



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:11 PM GMT

PDB ID : 1J86
Title : HUMAN HIGH AFFINITY FC RECEPTOR FC(EPSILON)RI(ALPHA),
MONOCLINIC CRYSTAL FORM 2
Authors : Garman, S.C.; Sechi, S.; Kinet, J.P.; Jardetzky, T.S.
Deposited on : 2001-05-20
Resolution : 3.20 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

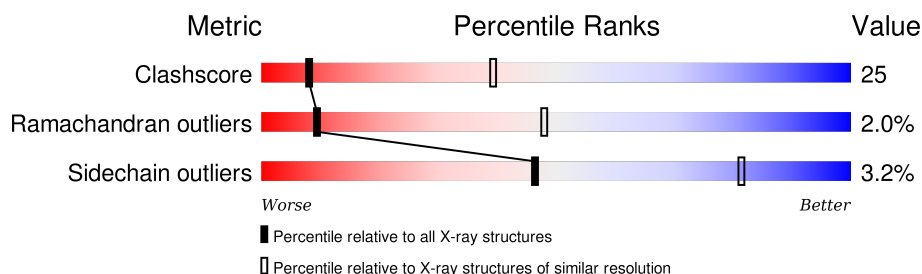
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	176	 <div>49%</div> <div>48%</div> <div>..</div>
1	B	176	 <div>55%</div> <div>41%</div> <div>..</div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3131 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 HIGH AFFINITY IMMUNOGLOBULIN EPSILON RECEPTOR ALPHA-SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1427	913	235	274	5			
1	B	173	Total	C	N	O	S	0	0	0
			1416	907	231	273	5			

- Molecule 2 is a polymer of unknown type called SUGAR (NAG-NAG).

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

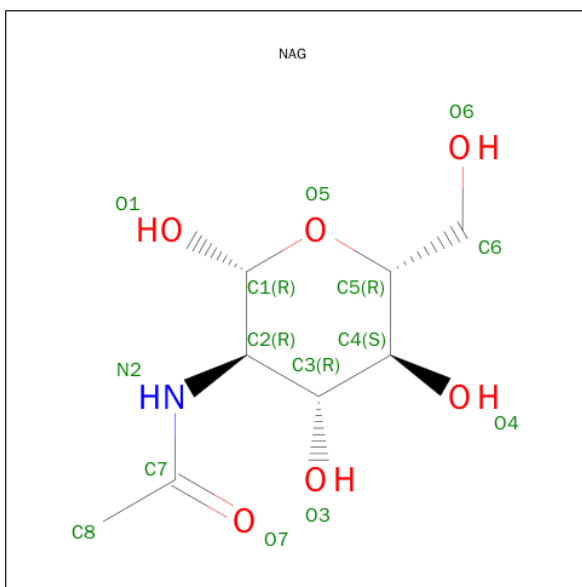
- Molecule 3 is a polymer of unknown type called SUGAR (NAG-NAG-MAN-MAN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	4	Total	C	N	O	0	0
			50	28	2	20		
3	B	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 is a polymer of unknown type called SUGAR (NAG-FUC-NAG).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is a polymer of unknown type called SUGAR (NAG-NAG-FUC).

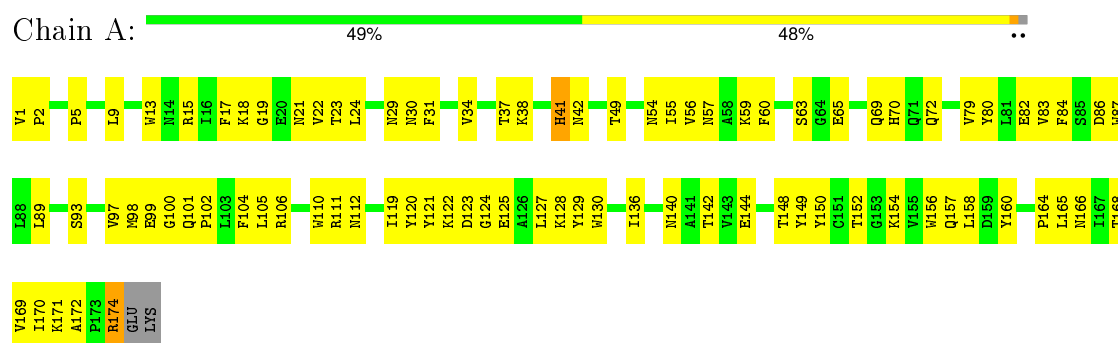
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	3	Total	C	N	O	0	0
			38	22	2	14		

3 Residue-property plots

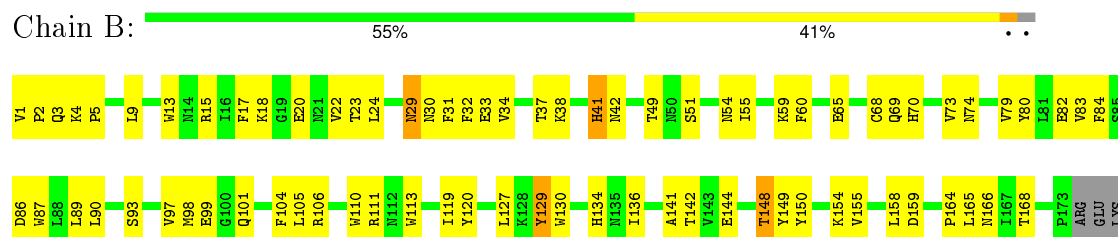
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: HIGH AFFINITY IMMUNOGLOBULIN EPSILON RECEPTOR ALPHA-SUBUNIT



• Molecule 1: HIGH AFFINITY IMMUNOGLOBULIN EPSILON RECEPTOR ALPHA-SUBUNIT



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.90 Å 73.79 Å 79.40 Å 90.00° 117.74° 90.00°	Depositor
Resolution (Å)	22.65 – 3.20	Depositor
% Data completeness (in resolution range)	99.5 (22.65-3.20)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.245 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3131	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

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: FCA, BMA, NAG, MAN

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	0.43	0/1469	0.64	0/2002
1	B	0.41	0/1458	0.64	0/1988
All	All	0.42	0/2927	0.64	0/3990

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	129	TYR	Sidechain

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	A	1427	0	1341	77	0
1	B	1416	0	1328	64	0
2	A	28	0	25	3	0
2	B	28	0	25	3	0
3	A	50	0	43	3	0
3	B	50	0	43	7	0
4	A	38	0	34	1	0
5	A	28	0	26	1	0
5	B	28	0	26	2	0
6	B	38	0	34	1	0
All	All	3131	0	2925	149	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 25.

All (149) 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:B:20:GLU:HA	5:B:221:NAG:H82	1.43	0.97
1:A:2:PRO:HB2	1:A:29:ASN:HD21	1.29	0.97
2:B:340:NAG:H61	2:B:341:NAG:H2	1.53	0.89
2:B:340:NAG:C6	2:B:341:NAG:H2	2.08	0.82
1:A:98:MET:HE1	1:A:170:ILE:HG13	1.61	0.82
1:A:72:GLN:O	4:A:274:NAG:H81	1.84	0.77
1:A:122:LYS:HB2	1:A:127:LEU:HD11	1.68	0.76
1:B:34:VAL:HG13	1:B:51:SER:HB3	1.68	0.76
1:A:148:THR:HG22	1:A:166:ASN:OD1	1.86	0.75
1:A:2:PRO:HB2	1:A:29:ASN:ND2	2.00	0.75
1:B:5:PRO:HG3	1:B:70:HIS:CE1	2.21	0.74
1:B:5:PRO:HG3	1:B:70:HIS:ND1	2.03	0.73
1:B:93:SER:HB3	1:B:104:PHE:HB3	1.70	0.73
1:A:93:SER:HB3	1:A:104:PHE:HB3	1.72	0.71
1:A:59:LYS:O	1:A:83:VAL:HG21	1.91	0.71
1:B:148:THR:HG22	1:B:166:ASN:OD1	1.91	0.71
1:A:15:ARG:CZ	1:A:165:LEU:HD13	2.22	0.70
1:A:119:ILE:HB	1:A:152:THR:HG22	1.73	0.69
1:B:3:GLN:HG3	1:B:29:ASN:OD1	1.93	0.69
1:A:17:PHE:CE2	1:A:89:LEU:HB2	2.29	0.68
1:B:17:PHE:CE2	1:B:89:LEU:HB2	2.28	0.67
1:A:9:LEU:HD22	1:A:24:LEU:CD2	2.24	0.67
1:B:70:HIS:CE1	1:B:73:VAL:HG11	2.31	0.66
1:B:9:LEU:HD22	1:B:24:LEU:CD2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ARG:CZ	1:B:165:LEU:HD13	2.28	0.64
1:B:20:GLU:HA	5:B:221:NAG:C8	2.25	0.64
1:A:98:MET:CE	1:A:170:ILE:HG13	2.28	0.63
1:B:59:LYS:O	1:B:83:VAL:HG21	1.99	0.62
1:A:42:ASN:HD22	3:A:242:NAG:C7	2.13	0.62
1:A:154:LYS:CE	1:A:157:GLN:HA	2.29	0.62
1:A:82:GLU:HG2	1:A:84:PHE:CE1	2.35	0.62
1:B:120:TYR:CG	1:B:136:ILE:HD11	2.35	0.61
1:B:18:LYS:HD2	1:B:60:PHE:CE1	2.35	0.61
1:A:154:LYS:HE2	1:A:157:GLN:HA	1.81	0.60
1:B:31:PHE:HD2	1:B:33:GLU:HB2	1.66	0.60
1:B:82:GLU:HG2	1:B:84:PHE:CE1	2.37	0.59
1:B:142:THR:HG22	1:B:144:GLU:H	1.68	0.58
1:B:154:LYS:HA	1:B:158:LEU:O	2.04	0.58
1:A:98:MET:HE1	1:A:170:ILE:CG1	2.33	0.57
1:A:174:ARG:HD3	1:A:174:ARG:N	2.20	0.56
1:A:119:ILE:HB	1:A:152:THR:CG2	2.33	0.56
1:B:38:LYS:HB2	1:B:69:GLN:O	2.05	0.56
1:B:38:LYS:O	1:B:68:CYS:HA	2.06	0.56
1:A:37:THR:HG22	1:A:38:LYS:N	2.20	0.56
1:A:21:ASN:OD1	1:A:56:VAL:HA	2.06	0.56
1:B:42:ASN:HD22	3:B:242:NAG:C7	2.18	0.55
1:B:154:LYS:HA	1:B:159:ASP:HA	1.88	0.55
1:A:99:GLU:OE1	1:A:171:LYS:HD2	2.07	0.55
1:B:97:VAL:CG1	1:B:101:GLN:HB2	2.36	0.55
1:A:98:MET:SD	1:A:170:ILE:HG13	2.47	0.55
1:A:18:LYS:HD2	1:A:60:PHE:CE1	2.42	0.55
1:A:142:THR:HG22	1:A:144:GLU:H	1.71	0.55
1:A:97:VAL:CG1	1:A:101:GLN:HB2	2.37	0.54
1:B:60:PHE:CB	3:B:243:NAG:H61	2.37	0.54
1:B:41:HIS:NE2	3:B:242:NAG:H82	2.22	0.54
1:B:110:TRP:NE1	1:B:111:ARG:HG3	2.22	0.54
1:A:130:TRP:CD2	1:A:136:ILE:HG23	2.43	0.54
1:B:70:HIS:O	1:B:73:VAL:HG12	2.08	0.54
2:A:221:NAG:H61	2:A:222:NAG:H82	1.89	0.53
1:A:120:TYR:CG	1:A:136:ILE:HD11	2.44	0.53
1:B:34:VAL:HG13	1:B:51:SER:CB	2.37	0.53
1:A:130:TRP:CE3	1:A:136:ILE:HG23	2.44	0.53
1:A:65:GLU:HB2	1:A:80:TYR:CE2	2.44	0.52
1:B:65:GLU:HB2	1:B:80:TYR:CE2	2.45	0.52
1:A:100:GLY:O	1:A:140:ASN:OD1	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:VAL:HG12	1:B:2:PRO:CD	2.40	0.51
2:A:221:NAG:H61	2:A:222:NAG:C7	2.41	0.51
1:B:60:PHE:HB3	3:B:243:NAG:H61	1.92	0.51
1:A:22:VAL:HG12	1:A:55:ILE:HB	1.92	0.51
1:B:37:THR:HG21	1:B:51:SER:HA	1.93	0.51
6:B:335:NAG:H61	6:B:336:NAG:C7	2.41	0.51
1:A:105:LEU:HB2	1:A:136:ILE:HB	1.92	0.51
1:A:150:TYR:HB3	1:A:164:PRO:HA	1.93	0.51
1:A:1:VAL:HB	1:A:2:PRO:HD3	1.93	0.50
1:A:123:ASP:C	1:A:125:GLU:H	2.15	0.50
2:A:221:NAG:H61	2:A:222:NAG:C8	2.42	0.50
1:B:13:TRP:NE1	1:B:106:ARG:NH1	2.60	0.49
1:B:1:VAL:HG12	1:B:2:PRO:HD2	1.94	0.49
1:A:128:LYS:O	1:A:129:TYR:C	2.51	0.49
1:B:22:VAL:HG12	1:B:55:ILE:HB	1.93	0.49
1:A:13:TRP:HH2	1:A:104:PHE:CD2	2.31	0.49
1:A:13:TRP:NE1	1:A:106:ARG:NH1	2.61	0.48
1:A:9:LEU:HD21	1:A:79:VAL:HG11	1.95	0.48
1:A:19:GLY:O	1:A:57:ASN:HA	2.13	0.48
1:B:4:LYS:HA	1:B:73:VAL:HG22	1.94	0.48
1:A:17:PHE:CZ	1:A:89:LEU:HB2	2.48	0.48
1:B:150:TYR:HB3	1:B:164:PRO:HA	1.96	0.48
1:A:34:VAL:HG11	1:A:70:HIS:CE1	2.48	0.48
1:A:13:TRP:HH2	1:A:104:PHE:HD2	1.62	0.48
1:A:23:THR:HG23	1:A:54:ASN:OD1	2.14	0.48
1:B:86:ASP:OD1	1:B:87:TRP:N	2.46	0.48
1:B:17:PHE:CZ	1:B:89:LEU:HB2	2.49	0.47
1:B:105:LEU:HB2	1:B:136:ILE:HB	1.96	0.47
1:B:70:HIS:NE2	1:B:73:VAL:HG11	2.30	0.47
1:A:156:TRP:CG	1:A:156:TRP:O	2.66	0.47
1:A:9:LEU:HD22	1:A:24:LEU:HD21	1.95	0.47
1:A:86:ASP:OD1	1:A:87:TRP:N	2.45	0.47
1:A:158:LEU:HB2	1:A:160:TYR:OH	2.14	0.47
1:B:97:VAL:HG13	1:B:101:GLN:HB2	1.97	0.47
1:A:140:ASN:OD1	5:A:340:NAG:C2	2.62	0.47
1:B:120:TYR:CB	1:B:136:ILE:HD11	2.44	0.46
1:B:13:TRP:HH2	1:B:104:PHE:CD2	2.33	0.46
1:B:105:LEU:HD23	1:B:105:LEU:HA	1.72	0.46
1:A:41:HIS:O	1:A:42:ASN:C	2.54	0.46
1:B:17:PHE:CE1	1:B:110:TRP:HA	2.51	0.46
1:A:154:LYS:HE3	1:A:157:GLN:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:TRP:CE2	1:A:136:ILE:HG23	2.51	0.46
1:A:42:ASN:ND2	3:A:242:NAG:C7	2.79	0.46
1:B:155:VAL:N	1:B:158:LEU:O	2.44	0.45
1:B:60:PHE:CE2	3:B:244:BMA:H5	2.51	0.45
1:A:130:TRP:CZ3	1:A:136:ILE:HG23	2.52	0.45
1:B:127:LEU:HD12	1:B:127:LEU:O	2.16	0.45
1:B:110:TRP:HD1	1:B:113:TRP:CZ3	2.34	0.45
1:B:60:PHE:HB2	3:B:243:NAG:H61	1.99	0.45
1:A:152:THR:HG23	1:A:152:THR:O	2.16	0.45
1:A:5:PRO:HG3	1:A:70:HIS:HD2	1.82	0.44
1:B:31:PHE:O	1:B:33:GLU:N	2.50	0.44
1:A:158:LEU:O	1:A:160:TYR:CE1	2.71	0.44
1:A:97:VAL:HG13	1:A:101:GLN:HB2	1.97	0.44
1:B:31:PHE:CD2	1:B:33:GLU:HB2	2.51	0.44
1:A:174:ARG:HH11	1:A:174:ARG:HG3	1.82	0.44
1:B:23:THR:HG23	1:B:54:ASN:OD1	2.18	0.44
1:B:31:PHE:C	1:B:33:GLU:N	2.71	0.43
1:A:42:ASN:ND2	3:A:242:NAG:O7	2.37	0.43
1:A:123:ASP:O	1:A:125:GLU:N	2.51	0.43
1:A:9:LEU:CD2	1:A:24:LEU:CD2	2.95	0.43
1:A:98:MET:CE	1:A:172:ALA:HB2	2.48	0.43
1:B:13:TRP:HH2	1:B:104:PHE:HD2	1.66	0.43
2:B:340:NAG:H62	2:B:341:NAG:H2	1.95	0.43
1:A:101:GLN:HB3	1:A:102:PRO:HD2	2.01	0.43
1:B:130:TRP:HB3	1:B:134:HIS:ND1	2.34	0.42
1:B:9:LEU:HD21	1:B:79:VAL:HG11	2.00	0.42
1:A:152:THR:CG2	1:A:152:THR:O	2.67	0.42
1:A:156:TRP:O	1:A:157:GLN:HB2	2.20	0.42
1:A:110:TRP:NE1	1:A:111:ARG:HG2	2.34	0.42
1:A:29:ASN:C	1:A:31:PHE:H	2.23	0.41
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.74	0.41
1:A:120:TYR:CB	1:A:136:ILE:HD11	2.50	0.41
1:B:149:TYR:O	1:B:150:TYR:HB3	2.20	0.41
1:A:97:VAL:O	1:A:169:VAL:HA	2.20	0.41
1:A:1:VAL:N	1:A:2:PRO:CD	2.84	0.41
1:A:41:HIS:HE1	1:A:63:SER:O	2.04	0.41
1:B:119:ILE:HG12	1:B:129:TYR:HD1	1.86	0.41
1:B:98:MET:O	1:B:99:GLU:C	2.60	0.41
1:A:121:TYR:O	1:A:149:TYR:HA	2.21	0.40
1:A:149:TYR:O	1:A:150:TYR:HB3	2.21	0.40
1:B:70:HIS:CD2	1:B:73:VAL:HG11	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:HD12	1:B:106:ARG:O	2.21	0.40
3:B:244:BMA:O2	3:B:245:MAN:H5	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	172/176 (98%)	147 (86%)	22 (13%)	3 (2%)	11	52
1	B	171/176 (97%)	150 (88%)	17 (10%)	4 (2%)	8	44
All	All	343/352 (97%)	297 (87%)	39 (11%)	7 (2%)	9	48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	30	ASN
1	B	74	ASN
1	B	32	PHE
1	A	112	ASN
1	A	124	GLY
1	B	141	ALA
1	A	30	ASN

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	159/161 (99%)	154 (97%)	5 (3%)	47	82
1	B	158/161 (98%)	153 (97%)	5 (3%)	46	81
All	All	317/322 (98%)	307 (97%)	10 (3%)	46	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	49	THR
1	A	69	GLN
1	A	168	THR
1	A	174	ARG
1	B	29	ASN
1	B	41	HIS
1	B	49	THR
1	B	148	THR
1	B	168	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	41	HIS
1	A	70	HIS
1	B	57	ASN

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 ⓘ

18 carbohydrates 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	$\# Z > 2$
2	NAG	A	221	1,2	14,14,15	0.56	0	15,19,21	1.10	2 (13%)
2	NAG	A	222	2	14,14,15	0.71	0	15,19,21	1.00	1 (6%)
3	NAG	A	242	1,3	14,14,15	0.74	0	15,19,21	0.76	0
3	NAG	A	243	3	14,14,15	0.50	0	15,19,21	1.08	1 (6%)
3	BMA	A	244	3	11,11,12	0.68	0	14,15,17	0.66	0
3	MAN	A	246	3	11,11,12	0.66	0	14,15,17	0.62	0
4	NAG	A	274	1,4	14,14,15	0.89	0	15,19,21	1.40	3 (20%)
4	FCA	A	275	4	10,10,11	1.45	1 (10%)	14,14,16	2.40	4 (28%)
4	NAG	A	276	4	14,14,15	0.72	0	15,19,21	0.90	1 (6%)
3	NAG	B	242	1,3	14,14,15	0.56	0	15,19,21	0.61	0
3	NAG	B	243	3	14,14,15	0.62	0	15,19,21	0.72	1 (6%)
3	BMA	B	244	3	11,11,12	0.66	0	14,15,17	0.36	0
3	MAN	B	245	3	11,11,12	0.55	0	14,15,17	0.76	0
6	NAG	B	335	1,6	14,14,15	0.56	0	15,19,21	0.91	1 (6%)
6	NAG	B	336	6	14,14,15	0.55	0	15,19,21	0.79	1 (6%)
6	FCA	B	337	6	10,10,11	1.42	1 (10%)	14,14,16	2.29	4 (28%)
2	NAG	B	340	1,2	14,14,15	0.85	1 (7%)	15,19,21	1.05	1 (6%)
2	NAG	B	341	2	14,14,15	0.52	0	15,19,21	0.67	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
2	NAG	A	221	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	222	2	-	0/6/23/26	0/1/1/1
3	NAG	A	242	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	243	3	-	0/6/23/26	0/1/1/1
3	BMA	A	244	3	-	0/2/19/22	0/1/1/1
3	MAN	A	246	3	-	0/2/19/22	0/1/1/1
4	NAG	A	274	1,4	-	0/6/23/26	0/1/1/1
4	FCA	A	275	4	-	0/0/17/20	0/1/1/1
4	NAG	A	276	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	242	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	243	3	-	0/6/23/26	0/1/1/1
3	BMA	B	244	3	-	0/2/19/22	0/1/1/1
3	MAN	B	245	3	-	0/2/19/22	0/1/1/1
6	NAG	B	335	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	336	6	-	0/6/23/26	0/1/1/1
6	FCA	B	337	6	-	0/0/17/20	0/1/1/1
2	NAG	B	340	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	341	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	337	FCA	C2-C3	-2.38	1.49	1.52
4	A	275	FCA	O2-C2	2.07	1.48	1.43
2	B	340	NAG	C4-C5	2.11	1.57	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	243	NAG	C2-N2-C7	-3.29	118.82	123.04
2	A	222	NAG	C2-N2-C7	-3.12	119.03	123.04
4	A	275	FCA	C3-C4-C5	-2.67	105.22	109.72
2	A	221	NAG	C2-N2-C7	-2.67	119.61	123.04
6	B	337	FCA	C3-C4-C5	-2.60	105.33	109.72
2	B	340	NAG	C2-N2-C7	-2.47	119.86	123.04
2	A	221	NAG	C4-C3-C2	-2.47	107.39	111.23
4	A	276	NAG	C2-N2-C7	-2.47	119.87	123.04
6	B	337	FCA	O5-C1-C2	-2.46	106.87	110.86
6	B	335	NAG	C2-N2-C7	-2.45	119.89	123.04
4	A	274	NAG	C2-N2-C7	-2.43	119.92	123.04
4	A	275	FCA	O5-C1-C2	-2.34	107.06	110.86
6	B	336	NAG	C2-N2-C7	-2.14	120.29	123.04
3	B	243	NAG	C2-N2-C7	-2.05	120.41	123.04
4	A	274	NAG	C3-C4-C5	2.53	114.62	110.20
4	A	274	NAG	C4-C3-C2	2.94	115.80	111.23
6	B	337	FCA	C1-C2-C3	3.44	113.61	109.54
4	A	275	FCA	C1-C2-C3	3.69	113.90	109.54
6	B	337	FCA	C1-O5-C5	6.35	122.18	112.38
4	A	275	FCA	C1-O5-C5	6.74	122.79	112.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	221	NAG	3	0
2	A	222	NAG	3	0
3	A	242	NAG	3	0
4	A	274	NAG	1	0
3	B	242	NAG	2	0
3	B	243	NAG	3	0
3	B	244	BMA	2	0
3	B	245	MAN	1	0
6	B	335	NAG	1	0
6	B	336	NAG	1	0
2	B	340	NAG	3	0
2	B	341	NAG	3	0

5.6 Ligand geometry

4 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	$\# Z > 2$
5	NAG	A	340	1	14,14,15	0.71	0	15,19,21	1.29	1 (6%)
5	NAG	A	366	1	14,14,15	0.52	0	15,19,21	0.88	1 (6%)
5	NAG	B	221	1	14,14,15	0.49	0	15,19,21	0.87	1 (6%)
5	NAG	B	366	1	14,14,15	0.53	0	15,19,21	0.78	1 (6%)

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	NAG	A	340	1	-	0/6/23/26	0/1/1/1
5	NAG	A	366	1	-	0/6/23/26	0/1/1/1
5	NAG	B	221	1	-	0/6/23/26	0/1/1/1
5	NAG	B	366	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	340	NAG	C2-N2-C7	-3.31	118.78	123.04
5	B	221	NAG	C2-N2-C7	-2.65	119.63	123.04
5	B	366	NAG	C2-N2-C7	-2.38	119.99	123.04
5	A	366	NAG	C2-N2-C7	-2.35	120.02	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	340	NAG	1	0
5	B	221	NAG	2	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.