Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:01 PM GMT

PDB ID	:	1RPQ
Title	:	High Affinity IgE Receptor (alpha chain) Complexed with Tight-Binding E131 'zeta' Peptide from Phage Display
Authors	:	Stamos, J.; Eigenbrot, C.; Nakamura, G.R.; Reynolds, M.E.; Yin, J.P.; Lowman, H.B.; Fairbrother, W.J.; Starovasnik, M.A.
Deposited on	:	2003-12-03
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
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:

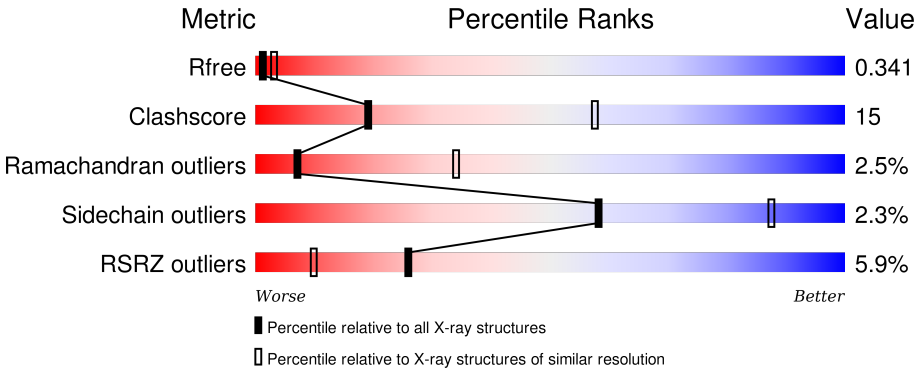
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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. 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	176	5% 68% 25% • 6%
1	B	176	6% 64% 29% • 7%
1	C	176	9% 61% 31% • 6%
1	D	176	3% 65% 28% • 5%
2	W	21	5% 86% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	X	21	62% 38%
2	Y	21	10% 67% 33%
2	Z	21	62% 38%

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
4	BMA	C	244	-	-	X	-
8	SO4	A	401	-	-	-	X
8	SO4	Z	402	-	-	-	X
9	CIT	C	403	-	-	-	X
9	CIT	D	404	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6757 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 precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	44	0	0
			1350	861	222	262	5			
1	B	164	Total	C	N	O	S	47	0	0
			1342	857	220	260	5			
1	C	166	Total	C	N	O	S	61	0	0
			1361	870	223	263	5			
1	D	167	Total	C	N	O	S	6	0	0
			1372	879	224	264	5			

- Molecule 2 is a protein called Peptide E131.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	21	Total	C	N	O	S	4	0	0
			175	114	24	33	4			
2	X	21	Total	C	N	O	S	0	0	0
			175	114	24	33	4			
2	Y	21	Total	C	N	O	S	0	0	0
			175	114	24	33	4			
2	Z	21	Total	C	N	O	S	0	0	0
			175	114	24	33	4			

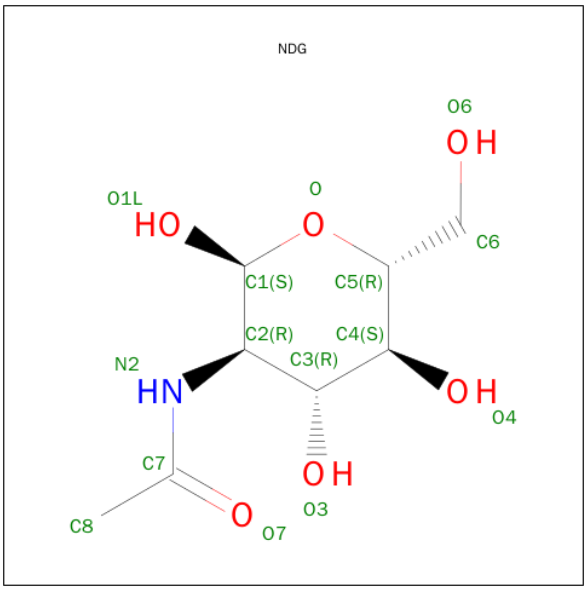
- Molecule 3 is a polymer of unknown type called SUGAR (NAG-NAG-NAG).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			42	24	3	15		
3	B	3	Total	C	N	O	0	0
			42	24	3	15		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total C N O 61 34 2 25	0	0
4	B	5	Total C N O 61 34 2 25	0	0
4	C	5	Total C N O 61 34 2 25	0	0
4	D	5	Total C N O 61 34 2 25	0	0

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total C N O 39 22 2 15	0	0

Continued on next page...

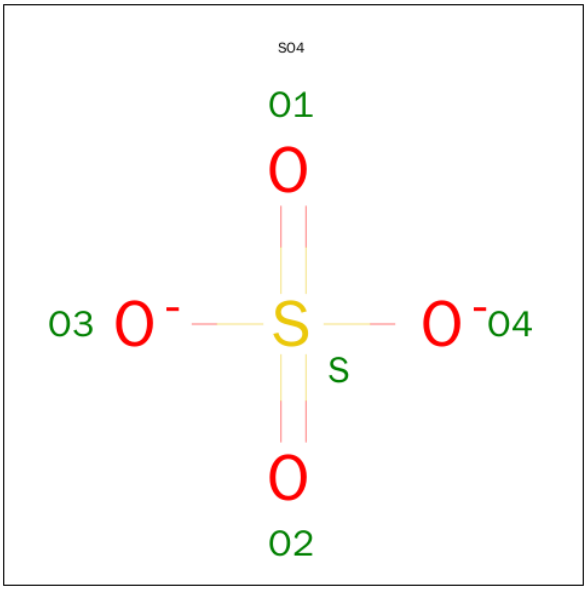
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	3	Total C N O 39 22 2 15	0	0
6	C	3	Total C N O 39 22 2 15	0	0
6	D	3	Total C N O 39 22 2 15	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (NAG-NAG).

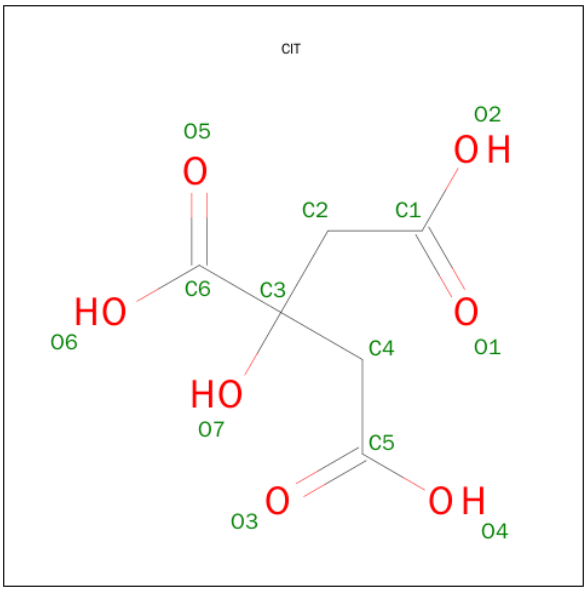
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	2	Total C N O 28 16 2 10	0	0
7	D	2	Total C N O 28 16 2 10	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O S 5 4 1	3	0
8	Z	1	Total O S 5 4 1	4	0

- Molecule 9 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



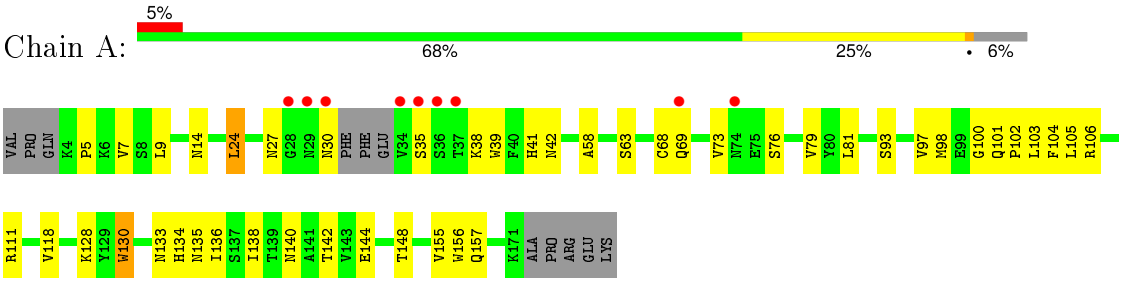
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O 13 6 7	0	0
9	D	1	Total C O 13 6 7	0	0

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.

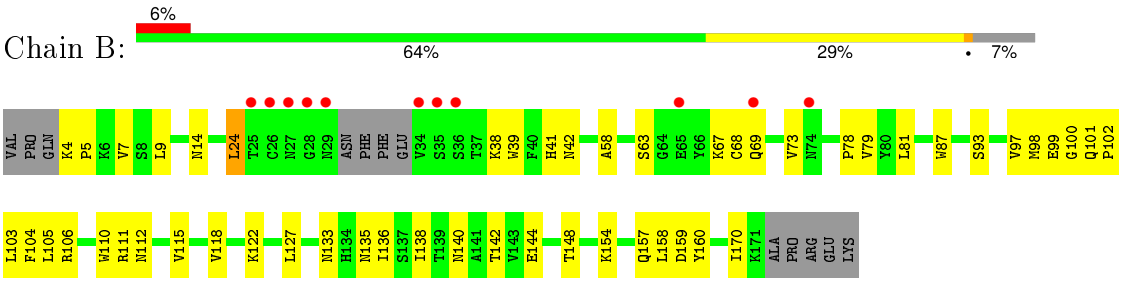
- Molecule 1: High affinity immunoglobulin epsilon receptor alpha-subunit precursor

Chain A:



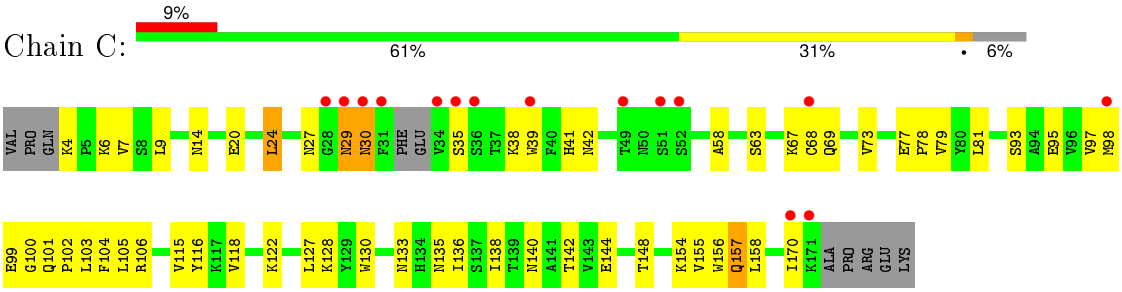
- Molecule 1: High affinity immunoglobulin epsilon receptor alpha-subunit precursor

Chain B:



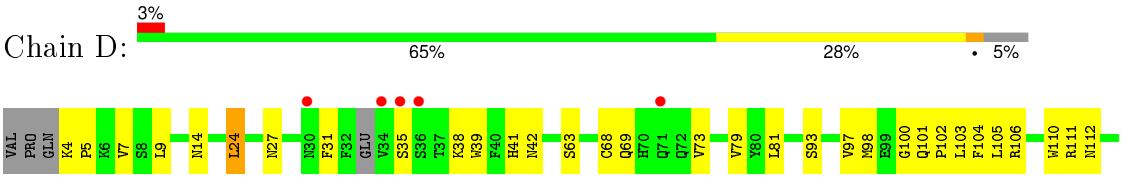
- Molecule 1: High affinity immunoglobulin epsilon receptor alpha-subunit precursor

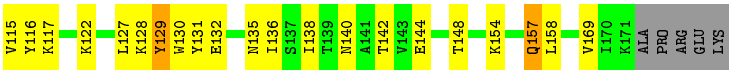
Chain C:



- Molecule 1: High affinity immunoglobulin epsilon receptor alpha-subunit precursor

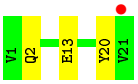
Chain D:





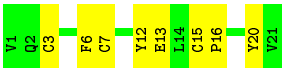
- Molecule 2: Peptide E131

Chain W:



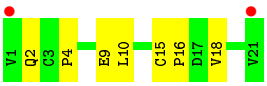
- Molecule 2: Peptide E131

Chain X:



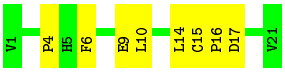
- Molecule 2: Peptide E131

Chain Y:



- Molecule 2: Peptide E131

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	199.70Å 149.70Å 104.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.02 – 3.01	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-3.00) 97.2 (30.02-3.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 3.00Å)	Xtriage
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.294 , 0.349 0.304 , 0.341	Depositor DCC
R_{free} test set	968 reflections (3.18%)	DCC
Wilson B-factor (Å^2)	79.8	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 36.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 30474 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6757	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.70% 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: SO4, BMA, NAG, NDG, CIT

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	0.42	0/1387	0.60	0/1888
1	B	0.42	0/1379	0.64	0/1877
1	C	0.44	0/1399	0.63	0/1904
1	D	0.65	1/1411 (0.1%)	0.71	3/1920 (0.2%)
2	W	0.44	0/181	0.67	0/248
2	X	0.48	0/181	0.80	1/248 (0.4%)
2	Y	0.44	0/181	0.79	0/248
2	Z	0.49	0/181	0.74	0/248
All	All	0.49	1/6300 (0.0%)	0.66	4/8581 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	31	PHE	CB-CG	-18.18	1.20	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	31	PHE	CB-CG-CD1	-9.34	114.27	120.80
1	D	31	PHE	CA-CB-CG	9.09	135.71	113.90
1	D	31	PHE	CB-CG-CD2	8.20	126.54	120.80
2	X	15	CYS	CA-CB-SG	-5.27	104.52	114.00

There are no chirality outliers.

There are no planarity outliers.

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	1350	0	1265	33	0
1	B	1342	0	1259	34	0
1	C	1361	0	1273	48	0
1	D	1372	0	1283	37	0
2	W	175	0	152	1	0
2	X	175	0	152	4	0
2	Y	175	0	152	4	0
2	Z	175	0	152	7	0
3	A	42	0	37	3	0
3	B	42	0	37	3	0
4	A	61	0	52	6	0
4	B	61	0	52	2	0
4	C	61	0	52	8	0
4	D	61	0	52	4	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
6	A	39	0	34	0	0
6	B	39	0	34	1	0
6	C	39	0	34	1	0
6	D	39	0	34	5	0
7	C	28	0	25	2	0
7	D	28	0	25	0	0
8	A	5	0	0	0	0
8	Z	5	0	0	0	0
9	C	13	0	5	5	0
9	D	13	0	5	3	0
All	All	6757	0	6218	192	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 (192) 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)
4:C:244:BMA:H61	4:C:245:BMA:O5	1.62	0.99
2:Z:6:PHE:HA	2:Z:9:GLU:HG2	1.42	0.99
3:A:222:NAG:H61	3:A:223:NAG:O5	1.67	0.95
4:D:244:BMA:H2	4:D:246:BMA:H2	1.50	0.91
4:D:244:BMA:C2	4:D:246:BMA:H2	2.10	0.82
4:B:244:BMA:H2	4:B:246:BMA:H2	1.64	0.80
1:D:105:LEU:HB2	1:D:136:ILE:CG2	2.16	0.76
1:C:157:GLN:HA	9:C:403:CIT:O4	1.86	0.75
1:C:105:LEU:HB2	1:C:136:ILE:CG2	2.15	0.75
1:A:105:LEU:HB2	1:A:136:ILE:CG2	2.17	0.74
1:B:105:LEU:HB2	1:B:136:ILE:CG2	2.16	0.74
1:A:30:ASN:C	6:D:366:NAG:H62	2.10	0.70
1:C:29:ASN:ND2	1:C:30:ASN:H	1.91	0.69
1:C:98:MET:O	1:C:101:GLN:HG2	1.92	0.68
1:B:14:ASN:O	1:B:81:LEU:HD12	1.94	0.65
1:D:110:TRP:CD1	1:D:111:ARG:HG3	2.32	0.65
1:A:98:MET:O	1:A:101:GLN:HG2	1.96	0.65
1:B:4:LYS:N	1:B:5:PRO:HD2	2.12	0.65
1:B:154:LYS:HA	1:B:158:LEU:O	1.96	0.64
1:C:118:VAL:HG21	1:C:133:ASN:HA	1.80	0.64
3:B:223:NAG:O7	3:B:223:NAG:C3	2.46	0.63
2:Z:4:PRO:HB2	2:Z:6:PHE:CD1	2.33	0.63
2:Z:15:CYS:HB3	2:Z:16:PRO:HD2	1.79	0.62
1:B:105:LEU:HB2	1:B:136:ILE:HG22	1.83	0.60
6:D:366:NAG:H61	6:D:367:NAG:H82	1.83	0.60
1:C:105:LEU:HB2	1:C:136:ILE:HG22	1.83	0.60
1:D:14:ASN:O	1:D:81:LEU:HD12	2.02	0.59
2:Y:16:PRO:HB2	2:Y:18:VAL:HG12	1.84	0.59
4:D:244:BMA:C2	4:D:246:BMA:C2	2.81	0.59
1:D:105:LEU:HB2	1:D:136:ILE:HG22	1.84	0.59
1:A:105:LEU:HB2	1:A:136:ILE:HG22	1.85	0.58
1:C:20:GLU:HA	7:C:221:NAG:H82	1.85	0.58
1:B:115:VAL:HB	1:B:133:ASN:HD22	1.69	0.57
1:C:116:TYR:CD1	9:C:403:CIT:H41	2.40	0.57
1:B:9:LEU:HD22	1:B:24:LEU:HD22	1.87	0.57
4:A:244:BMA:C6	4:A:245:BMA:C1	2.82	0.56
1:D:158:LEU:HD12	2:Z:4:PRO:HD3	1.87	0.56
1:C:98:MET:H	1:C:101:GLN:NE2	2.03	0.56
1:C:9:LEU:HD22	1:C:24:LEU:HD22	1.86	0.56
1:A:38:LYS:O	1:A:68:CYS:HA	2.06	0.56
1:C:116:TYR:HD1	9:C:403:CIT:O3	1.89	0.56
1:C:38:LYS:O	1:C:68:CYS:HA	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:THR:HG22	1:D:144:GLU:H	1.71	0.56
1:D:38:LYS:O	1:D:68:CYS:HA	2.05	0.56
1:C:14:ASN:O	1:C:81:LEU:HD12	2.06	0.56
1:C:142:THR:HG22	1:C:144:GLU:H	1.71	0.56
1:B:38:LYS:O	1:B:68:CYS:HA	2.05	0.56
1:B:118:VAL:HG21	1:B:133:ASN:HA	1.87	0.56
1:A:9:LEU:HD22	1:A:24:LEU:HD22	1.87	0.56
1:C:155:VAL:HG12	1:C:156:TRP:CD1	2.41	0.55
4:A:244:BMA:H61	4:A:245:BMA:O5	2.06	0.55
1:C:128:LYS:HD3	1:C:130:TRP:CH2	2.41	0.55
4:B:244:BMA:C2	4:B:246:BMA:H2	2.35	0.55
1:D:9:LEU:HD22	1:D:24:LEU:HD22	1.87	0.55
1:C:99:GLU:HB2	1:C:170:ILE:O	2.07	0.55
1:B:142:THR:HG22	1:B:144:GLU:H	1.72	0.54
3:B:223:NAG:O7	3:B:223:NAG:H3	2.08	0.54
4:C:243:NAG:O3	4:C:244:BMA:H2	2.08	0.53
6:B:367:NAG:O7	6:B:367:NAG:H3	2.08	0.53
1:A:142:THR:HG22	1:A:144:GLU:H	1.73	0.53
2:Z:10:LEU:HD12	2:Z:14:LEU:HD22	1.91	0.53
1:D:98:MET:O	1:D:101:GLN:HG2	2.09	0.52
1:A:157:GLN:HA	1:A:157:GLN:HE21	1.73	0.52
1:D:117:LYS:HE3	9:D:404:CIT:O6	2.09	0.52
4:C:244:BMA:H61	4:C:245:BMA:O6	2.10	0.52
1:A:103:LEU:HD23	1:A:138:ILE:HD12	1.92	0.52
1:A:106:ARG:HB2	1:A:135:ASN:ND2	2.25	0.51
1:D:131:TYR:HD2	1:D:132:GLU:HG2	1.75	0.51
1:C:158:LEU:HD12	2:Y:4:PRO:HD3	1.93	0.51
1:B:39:TRP:CZ3	1:B:68:CYS:HB3	2.46	0.51
1:D:106:ARG:HB2	1:D:135:ASN:ND2	2.26	0.51
1:D:39:TRP:CZ3	1:D:68:CYS:HB3	2.46	0.50
1:C:106:ARG:HB2	1:C:135:ASN:ND2	2.26	0.50
1:D:38:LYS:HB2	1:D:69:GLN:HB3	1.93	0.50
1:B:4:LYS:N	1:B:5:PRO:CD	2.75	0.50
1:C:39:TRP:CZ3	1:C:68:CYS:HB3	2.47	0.50
1:B:98:MET:O	1:B:101:GLN:HG2	2.11	0.50
1:D:103:LEU:HD23	1:D:138:ILE:HD12	1.93	0.50
1:A:39:TRP:CZ3	1:A:68:CYS:HB3	2.46	0.50
1:B:103:LEU:HD23	1:B:138:ILE:HD12	1.93	0.50
1:C:103:LEU:HD23	1:C:138:ILE:HD12	1.94	0.50
1:D:97:VAL:O	1:D:169:VAL:HA	2.11	0.50
1:C:157:GLN:CA	9:C:403:CIT:O4	2.57	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LYS:HB2	1:B:69:GLN:HB3	1.94	0.49
1:C:128:LYS:HD3	1:C:130:TRP:HH2	1.77	0.49
1:B:87:TRP:CD1	1:B:160:TYR:CE2	3.00	0.49
1:C:38:LYS:HB2	1:C:69:GLN:HB3	1.94	0.49
2:Y:9:GLU:O	2:Y:10:LEU:HB3	2.12	0.49
2:W:13:GLU:HB3	2:W:20:TYR:CZ	2.47	0.49
1:A:38:LYS:HB2	1:A:69:GLN:HB3	1.94	0.49
1:C:6:LYS:H	1:C:27:ASN:CB	2.26	0.49
1:C:29:ASN:HD22	1:C:30:ASN:H	1.58	0.49
1:B:106:ARG:HB2	1:B:135:ASN:ND2	2.28	0.49
1:C:4:LYS:HE3	1:C:77:GLU:HG2	1.94	0.49
1:A:5:PRO:HG2	1:A:76:SER:HB3	1.95	0.48
1:D:129:TYR:C	1:D:129:TYR:CD2	2.87	0.48
1:D:101:GLN:HB2	1:D:102:PRO:HD2	1.95	0.48
4:C:244:BMA:C6	4:C:245:BMA:O5	2.48	0.48
1:C:105:LEU:HB2	1:C:136:ILE:HG23	1.96	0.48
1:B:157:GLN:HA	1:B:157:GLN:HE21	1.79	0.47
4:C:242:NAG:O3	4:C:243:NAG:O5	2.30	0.47
4:C:244:BMA:H61	4:C:245:BMA:C5	2.44	0.47
4:C:244:BMA:C6	4:C:245:BMA:O6	2.63	0.47
1:A:101:GLN:HB2	1:A:102:PRO:HD2	1.97	0.47
1:D:103:LEU:HB3	1:D:138:ILE:HB	1.97	0.47
1:A:42:ASN:HD22	4:A:242:NAG:C7	2.28	0.46
1:B:110:TRP:CG	2:X:16:PRO:HG3	2.51	0.46
1:D:7:VAL:HB	1:D:79:VAL:HG21	1.98	0.46
1:A:155:VAL:HG12	1:A:156:TRP:CD1	2.50	0.46
1:A:118:VAL:HG21	1:A:133:ASN:HA	1.97	0.46
1:A:156:TRP:O	1:A:157:GLN:HB2	2.15	0.46
1:C:101:GLN:HB2	1:C:102:PRO:HD2	1.96	0.46
1:B:101:GLN:HB2	1:B:102:PRO:HD2	1.97	0.46
1:B:110:TRP:CD1	1:B:111:ARG:HG3	2.50	0.46
6:D:366:NAG:H61	6:D:367:NAG:C7	2.45	0.46
4:A:244:BMA:C6	4:A:245:BMA:O5	2.63	0.46
1:C:103:LEU:HB3	1:C:138:ILE:HB	1.97	0.46
1:B:103:LEU:HB3	1:B:138:ILE:HB	1.98	0.46
1:C:41:HIS:HE1	1:C:63:SER:O	1.99	0.46
2:X:13:GLU:HB3	2:X:20:TYR:CE1	2.51	0.46
6:C:366:NAG:O3	6:C:367:NAG:N2	2.46	0.46
1:C:7:VAL:HB	1:C:79:VAL:HG21	1.98	0.45
1:A:7:VAL:HB	1:A:79:VAL:HG21	1.98	0.45
4:A:244:BMA:H61	4:A:245:BMA:C1	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:TYR:CD1	9:D:404:CIT:H41	2.51	0.45
1:B:7:VAL:HB	1:B:79:VAL:HG21	1.99	0.45
1:C:100:GLY:HA2	1:C:140:ASN:OD1	2.17	0.45
1:C:97:VAL:HG21	1:C:103:LEU:HD13	1.98	0.45
1:D:128:LYS:HD3	1:D:130:TRP:CH2	2.52	0.45
1:B:105:LEU:HB2	1:B:136:ILE:HG23	1.97	0.45
1:D:131:TYR:CD2	1:D:132:GLU:HG2	2.52	0.45
1:C:14:ASN:ND2	1:C:95:GLU:OE1	2.50	0.45
1:B:97:VAL:HG21	1:B:103:LEU:HD13	1.99	0.45
1:A:98:MET:H	1:A:101:GLN:NE2	2.15	0.44
1:D:105:LEU:HB2	1:D:136:ILE:HG23	1.97	0.44
1:A:105:LEU:HB2	1:A:136:ILE:HG23	1.98	0.44
1:A:103:LEU:HB3	1:A:138:ILE:HB	1.98	0.44
1:D:97:VAL:HG21	1:D:103:LEU:HD13	1.99	0.44
2:Y:15:CYS:HB3	2:Y:16:PRO:CD	2.48	0.44
1:D:4:LYS:HB3	1:D:5:PRO:HD3	2.00	0.44
1:C:93:SER:HB3	1:C:104:PHE:HB2	2.00	0.44
1:B:41:HIS:HE1	1:B:63:SER:O	2.01	0.43
1:C:97:VAL:CG1	1:C:101:GLN:HG3	2.48	0.43
4:A:244:BMA:H61	4:A:245:BMA:C5	2.48	0.43
1:D:157:GLN:HA	9:D:404:CIT:O4	2.18	0.43
1:C:6:LYS:H	1:C:27:ASN:HB2	1.84	0.43
1:A:97:VAL:HG12	1:A:101:GLN:HG3	2.01	0.43
1:D:110:TRP:CD1	2:Z:16:PRO:HD3	2.54	0.43
7:C:221:NAG:O3	7:C:222:NAG:C1	2.67	0.43
1:A:128:LYS:HD3	1:A:130:TRP:CH2	2.54	0.43
1:B:93:SER:HB3	1:B:104:PHE:HB2	2.00	0.43
1:A:156:TRP:HZ3	1:C:116:TYR:HE1	1.67	0.42
1:D:110:TRP:NE1	1:D:111:ARG:HG3	2.34	0.42
1:A:41:HIS:HE1	1:A:63:SER:O	2.02	0.42
1:D:41:HIS:HE1	1:D:63:SER:O	2.02	0.42
1:B:99:GLU:HB2	1:B:170:ILE:O	2.19	0.42
1:A:41:HIS:O	1:A:42:ASN:HB2	2.19	0.42
6:D:366:NAG:H61	6:D:367:NAG:C8	2.48	0.42
1:B:41:HIS:O	1:B:42:ASN:HB2	2.19	0.42
1:B:100:GLY:HA2	1:B:140:ASN:OD1	2.19	0.42
1:D:154:LYS:HB3	1:D:154:LYS:HE2	1.76	0.42
1:D:115:VAL:HA	1:D:154:LYS:O	2.18	0.42
1:A:97:VAL:CG1	1:A:101:GLN:HG3	2.49	0.42
1:A:14:ASN:O	1:A:81:LEU:HD12	2.19	0.42
1:A:93:SER:HB3	1:A:104:PHE:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:LYS:HD3	9:C:403:CIT:O6	2.20	0.42
1:B:97:VAL:HG13	1:B:101:GLN:HE21	1.84	0.42
1:C:122:LYS:HB2	1:C:127:LEU:HD11	2.01	0.42
3:A:222:NAG:H61	3:A:223:NAG:O6	2.19	0.41
1:C:115:VAL:HA	1:C:154:LYS:O	2.20	0.41
6:D:367:NAG:H62	6:D:368:BMA:C1	2.50	0.41
1:D:122:LYS:HB2	1:D:127:LEU:HD11	2.02	0.41
1:C:41:HIS:O	1:C:42:ASN:HB2	2.20	0.41
1:C:97:VAL:HG13	1:C:101:GLN:HE21	1.85	0.41
1:D:93:SER:HB3	1:D:104:PHE:HB2	2.01	0.41
1:D:100:GLY:HA2	1:D:140:ASN:OD1	2.20	0.41
3:A:222:NAG:C6	3:A:223:NAG:O5	2.53	0.41
1:B:122:LYS:HB2	1:B:127:LEU:HD11	2.01	0.41
1:C:42:ASN:HD22	4:C:242:NAG:C7	2.31	0.41
3:B:223:NAG:O7	3:B:223:NAG:O3	2.37	0.41
1:A:9:LEU:CD2	1:A:24:LEU:HD22	2.51	0.41
1:D:41:HIS:O	1:D:42:ASN:HB2	2.20	0.41
1:C:97:VAL:HG12	1:C:101:GLN:HG3	2.03	0.40
1:C:98:MET:SD	1:C:99:GLU:O	2.79	0.40
1:B:9:LEU:CD2	1:B:24:LEU:HD22	2.51	0.40
1:A:130:TRP:CE2	1:A:134:HIS:HD2	2.40	0.40
1:B:67:LYS:HE2	1:B:78:PRO:HG3	2.04	0.40
1:A:100:GLY:HA2	1:A:140:ASN:OD1	2.21	0.40
1:D:42:ASN:HD22	4:D:242:NAG:C7	2.33	0.40
2:X:3:CYS:HB3	2:X:7:CYS:SG	2.61	0.40
1:C:67:LYS:HE2	1:C:78:PRO:HG3	2.04	0.40
2:X:12:TYR:CG	2:Z:10:LEU:HD11	2.57	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	161/176 (92%)	147 (91%)	9 (6%)	5 (3%)	5 28
1	B	160/176 (91%)	146 (91%)	12 (8%)	2 (1%)	15 53
1	C	162/176 (92%)	150 (93%)	7 (4%)	5 (3%)	5 28
1	D	163/176 (93%)	150 (92%)	10 (6%)	3 (2%)	11 45
2	W	19/21 (90%)	15 (79%)	4 (21%)	0	100 100
2	X	19/21 (90%)	16 (84%)	2 (10%)	1 (5%)	2 14
2	Y	19/21 (90%)	11 (58%)	7 (37%)	1 (5%)	2 14
2	Z	19/21 (90%)	18 (95%)	0	1 (5%)	2 14
All	All	722/788 (92%)	653 (90%)	51 (7%)	18 (2%)	7 34

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	27	ASN
1	A	27	ASN
2	Y	2	GLN
1	C	29	ASN
1	A	35	SER
1	C	30	ASN
1	C	35	SER
1	D	35	SER
2	Z	17	ASP
1	A	73	VAL
1	A	111	ARG
2	X	6	PHE
1	A	58	ALA
1	B	58	ALA
1	C	58	ALA
1	B	73	VAL
1	D	73	VAL
1	C	73	VAL

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	151/161 (94%)	148 (98%)	3 (2%)	63 89
1	B	150/161 (93%)	146 (97%)	4 (3%)	52 85
1	C	152/161 (94%)	149 (98%)	3 (2%)	63 89
1	D	153/161 (95%)	148 (97%)	5 (3%)	45 82
2	W	21/21 (100%)	20 (95%)	1 (5%)	31 71
2	X	21/21 (100%)	21 (100%)	0	100 100
2	Y	21/21 (100%)	21 (100%)	0	100 100
2	Z	21/21 (100%)	21 (100%)	0	100 100
All	All	690/728 (95%)	674 (98%)	16 (2%)	58 87

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	130	TRP
1	A	148	THR
1	B	24	LEU
1	B	112	ASN
1	B	148	THR
1	B	159	ASP
1	C	24	LEU
1	C	148	THR
1	C	157	GLN
1	D	24	LEU
1	D	112	ASN
1	D	129	TYR
1	D	148	THR
1	D	157	GLN
2	W	2	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	57	ASN
1	A	101	GLN
1	A	134	HIS
1	A	135	ASN
1	A	157	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	41	HIS
1	B	101	GLN
1	B	135	ASN
1	B	157	GLN
1	C	29	ASN
1	C	41	HIS
1	C	101	GLN
1	C	135	ASN
1	D	27	ASN
1	D	41	HIS
1	D	135	ASN
2	W	2	GLN
2	X	2	GLN

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

42 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	$\#\|Z\| > 2$
3	NAG	A	221	1,3	14,14,15	0.73	0	15,19,21	1.07	1 (6%)
3	NAG	A	222	3	14,14,15	0.77	0	15,19,21	0.99	1 (6%)
3	NAG	A	223	3	14,14,15	0.57	0	15,19,21	0.83	1 (6%)
4	NAG	A	242	1,4	14,14,15	0.45	0	15,19,21	0.78	0
4	NAG	A	243	4	14,14,15	0.65	0	15,19,21	1.70	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BMA	A	244	4	11,11,12	0.87	1 (9%)	14,15,17	1.80	3 (21%)
4	BMA	A	245	4	11,11,12	0.43	0	14,15,17	0.33	0
4	BMA	A	246	4	11,11,12	0.49	0	14,15,17	0.37	0
6	NAG	A	366	1,6	14,14,15	0.57	0	15,19,21	0.87	1 (6%)
6	NAG	A	367	6	14,14,15	0.37	0	15,19,21	0.75	1 (6%)
6	BMA	A	368	6	11,11,12	0.35	0	14,15,17	0.29	0
3	NAG	B	221	1,3	14,14,15	0.56	0	15,19,21	0.89	1 (6%)
3	NAG	B	222	3	14,14,15	0.61	0	15,19,21	0.62	0
3	NAG	B	223	3	14,14,15	0.54	0	15,19,21	0.61	0
4	NAG	B	242	1,4	14,14,15	0.63	0	15,19,21	0.93	1 (6%)
4	NAG	B	243	4	14,14,15	0.70	0	15,19,21	2.03	4 (26%)
4	BMA	B	244	4	11,11,12	0.52	0	14,15,17	1.25	1 (7%)
4	BMA	B	245	4	11,11,12	0.35	0	14,15,17	0.50	0
4	BMA	B	246	4	11,11,12	0.39	0	14,15,17	0.62	0
6	NAG	B	366	1,6	14,14,15	0.63	0	15,19,21	0.76	0
6	NAG	B	367	6	14,14,15	0.46	0	15,19,21	0.62	0
6	BMA	B	368	6	11,11,12	0.33	0	14,15,17	0.48	0
7	NAG	C	221	1,7	14,14,15	0.62	0	15,19,21	0.87	1 (6%)
7	NAG	C	222	7	14,14,15	0.38	0	15,19,21	0.70	1 (6%)
4	NAG	C	242	1,4	14,14,15	0.56	0	15,19,21	0.62	0
4	NAG	C	243	4	14,14,15	0.70	0	15,19,21	2.08	3 (20%)
4	BMA	C	244	4	11,11,12	0.68	0	14,15,17	1.10	1 (7%)
4	BMA	C	245	4	11,11,12	0.51	0	14,15,17	0.39	0
4	BMA	C	246	4	11,11,12	0.53	0	14,15,17	0.69	1 (7%)
6	NAG	C	366	1,6	14,14,15	0.64	0	15,19,21	1.15	2 (13%)
6	NAG	C	367	6	14,14,15	0.65	0	15,19,21	0.73	0
6	BMA	C	368	6	11,11,12	0.37	0	14,15,17	0.26	0
7	NAG	D	221	1,7	14,14,15	0.62	0	15,19,21	0.80	0
7	NAG	D	222	7	14,14,15	0.56	0	15,19,21	0.76	1 (6%)
4	NAG	D	242	1,4	14,14,15	0.55	0	15,19,21	0.89	1 (6%)
4	NAG	D	243	4	14,14,15	0.81	0	15,19,21	2.07	3 (20%)
4	BMA	D	244	4	11,11,12	0.57	0	14,15,17	1.19	2 (14%)
4	BMA	D	245	4	11,11,12	0.34	0	14,15,17	0.37	0
4	BMA	D	246	4	11,11,12	0.38	0	14,15,17	0.49	0
6	NAG	D	366	1,6	14,14,15	0.71	0	15,19,21	0.76	1 (6%)
6	NAG	D	367	6	14,14,15	0.48	0	15,19,21	0.67	0
6	BMA	D	368	6	11,11,12	0.36	0	14,15,17	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	221	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	222	3	-	0/6/23/26	0/1/1/1
3	NAG	A	223	3	-	0/6/23/26	0/1/1/1
4	NAG	A	242	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	243	4	-	0/6/23/26	0/1/1/1
4	BMA	A	244	4	-	0/2/19/22	0/1/1/1
4	BMA	A	245	4	-	0/2/19/22	0/1/1/1
4	BMA	A	246	4	-	0/2/19/22	0/1/1/1
6	NAG	A	366	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	367	6	-	0/6/23/26	0/1/1/1
6	BMA	A	368	6	-	0/2/19/22	0/1/1/1
3	NAG	B	221	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	222	3	-	0/6/23/26	0/1/1/1
3	NAG	B	223	3	-	0/6/23/26	0/1/1/1
4	NAG	B	242	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	243	4	-	0/6/23/26	0/1/1/1
4	BMA	B	244	4	-	0/2/19/22	0/1/1/1
4	BMA	B	245	4	-	0/2/19/22	0/1/1/1
4	BMA	B	246	4	-	0/2/19/22	0/1/1/1
6	NAG	B	366	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	367	6	-	0/6/23/26	0/1/1/1
6	BMA	B	368	6	-	0/2/19/22	0/1/1/1
7	NAG	C	221	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	222	7	-	0/6/23/26	0/1/1/1
4	NAG	C	242	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	243	4	-	0/6/23/26	0/1/1/1
4	BMA	C	244	4	-	0/2/19/22	0/1/1/1
4	BMA	C	245	4	-	0/2/19/22	0/1/1/1
4	BMA	C	246	4	-	0/2/19/22	0/1/1/1
6	NAG	C	366	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	367	6	-	0/6/23/26	0/1/1/1
6	BMA	C	368	6	-	0/2/19/22	0/1/1/1
7	NAG	D	221	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	222	7	-	0/6/23/26	0/1/1/1
4	NAG	D	242	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	243	4	-	0/6/23/26	0/1/1/1
4	BMA	D	244	4	-	0/2/19/22	0/1/1/1
4	BMA	D	245	4	-	0/2/19/22	0/1/1/1
4	BMA	D	246	4	-	0/2/19/22	0/1/1/1
6	NAG	D	366	1,6	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	D	367	6	-	0/6/23/26	0/1/1/1
6	BMA	D	368	6	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	244	BMA	C1-C2	2.26	1.57	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	243	NAG	C4-C3-C2	-6.32	101.41	111.23
4	D	243	NAG	C4-C3-C2	-6.22	101.56	111.23
4	B	243	NAG	C4-C3-C2	-6.21	101.58	111.23
4	A	243	NAG	C4-C3-C2	-4.95	103.54	111.23
4	D	243	NAG	C2-N2-C7	-3.19	118.94	123.04
4	A	243	NAG	C2-N2-C7	-3.10	119.06	123.04
4	C	243	NAG	C2-N2-C7	-3.06	119.10	123.04
6	C	366	NAG	C4-C3-C2	-3.04	106.51	111.23
4	B	242	NAG	C2-N2-C7	-2.93	119.28	123.04
7	C	221	NAG	C2-N2-C7	-2.66	119.62	123.04
4	B	243	NAG	C2-N2-C7	-2.63	119.66	123.04
3	B	221	NAG	C2-N2-C7	-2.56	119.75	123.04
6	C	366	NAG	C2-N2-C7	-2.47	119.86	123.04
3	A	222	NAG	O4-C4-C3	-2.41	104.91	110.34
3	A	221	NAG	C2-N2-C7	-2.39	119.97	123.04
4	D	242	NAG	C2-N2-C7	-2.32	120.06	123.04
6	A	367	NAG	C2-N2-C7	-2.19	120.22	123.04
6	A	366	NAG	C2-N2-C7	-2.17	120.25	123.04
7	C	222	NAG	C2-N2-C7	-2.14	120.30	123.04
6	D	366	NAG	C2-N2-C7	-2.11	120.32	123.04
7	D	222	NAG	C2-N2-C7	-2.10	120.34	123.04
4	A	244	BMA	C3-C4-C5	-2.08	106.58	110.20
4	D	244	BMA	C3-C4-C5	-2.07	106.59	110.20
3	A	223	NAG	C1-O5-C5	-2.02	109.68	112.25
4	D	243	NAG	C1-O5-C5	2.10	114.91	112.25
4	C	246	BMA	C1-O5-C5	2.26	115.12	112.25
4	B	243	NAG	O4-C4-C3	2.29	115.50	110.34
4	B	243	NAG	O4-C4-C5	2.35	115.48	109.24
4	C	243	NAG	O4-C4-C3	2.97	117.03	110.34
4	A	244	BMA	C1-O5-C5	2.98	116.03	112.25
4	C	244	BMA	C1-C2-C3	3.28	113.43	109.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	244	BMA	C1-C2-C3	3.61	113.81	109.54
4	B	244	BMA	C1-C2-C3	3.75	113.98	109.54
4	A	244	BMA	C1-C2-C3	5.31	115.82	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	222	NAG	3	0
3	A	223	NAG	3	0
4	A	242	NAG	1	0
4	A	244	BMA	5	0
4	A	245	BMA	5	0
3	B	223	NAG	3	0
4	B	244	BMA	2	0
4	B	246	BMA	2	0
6	B	367	NAG	1	0
7	C	221	NAG	2	0
7	C	222	NAG	1	0
4	C	242	NAG	2	0
4	C	243	NAG	2	0
4	C	244	BMA	6	0
4	C	245	BMA	5	0
6	C	366	NAG	1	0
6	C	367	NAG	1	0
4	D	242	NAG	1	0
4	D	244	BMA	3	0
4	D	246	BMA	3	0
6	D	366	NAG	4	0
6	D	367	NAG	4	0
6	D	368	BMA	1	0

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
5	NDG	A	340	1	14,14,15	0.69	0	15,19,21	0.92	0
8	SO4	A	401	-	4,4,4	0.15	0	6,6,6	0.18	0
5	NDG	B	340	1	14,14,15	0.54	0	15,19,21	0.83	1 (6%)
5	NDG	C	340	1	14,14,15	0.40	0	15,19,21	0.71	1 (6%)
9	CIT	C	403	-	3,12,12	1.10	0	3,17,17	1.76	1 (33%)
5	NDG	D	340	1	14,14,15	0.38	0	15,19,21	0.81	1 (6%)
9	CIT	D	404	-	3,12,12	1.35	1 (33%)	3,17,17	1.96	1 (33%)
8	SO4	Z	402	-	4,4,4	0.20	0	6,6,6	0.17	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
5	NDG	A	340	1	-	0/6/23/26	0/1/1/1
8	SO4	A	401	-	-	0/0/0/0	0/0/0/0
5	NDG	B	340	1	-	0/6/23/26	0/1/1/1
5	NDG	C	340	1	-	0/6/23/26	0/1/1/1
9	CIT	C	403	-	-	0/6/16/16	0/0/0/0
5	NDG	D	340	1	-	0/6/23/26	0/1/1/1
9	CIT	D	404	-	-	0/6/16/16	0/0/0/0
8	SO4	Z	402	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	404	CIT	O7-C3	2.15	1.46	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	340	NDG	C2-N2-C7	-2.63	119.66	123.04
5	D	340	NDG	C2-N2-C7	-2.42	119.92	123.04
5	C	340	NDG	C2-N2-C7	-2.12	120.31	123.04
9	C	403	CIT	C3-C2-C1	2.98	119.72	114.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	404	CIT	C3-C2-C1	3.32	120.27	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	403	CIT	5	0
9	D	404	CIT	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	161/176 (91%)	0.01	9 (5%) 28 11	29, 62, 111, 118	8 (4%)
1	B	160/176 (90%)	0.05	11 (6%) 20 7	34, 64, 110, 117	7 (4%)
1	C	162/176 (92%)	0.15	15 (9%) 11 4	32, 66, 110, 114	11 (6%)
1	D	167/176 (94%)	0.03	5 (2%) 54 25	31, 65, 111, 116	8 (4%)
2	W	21/21 (100%)	-0.11	1 (4%) 34 14	50, 66, 92, 96	1 (4%)
2	X	21/21 (100%)	-0.15	0 100 100	50, 67, 93, 94	0
2	Y	21/21 (100%)	0.14	2 (9%) 10 4	48, 65, 93, 98	0
2	Z	21/21 (100%)	-0.22	0 100 100	49, 68, 92, 99	0
All	All	734/788 (93%)	0.04	43 (5%) 26 10	29, 65, 110, 118	35 (4%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	34	VAL	17.8
1	D	35	SER	13.7
1	C	34	VAL	13.1
1	D	34	VAL	9.6
1	C	35	SER	8.7
1	B	28	GLY	7.0
1	A	30	ASN	6.1
1	B	35	SER	6.1
1	A	29	ASN	5.4
1	A	36	SER	5.2
1	B	74	ASN	4.4
1	B	27	ASN	4.1
1	C	30	ASN	3.8
1	A	35	SER	3.7
1	B	36	SER	3.5
2	Y	1	VAL	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	W	21	VAL	3.4
1	A	34	VAL	3.3
1	A	69	GLN	3.3
1	B	26	CYS	3.3
1	C	36	SER	3.3
1	C	29	ASN	3.2
1	B	29	ASN	3.2
1	C	51	SER	3.1
2	Y	21	VAL	3.0
1	B	69	GLN	3.0
1	C	68	CYS	2.9
1	A	74	ASN	2.8
1	C	98	MET	2.7
1	C	39	TRP	2.6
1	D	71	GLN	2.6
1	C	31	PHE	2.5
1	D	30	ASN	2.5
1	C	170	ILE	2.4
1	C	171	LYS	2.4
1	C	28	GLY	2.4
1	C	49	THR	2.2
1	B	65	GLU	2.2
1	A	28	GLY	2.1
1	C	52	SER	2.1
1	A	37	THR	2.1
1	B	25	THR	2.1
1	D	36	SER	2.1

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
3	NAG	B	223	14/15	0.75	0.29	0.14	41,46,48,49	14
3	NAG	A	221	14/15	0.90	0.24	0.13	72,76,83,83	0
4	NAG	A	242	14/15	0.97	0.18	-0.64	53,55,63,66	0
4	NAG	B	242	14/15	0.94	0.15	-0.68	59,61,69,69	0
4	NAG	D	242	14/15	0.96	0.19	-0.82	60,62,67,69	0
4	NAG	C	242	14/15	0.92	0.14	-1.53	51,55,59,62	0
4	BMA	A	245	11/12	0.25	0.35	-	78,85,86,86	11
6	NAG	D	366	14/15	0.81	0.37	-	80,84,85,85	14
6	NAG	A	366	14/15	0.78	0.23	-	69,75,77,78	0
3	NAG	A	223	14/15	0.76	0.26	-	72,79,85,91	0
3	NAG	B	222	14/15	0.91	0.26	-	44,49,52,53	14
6	NAG	C	367	14/15	0.32	0.60	-	70,74,76,76	14
3	NAG	A	222	14/15	0.88	0.23	-	60,75,81,82	0
4	BMA	D	244	11/12	0.80	0.20	-	71,73,75,76	0
4	BMA	D	246	11/12	0.57	0.49	-	59,62,64,65	11
7	NAG	D	221	14/15	0.85	0.17	-	82,88,94,97	0
3	NAG	B	221	14/15	0.86	0.24	-	61,76,82,82	0
6	BMA	C	368	11/12	0.21	1.27	-	67,67,68,68	11
4	BMA	D	245	11/12	0.61	0.52	-	64,67,69,69	11
4	NAG	A	243	14/15	0.92	0.25	-	55,61,63,71	0
4	BMA	A	246	11/12	0.64	0.35	-	56,61,63,65	11
4	BMA	C	246	11/12	0.77	0.24	-	96,101,102,102	0
6	NAG	A	367	14/15	0.55	0.46	-	53,57,61,62	14
4	BMA	B	244	11/12	0.49	0.62	-	46,51,54,56	11
6	BMA	D	368	11/12	0.25	0.88	-	70,71,71,72	11
4	BMA	C	244	11/12	0.74	0.31	-	88,92,97,97	0
6	NAG	C	366	14/15	0.77	0.31	-	75,81,84,84	14
4	NAG	D	243	14/15	0.89	0.21	-	64,70,79,80	0
4	BMA	C	245	11/12	0.37	0.47	-	88,93,95,95	11
6	NAG	B	367	14/15	0.60	0.55	-	59,65,65,66	14
6	NAG	D	367	14/15	0.47	0.72	-	70,73,75,76	14
6	BMA	A	368	11/12	0.24	0.73	-	52,54,55,56	11
4	BMA	B	246	11/12	0.52	0.55	-	36,39,41,42	11
4	BMA	A	244	11/12	0.71	0.30	-	71,79,87,89	0
4	NAG	B	243	14/15	0.92	0.19	-	63,69,79,80	0
4	NAG	C	243	14/15	0.90	0.21	-	67,71,76,80	0
6	NAG	B	366	14/15	0.81	0.23	-	68,75,85,86	14
6	BMA	B	368	11/12	0.08	1.19	-	64,66,67,67	11
7	NAG	D	222	14/15	0.70	0.47	-	89,89,91,91	14
4	BMA	B	245	11/12	-0.12	1.14	-	50,51,52,53	11
7	NAG	C	222	14/15	0.80	0.37	-	95,96,97,97	14
7	NAG	C	221	14/15	0.92	0.17	-	92,96,100,101	0

6.4 Ligands

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
8	SO4	Z	402	5/5	0.94	0.69	16.69	25,25,26,26	5
8	SO4	A	401	5/5	0.33	1.27	14.33	119,120,120,120	5
9	CIT	C	403	13/13	0.79	0.44	7.90	107,109,110,110	0
9	CIT	D	404	13/13	0.78	0.38	5.00	118,119,120,120	0
5	NDG	B	340	14/15	0.77	0.28	-	60,67,69,69	14
5	NDG	C	340	14/15	0.43	0.41	-	71,73,75,76	14
5	NDG	D	340	14/15	0.44	0.54	-	70,73,76,77	14
5	NDG	A	340	14/15	0.71	0.33	-	45,47,51,53	14

6.5 Other polymers

There are no such residues in this entry.