	PRO	2.6
1	A	203	PRO	2.5
1	A	842	GLN	2.5
1	A	517	ASN	2.5
1	A	188	THR	2.5
1	A	409	LEU	2.5
1	A	93	THR	2.5
1	A	212	PRO	2.5
1	A	186	PRO	2.4
1	A	757	ARG	2.4
1	A	685	GLU	2.4
1	A	169	ASN	2.3
1	A	94	ASN	2.3
1	A	405	ASP	2.3
1	A	297	PRO	2.3
1	A	818	ILE	2.3
1	A	408	ASN	2.2
2	H	41	HIS	2.2
1	A	640	ILE	2.2
1	A	211	ALA	2.2
1	A	286	SER	2.1
1	A	344	LEU	2.1
1	A	171	TYR	2.1
1	A	330	LEU	2.1
2	H	68	ALA	2.1
1	A	190	GLY	2.1
1	A	807	PRO	2.0
1	A	877	ALA	2.0
1	A	406	HIS	2.0
1	A	559	VAL	2.0
3	L	32	ASN	2.0

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

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

6.3 Carbohydrates [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
4	NAG	C	2	14/15	0.80	0.17	127,152,163,165	0
4	NAG	B	1	14/15	0.81	0.18	116,137,146,148	0
4	NAG	B	2	14/15	0.82	0.30	159,181,191,191	0
4	NAG	C	1	14/15	0.94	0.13	87,107,121,138	0

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
6	MLT	A	1003	9/9	0.41	0.61	104,136,146,147	0
7	NAG	A	1011	14/15	0.73	0.36	114,156,162,167	0
7	NAG	A	1004	14/15	0.75	0.23	126,151,165,167	0
7	NAG	A	1010	14/15	0.81	0.19	106,148,155,158	0
7	NAG	A	1007	14/15	0.83	0.40	129,144,153,153	0
6	MLT	A	1002	9/9	0.83	0.21	99,114,136,137	0
8	IMD	H	201	5/5	0.86	0.21	89,92,99,103	0
5	SO4	A	1001	5/5	0.88	0.17	120,145,158,159	0

6.5 Other polymers [i](#)

There are no such residues in this entry.