Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:53 PM GMT

PDB ID	:	1YY9
Title	:	Structure of the extracellular domain of the epidermal growth factor receptor in complex with the Fab fragment of cetuximab/Erbitux/IMC-C225
Authors	:	Li, S.; Schmitz, K.R.; Jeffrey, P.D.; Wiltzius, J.J.W.; Kussie, P.; Ferguson, K.M.
Deposited on	:	2005-02-24
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

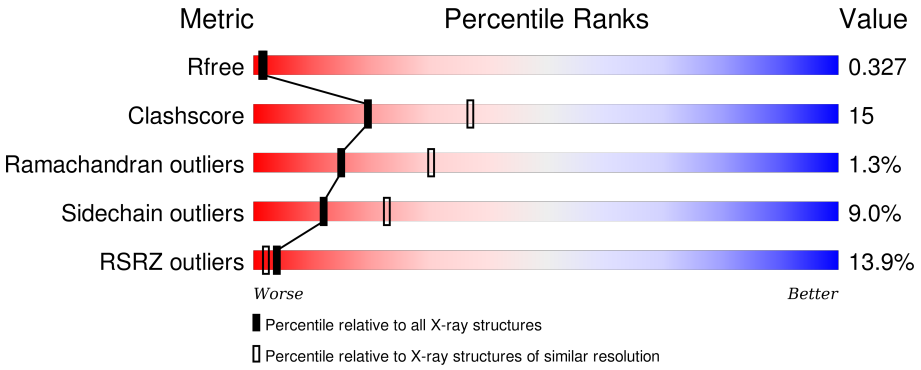
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 <=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	624	14% 68% 27%
2	C	213	10% 62% 31% 5%
3	D	221	17% 68% 26% 5%

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	NAG	A	5791	X	-	-	-
6	NAG	A	5792	X	-	-	-
7	NAG	A	5041	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8225 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 Epidermal Growth Factor Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	0	0
			4653	2879	828	886	60			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	474	LYS	SER	CONFLICT	UNP P00533
A	610	ARG	GLU	CONFLICT	UNP P00533
A	619	HIS	-	EXPRESSION TAG	UNP P00533
A	620	HIS	-	EXPRESSION TAG	UNP P00533
A	621	HIS	-	EXPRESSION TAG	UNP P00533
A	622	HIS	-	EXPRESSION TAG	UNP P00533
A	623	HIS	-	EXPRESSION TAG	UNP P00533
A	624	HIS	-	EXPRESSION TAG	UNP P00533

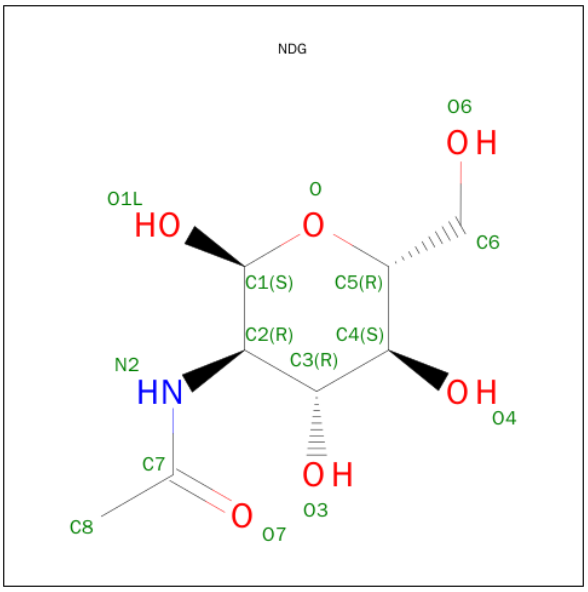
- Molecule 2 is a protein called Cetuximab Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	211	Total	C	N	O	S	0	0	0
			1609	1003	270	332	4			

- Molecule 3 is a protein called Cetuximab Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	220	Total	C	N	O	S	0	0	0
			1648	1046	271	326	5			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



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

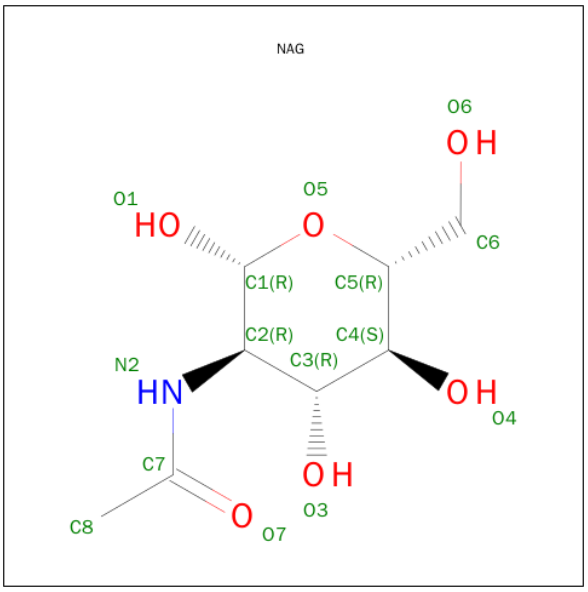
- Molecule 5 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	9	Total C N O 105 58 2 45	0	0

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is water.

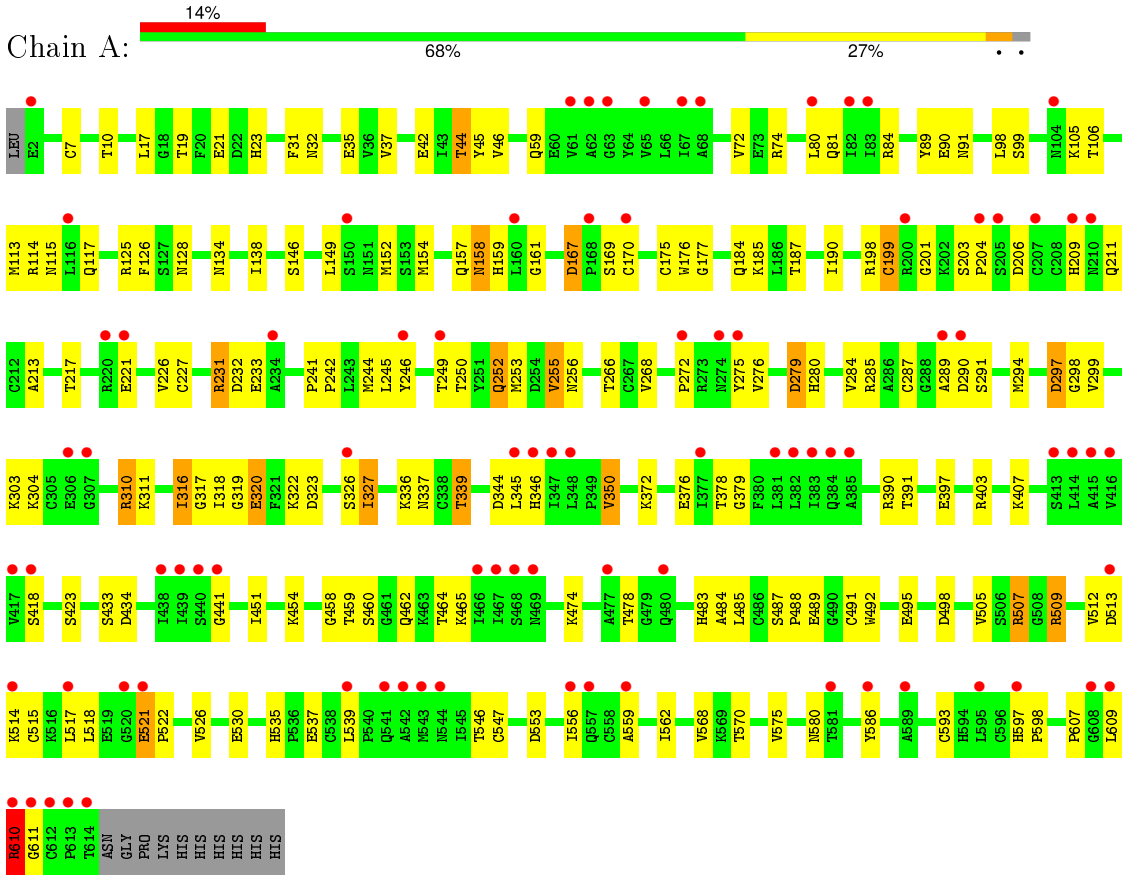
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	35	Total O 35 35	0	0
8	C	6	Total O 6 6	0	0
8	D	15	Total O 15 15	0	0

3 Residue-property plots (i)

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.

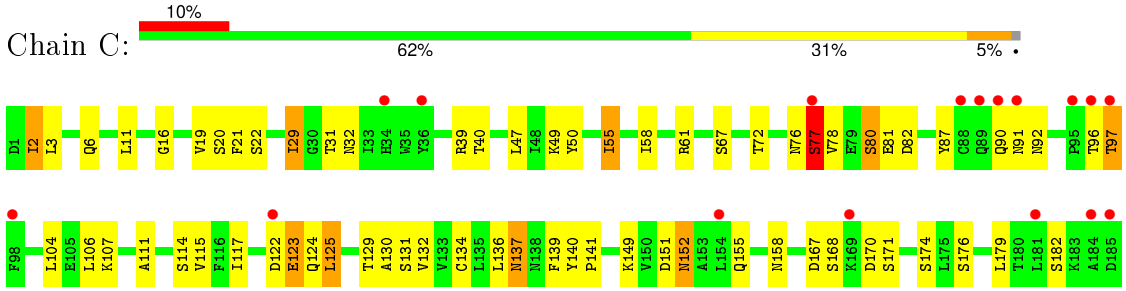
- Molecule 1: Epidermal Growth Factor Receptor

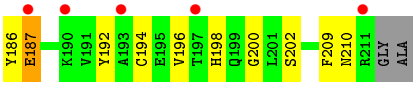
Chain A:



- Molecule 2: Cetuximab Fab Light chain

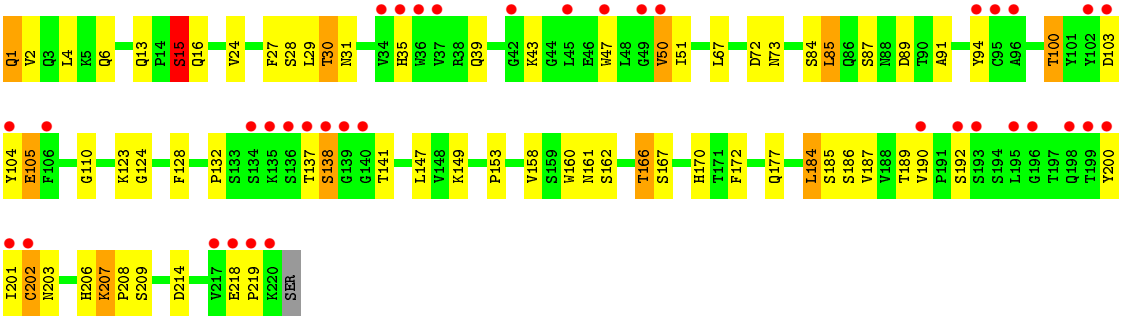
Chain C:





- Molecule 3: Cetuximab Fab Heavy chain

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.82Å 70.86Å 147.12Å 90.00° 102.48° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 30.06 – 2.61	Depositor EDS
% Data completeness (in resolution range)	98.2 (40.00-2.60) 98.3 (30.06-2.61)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.239 , 0.289 0.289 , 0.327	Depositor DCC
R_{free} test set	2349 reflections (4.98%)	DCC
Wilson B-factor (Å^2)	51.6	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.5	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	3 of 47331 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	8225	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: BMA, NAG, NDG, 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	0.66	0/4745	0.76	0/6426
2	C	0.65	0/1643	0.79	0/2237
3	D	0.68	0/1692	0.76	0/2316
All	All	0.66	0/8080	0.77	0/10979

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
6	A	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	5791	NAG	C1
6	A	5792	NAG	C1

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	4653	0	4451	120	0
2	C	1609	0	1535	58	0
3	D	1648	0	1584	65	0
4	A	14	0	13	0	0
4	D	14	0	13	0	0
5	A	105	0	88	5	0
6	A	84	0	75	0	0
7	A	42	0	39	1	0
8	A	35	0	0	3	0
8	C	6	0	0	0	0
8	D	15	0	0	0	0
All	All	8225	0	7798	239	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 15.

All (239) 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)
5:A:3288:MAN:O6	5:A:3288:MAN:C6	1.92	1.18
1:A:10:THR:HG22	1:A:42:GLU:OE1	1.56	1.05
1:A:157:GLN:HB3	1:A:159:HIS:NE2	1.80	0.96
2:C:136:LEU:HD21	2:C:196:VAL:HG21	1.48	0.95
1:A:44:THR:HG23	1:A:45:TYR:CD1	2.08	0.87
1:A:23:HIS:CE1	1:A:44:THR:HG22	2.13	0.84
2:C:80:SER:HA	2:C:106:LEU:HD11	1.63	0.80
2:C:115:VAL:HG22	2:C:136:LEU:HD22	1.61	0.80
1:A:209:HIS:HD2	1:A:211:GLN:H	1.30	0.79
1:A:17:LEU:H	1:A:23:HIS:HD2	1.31	0.79
1:A:227:CYS:SG	1:A:231:ARG:HB3	2.22	0.79
5:A:3284:MAN:H61	5:A:3287:MAN:H5	1.63	0.78
2:C:186:TYR:O	2:C:187:GLU:HB2	1.83	0.78
3:D:1:GLN:H1	3:D:1:GLN:HE21	1.31	0.78
1:A:458:GLY:H	1:A:462:GLN:HE22	1.32	0.78
1:A:232:ASP:O	1:A:233:GLU:HG2	1.85	0.76
1:A:515:CYS:SG	1:A:526:VAL:HG22	2.25	0.76
1:A:521:GLU:CB	1:A:522:PRO:CD	2.64	0.76
3:D:4:LEU:HD22	3:D:24:VAL:HG22	1.68	0.75
1:A:44:THR:CG2	1:A:45:TYR:HD1	1.99	0.75
2:C:32:ASN:HB3	2:C:91:ASN:HB3	1.69	0.74
1:A:244:MET:HE2	1:A:255:VAL:HA	1.70	0.73
1:A:465:LYS:NZ	3:D:100:THR:HG21	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:167:ASP:O	2:C:171:SER:HA	1.88	0.73
1:A:483:HIS:HD2	1:A:485:LEU:H	1.34	0.73
2:C:115:VAL:HG22	2:C:136:LEU:CD2	2.19	0.72
3:D:184:LEU:HG	3:D:185:SER:H	1.53	0.72
1:A:521:GLU:CB	1:A:522:PRO:HD3	2.19	0.72
3:D:13:GLN:HB2	3:D:16:GLN:CG	2.18	0.72
3:D:35:HIS:ND1	3:D:50:VAL:HG13	2.05	0.71
1:A:253:MET:HE1	1:A:575:VAL:HG11	1.73	0.70
3:D:162:SER:H	3:D:203:ASN:ND2	1.88	0.70
3:D:1:GLN:N	3:D:1:GLN:HE21	1.89	0.70
1:A:99:SER:HA	1:A:128:ASN:O	1.92	0.70
3:D:13:GLN:HB2	3:D:16:GLN:HG2	1.74	0.69
1:A:376:GLU:OE1	1:A:403:ARG:NH1	2.27	0.68
2:C:82:ASP:O	2:C:104:LEU:HD23	1.94	0.68
1:A:44:THR:CG2	1:A:45:TYR:CD1	2.75	0.68
1:A:459:THR:H	1:A:462:GLN:HE21	1.41	0.67
1:A:138:ILE:HD12	1:A:184:GLN:HG3	1.77	0.67
1:A:327:ILE:HD11	1:A:345:LEU:HD22	1.76	0.66
1:A:459:THR:H	1:A:462:GLN:NE2	1.93	0.66
1:A:291:SER:HB2	1:A:303:LYS:O	1.96	0.66
1:A:17:LEU:H	1:A:23:HIS:CD2	2.14	0.66
1:A:297:ASP:O	1:A:299:VAL:N	2.29	0.66
1:A:289:ALA:O	1:A:290:ASP:HB2	1.95	0.65
1:A:289:ALA:O	1:A:290:ASP:CB	2.45	0.65
1:A:326:SER:HB2	1:A:346:HIS:O	1.97	0.65
1:A:320:GLU:N	1:A:320:GLU:OE1	2.25	0.64
2:C:115:VAL:HG13	2:C:136:LEU:CD2	2.28	0.64
3:D:35:HIS:CE1	3:D:50:VAL:CG1	2.80	0.63
1:A:509:ARG:CD	1:A:509:ARG:H	2.10	0.63
3:D:137:THR:HG22	3:D:138:SER:H	1.63	0.63
1:A:607:PRO:O	1:A:610:ARG:HG2	1.98	0.63
1:A:157:GLN:HB3	1:A:159:HIS:CE1	2.34	0.62
1:A:336:LYS:O	1:A:337:ASN:HB2	2.00	0.61
1:A:535:HIS:CD2	1:A:537:GLU:H	2.17	0.61
3:D:28:SER:OG	3:D:30:THR:HB	2.01	0.61
2:C:90:GLN:HE21	2:C:97:THR:HB	1.66	0.60
2:C:137:ASN:HD21	3:D:170:HIS:HD2	1.49	0.60
3:D:162:SER:H	3:D:203:ASN:HD21	1.48	0.60
5:A:3284:MAN:H61	5:A:3287:MAN:C5	2.30	0.60
1:A:89:TYR:CD2	1:A:90:GLU:HB2	2.37	0.60
1:A:114:ARG:HA	1:A:176:TRP:CD1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:136:LEU:CD2	2:C:196:VAL:HG21	2.28	0.60
1:A:80:LEU:HD23	1:A:113:MET:HE2	1.84	0.60
1:A:535:HIS:CD2	1:A:537:GLU:HB2	2.37	0.59
1:A:149:LEU:HA	1:A:152:MET:HE1	1.84	0.59
1:A:465:LYS:HZ1	3:D:100:THR:HG21	1.67	0.59
1:A:272:PRO:HG2	1:A:275:TYR:CD1	2.37	0.59
1:A:198:ARG:HG3	1:A:213:ALA:O	2.03	0.59
1:A:17:LEU:N	1:A:23:HIS:HD2	2.00	0.58
3:D:184:LEU:HG	3:D:185:SER:N	2.19	0.58
1:A:244:MET:CE	1:A:255:VAL:HA	2.32	0.58
2:C:6:GLN:HE22	2:C:87:TYR:HA	1.69	0.58
2:C:136:LEU:HD21	2:C:196:VAL:CG2	2.29	0.58
3:D:35:HIS:CE1	3:D:50:VAL:HG11	2.39	0.57
1:A:201:GLY:HA3	1:A:206:ASP:OD1	2.04	0.57
1:A:134:ASN:ND2	1:A:177:GLY:HA2	2.19	0.57
1:A:19:THR:HG22	1:A:21:GLU:H	1.68	0.57
1:A:316:ILE:HD11	1:A:327:ILE:HG12	1.85	0.57
3:D:16:GLN:HA	3:D:16:GLN:OE1	2.04	0.57
3:D:147:LEU:HD12	3:D:184:LEU:O	2.05	0.57
3:D:13:GLN:HB2	3:D:16:GLN:HG3	1.86	0.57
1:A:217:THR:O	1:A:217:THR:HG22	2.04	0.56
3:D:1:GLN:H1	3:D:1:GLN:NE2	2.00	0.56
1:A:546:THR:HG22	1:A:546:THR:O	2.06	0.56
1:A:317:GLY:O	1:A:322:LYS:HA	2.06	0.56
1:A:245:LEU:HG	1:A:256:ASN:HB2	1.87	0.56
2:C:155:GLN:HB3	2:C:158:ASN:HD21	1.71	0.56
1:A:149:LEU:HA	1:A:152:MET:CE	2.36	0.56
1:A:597:HIS:ND1	1:A:598:PRO:HD2	2.21	0.55
3:D:172:PHE:O	3:D:184:LEU:HD11	2.06	0.55
1:A:483:HIS:CD2	1:A:485:LEU:H	2.20	0.55
1:A:451:ILE:HD11	1:A:491:CYS:O	2.07	0.55
2:C:117:ILE:HD12	2:C:194:CYS:HB2	1.89	0.55
1:A:209:HIS:CD2	1:A:211:GLN:H	2.19	0.55
2:C:115:VAL:HG13	2:C:136:LEU:HD21	1.88	0.55
3:D:47:TRP:HZ2	3:D:50:VAL:HG22	1.71	0.55
8:A:5797:HOH:O	3:D:100:THR:CG2	2.55	0.54
1:A:246:TYR:HD1	1:A:253:MET:HE1	1.72	0.54
1:A:407:LYS:HZ1	1:A:434:ASP:CG	2.10	0.54
1:A:46:VAL:HG12	1:A:72:VAL:HB	1.89	0.54
1:A:90:GLU:O	1:A:91:ASN:C	2.45	0.53
7:A:3891:NAG:H3	7:A:3891:NAG:H83	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ASN:HD21	1:A:161:GLY:H	1.57	0.53
1:A:310:ARG:HA	1:A:339:THR:HG21	1.90	0.53
1:A:284:VAL:HG12	1:A:285:ARG:N	2.24	0.53
1:A:213:ALA:HB3	1:A:226:VAL:HG13	1.90	0.53
1:A:23:HIS:HE1	1:A:44:THR:HG22	1.65	0.53
1:A:80:LEU:HD23	1:A:113:MET:CE	2.39	0.53
3:D:161:ASN:HD21	3:D:200:TYR:HA	1.74	0.53
2:C:209:PHE:HD1	2:C:210:ASN:HB2	1.75	0.52
2:C:137:ASN:HD21	3:D:170:HIS:CD2	2.27	0.52
3:D:206:HIS:CE1	3:D:208:PRO:HG2	2.45	0.52
1:A:81:GLN:HA	1:A:115:ASN:O	2.08	0.52
3:D:1:GLN:N	3:D:1:GLN:NE2	2.57	0.52
2:C:2:ILE:HD13	2:C:29:ILE:HD11	1.91	0.52
2:C:31:THR:O	2:C:50:TYR:HA	2.10	0.52
2:C:151:ASP:O	2:C:152:ASN:HB2	2.09	0.52
3:D:29:LEU:HB2	3:D:73:ASN:OD1	2.10	0.51
2:C:29:ILE:O	2:C:29:ILE:HG23	2.09	0.51
2:C:198:HIS:CD2	2:C:200:GLY:H	2.28	0.51
3:D:149:LYS:HE2	3:D:177:GLN:HE22	1.75	0.51
1:A:276:VAL:HG11	1:A:287:CYS:SG	2.51	0.51
1:A:316:ILE:CD1	1:A:327:ILE:HG12	2.41	0.51
1:A:539:LEU:HG	1:A:559:ALA:HA	1.92	0.51
1:A:372:LYS:HE2	1:A:397:GLU:OE2	2.11	0.51
1:A:483:HIS:CD2	1:A:484:ALA:N	2.79	0.50
1:A:246:TYR:HD1	1:A:253:MET:CE	2.23	0.50
2:C:209:PHE:HD1	2:C:210:ASN:CB	2.24	0.50
1:A:190:ILE:O	1:A:190:ILE:HG23	2.12	0.50
3:D:30:THR:HG22	3:D:31:ASN:OD1	2.11	0.50
1:A:322:LYS:O	1:A:323:ASP:HB2	2.12	0.50
3:D:35:HIS:ND1	3:D:50:VAL:CG1	2.74	0.50
2:C:124:GLN:HE22	2:C:131:SER:HB2	1.77	0.50
1:A:31:PHE:O	1:A:32:ASN:C	2.51	0.49
1:A:203:SER:HB2	1:A:204:PRO:HD2	1.94	0.49
2:C:129:THR:HG22	2:C:130:ALA:N	2.28	0.49
2:C:115:VAL:HG13	2:C:136:LEU:HD23	1.94	0.49
3:D:170:HIS:O	3:D:187:VAL:HG22	2.12	0.49
3:D:161:ASN:ND2	3:D:201:ILE:H	2.08	0.49
3:D:158:VAL:HG11	3:D:186:SER:CB	2.43	0.49
3:D:202:CYS:O	3:D:214:ASP:HA	2.12	0.49
3:D:85:LEU:HD13	3:D:89:ASP:HB3	1.94	0.49
3:D:6:GLN:HE21	3:D:110:GLY:HA3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLN:NE2	1:A:185:LYS:HB2	2.29	0.48
1:A:403:ARG:O	1:A:433:SER:HB2	2.13	0.48
1:A:407:LYS:NZ	1:A:434:ASP:CG	2.67	0.48
3:D:123:LYS:HE2	3:D:124:GLY:O	2.13	0.48
1:A:418:SER:HA	1:A:441:GLY:O	2.14	0.48
2:C:141:PRO:O	2:C:198:HIS:HE1	1.96	0.47
2:C:50:TYR:OH	3:D:103:ASP:OD2	2.27	0.47
2:C:129:THR:HA	2:C:182:SER:HA	1.96	0.47
3:D:153:PRO:O	3:D:206:HIS:HE1	1.97	0.47
2:C:55:ILE:HG22	2:C:58:ILE:HD13	1.97	0.47
2:C:32:ASN:HD22	2:C:92:ASN:HD22	1.62	0.47
3:D:207:LYS:N	3:D:208:PRO:HD2	2.28	0.47
1:A:84:ARG:NH2	1:A:227:CYS:O	2.48	0.47
2:C:167:ASP:HB3	2:C:170:ASP:OD1	2.15	0.47
2:C:174:SER:O	3:D:172:PHE:HE2	1.97	0.47
2:C:76:ASN:O	2:C:77:SER:C	2.51	0.47
2:C:125:LEU:HD21	2:C:186:TYR:HD2	1.80	0.47
2:C:124:GLN:HG3	3:D:128:PHE:CZ	2.50	0.47
1:A:458:GLY:H	1:A:462:GLN:NE2	2.07	0.46
3:D:15:SER:HA	3:D:84:SER:HA	1.97	0.46
3:D:35:HIS:CE1	3:D:50:VAL:HG13	2.50	0.46
2:C:123:GLU:HG2	2:C:124:GLN:N	2.30	0.46
3:D:170:HIS:HB2	3:D:187:VAL:HG23	1.98	0.45
1:A:546:THR:O	1:A:547:CYS:HB3	2.17	0.45
3:D:206:HIS:HD2	3:D:209:SER:OG	2.00	0.45
3:D:6:GLN:HE22	3:D:94:TYR:HA	1.80	0.45
5:A:3288:MAN:C5	5:A:3288:MAN:O6	2.64	0.45
1:A:318:ILE:HG22	1:A:319:GLY:N	2.31	0.45
1:A:311:LYS:H	1:A:339:THR:HB	1.81	0.44
1:A:154:MET:HA	1:A:154:MET:HE2	1.98	0.44
2:C:132:VAL:HB	2:C:179:LEU:HB3	1.98	0.44
1:A:126:PHE:H	1:A:154:MET:HE2	1.82	0.44
3:D:166:THR:HG22	3:D:167:SER:N	2.33	0.44
1:A:170:CYS:SG	1:A:175:CYS:HB3	2.58	0.44
1:A:495:GLU:O	1:A:498:ASP:HB2	2.18	0.44
3:D:149:LYS:HE2	3:D:177:GLN:NE2	2.32	0.44
2:C:2:ILE:HD11	2:C:29:ILE:HD12	1.99	0.44
3:D:47:TRP:CZ2	3:D:50:VAL:HG22	2.51	0.44
1:A:146:SER:HA	1:A:149:LEU:HG	1.99	0.44
1:A:485:LEU:HD13	1:A:512:VAL:HA	2.00	0.43
2:C:192:TYR:HB2	2:C:209:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:96:THR:HG21	3:D:104:TYR:CG	2.53	0.43
3:D:105:GLU:O	3:D:105:GLU:HG2	2.19	0.43
1:A:284:VAL:CG1	1:A:285:ARG:N	2.82	0.43
3:D:172:PHE:HE1	3:D:187:VAL:HG22	1.83	0.43
2:C:39:ARG:O	2:C:40:THR:C	2.56	0.43
1:A:546:THR:O	1:A:546:THR:CG2	2.66	0.43
3:D:2:VAL:HG13	3:D:27:PHE:CD2	2.53	0.43
2:C:124:GLN:HG3	3:D:128:PHE:CE1	2.54	0.43
1:A:241:PRO:HA	1:A:242:PRO:HD3	1.77	0.43
1:A:586:TYR:O	1:A:593:CYS:HA	2.18	0.43
1:A:167:ASP:OD1	1:A:169:SER:HB2	2.17	0.43
2:C:16:GLY:C	2:C:77:SER:HA	2.39	0.42
3:D:51:ILE:HG23	3:D:51:ILE:O	2.18	0.42
1:A:609:LEU:C	1:A:611:GLY:H	2.22	0.42
3:D:72:ASP:OD1	3:D:72:ASP:C	2.57	0.42
1:A:35:GLU:OE1	1:A:59:GLN:NE2	2.50	0.42
3:D:39:GLN:O	3:D:91:ALA:HB1	2.19	0.42
3:D:132:PRO:HG2	3:D:219:PRO:HD3	2.01	0.42
2:C:11:LEU:HD21	2:C:19:VAL:CG1	2.49	0.42
2:C:186:TYR:O	2:C:187:GLU:CB	2.59	0.42
1:A:526:VAL:HA	1:A:530:GLU:O	2.19	0.42
1:A:252:GLN:HE21	1:A:252:GLN:CA	2.33	0.42
1:A:350:VAL:HG22	8:A:5798:HOH:O	2.19	0.42
2:C:80:SER:HA	2:C:106:LEU:CD1	2.43	0.42
2:C:16:GLY:O	2:C:77:SER:HA	2.20	0.42
3:D:160:TRP:HZ2	3:D:186:SER:O	2.03	0.42
2:C:21:PHE:O	2:C:72:THR:HA	2.19	0.42
2:C:107:LYS:HA	2:C:140:TYR:OH	2.19	0.42
1:A:98:LEU:HD21	1:A:125:ARG:HG2	2.01	0.42
2:C:174:SER:O	3:D:172:PHE:CE2	2.73	0.41
1:A:344:ASP:OD1	1:A:379:GLY:HA3	2.20	0.41
3:D:172:PHE:HE1	3:D:187:VAL:CG2	2.33	0.41
2:C:47:LEU:HA	2:C:58:ILE:HG12	2.01	0.41
1:A:7:CYS:SG	1:A:37:VAL:HG22	2.60	0.41
2:C:3:LEU:HD23	2:C:3:LEU:HA	1.86	0.41
1:A:513:ASP:OD1	1:A:513:ASP:N	2.48	0.41
3:D:67:LEU:HA	3:D:67:LEU:HD12	1.71	0.41
1:A:209:HIS:HD2	1:A:211:GLN:N	2.07	0.41
1:A:509:ARG:NE	1:A:509:ARG:H	2.19	0.41
1:A:517:LEU:O	1:A:518:LEU:HB2	2.19	0.41
5:A:3284:MAN:C6	5:A:3287:MAN:H5	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ILE:CD1	1:A:184:GLN:HG3	2.49	0.41
2:C:122:ASP:O	2:C:123:GLU:HB3	2.21	0.41
1:A:187:THR:O	1:A:199:CYS:SG	2.79	0.41
1:A:568:VAL:HG11	8:A:5818:HOH:O	2.21	0.41
1:A:454:LYS:HD2	1:A:454:LYS:N	2.36	0.41
2:C:111:ALA:O	2:C:139:PHE:HA	2.21	0.41
1:A:252:GLN:HE21	1:A:252:GLN:C	2.24	0.40
2:C:149:LYS:HB3	2:C:152:ASN:HA	2.01	0.40
1:A:487:SER:C	1:A:489:GLU:H	2.24	0.40
1:A:517:LEU:O	1:A:518:LEU:CB	2.69	0.40
1:A:423:SER:HB2	1:A:492:TRP: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	611/624 (98%)	543 (89%)	60 (10%)	8 (1%)	15	30
2	C	209/213 (98%)	189 (90%)	17 (8%)	3 (1%)	14	28
3	D	218/221 (99%)	200 (92%)	16 (7%)	2 (1%)	21	42
All	All	1038/1058 (98%)	932 (90%)	93 (9%)	13 (1%)	15	30

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	GLY
2	C	187	GLU
3	D	138	SER
1	A	507	ARG
2	C	77	SER
2	C	152	ASN

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Mol	Chain	Res	Type
1	A	221	GLU
1	A	297	ASP
1	A	610	ARG
1	A	279	ASP
1	A	521	GLU
3	D	15	SER
1	A	488	PRO

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	520/545 (95%)	479 (92%)	41 (8%)	15 30
2	C	184/188 (98%)	163 (89%)	21 (11%)	7 12
3	D	186/191 (97%)	168 (90%)	18 (10%)	10 19
All	All	890/924 (96%)	810 (91%)	80 (9%)	12 23

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	74	ARG
1	A	105	LYS
1	A	106	THR
1	A	158	ASN
1	A	167	ASP
1	A	199	CYS
1	A	231	ARG
1	A	249	THR
1	A	250	THR
1	A	252	GLN
1	A	255	VAL
1	A	266	THR
1	A	268	VAL
1	A	279	ASP

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Mol	Chain	Res	Type
1	A	280	HIS
1	A	294	MET
1	A	304	LYS
1	A	310	ARG
1	A	316	ILE
1	A	320	GLU
1	A	327	ILE
1	A	339	THR
1	A	350	VAL
1	A	378	THR
1	A	390	ARG
1	A	391	THR
1	A	460	SER
1	A	464	THR
1	A	474	LYS
1	A	478	THR
1	A	505	VAL
1	A	507	ARG
1	A	509	ARG
1	A	514	LYS
1	A	553	ASP
1	A	556	ILE
1	A	562	ILE
1	A	570	THR
1	A	580	ASN
1	A	610	ARG
2	C	2	ILE
2	C	20	SER
2	C	22	SER
2	C	29	ILE
2	C	49	LYS
2	C	55	ILE
2	C	61	ARG
2	C	67	SER
2	C	77	SER
2	C	78	VAL
2	C	80	SER
2	C	81	GLU
2	C	97	THR
2	C	114	SER
2	C	123	GLU
2	C	125	LEU

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Mol	Chain	Res	Type
2	C	134	CYS
2	C	137	ASN
2	C	168	SER
2	C	176	SER
2	C	202	SER
3	D	1	GLN
3	D	15	SER
3	D	30	THR
3	D	43	LYS
3	D	50	VAL
3	D	85	LEU
3	D	87	SER
3	D	100	THR
3	D	105	GLU
3	D	141	THR
3	D	166	THR
3	D	184	LEU
3	D	189	THR
3	D	190	VAL
3	D	192	SER
3	D	202	CYS
3	D	207	LYS
3	D	218	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	134	ASN
1	A	158	ASN
1	A	209	HIS
1	A	252	GLN
1	A	280	HIS
1	A	462	GLN
1	A	483	HIS
1	A	535	HIS
1	A	541	GLN
1	A	580	ASN
2	C	6	GLN
2	C	92	ASN
2	C	137	ASN
2	C	160	GLN

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Mol	Chain	Res	Type
2	C	198	HIS
3	D	1	GLN
3	D	6	GLN
3	D	70	ASN
3	D	161	ASN
3	D	177	GLN
3	D	203	ASN
3	D	206	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

15 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	$\#\|Z\| > 2$
5	NAG	A	3281	1,5	14,14,15	0.54	0	15,19,21	1.46	2 (13%)
5	NAG	A	3282	5	14,14,15	0.63	0	15,19,21	1.56	1 (6%)
5	BMA	A	3283	5	11,11,12	0.72	0	14,15,17	1.51	3 (21%)
5	MAN	A	3284	5	11,11,12	0.91	0	14,15,17	1.71	5 (35%)
5	MAN	A	3285	5	11,11,12	1.43	1 (9%)	14,15,17	2.51	7 (50%)
5	MAN	A	3286	5	11,11,12	1.50	2 (18%)	14,15,17	1.35	1 (7%)
5	MAN	A	3287	5	11,11,12	0.95	1 (9%)	14,15,17	2.57	3 (21%)
5	MAN	A	3288	5	11,11,12	3.63	2 (18%)	14,15,17	2.21	3 (21%)
5	MAN	A	3289	5	11,11,12	0.61	0	14,15,17	1.09	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	A	3371	1,6	14,14,15	0.49	0	15,19,21	1.60	3 (20%)
6	NAG	A	3372	6	14,14,15	0.55	0	15,19,21	1.19	0
6	NAG	A	4201	1,6	14,14,15	0.71	0	15,19,21	1.12	0
6	NAG	A	4202	6	14,14,15	0.51	0	15,19,21	1.45	1 (6%)
6	NAG	A	5791	1,6	14,14,15	0.82	1 (7%)	15,19,21	1.26	2 (13%)
6	NAG	A	5792	6	14,14,15	0.47	0	15,19,21	1.36	2 (13%)

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	3281	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	3282	5	-	0/6/23/26	0/1/1/1
5	BMA	A	3283	5	-	0/2/19/22	0/1/1/1
5	MAN	A	3284	5	-	0/2/19/22	0/1/1/1
5	MAN	A	3285	5	-	0/2/19/22	0/1/1/1
5	MAN	A	3286	5	-	0/2/19/22	1/1/1/1
5	MAN	A	3287	5	-	0/2/19/22	0/1/1/1
5	MAN	A	3288	5	-	0/2/19/22	1/1/1/1
5	MAN	A	3289	5	-	0/2/19/22	0/1/1/1
6	NAG	A	3371	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	3372	6	-	0/6/23/26	0/1/1/1
6	NAG	A	4201	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	4202	6	-	1/6/23/26	0/1/1/1
6	NAG	A	5791	1,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	A	5792	6	1/1/5/7	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	5791	NAG	C1-C2	2.37	1.55	1.52
5	A	3286	MAN	O5-C5	2.46	1.48	1.43
5	A	3287	MAN	O6-C6	2.75	1.54	1.42
5	A	3288	MAN	C6-C5	2.77	1.61	1.51
5	A	3286	MAN	C2-C3	2.77	1.56	1.52
5	A	3285	MAN	O5-C1	3.02	1.48	1.43
5	A	3288	MAN	O6-C6	11.55	1.92	1.42

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	3288	MAN	O6-C6-C5	-4.57	96.23	111.33
5	A	3285	MAN	O5-C1-C2	-4.04	104.30	110.86
5	A	3287	MAN	O2-C2-C3	-3.69	102.69	110.12
5	A	3285	MAN	O3-C3-C2	-3.59	103.51	110.00
5	A	3281	NAG	O7-C7-C8	-3.26	116.08	122.06
5	A	3283	BMA	O5-C1-C2	-3.26	105.57	110.86
5	A	3284	MAN	C2-C3-C4	-2.79	106.31	111.04
5	A	3285	MAN	C2-C3-C4	-2.34	107.07	111.04
6	A	3371	NAG	O4-C4-C3	-2.12	105.56	110.34
5	A	3285	MAN	O2-C2-C1	-2.02	105.16	109.21
5	A	3284	MAN	O3-C3-C2	2.09	113.77	110.00
5	A	3289	MAN	C1-C2-C3	2.12	112.05	109.54
6	A	5791	NAG	O4-C4-C3	2.23	115.36	110.34
5	A	3289	MAN	O5-C5-C6	2.31	112.35	107.35
5	A	3288	MAN	O5-C5-C6	2.31	112.36	107.35
5	A	3283	BMA	O5-C5-C6	2.38	112.49	107.35
5	A	3286	MAN	O5-C1-C2	2.39	114.74	110.86
5	A	3284	MAN	O2-C2-C1	2.55	114.32	109.21
5	A	3285	MAN	O6-C6-C5	2.55	119.77	111.33
5	A	3285	MAN	C3-C4-C5	2.56	114.66	110.20
5	A	3283	BMA	C1-C2-C3	2.59	112.61	109.54
6	A	3371	NAG	C4-C3-C2	2.68	115.39	111.23
5	A	3284	MAN	O3-C3-C4	2.70	116.43	110.34
5	A	3281	NAG	C1-O5-C5	2.74	115.73	112.25
6	A	5792	NAG	C3-C4-C5	2.74	114.97	110.20
5	A	3284	MAN	C1-O5-C5	2.83	115.84	112.25
6	A	5791	NAG	C1-O5-C5	3.04	116.11	112.25
6	A	5792	NAG	C1-O5-C5	3.28	116.41	112.25
6	A	4202	NAG	C1-O5-C5	3.76	117.02	112.25
5	A	3282	NAG	C1-O5-C5	4.49	117.94	112.25
6	A	3371	NAG	C1-O5-C5	4.56	118.04	112.25
5	A	3287	MAN	O2-C2-C1	5.14	119.52	109.21
5	A	3285	MAN	O3-C3-C4	5.66	123.08	110.34
5	A	3287	MAN	C1-O5-C5	6.21	120.13	112.25
5	A	3288	MAN	C1-O5-C5	6.29	120.24	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	5791	NAG	C1
6	A	5792	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	4202	NAG	O7-C7-N2-C2

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3286	MAN	C1-C2-C3-C4-C5-O5
5	A	3288	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3284	MAN	3	0
5	A	3287	MAN	3	0
5	A	3288	MAN	2	0

5.6 Ligand geometry

5 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	3891	1	14,14,15	0.73	0	15,19,21	1.60	3 (20%)
7	NAG	A	5041	1	14,14,15	0.86	1 (7%)	15,19,21	1.55	2 (13%)
7	NAG	A	5441	1	14,14,15	0.69	0	15,19,21	1.53	2 (13%)
4	NDG	A	625	1	14,14,15	0.99	1 (7%)	15,19,21	1.49	3 (20%)
4	NDG	D	881	3	14,14,15	0.59	0	15,19,21	1.81	2 (13%)

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	3891	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	5041	1	1/1/5/7	1/6/23/26	0/1/1/1
7	NAG	A	5441	1	-	0/6/23/26	0/1/1/1
4	NDG	A	625	1	-	0/6/23/26	0/1/1/1
4	NDG	D	881	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	5041	NAG	C1-C2	2.34	1.55	1.52
4	A	625	NDG	C1-C2	2.93	1.56	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	625	NDG	C1-O-C5	-3.06	108.37	112.25
7	A	3891	NAG	O7-C7-C8	-2.24	117.95	122.06
4	A	625	NDG	C3-C4-C5	-2.09	106.55	110.20
7	A	5441	NAG	C2-N2-C7	2.02	125.63	123.04
4	A	625	NDG	O-C5-C6	2.04	111.76	107.35
7	A	3891	NAG	C8-C7-N2	2.22	120.36	116.11
7	A	5041	NAG	C3-C2-N2	2.36	116.22	110.56
7	A	5041	NAG	O3-C3-C2	3.31	115.67	109.11
4	D	881	NDG	C2-N2-C7	3.70	127.79	123.04
7	A	5441	NAG	C1-O5-C5	4.37	117.79	112.25
7	A	3891	NAG	C2-N2-C7	4.43	128.74	123.04
4	D	881	NDG	C1-O-C5	4.97	118.56	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	5041	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	5041	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	3891	NAG	1	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, 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	613/624 (98%)	0.82	86 (14%)	4 2	15, 32, 42, 50	0
2	C	211/213 (99%)	0.62	22 (10%)	8 5	25, 37, 43, 52	0
3	D	220/221 (99%)	1.01	37 (16%)	2 1	28, 38, 45, 54	0
All	All	1044/1058 (98%)	0.82	145 (13%)	4 2	15, 34, 43, 54	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	137	THR	9.1
3	D	196	GLY	6.8
3	D	136	SER	6.5
1	A	589	ALA	6.2
3	D	199	THR	5.9
1	A	416	VAL	5.3
1	A	272	PRO	4.7
1	A	614	THR	4.4
3	D	104	TYR	4.3
1	A	383	ILE	4.2
3	D	200	TYR	4.1
1	A	83	ILE	4.1
1	A	249	THR	4.1
1	A	611	GLY	4.0
3	D	220	LYS	4.0
1	A	415	ALA	3.9
1	A	609	LEU	3.8
1	A	613	PRO	3.8
3	D	106	PHE	3.8
1	A	220	ARG	3.7
3	D	201	ILE	3.7
1	A	417	VAL	3.7
3	D	49	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
3	D	135	LYS	3.7
3	D	140	GLY	3.6
1	A	440	SER	3.6
1	A	439	ILE	3.5
1	A	116	LEU	3.4
1	A	514	LYS	3.4
3	D	47	TRP	3.4
3	D	35	HIS	3.4
1	A	544	ASN	3.4
1	A	275	TYR	3.3
1	A	82	ILE	3.3
2	C	184	ALA	3.3
1	A	307	GLY	3.2
1	A	345	LEU	3.2
3	D	102	TYR	3.2
2	C	36	TYR	3.2
1	A	467	ILE	3.2
3	D	198	GLN	3.2
3	D	103	ASP	3.2
1	A	438	ILE	3.2
1	A	80	LEU	3.1
2	C	96	THR	3.1
1	A	521	GLU	3.1
3	D	218	GLU	3.1
1	A	543	MET	3.1
1	A	65	VAL	3.1
2	C	91	ASN	3.0
2	C	154	LEU	3.0
1	A	221	GLU	3.0
1	A	539	LEU	3.0
1	A	418	SER	3.0
3	D	219	PRO	3.0
1	A	381	LEU	2.9
1	A	610	ARG	2.9
1	A	556	ILE	2.9
1	A	61	VAL	2.9
1	A	205	SER	2.9
1	A	441	GLY	2.8
3	D	139	GLY	2.8
2	C	193	ALA	2.8
3	D	37	VAL	2.8
1	A	209	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	608	GLY	2.8
3	D	50	VAL	2.7
1	A	597	HIS	2.7
2	C	190	LYS	2.7
2	C	185	ASP	2.7
3	D	193	SER	2.7
2	C	89	GLN	2.7
1	A	67	ILE	2.7
1	A	2	GLU	2.7
3	D	138	SER	2.7
1	A	382	LEU	2.6
3	D	34	VAL	2.6
2	C	98	PHE	2.6
1	A	384	GLN	2.6
1	A	63	GLY	2.6
3	D	95	CYS	2.6
1	A	160	LEU	2.5
3	D	36	TRP	2.5
1	A	477	ALA	2.5
3	D	190	VAL	2.5
1	A	246	TYR	2.5
2	C	77	SER	2.5
1	A	326	SER	2.5
3	D	195	LEU	2.5
1	A	347	ILE	2.5
1	A	559	ALA	2.5
1	A	557	GLN	2.4
2	C	97	THR	2.4
3	D	202	CYS	2.4
1	A	468	SER	2.4
2	C	187	GLU	2.4
3	D	42	GLY	2.4
1	A	346	HIS	2.4
1	A	520	GLY	2.3
2	C	34	HIS	2.3
1	A	517	LEU	2.3
1	A	234	ALA	2.3
1	A	466	ILE	2.3
1	A	414	LEU	2.3
1	A	62	ALA	2.3
2	C	90	GLN	2.3
1	A	542	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	204	PRO	2.3
1	A	104	ASN	2.3
1	A	586	TYR	2.3
3	D	217	VAL	2.3
1	A	290	ASP	2.3
1	A	150	SER	2.3
1	A	207	CYS	2.3
1	A	170	CYS	2.2
1	A	348	LEU	2.2
2	C	181	LEU	2.2
1	A	168	PRO	2.2
1	A	513	ASP	2.2
1	A	68	ALA	2.2
3	D	94	TYR	2.2
1	A	210	ASN	2.2
2	C	211	ARG	2.2
1	A	377	ILE	2.2
1	A	595	LEU	2.2
1	A	612	CYS	2.2
1	A	385	ALA	2.2
3	D	96	ALA	2.2
1	A	306	GLU	2.1
2	C	122	ASP	2.1
1	A	413	SER	2.1
2	C	88	CYS	2.1
2	C	95	PRO	2.1
1	A	480	GLN	2.1
3	D	45	LEU	2.1
1	A	469	ASN	2.1
2	C	169	LYS	2.1
1	A	541	GLN	2.1
3	D	192	SER	2.1
1	A	274	ASN	2.0
1	A	200	ARG	2.0
3	D	134	SER	2.0
2	C	197	THR	2.0
1	A	289	ALA	2.0
1	A	581	THR	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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
6	NAG	A	4201	14/15	0.94	0.19	0.13	28,32,36,39	0
5	NAG	A	3282	14/15	0.95	0.20	-0.22	32,34,38,41	0
5	NAG	A	3281	14/15	0.96	0.19	-0.53	24,31,33,34	0
5	BMA	A	3283	11/12	0.88	0.19	-	37,38,39,41	0
5	MAN	A	3287	11/12	0.87	0.26	-	23,26,26,27	0
5	MAN	A	3286	11/12	0.69	0.42	-	26,33,34,36	0
5	MAN	A	3284	11/12	0.86	0.18	-	28,32,33,33	0
6	NAG	A	5791	14/15	0.71	0.50	-	66,70,71,74	0
6	NAG	A	4202	14/15	0.86	0.36	-	44,47,49,49	0
5	MAN	A	3288	11/12	0.82	0.29	-	15,19,20,21	0
5	MAN	A	3285	11/12	0.74	0.32	-	23,31,33,35	0
6	NAG	A	3371	14/15	0.79	0.26	-	52,56,57,59	0
6	NAG	A	3372	14/15	0.81	0.37	-	59,60,61,61	0
5	MAN	A	3289	11/12	0.83	0.42	-	47,48,49,50	0
6	NAG	A	5792	14/15	0.76	0.42	-	75,76,76,77	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
7	NAG	A	5441	14/15	0.39	0.50	-	51,53,54,54	0
7	NAG	A	3891	14/15	0.84	0.22	-	48,51,52,54	0
7	NAG	A	5041	14/15	0.64	0.44	-	48,49,50,50	0
4	NDG	A	625	14/15	0.69	0.26	-	41,44,44,46	0
4	NDG	D	881	14/15	0.68	0.39	-	57,59,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.