Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:26 AM GMT

PDB ID	:	3LTF
Title	:	Crystal Structure of the Drosophila Epidermal Growth Factor Receptor ectodomain in complex with Spitz
Authors	:	Alvarado, D.; Klein, D.E.; Lemmon, M.A.
Deposited on	:	2010-02-15
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 (i) symbol.

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

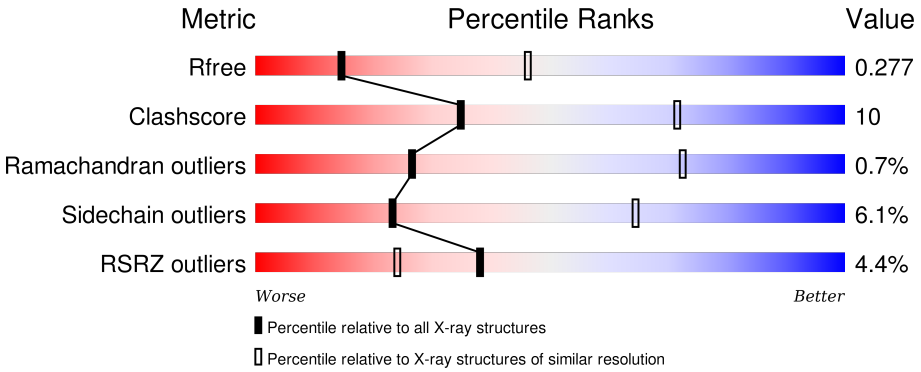
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	601	4% 66% 19% • 13%
1	C	601	3% 65% 21% • 12%
2	B	58	10% 84% 12% • •
2	D	58	83% 12% • •

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
3	MAN	A	4702	X	-	-	-
3	MAN	A	4703	X	-	-	-
3	MAN	A	4704	X	-	-	-
3	MAN	A	4705	X	-	-	-
4	NAG	C	596	X	-	-	-
6	MAN	C	4702	X	-	-	-
6	MAN	C	4703	X	-	-	-
7	MLI	A	596	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9221 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	522	Total	C	N	O	S	0	0	0
			4007	2495	707	757	48			
1	C	531	Total	C	N	O	S	0	1	0
			4109	2559	732	768	50			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP P04412
A	-4	HIS	-	EXPRESSION TAG	UNP P04412
A	-3	HIS	-	EXPRESSION TAG	UNP P04412
A	-2	HIS	-	EXPRESSION TAG	UNP P04412
A	-1	HIS	-	EXPRESSION TAG	UNP P04412
A	0	HIS	-	EXPRESSION TAG	UNP P04412
A	38	GLU	LYS	CONFLICT	UNP P04412
A	230	GLY	ALA	CONFLICT	UNP P04412
A	232	CYS	SER	CONFLICT	UNP P04412
A	359	LEU	ARG	CONFLICT	UNP P04412
A	493	ASN	THR	CONFLICT	UNP P04412
A	590	HIS	-	EXPRESSION TAG	UNP P04412
A	591	HIS	-	EXPRESSION TAG	UNP P04412
A	592	HIS	-	EXPRESSION TAG	UNP P04412
A	593	HIS	-	EXPRESSION TAG	UNP P04412
A	594	HIS	-	EXPRESSION TAG	UNP P04412
A	595	HIS	-	EXPRESSION TAG	UNP P04412
C	-5	HIS	-	EXPRESSION TAG	UNP P04412
C	-4	HIS	-	EXPRESSION TAG	UNP P04412
C	-3	HIS	-	EXPRESSION TAG	UNP P04412
C	-2	HIS	-	EXPRESSION TAG	UNP P04412
C	-1	HIS	-	EXPRESSION TAG	UNP P04412
C	0	HIS	-	EXPRESSION TAG	UNP P04412
C	38	GLU	LYS	CONFLICT	UNP P04412
C	230	GLY	ALA	CONFLICT	UNP P04412

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	232	CYS	SER	CONFLICT	UNP P04412
C	359	LEU	ARG	CONFLICT	UNP P04412
C	493	ASN	THR	CONFLICT	UNP P04412
C	590	HIS	-	EXPRESSION TAG	UNP P04412
C	591	HIS	-	EXPRESSION TAG	UNP P04412
C	592	HIS	-	EXPRESSION TAG	UNP P04412
C	593	HIS	-	EXPRESSION TAG	UNP P04412
C	594	HIS	-	EXPRESSION TAG	UNP P04412
C	595	HIS	-	EXPRESSION TAG	UNP P04412

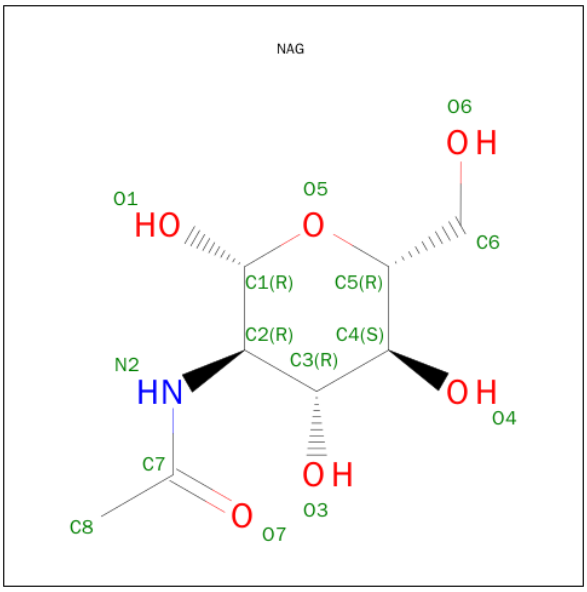
- Molecule 2 is a protein called Protein spitz.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	57	Total	C	N	O	S	0	0	0
			450	290	70	83	7			
2	B	57	Total	C	N	O	S	0	0	0
			456	296	70	83	7			

- Molecule 3 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	6	Total	C	N	O	0	0
			72	40	2	30		

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



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

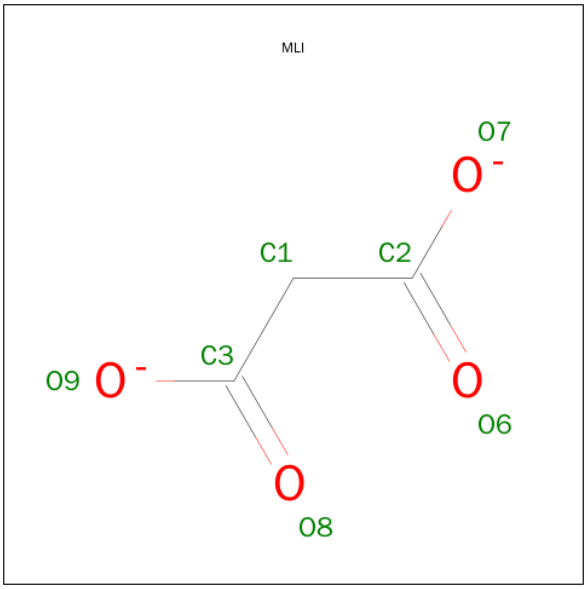
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 7 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



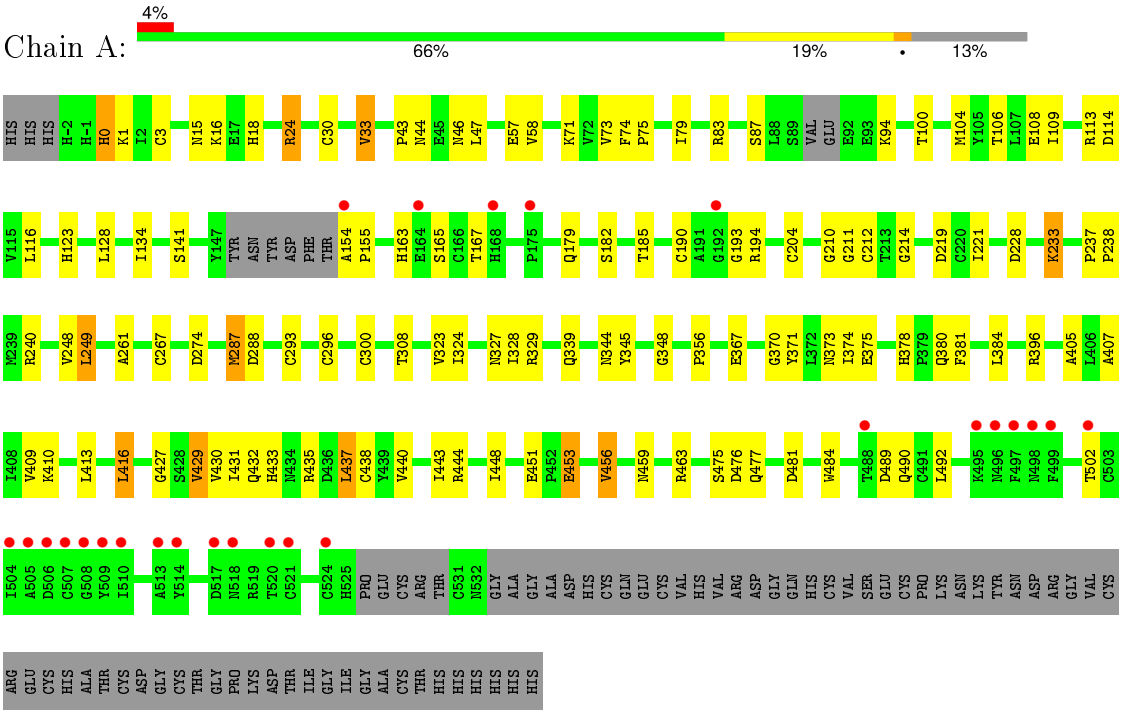
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	3	4		

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.

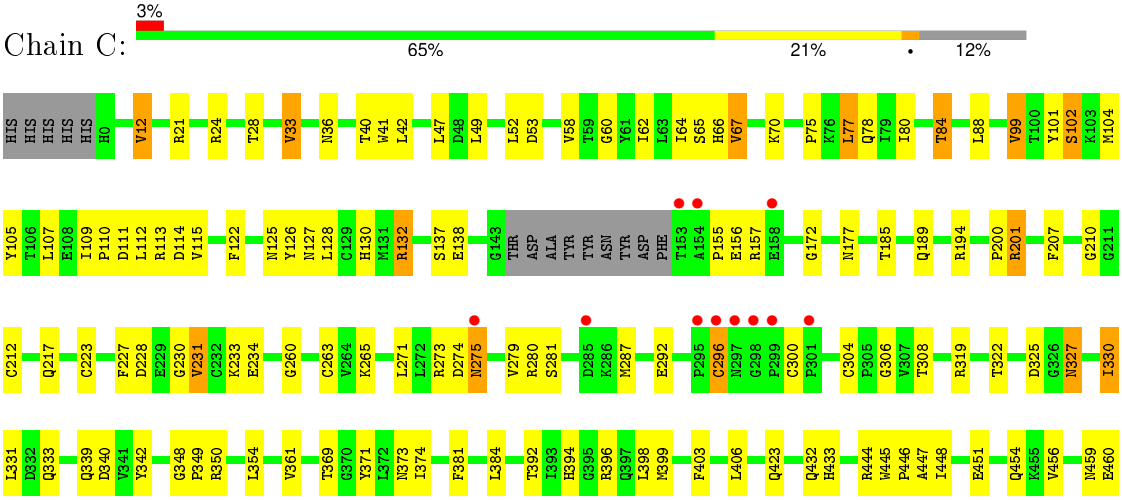
- Molecule 1: Epidermal growth factor receptor

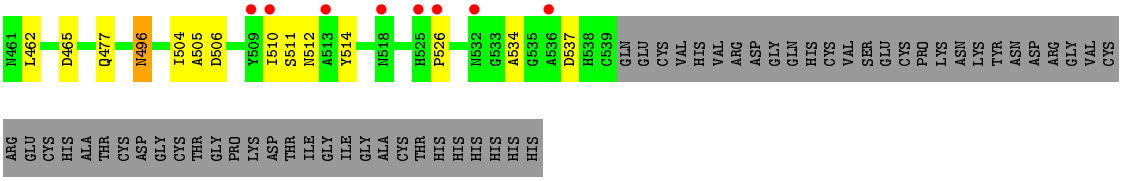
Chain A:



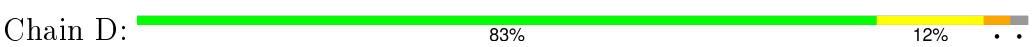
- Molecule 1: Epidermal growth factor receptor

Chain C:

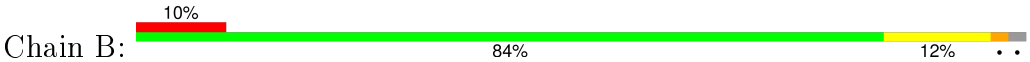


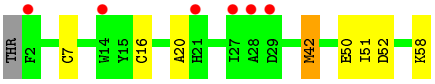


- Molecule 2: Protein spitz



- Molecule 2: Protein spitz





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	118.21Å 124.24Å 186.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 36.05 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-3.20) 99.8 (36.05-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.237 , 0.275 0.238 , 0.277	Depositor DCC
R_{free} test set	4589 reflections (11.11%)	DCC
Wilson B-factor (Å^2)	82.8	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.0	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 45879 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9221	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: MLI, 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	0.37	1/4097 (0.0%)	0.55	0/5558
1	C	0.36	0/4205	0.55	0/5699
2	B	0.40	0/471	0.48	0/640
2	D	0.40	0/464	0.57	1/631 (0.2%)
All	All	0.37	1/9237 (0.0%)	0.55	1/12528 (0.0%)

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
3	A	4	0
6	C	2	0
All	All	6	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	CYS	CB-SG	-5.65	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	16	CYS	CA-CB-SG	-5.23	104.58	114.00

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	4702	MAN	C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
3	A	4703	MAN	C1
3	A	4704	MAN	C1
3	A	4705	MAN	C1
6	C	4702	MAN	C1
6	C	4703	MAN	C1

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	4007	0	3741	83	0
1	C	4109	0	3884	93	0
2	B	456	0	413	5	0
2	D	450	0	406	10	0
3	A	72	0	61	3	0
4	A	14	0	13	0	0
4	C	28	0	26	0	0
5	C	28	0	25	0	0
6	C	50	0	43	0	0
7	A	7	0	2	0	0
All	All	9221	0	8614	176	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 10.

All (176) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ARG:HH11	1:A:24:ARG:HG2	1.35	0.91
1:C:373:ASN:HB2	1:C:399:MET:HE3	1.58	0.85
1:A:194:ARG:HD3	1:A:210:GLY:O	1.77	0.83
1:C:333:GLN:NE2	2:D:47:GLU:HB2	1.92	0.83
1:A:194:ARG:O	1:A:204:CYS:HB2	1.77	0.83
1:A:15:ASN:CG	1:A:18:HIS:HD2	1.83	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:THR:HG22	1:C:423:GLN:HB3	1.64	0.78
1:A:73:VAL:HG12	1:A:108:GLU:HB2	1.65	0.78
1:A:163:HIS:HD2	1:A:165:SER:H	1.34	0.75
1:C:36:ASN:HD21	1:C:84:THR:HB	1.52	0.75
1:A:100:THR:HG22	1:A:123:HIS:HB3	1.71	0.72
1:C:374:ILE:HD13	1:C:384:LEU:HD21	1.71	0.72
1:C:330:ILE:HD11	1:C:381:PHE:CZ	2.24	0.72
1:A:204:CYS:O	1:C:201:ARG:NH2	2.25	0.69
1:C:101:TYR:HE2	2:D:27:ILE:HG22	1.59	0.68
1:C:333:GLN:HE22	2:D:47:GLU:HB2	1.58	0.67
1:A:484:TRP:HB2	1:A:490:GLN:HG3	1.75	0.67
1:A:214:GLY:H	1:A:219:ASP:HB3	1.59	0.66
1:A:327:ASN:ND2	1:A:370:GLY:HA3	2.11	0.65
1:C:371:TYR:CE1	1:C:399:MET:HE2	2.32	0.65
1:A:443:ILE:HG23	1:A:492:LEU:HD11	1.79	0.64
1:C:99:VAL:HG22	1:C:122:PHE:CD2	2.34	0.63
1:C:373:ASN:CB	1:C:399:MET:HE3	2.27	0.63
1:A:33:VAL:CG1	1:A:58:VAL:HG22	2.30	0.61
1:A:327:ASN:HD22	1:A:370:GLY:HA3	1.65	0.61
1:C:373:ASN:HB2	1:C:399:MET:CE	2.28	0.60
1:C:227:PHE:CZ	1:C:230:GLY:HA2	2.36	0.60
1:C:274:ASP:HB2	1:C:279:VAL:HG21	1.84	0.59
1:C:113:ARG:HG3	1:C:113:ARG:HH11	1.66	0.59
1:C:130:HIS:H	1:C:132:ARG:HH11	1.49	0.59
1:C:350[B]:ARG:NH1	1:C:350[B]:ARG:HB2	2.17	0.59
1:A:287:MET:HB2	1:A:296:CYS:HB3	1.85	0.59
1:C:228:ASP:HB2	1:C:263:CYS:HB2	1.86	0.58
1:C:398:LEU:HD23	1:C:403:PHE:HB3	1.85	0.58
1:A:444:ARG:HG2	1:A:481:ASP:HA	1.86	0.57
1:A:324:ILE:HD13	1:A:328:ILE:HD11	1.85	0.57
1:A:24:ARG:HH11	1:A:24:ARG:CG	2.13	0.56
1:A:409:VAL:HG21	2:B:51:ILE:HG12	1.87	0.56
1:A:344:ASN:O	1:A:345:TYR:HB2	2.05	0.56
1:C:127:ASN:O	1:C:157:ARG:NH1	2.38	0.56
1:C:207:PHE:CE1	1:C:234:GLU:HB2	2.40	0.56
1:A:431:ILE:HG21	1:A:440:VAL:HG11	1.88	0.55
1:C:287:MET:HE2	1:C:296:CYS:HB3	1.88	0.55
1:C:36:ASN:HD22	1:C:60:GLY:HA3	1.71	0.55
1:A:33:VAL:HG13	1:A:58:VAL:HG22	1.88	0.55
1:C:444:ARG:NH1	1:C:447:ALA:HB2	2.22	0.55
1:A:228:ASP:HB3	1:A:233:LYS:HD3	1.87	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:514:TYR:CZ	1:C:534:ALA:HB2	2.41	0.54
1:A:432:GLN:HA	1:A:459:ASN:O	2.07	0.54
1:A:163:HIS:CD2	1:A:165:SER:H	2.20	0.54
1:C:306:GLY:N	1:C:325:ASP:O	2.39	0.54
1:C:65:SER:OG	1:C:66:HIS:HD2	1.91	0.54
1:C:42:LEU:HD23	1:C:49:LEU:HD11	1.88	0.54
1:C:432:GLN:HA	1:C:459:ASN:O	2.07	0.54
1:A:240:ARG:HB3	1:A:249:LEU:HD22	1.91	0.53
1:C:138:GLU:O	1:C:194:ARG:NH2	2.42	0.53
1:C:510:ILE:O	1:C:512:ASN:N	2.40	0.52
1:C:99:VAL:HG22	1:C:122:PHE:HD2	1.73	0.52
1:C:504:ILE:HG22	1:C:506:ASP:H	1.74	0.52
1:A:324:ILE:CD1	1:A:328:ILE:HD11	2.39	0.52
1:C:21:ARG:HG3	1:C:24:ARG:NH2	2.24	0.52
1:A:329:ARG:HD2	1:A:373:ASN:HB3	1.92	0.52
1:C:333:GLN:HE22	2:D:47:GLU:CB	2.22	0.51
1:C:114:ASP:HB2	1:C:210:GLY:HA2	1.92	0.51
1:C:279:VAL:HG12	1:C:281:SER:H	1.75	0.51
1:A:413:LEU:HB3	1:A:437:LEU:HD22	1.93	0.51
1:A:57:GLU:HG3	1:A:79:ILE:HB	1.91	0.51
1:A:15:ASN:CG	1:A:18:HIS:CD2	2.75	0.51
1:C:101:TYR:CE2	2:D:27:ILE:HG22	2.42	0.51
1:A:323:VAL:HG22	1:A:367:GLU:HB2	1.91	0.51
1:C:271:LEU:HD23	1:C:396:ARG:HG2	1.93	0.51
1:C:40:THR:HA	1:C:65:SER:O	2.11	0.51
1:C:333:GLN:HE21	2:D:47:GLU:HB2	1.75	0.50
1:C:456:VAL:HG23	2:D:58:LYS:HB2	1.94	0.50
1:A:190:CYS:HB2	1:C:201:ARG:NH1	2.26	0.50
1:A:448:ILE:HD11	1:A:484:TRP:CZ2	2.47	0.50
1:A:248:VAL:HA	1:C:279:VAL:HG13	1.93	0.50
1:C:340:ASP:HB3	1:C:349:PRO:HD2	1.94	0.49
1:A:18:HIS:CE1	2:B:52:ASP:HA	2.48	0.49
1:A:432:GLN:HE22	2:B:52:ASP:H	1.61	0.49
1:C:67:VAL:HG13	1:C:102:SER:OG	2.13	0.49
1:C:279:VAL:HG12	1:C:280:ARG:N	2.28	0.48
1:C:64:ILE:HG23	1:C:67:VAL:HG11	1.94	0.48
1:C:339:GLN:OE1	1:C:350[B]:ARG:NH2	2.47	0.48
1:C:78:GLN:HA	1:C:112:LEU:HA	1.96	0.48
1:A:374:ILE:HD13	1:A:384:LEU:HD21	1.94	0.48
1:C:327:ASN:HB3	1:C:371:TYR:H	1.79	0.48
1:C:200:PRO:O	1:C:201:ARG:CB	2.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LEU:HD13	1:A:438:CYS:H	1.77	0.48
1:C:189:GLN:OE1	1:C:200:PRO:HB3	2.14	0.48
1:A:308:THR:O	1:A:329:ARG:HG3	2.13	0.48
1:C:228:ASP:OD2	1:C:233:LYS:HE3	2.14	0.48
1:A:288:ASP:OD2	1:A:396:ARG:NH2	2.46	0.48
1:A:451:GLU:HB3	1:A:453:GLU:OE2	2.13	0.48
1:C:24:ARG:O	1:C:28:THR:HB	2.14	0.48
1:C:217:GLN:HB2	1:C:231:VAL:HG23	1.96	0.48
1:C:33:VAL:CG1	1:C:58:VAL:HG22	2.44	0.48
1:C:33:VAL:HG13	1:C:58:VAL:HG22	1.95	0.48
1:C:504:ILE:HG22	1:C:505:ALA:N	2.28	0.47
1:A:327:ASN:ND2	1:A:371:TYR:H	2.12	0.47
1:A:475:SER:C	1:A:477:GLN:H	2.17	0.47
1:C:451:GLU:H	1:C:454:GLN:NE2	2.12	0.47
1:A:100:THR:HA	1:A:123:HIS:O	2.14	0.47
1:A:435:ARG:HH22	3:A:4705:MAN:H2	1.79	0.47
1:C:373:ASN:CG	1:C:399:MET:CE	2.83	0.47
1:A:134:ILE:O	1:A:179:GLN:OE1	2.33	0.47
1:C:477:GLN:HE22	1:C:505:ALA:HB2	1.80	0.47
1:A:87:SER:HB3	1:A:94:LYS:HA	1.98	0.46
1:A:83:ARG:HH21	1:A:261:ALA:HB2	1.81	0.46
1:A:1:LYS:HG2	1:A:30:CYS:HA	1.96	0.46
1:A:274:ASP:HB2	1:A:293:CYS:HB2	1.97	0.46
1:A:410:LYS:HD2	1:A:433:HIS:HB3	1.97	0.46
1:C:496:ASN:ND2	1:C:496:ASN:N	2.64	0.46
1:A:429:VAL:HG13	1:A:456:VAL:HB	1.98	0.46
1:A:378:HIS:CD2	1:A:380:GLN:H	2.33	0.45
1:C:445:TRP:HB2	1:C:456:VAL:HG11	1.96	0.45
1:C:109:ILE:HG22	1:C:112:LEU:HB2	1.98	0.45
1:C:70:LYS:HG3	1:C:105:TYR:CD1	2.52	0.45
1:A:113:ARG:NH2	1:A:182:SER:OG	2.50	0.45
1:C:369:THR:HA	1:C:394:HIS:HB2	1.99	0.45
1:C:36:ASN:ND2	1:C:60:GLY:HA3	2.30	0.45
1:A:405:ALA:HB2	1:A:427:GLY:HA3	1.99	0.45
2:B:16:CYS:HB3	2:B:20:ALA:HB3	1.98	0.45
1:C:445:TRP:N	1:C:446:PRO:HD2	2.32	0.45
1:C:88:LEU:HD21	2:D:27:ILE:HD11	1.99	0.45
1:C:496:ASN:H	1:C:496:ASN:ND2	2.15	0.45
1:A:416:LEU:HD21	1:A:440:VAL:CG1	2.47	0.45
1:C:12:VAL:CG1	1:C:41:TRP:CD1	3.00	0.45
1:C:373:ASN:CG	1:C:399:MET:HE3	2.38	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ARG:HD3	1:C:132:ARG:H	1.82	0.45
1:C:200:PRO:O	1:C:201:ARG:HB2	2.17	0.44
1:C:342:TYR:CE1	1:C:348:GLY:HA2	2.52	0.44
2:D:8:PRO:HD2	2:D:33:TYR:CE2	2.53	0.44
1:A:339:GLN:NE2	1:A:348:GLY:O	2.50	0.44
1:A:114:ASP:HB2	1:A:210:GLY:HA2	1.99	0.44
1:A:433:HIS:CE1	3:A:4703:MAN:H62	2.52	0.44
1:A:329:ARG:HD3	1:A:371:TYR:HE1	1.81	0.44
2:B:42:MET:HG2	2:B:50:GLU:HG3	1.99	0.44
1:C:40:THR:HG22	1:C:65:SER:HB3	2.00	0.44
1:C:53:ASP:HA	1:C:75:PRO:HD2	2.01	0.43
1:A:193:GLY:HA3	1:C:201:ARG:NH1	2.33	0.43
1:A:24:ARG:NH1	1:A:24:ARG:HG2	2.15	0.43
1:C:110:PRO:O	1:C:111:ASP:CB	2.66	0.43
1:A:433:HIS:HE1	3:A:4703:MAN:H62	1.83	0.43
1:A:44:ASN:HD21	1:A:46:ASN:HB2	1.82	0.43
1:C:373:ASN:CB	1:C:399:MET:CE	2.94	0.43
1:C:433:HIS:CE1	1:C:460:GLU:HG3	2.53	0.42
1:A:73:VAL:O	1:A:75:PRO:HD3	2.19	0.42
1:A:211:GLY:HA3	1:A:221:ILE:HD12	2.02	0.42
1:C:274:ASP:O	1:C:275:ASN:C	2.57	0.42
1:C:126:TYR:O	1:C:155:PRO:O	2.38	0.42
1:A:329:ARG:HD3	1:A:371:TYR:CE1	2.54	0.42
1:A:378:HIS:HD2	1:A:380:GLN:H	1.67	0.42
1:A:116:LEU:HA	1:A:141:SER:HB3	2.01	0.42
1:A:409:VAL:HG12	1:A:410:LYS:HD3	2.02	0.42
1:A:44:ASN:HB3	1:A:47:LEU:HG	2.02	0.42
1:C:319:ARG:HA	1:C:361:VAL:HG13	2.02	0.42
1:C:172:GLY:H	1:C:177:ASN:HB3	1.85	0.42
1:A:71:LYS:HB3	1:A:71:LYS:HE2	1.91	0.42
1:A:416:LEU:HD21	1:A:440:VAL:HG12	2.01	0.42
1:C:273:ARG:HD3	1:C:292:GLU:OE2	2.20	0.41
1:A:154:ALA:HA	1:A:155:PRO:HD3	1.86	0.41
1:C:64:ILE:O	1:C:99:VAL:HA	2.20	0.41
1:C:423:GLN:HA	1:C:448:ILE:O	2.20	0.41
1:A:407:ALA:HA	1:A:430:VAL:O	2.20	0.41
1:A:237:PRO:HA	1:A:238:PRO:HD3	1.92	0.41
2:D:16:CYS:HB3	2:D:20:ALA:HB3	2.02	0.41
1:A:327:ASN:HD22	1:A:371:TYR:H	1.69	0.41
1:C:113:ARG:NH1	1:C:113:ARG:HG3	2.34	0.41
1:C:62:ILE:CD1	1:C:77:LEU:HD11	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LYS:HG2	1:A:43:PRO:HG3	2.03	0.41
1:A:71:LYS:HG2	1:A:106:THR:CG2	2.51	0.40
1:A:74:PHE:HB2	1:A:109:ILE:HG23	2.03	0.40
1:C:80:ILE:HB	1:C:115:VAL:HG22	2.03	0.40
1:A:356:PRO:HG3	1:A:381:PHE:HB2	2.03	0.40
1:A:489:ASP:HB3	1:A:502:THR:HG22	2.04	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	514/601 (86%)	473 (92%)	38 (7%)	3 (1%)	30 75
1	C	528/601 (88%)	492 (93%)	31 (6%)	5 (1%)	21 67
2	B	55/58 (95%)	51 (93%)	4 (7%)	0	100 100
2	D	55/58 (95%)	52 (94%)	3 (6%)	0	100 100
All	All	1152/1318 (87%)	1068 (93%)	76 (7%)	8 (1%)	26 72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	CYS
1	C	511	SER
1	A	0	HIS
1	A	476	ASP
1	C	212	CYS
1	C	275	ASN
1	C	260	GLY
1	C	526	PRO

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	438/531 (82%)	419 (96%)	19 (4%)	35 75
1	C	452/531 (85%)	417 (92%)	35 (8%)	16 54
2	B	48/51 (94%)	45 (94%)	3 (6%)	22 63
2	D	47/51 (92%)	44 (94%)	3 (6%)	22 62
All	All	985/1164 (85%)	925 (94%)	60 (6%)	23 64

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	24	ARG
1	A	33	VAL
1	A	104	MET
1	A	128	LEU
1	A	167	THR
1	A	185	THR
1	A	233	LYS
1	A	249	LEU
1	A	267	CYS
1	A	287	MET
1	A	300	CYS
1	A	375	GLU
1	A	416	LEU
1	A	429	VAL
1	A	437	LEU
1	A	453	GLU
1	A	456	VAL
1	A	463	ARG
1	C	12	VAL
1	C	33	VAL
1	C	47	LEU
1	C	52	LEU
1	C	67	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	77	LEU
1	C	84	THR
1	C	99	VAL
1	C	102	SER
1	C	104	MET
1	C	107	LEU
1	C	125	ASN
1	C	128	LEU
1	C	132	ARG
1	C	137	SER
1	C	156	GLU
1	C	185	THR
1	C	201	ARG
1	C	223	CYS
1	C	231	VAL
1	C	265	LYS
1	C	296	CYS
1	C	300	CYS
1	C	304	CYS
1	C	308	THR
1	C	322	THR
1	C	327	ASN
1	C	330	ILE
1	C	331	LEU
1	C	354	LEU
1	C	406	LEU
1	C	462	LEU
1	C	465	ASP
1	C	496	ASN
1	C	537	ASP
2	D	4	THR
2	D	27	ILE
2	D	42	MET
2	B	7	CYS
2	B	42	MET
2	B	58	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	163	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	177	ASN
1	A	275	ASN
1	A	327	ASN
1	A	378	HIS
1	A	394	HIS
1	A	420	ASN
1	A	449	GLN
1	A	454	GLN
1	C	36	ASN
1	C	54	ASN
1	C	66	HIS
1	C	177	ASN
1	C	205	HIS
1	C	327	ASN
1	C	333	GLN
1	C	373	ASN
1	C	394	HIS
1	C	420	ASN
1	C	433	HIS
1	C	454	GLN
1	C	496	ASN
1	C	498	ASN
2	D	44	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

12 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	4700	1,3	14,14,15	0.61	0	15,19,21	1.70	2 (13%)
3	NAG	A	4701	3	14,14,15	0.60	0	15,19,21	0.74	0
3	MAN	A	4702	3	11,11,12	0.68	0	14,15,17	1.70	4 (28%)
3	MAN	A	4703	3	11,11,12	0.85	0	14,15,17	2.66	8 (57%)
3	MAN	A	4704	3	11,11,12	0.67	0	14,15,17	0.62	0
3	MAN	A	4705	3	11,11,12	0.66	0	14,15,17	1.29	2 (14%)
5	NAG	C	3830	1,5	14,14,15	0.60	0	15,19,21	1.07	1 (6%)
5	NAG	C	3831	5	14,14,15	0.46	0	15,19,21	1.18	2 (13%)
6	NAG	C	4700	1,6	14,14,15	0.48	0	15,19,21	1.31	2 (13%)
6	NAG	C	4701	6	14,14,15	0.45	0	15,19,21	1.02	1 (6%)
6	MAN	C	4702	6	11,11,12	0.70	0	14,15,17	1.34	1 (7%)
6	MAN	C	4703	6	11,11,12	0.69	0	14,15,17	1.59	3 (21%)

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	4700	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	4701	3	-	0/6/23/26	0/1/1/1
3	MAN	A	4702	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	A	4703	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	A	4704	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	A	4705	3	1/1/4/5	0/2/19/22	0/1/1/1
5	NAG	C	3830	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	3831	5	-	0/6/23/26	0/1/1/1
6	NAG	C	4700	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	4701	6	-	0/6/23/26	0/1/1/1
6	MAN	C	4702	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	C	4703	6	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	4703	MAN	C1-O5-C5	-5.99	104.64	112.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	4703	MAN	C1-O5-C5	-3.10	108.31	112.25
3	A	4703	MAN	O4-C4-C5	-2.82	101.76	109.24
3	A	4702	MAN	O3-C3-C2	-2.81	104.93	110.00
3	A	4703	MAN	O5-C1-C2	-2.78	106.35	110.86
3	A	4702	MAN	O3-C3-C4	-2.49	104.72	110.34
3	A	4703	MAN	C1-C2-C3	-2.01	107.16	109.54
5	C	3831	NAG	C3-C4-C5	2.19	114.01	110.20
3	A	4702	MAN	O5-C5-C6	2.24	112.20	107.35
3	A	4703	MAN	O5-C5-C6	2.37	112.47	107.35
3	A	4705	MAN	C2-C3-C4	2.41	115.13	111.04
3	A	4700	NAG	O7-C7-N2	2.46	126.88	121.86
6	C	4703	MAN	C2-C3-C4	2.52	115.31	111.04
5	C	3830	NAG	C4-C3-C2	2.60	115.27	111.23
6	C	4700	NAG	C1-O5-C5	2.66	115.62	112.25
3	A	4703	MAN	O4-C4-C3	2.67	116.34	110.34
6	C	4702	MAN	O3-C3-C2	2.74	114.94	110.00
3	A	4705	MAN	C3-C4-C5	2.74	114.97	110.20
6	C	4703	MAN	C3-C4-C5	2.74	114.98	110.20
6	C	4701	NAG	C1-O5-C5	2.75	115.74	112.25
5	C	3831	NAG	C1-O5-C5	3.12	116.21	112.25
6	C	4700	NAG	C2-N2-C7	3.32	127.30	123.04
3	A	4703	MAN	C3-C4-C5	3.38	116.09	110.20
3	A	4702	MAN	C1-C2-C3	3.50	113.69	109.54
3	A	4703	MAN	C2-C3-C4	3.64	117.23	111.04
3	A	4700	NAG	C2-N2-C7	5.42	130.00	123.04

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	4705	MAN	C1
3	A	4704	MAN	C1
3	A	4703	MAN	C1
6	C	4703	MAN	C1
3	A	4702	MAN	C1
6	C	4702	MAN	C1

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
3	A	4703	MAN	2	0
3	A	4705	MAN	1	0

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	NAG	A	3830	1	14,14,15	0.46	0	15,19,21	0.98	1 (6%)
7	MLI	A	596	-	0,6,6	0.00	-	0,7,7	0.00	-
4	NAG	C	3440	1	14,14,15	0.64	0	15,19,21	1.01	1 (6%)
4	NAG	C	596	1	14,14,15	0.63	0	15,19,21	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	3830	1	-	0/6/23/26	0/1/1/1
7	MLI	A	596	-	-	0/0/4/4	0/0/0/0
4	NAG	C	3440	1	-	0/6/23/26	0/1/1/1
4	NAG	C	596	1	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	3440	NAG	C1-O5-C5	2.14	114.97	112.25
4	A	3830	NAG	C1-O5-C5	3.26	116.39	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	596	NAG	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	522/601 (86%)	0.13	26 (4%) 32 19	58, 81, 119, 169	0
1	C	531/601 (88%)	0.18	19 (3%) 46 31	52, 74, 121, 166	0
2	B	57/58 (98%)	0.27	6 (10%) 8 5	70, 103, 136, 144	0
2	D	57/58 (98%)	-0.09	0 100 100	58, 72, 95, 112	0
All	All	1167/1318 (88%)	0.15	51 (4%) 38 24	52, 78, 124, 169	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	507	CYS	6.5
1	C	299	PRO	5.0
1	A	506	ASP	4.9
1	A	508	GLY	4.0
1	A	518	ASN	3.8
2	B	14	TRP	3.7
1	A	521	CYS	3.6
1	C	526	PRO	3.5
1	C	296	CYS	3.4
1	A	499	PHE	3.2
1	A	510	ILE	3.1
1	A	505	ALA	3.0
2	B	2	PHE	3.0
1	A	168	HIS	2.9
1	C	153	THR	2.9
1	C	158	GLU	2.9
1	A	175	PRO	2.9
1	A	498	ASN	2.8
1	C	532	ASN	2.8
1	A	509	TYR	2.8
1	C	297	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	524	CYS	2.8
1	C	518	ASN	2.7
1	A	154	ALA	2.7
2	B	21	HIS	2.6
1	A	192	GLY	2.6
1	C	536	ALA	2.6
1	A	164	GLU	2.6
1	A	495	LYS	2.6
1	A	502	THR	2.5
2	B	28	ALA	2.5
1	A	520	THR	2.5
1	A	497	PHE	2.5
1	A	496	ASN	2.5
1	C	301	PRO	2.5
1	C	510	ILE	2.4
2	B	29	ASP	2.3
2	B	27	ILE	2.3
1	C	509	TYR	2.3
1	C	525	HIS	2.3
1	C	298	GLY	2.3
1	A	517	ASP	2.2
1	C	295	PRO	2.2
1	A	488	THR	2.2
1	A	504	ILE	2.2
1	A	514	TYR	2.1
1	C	275	ASN	2.1
1	C	285	ASP	2.1
1	A	513	ALA	2.0
1	C	154	ALA	2.0
1	C	513	ALA	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	C	4700	14/15	0.97	0.28	1.47	59,61,63,64	0
3	NAG	A	4700	14/15	0.94	0.23	-0.27	66,69,71,71	0
5	NAG	C	3830	14/15	0.90	0.18	-1.02	73,78,80,83	0
3	NAG	A	4701	14/15	0.95	0.23	-	73,74,76,79	0
6	NAG	C	4701	14/15	0.96	0.28	-	65,66,67,68	0
3	MAN	A	4705	11/12	0.73	0.40	-	94,95,95,96	0
3	MAN	A	4703	11/12	0.82	0.31	-	88,90,91,91	0
6	MAN	C	4703	11/12	0.84	0.25	-	70,72,73,73	0
5	NAG	C	3831	14/15	0.92	0.21	-	85,87,87,88	0
3	MAN	A	4702	11/12	0.87	0.28	-	82,85,89,92	0
3	MAN	A	4704	11/12	0.88	0.30	-	90,91,91,91	0
6	MAN	C	4702	11/12	0.90	0.24	-	69,70,71,71	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
7	MLI	A	596	7/7	0.76	0.41	4.88	69,70,70,71	0
4	NAG	A	3830	14/15	0.88	0.21	-0.61	76,79,80,80	0
4	NAG	C	3440	14/15	0.81	0.30	-	87,90,92,93	0
4	NAG	C	596	14/15	0.88	0.40	-	81,84,85,85	0

6.5 Other polymers

There are no such residues in this entry.