Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:53 AM GMT

PDB ID	:	2YPG
Title	:	Haemagglutinin of 1968 Human H3N2 Virus in Complex with Human Receptor Analogue LSTc
Authors	:	Liu, J.; Xiong, X.; Haire, L.F.; Lin, Y.P.; Wharton, S.A.; Martin, S.R.; Coombs, P.J.; Vachieri, S.G.; Christodoulou, E.; Walker, P.A.; Skehel, J.J.; Gamblin, S.J.; Hay, A.J.; Daniels, R.S.; McCauley, J.W.
Deposited on	:	2012-10-30
Resolution	:	2.85 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:

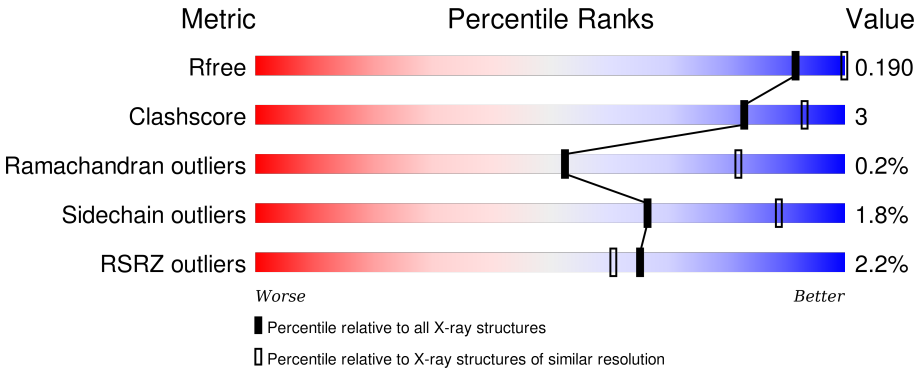
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	328	2% 88% 9%
1	C	328	3% 89% 8%
1	E	328	% 89% 7%
2	B	175	3% 93% 5%
2	D	175	2% 93%

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Mol	Chain	Length	Quality of chain
2	F	175	2% 94%

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
8	FLC	B	1176	-	-	-	X
8	FLC	B	1177	-	-	-	X
8	FLC	C	1339	-	-	-	X
8	FLC	D	1174	-	-	-	X
8	FLC	E	1336	-	-	-	X
8	FLC	E	1337	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 12735 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.

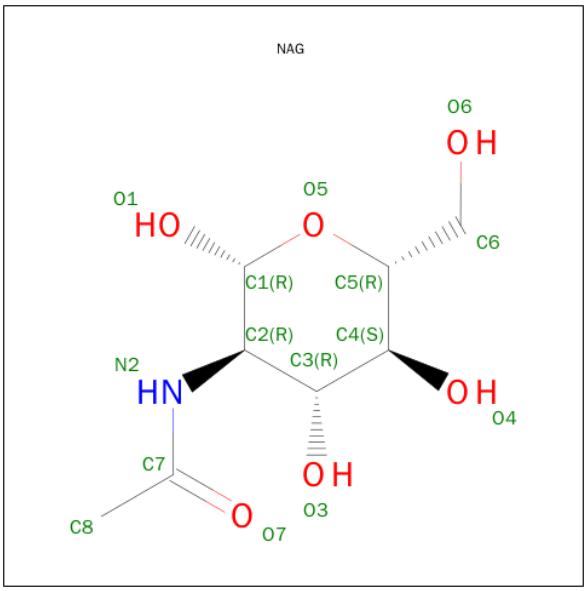
- Molecule 1 is a protein called HEMAGGLUTININ HA1 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2446	1532	429	472	13			
1	C	320	Total	C	N	O	S	0	0	0
			2472	1547	435	477	13			
1	E	318	Total	C	N	O	S	0	0	0
			2455	1538	431	473	13			

- Molecule 2 is a protein called HEMAGGLUTININ HA2 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1407	874	247	280	6			
2	D	172	Total	C	N	O	S	0	0	0
			1399	868	246	279	6			
2	F	173	Total	C	N	O	S	0	0	0
			1407	874	247	280	6			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

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

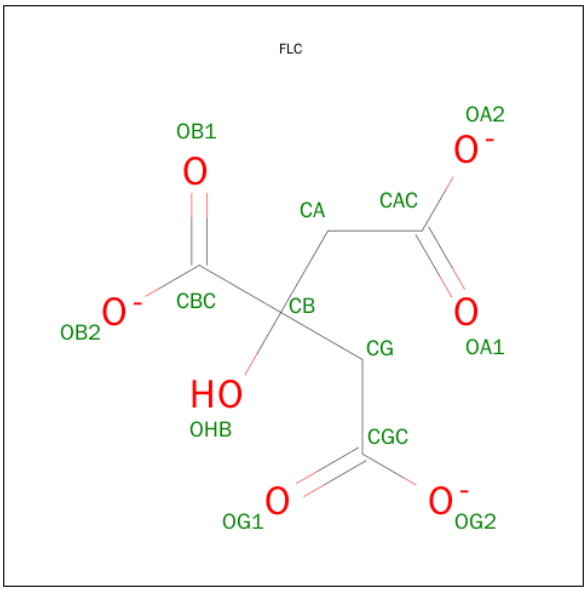
- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	5	Total C N O 68 37 2 29	0	0
7	E	5	Total C N O 68 37 2 29	0	0

- Molecule 8 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 13 6 7	0	0
8	A	1	Total C O 13 6 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 13 6 7	0	0
8	B	1	Total C O 13 6 7	0	0
8	B	1	Total C O 13 6 7	0	0
8	C	1	Total C O 13 6 7	0	0
8	C	1	Total C O 13 6 7	0	0
8	C	1	Total C O 13 6 7	0	0
8	D	1	Total C O 13 6 7	0	0
8	E	1	Total C O 13 6 7	0	0
8	E	1	Total C O 13 6 7	0	0
8	E	1	Total C O 13 6 7	0	0
8	F	1	Total C O 13 6 7	0	0

- Molecule 9 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	4	Total C N O 46 25 2 19	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	96	Total O 96 96	0	0
10	B	61	Total O 61 61	0	0
10	C	83	Total O 83 83	0	0
10	D	61	Total O 61 61	0	0
10	E	93	Total O 93 93	0	0

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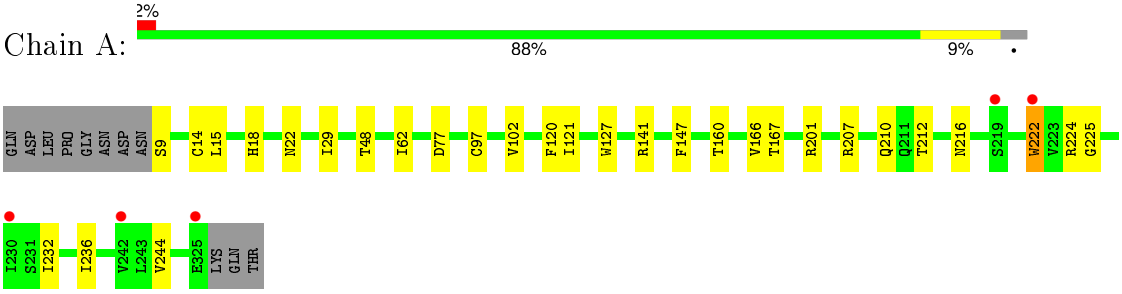
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	F	39	Total O 39 39	0	0

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.

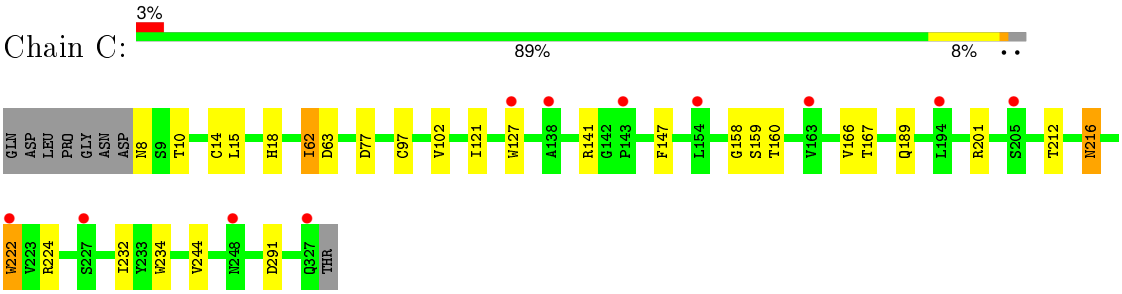
- Molecule 1: HEMAGGLUTININ HA1 CHAIN

Chain A:



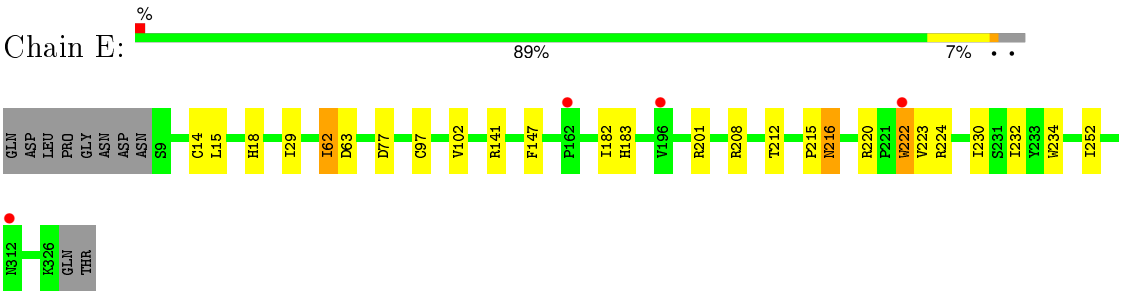
- Molecule 1: HEMAGGLUTININ HA1 CHAIN

Chain C:



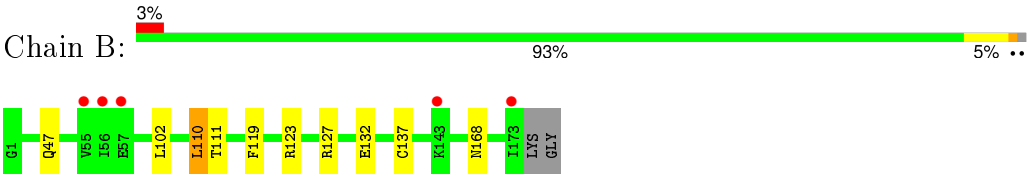
- Molecule 1: HEMAGGLUTININ HA1 CHAIN

Chain E:



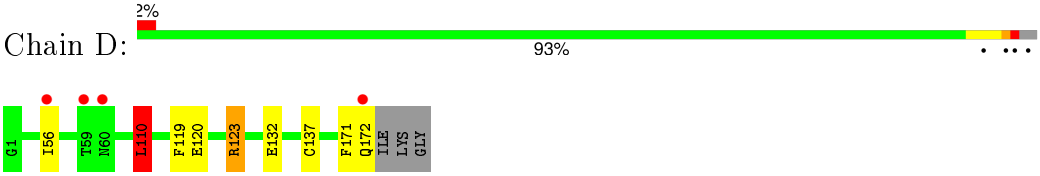
- Molecule 2: HEMAGGLUTININ HA2 CHAIN

Chain B:



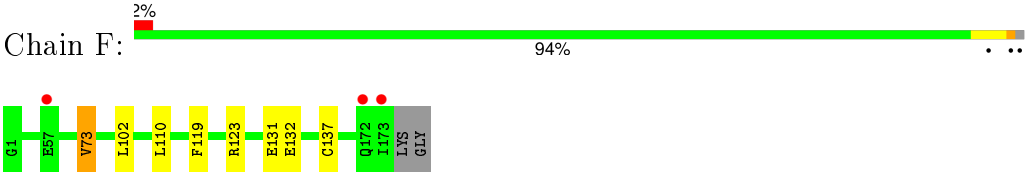
• Molecule 2: HEMAGGLUTININ HA2 CHAIN

Chain D:



• Molecule 2: HEMAGGLUTININ HA2 CHAIN

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	160.77Å 160.77Å 177.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	160.77 – 2.85 160.77 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (160.77-2.85) 100.0 (160.77-2.85)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.177 , 0.190 0.177 , 0.190	Depositor DCC
R_{free} test set	5238 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	47.4	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.6	EDS
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 104850 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12735	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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: BGC, NAG, SIA, GAL, BMA, FLC, FUL

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	0.48	1/2502 (0.0%)	0.57	0/3410
1	C	0.48	2/2528 (0.1%)	0.56	0/3444
1	E	0.48	2/2511 (0.1%)	0.55	0/3421
2	B	0.48	0/1431	0.61	1/1923 (0.1%)
2	D	0.49	0/1423	0.61	2/1912 (0.1%)
2	F	0.50	0/1431	0.60	1/1923 (0.1%)
All	All	0.48	5/11826 (0.0%)	0.57	4/16033 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	222	TRP	CD2-CE2	5.99	1.48	1.41
1	E	222	TRP	CD2-CE2	5.77	1.48	1.41
1	A	222	TRP	CD2-CE2	5.27	1.47	1.41
1	C	234	TRP	CD2-CE2	5.19	1.47	1.41
1	E	234	TRP	CD2-CE2	5.05	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	123	ARG	NE-CZ-NH1	6.75	123.68	120.30
2	F	123	ARG	NE-CZ-NH1	6.51	123.56	120.30
2	D	110	LEU	CA-CB-CG	6.19	129.54	115.30
2	D	123	ARG	NE-CZ-NH1	5.15	122.87	120.30

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	2446	0	2393	29	0
1	C	2472	0	2419	24	0
1	E	2455	0	2406	15	0
2	B	1407	0	1329	6	0
2	D	1399	0	1318	9	0
2	F	1407	0	1329	6	0
3	A	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
3	E	14	0	13	0	0
3	F	14	0	13	0	0
4	A	38	0	34	1	0
5	A	39	0	34	2	0
5	C	39	0	34	1	0
5	E	39	0	32	2	0
6	A	28	0	25	0	0
6	B	28	0	25	0	0
6	C	56	0	50	0	0
6	E	28	0	25	0	0
7	A	68	0	58	0	0
7	E	68	0	58	0	0
8	A	26	0	10	0	0
8	B	39	0	15	4	0
8	C	39	0	15	0	0
8	D	13	0	5	0	0
8	E	39	0	15	0	0
8	F	13	0	5	0	0
9	C	46	0	38	0	0
10	A	96	0	0	2	0
10	B	61	0	0	1	0
10	C	83	0	0	0	0
10	D	61	0	0	0	0
10	E	93	0	0	0	0
10	F	39	0	0	0	0
All	All	12735	0	11737	75	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 3.

All (75) 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:216:ASN:ND2	1:C:212:THR:HG21	1.53	1.22
1:C:216:ASN:HB3	1:E:212:THR:HG21	1.46	0.97
1:A:216:ASN:ND2	1:C:212:THR:CG2	2.28	0.95
1:A:216:ASN:HD22	1:C:212:THR:HG21	1.23	0.93
1:C:167:THR:HG22	1:C:244:VAL:HG22	1.54	0.89
1:A:167:THR:HG22	1:A:244:VAL:HG22	1.63	0.80
1:E:230:ILE:HD12	1:E:252:ILE:HG13	1.64	0.77
1:A:222:TRP:CZ2	1:A:225:GLY:HA2	2.28	0.68
5:E:1328:NAG:O4	5:E:1329:NAG:C7	2.42	0.68
1:A:216:ASN:HD22	1:C:212:THR:CG2	2.00	0.66
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.78	0.66
1:A:167:THR:HG21	5:A:1329:NAG:H61	1.79	0.65
8:B:1177:FLC:OG2	10:B:2060:HOH:O	2.15	0.65
1:A:97:CYS:O	1:A:224:ARG:NH1	2.31	0.64
1:E:97:CYS:O	1:E:224:ARG:NH1	2.31	0.63
1:C:97:CYS:O	1:C:224:ARG:NH1	2.31	0.62
1:C:15:LEU:HD22	2:D:119:PHE:HA	1.81	0.61
1:A:212:THR:HG21	1:E:216:ASN:HB3	1.82	0.61
1:A:236:ILE:CD1	2:F:73:VAL:HG22	2.31	0.61
1:A:141:ARG:NH2	1:A:147:PHE:O	2.35	0.60
1:A:216:ASN:CG	1:C:212:THR:HG21	2.19	0.60
1:E:141:ARG:NH2	1:E:147:PHE:O	2.35	0.60
1:A:236:ILE:HD12	2:F:73:VAL:HG22	1.84	0.59
5:E:1328:NAG:O4	5:E:1329:NAG:N2	2.36	0.59
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.86	0.58
1:C:167:THR:HG21	5:C:1331:NAG:H62	1.86	0.58
1:C:141:ARG:NH2	1:C:147:PHE:O	2.35	0.58
1:A:207:ARG:HG3	1:E:223:VAL:HG22	1.90	0.54
1:E:183:HIS:HA	1:E:230:ILE:HD13	1.88	0.53
1:A:29:ILE:HD11	2:B:102:LEU:HD23	1.92	0.52
8:B:1178:FLC:CGC	8:B:1178:FLC:OB1	2.56	0.52
1:A:167:THR:CG2	5:A:1329:NAG:H61	2.40	0.51
1:C:127:TRP:CZ3	1:C:166:VAL:HG21	2.46	0.51
1:C:291:ASP:O	2:D:56:ILE:HG23	2.11	0.50
1:E:29:ILE:HD11	2:F:102:LEU:HD23	1.92	0.50
2:D:119:PHE:HZ	2:D:132:GLU:HG3	1.77	0.50
1:A:222:TRP:CE2	1:A:225:GLY:HA2	2.47	0.49
2:D:120:GLU:CD	2:D:123:ARG:HH21	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:119:PHE:HZ	2:F:132:GLU:CG	2.25	0.49
1:A:48:THR:HG23	10:A:2015:HOH:O	2.12	0.49
2:B:110:LEU:HD23	2:B:111:THR:N	2.28	0.48
8:B:1176:FLC:OHB	8:B:1176:FLC:OA1	2.31	0.48
2:B:127:ARG:NH1	2:F:131:GLU:OE1	2.44	0.48
1:A:127:TRP:CH2	1:A:166:VAL:HG21	2.49	0.48
1:C:121:ILE:N	1:C:121:ILE:HD12	2.28	0.48
2:D:110:LEU:HD23	2:D:110:LEU:C	2.34	0.47
1:C:62:ILE:HG22	1:C:63:ASP:N	2.31	0.45
1:C:167:THR:CG2	1:C:244:VAL:HG22	2.36	0.45
1:C:216:ASN:CB	1:E:212:THR:HG21	2.33	0.45
1:A:121:ILE:N	1:A:121:ILE:HD12	2.32	0.45
1:A:14:CYS:HA	2:B:137:CYS:HA	1.99	0.45
1:A:77:ASP:OD2	1:A:141:ARG:NH1	2.50	0.44
2:D:120:GLU:OE1	2:D:123:ARG:NH2	2.50	0.44
1:E:102:VAL:HG22	1:E:232:ILE:HB	1.99	0.44
1:E:77:ASP:OD2	1:E:141:ARG:NH1	2.51	0.44
2:D:110:LEU:C	2:D:110:LEU:CD2	2.86	0.44
8:B:1177:FLC:OB2	8:B:1177:FLC:CGC	2.66	0.43
4:A:1328:NAG:H82	4:A:1328:NAG:O3	2.18	0.43
1:E:182:ILE:HD11	1:E:215:PRO:HD3	2.00	0.43
1:C:14:CYS:HA	2:D:137:CYS:HA	2.01	0.43
1:C:127:TRP:CE3	1:C:166:VAL:HG21	2.54	0.43
1:A:102:VAL:HG22	1:A:232:ILE:HB	2.00	0.42
1:C:77:ASP:OD2	1:C:141:ARG:NH1	2.51	0.42
1:E:14:CYS:HA	2:F:137:CYS:HA	2.02	0.42
1:A:120:PHE:C	1:A:121:ILE:HD12	2.40	0.42
1:C:8:ASN:HA	1:C:10:THR:H	1.84	0.42
2:D:171:PHE:O	2:D:172:GLN:CB	2.68	0.42
1:A:167:THR:CG2	1:A:244:VAL:HG22	2.42	0.41
1:E:62:ILE:HG22	1:E:63:ASP:N	2.35	0.41
1:C:158:GLY:O	1:C:159:SER:OG	2.20	0.41
2:B:47:GLN:HB3	2:B:110:LEU:HD11	2.01	0.41
1:A:224:ARG:NH2	10:A:2066:HOH:O	2.54	0.41
1:C:15:LEU:N	1:C:15:LEU:HD12	2.36	0.40
1:A:127:TRP:CZ3	1:A:166:VAL:HG21	2.56	0.40
1:A:210:GLN:OE1	1:E:220:ARG:NH2	2.55	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	315/328 (96%)	307 (98%)	7 (2%)	1 (0%)	46 76
1	C	318/328 (97%)	309 (97%)	8 (2%)	1 (0%)	46 76
1	E	316/328 (96%)	309 (98%)	6 (2%)	1 (0%)	46 76
2	B	171/175 (98%)	162 (95%)	9 (5%)	0	100 100
2	D	170/175 (97%)	162 (95%)	8 (5%)	0	100 100
2	F	171/175 (98%)	164 (96%)	7 (4%)	0	100 100
All	All	1461/1509 (97%)	1413 (97%)	45 (3%)	3 (0%)	52 82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	C	62	ILE
1	E	62	ILE

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	279/289 (96%)	274 (98%)	5 (2%)	66 89
1	C	282/289 (98%)	276 (98%)	6 (2%)	61 86
1	E	280/289 (97%)	274 (98%)	6 (2%)	61 86
2	B	148/149 (99%)	145 (98%)	3 (2%)	63 87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	147/149 (99%)	146 (99%)	1 (1%)	88 96
2	F	148/149 (99%)	146 (99%)	2 (1%)	74 91
All	All	1284/1314 (98%)	1261 (98%)	23 (2%)	66 89

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	18	HIS
1	A	22	ASN
1	A	160	THR
1	A	201	ARG
2	B	110	LEU
2	B	132	GLU
2	B	168	ASN
1	C	18	HIS
1	C	160	THR
1	C	189	GLN
1	C	201	ARG
1	C	216	ASN
1	C	222	TRP
2	D	110	LEU
1	E	15	LEU
1	E	18	HIS
1	E	201	ARG
1	E	208	ARG
1	E	216	ASN
1	E	222	TRP
2	F	73	VAL
2	F	110	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	197	GLN
1	A	216	ASN
2	B	26	HIS
1	C	171	ASN
1	C	197	GLN

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Mol	Chain	Res	Type
2	D	26	HIS
1	E	54	ASN
1	E	171	ASN
1	E	197	GLN
2	F	26	HIS
2	F	60	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

Of 36 carbohydrates modelled in this entry, 1 is modelled with single atom - leaving 35 for Mogul analysis.

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	1327	1,4	14,14,15	0.51	0	15,19,21	1.39	2 (13%)
4	NAG	A	1328	4	14,14,15	0.68	0	15,19,21	1.21	1 (6%)
5	NAG	A	1329	1,5	14,14,15	1.83	1 (7%)	15,19,21	1.28	1 (6%)
5	NAG	A	1330	5	14,14,15	0.55	0	15,19,21	1.12	1 (6%)
5	BMA	A	1331	5	11,11,12	0.62	0	14,15,17	1.06	2 (14%)
6	NAG	A	1332	1,6	14,14,15	0.51	0	15,19,21	1.15	1 (6%)
6	NAG	A	1333	6	14,14,15	0.47	0	15,19,21	0.83	1 (6%)
4	FUL	A	1334	4	10,10,11	0.68	0	14,14,16	1.70	3 (21%)
7	SIA	A	1335	7	16,20,21	0.31	0	18,28,31	0.93	1 (5%)
7	GAL	A	1336	7	11,11,12	0.29	0	14,15,17	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BGC	A	1337	7	12,12,12	0.43	0	17,17,17	0.57	0
7	NAG	A	1340	7	14,14,15	0.33	0	15,19,21	0.70	0
7	GAL	A	1341	7	11,11,12	0.32	0	14,15,17	0.63	0
6	NAG	B	1174	2,6	14,14,15	0.49	0	15,19,21	0.71	0
6	NAG	B	1175	6	14,14,15	0.45	0	15,19,21	1.01	0
6	NAG	C	1329	1,6	14,14,15	1.60	1 (7%)	15,19,21	1.57	2 (13%)
6	NAG	C	1330	6	14,14,15	0.72	0	15,19,21	1.13	2 (13%)
5	NAG	C	1331	1,5	14,14,15	0.67	0	15,19,21	1.37	1 (6%)
5	NAG	C	1332	5	14,14,15	0.54	0	15,19,21	0.62	0
5	BMA	C	1333	5	11,11,12	0.53	0	14,15,17	0.73	0
6	NAG	C	1334	1,6	14,14,15	1.95	1 (7%)	15,19,21	1.91	2 (13%)
6	NAG	C	1335	6	14,14,15	0.50	0	15,19,21	0.68	0
9	SIA	C	1336	9	16,20,21	0.40	0	18,28,31	0.90	1 (5%)
9	GAL	C	1337	9	11,11,12	0.33	0	14,15,17	0.68	0
9	NAG	C	1341	9	14,14,15	0.37	0	15,19,21	0.98	1 (6%)
5	NAG	E	1328	1,5	14,14,15	0.71	0	15,19,21	1.86	6 (40%)
5	NAG	E	1329	5	14,14,15	0.87	1 (7%)	15,19,21	2.28	3 (20%)
5	BMA	E	1330	5	11,11,12	0.46	0	14,15,17	1.23	1 (7%)
6	NAG	E	1331	1,6	14,14,15	0.54	0	15,19,21	1.18	1 (6%)
6	NAG	E	1332	6	14,14,15	0.48	0	15,19,21	0.87	0
7	SIA	E	1333	7	16,20,21	0.34	0	18,28,31	1.01	1 (5%)
7	GAL	E	1334	7	11,11,12	0.39	0	14,15,17	0.75	1 (7%)
7	NAG	E	1338	7	14,14,15	0.45	0	15,19,21	0.90	0
7	GAL	E	1339	7	11,11,12	0.47	0	14,15,17	0.80	1 (7%)
7	BGC	E	1340	7	12,12,12	0.43	0	17,17,17	0.60	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	1327	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1328	4	-	0/6/23/26	0/1/1/1
5	NAG	A	1329	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1330	5	-	0/6/23/26	0/1/1/1
5	BMA	A	1331	5	-	0/2/19/22	0/1/1/1
6	NAG	A	1332	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1333	6	-	0/6/23/26	0/1/1/1
4	FUL	A	1334	4	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SIA	A	1335	7	-	0/14/34/38	0/1/1/1
7	GAL	A	1336	7	-	0/2/19/22	0/1/1/1
7	BGC	A	1337	7	-	0/2/22/22	0/1/1/1
7	NAG	A	1340	7	-	0/6/23/26	0/1/1/1
7	GAL	A	1341	7	-	0/2/19/22	0/1/1/1
6	NAG	B	1174	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1175	6	-	0/6/23/26	0/1/1/1
6	NAG	C	1329	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	1330	6	-	0/6/23/26	0/1/1/1
5	NAG	C	1331	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1332	5	-	0/6/23/26	0/1/1/1
5	BMA	C	1333	5	-	0/2/19/22	0/1/1/1
6	NAG	C	1334	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	1335	6	-	0/6/23/26	0/1/1/1
9	SIA	C	1336	9	-	0/14/34/38	0/1/1/1
9	GAL	C	1337	9	-	0/2/19/22	0/1/1/1
9	NAG	C	1341	9	-	0/6/23/26	0/1/1/1
5	NAG	E	1328	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1329	5	-	0/6/23/26	0/1/1/1
5	BMA	E	1330	5	-	0/2/19/22	0/1/1/1
6	NAG	E	1331	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	1332	6	-	0/6/23/26	0/1/1/1
7	SIA	E	1333	7	-	0/14/34/38	0/1/1/1
7	GAL	E	1334	7	-	0/2/19/22	0/1/1/1
7	NAG	E	1338	7	-	0/6/23/26	0/1/1/1
7	GAL	E	1339	7	-	0/2/19/22	0/1/1/1
7	BGC	E	1340	7	-	0/2/22/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1334	NAG	O5-C1	-7.04	1.31	1.43
5	A	1329	NAG	O5-C1	-6.46	1.32	1.43
6	C	1329	NAG	O5-C1	-5.63	1.34	1.43
5	E	1329	NAG	C1-C2	2.45	1.55	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1334	NAG	C1-O5-C5	-5.67	105.06	112.25
5	E	1329	NAG	C3-C2-N2	-5.64	97.05	110.56
4	A	1327	NAG	O4-C4-C3	-4.15	101.00	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1329	NAG	C1-O5-C5	-3.45	107.87	112.25
5	E	1328	NAG	O4-C4-C3	-3.22	103.09	110.34
9	C	1336	SIA	C4-C5-N5	-2.91	104.09	110.41
7	E	1333	SIA	C6-C5-N5	-2.36	106.95	111.07
7	A	1335	SIA	C4-C5-N5	-2.35	105.31	110.41
4	A	1334	FUL	O2-C2-C3	-2.18	105.74	110.12
6	C	1334	NAG	C4-C3-C2	-2.10	107.96	111.23
5	E	1328	NAG	O7-C7-C8	-2.08	118.25	122.06
6	C	1329	NAG	O4-C4-C3	-2.06	105.71	110.34
4	A	1328	NAG	C8-C7-N2	2.04	120.01	116.11
7	E	1334	GAL	C1-C2-C3	2.07	112.00	109.54
6	A	1333	NAG	C1-O5-C5	2.16	114.99	112.25
5	A	1331	BMA	C1-O5-C5	2.26	115.11	112.25
5	E	1329	NAG	C4-C3-C2	2.33	114.85	111.23
6	C	1330	NAG	C3-C4-C5	2.34	114.27	110.20
7	E	1339	GAL	C1-C2-C3	2.38	112.36	109.54
5	E	1328	NAG	O3-C3-C2	2.38	113.83	109.11
5	E	1328	NAG	C4-C3-C2	2.40	114.95	111.23
4	A	1327	NAG	C4-C3-C2	2.54	115.18	111.23
5	E	1328	NAG	C3-C4-C5	2.55	114.64	110.20
9	C	1341	NAG	C3-C4-C5	2.63	114.79	110.20
5	A	1331	BMA	C1-C2-C3	2.64	112.67	109.54
6	C	1330	NAG	C4-C3-C2	2.65	115.34	111.23
5	A	1330	NAG	C1-O5-C5	2.72	115.70	112.25
6	A	1332	NAG	C1-O5-C5	2.94	115.98	112.25
6	E	1331	NAG	C1-O5-C5	3.21	116.32	112.25
4	A	1334	FUL	O5-C5-C6	3.25	111.50	106.13
5	E	1328	NAG	O5-C5-C6	3.58	115.09	107.35
5	C	1331	NAG	C1-O5-C5	3.74	117.00	112.25
5	E	1330	BMA	C1-O5-C5	3.81	117.08	112.25
4	A	1334	FUL	C1-C2-C3	4.16	114.46	109.54
6	C	1329	NAG	C3-C4-C5	4.26	117.63	110.20
5	E	1329	NAG	C1-O5-C5	5.05	118.66	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1328	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1329	NAG	2	0
5	C	1331	NAG	1	0
5	E	1328	NAG	2	0
5	E	1329	NAG	2	0

5.6 Ligand geometry

18 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	$\#\|Z\| > 2$
3	NAG	A	1326	1	14,14,15	0.65	0	15,19,21	1.37	2 (13%)
8	FLC	A	1338	-	3,12,12	0.63	0	3,17,17	1.29	0
8	FLC	A	1339	-	3,12,12	0.83	0	3,17,17	2.90	1 (33%)
8	FLC	B	1176	-	3,12,12	0.72	0	3,17,17	2.28	2 (66%)
8	FLC	B	1177	-	3,12,12	0.63	0	3,17,17	1.30	1 (33%)
8	FLC	B	1178	-	3,12,12	0.85	0	3,17,17	1.43	1 (33%)
3	NAG	C	1328	1	14,14,15	0.54	0	15,19,21	1.50	1 (6%)
8	FLC	C	1338	-	3,12,12	0.49	0	3,17,17	1.12	0
8	FLC	C	1339	-	3,12,12	0.18	0	3,17,17	0.70	0
8	FLC	C	1340	-	3,12,12	0.67	0	3,17,17	1.60	1 (33%)
3	NAG	D	1173	2	14,14,15	0.49	0	15,19,21	0.85	0
8	FLC	D	1174	-	3,12,12	0.35	0	3,17,17	1.26	1 (33%)
3	NAG	E	1327	1	14,14,15	0.44	0	15,19,21	1.94	1 (6%)
8	FLC	E	1335	-	3,12,12	0.45	0	3,17,17	1.12	0
8	FLC	E	1336	-	3,12,12	0.57	0	3,17,17	0.73	0
8	FLC	E	1337	-	3,12,12	0.14	0	3,17,17	0.90	0
3	NAG	F	1174	2	14,14,15	0.50	0	15,19,21	0.84	0
8	FLC	F	1175	-	3,12,12	0.58	0	3,17,17	1.38	1 (33%)

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	1326	1	-	0/6/23/26	0/1/1/1
8	FLC	A	1338	-	-	0/6/16/16	0/0/0/0
8	FLC	A	1339	-	-	0/6/16/16	0/0/0/0
8	FLC	B	1176	-	-	0/6/16/16	0/0/0/0
8	FLC	B	1177	-	-	0/6/16/16	0/0/0/0
8	FLC	B	1178	-	-	0/6/16/16	0/0/0/0
3	NAG	C	1328	1	-	0/6/23/26	0/1/1/1
8	FLC	C	1338	-	-	0/6/16/16	0/0/0/0
8	FLC	C	1339	-	-	0/6/16/16	0/0/0/0
8	FLC	C	1340	-	-	0/6/16/16	0/0/0/0
3	NAG	D	1173	2	-	0/6/23/26	0/1/1/1
8	FLC	D	1174	-	-	0/6/16/16	0/0/0/0
3	NAG	E	1327	1	-	0/6/23/26	0/1/1/1
8	FLC	E	1335	-	-	0/6/16/16	0/0/0/0
8	FLC	E	1336	-	-	0/6/16/16	0/0/0/0
8	FLC	E	1337	-	-	0/6/16/16	0/0/0/0
3	NAG	F	1174	2	-	0/6/23/26	0/1/1/1
8	FLC	F	1175	-	-	0/6/16/16	0/0/0/0

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1176	FLC	CB-CG-CGC	-3.03	110.11	114.96
8	C	1340	FLC	CB-CA-CAC	-2.53	110.92	114.96
8	F	1175	FLC	CB-CG-CGC	-2.05	111.68	114.96
8	B	1178	FLC	CB-CG-CGC	2.02	118.19	114.96
8	D	1174	FLC	CB-CA-CAC	2.04	118.22	114.96
8	B	1177	FLC	CG-CB-CA	2.10	114.83	109.81
8	B	1176	FLC	CG-CB-CA	2.30	115.31	109.81
3	A	1326	NAG	C4-C3-C2	2.79	115.56	111.23
3	A	1326	NAG	C1-O5-C5	2.88	115.91	112.25
8	A	1339	FLC	CG-CB-CA	4.50	120.58	109.81
3	C	1328	NAG	C1-O5-C5	4.95	118.53	112.25
3	E	1327	NAG	C1-O5-C5	6.98	121.10	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1176	FLC	1	0
8	B	1177	FLC	2	0
8	B	1178	FLC	1	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	317/328 (96%)	0.75	5 (1%) 74 72	27, 42, 67, 88	0
1	C	320/328 (97%)	0.84	11 (3%) 49 41	27, 47, 76, 95	0
1	E	318/328 (96%)	0.73	4 (1%) 79 77	27, 40, 61, 90	0
2	B	173/175 (98%)	0.69	5 (2%) 55 49	26, 42, 74, 104	0
2	D	172/175 (98%)	0.62	4 (2%) 64 59	24, 38, 62, 150	0
2	F	173/175 (98%)	0.67	3 (1%) 73 70	23, 40, 62, 104	0
All	All	1473/1509 (97%)	0.73	32 (2%) 65 61	23, 42, 71, 150	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	173	ILE	4.2
1	E	222	TRP	3.3
2	F	173	ILE	3.3
2	F	57	GLU	3.2
1	C	248	ASN	3.0
1	C	222	TRP	2.9
2	D	60	ASN	2.8
2	B	143	LYS	2.8
1	C	127	TRP	2.6
2	B	57	GLU	2.6
1	C	143	PRO	2.6
1	A	325	GLU	2.5
2	D	56	ILE	2.5
1	C	194	LEU	2.5
2	B	56	ILE	2.3
1	C	205	SER	2.3
1	C	327	GLN	2.2
1	C	138	ALA	2.2
2	B	55	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	162	PRO	2.2
1	E	312	ASN	2.2
1	A	219	SER	2.1
1	C	227	SER	2.1
2	D	59	THR	2.1
1	C	163	VAL	2.1
2	D	172	GLN	2.1
1	A	230	ILE	2.1
1	C	154	LEU	2.1
1	A	242	VAL	2.1
1	A	222	TRP	2.1
2	F	172	GLN	2.0
1	E	196	VAL	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	E	1331	14/15	0.94	0.29	1.65	55,63,74,84	0
5	NAG	C	1332	14/15	0.96	0.31	0.74	58,61,70,74	0
9	SIA	C	1336	20/21	0.94	0.32	0.56	68,86,90,91	0
6	NAG	A	1332	14/15	0.95	0.23	0.16	52,58,69,80	0
5	NAG	E	1328	14/15	0.85	0.28	-0.16	47,58,67,71	0
7	SIA	A	1335	20/21	0.98	0.25	-0.20	48,56,59,60	0
5	NAG	C	1331	14/15	0.96	0.28	-0.22	47,53,63,69	0
6	NAG	C	1334	14/15	0.94	0.22	-0.38	50,57,62,72	0
5	NAG	A	1329	14/15	0.96	0.23	-0.43	50,51,59,61	0
7	SIA	E	1333	20/21	0.97	0.23	-0.62	44,50,55,55	0
6	NAG	B	1174	14/15	0.93	0.19	-0.67	68,75,85,95	0
5	NAG	A	1330	14/15	0.94	0.26	-0.70	52,57,60,69	0
4	NAG	A	1327	14/15	0.94	0.23	-0.86	50,61,77,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	NAG	C	1329	14/15	0.88	0.21	-1.83	64,71,82,99	0
5	NAG	E	1329	14/15	0.94	0.22	-2.20	60,73,80,90	0
7	NAG	A	1340	14/15	0.92	0.27	-	96,104,111,113	0
5	BMA	E	1330	11/12	0.71	0.20	-	92,102,107,111	0
9	GAL	C	1342	1/12	0.82	0.67	-	144,144,144,144	0
7	GAL	E	1339	11/12	0.79	0.41	-	134,143,152,152	0
7	GAL	E	1334	11/12	0.94	0.21	-	61,83,91,92	0
7	GAL	A	1336	11/12	0.96	0.20	-	64,81,87,88	0
4	FUL	A	1334	10/11	0.88	0.26	-	73,82,87,89	0
6	NAG	A	1333	14/15	0.81	0.39	-	78,98,104,105	0
6	NAG	C	1335	14/15	0.87	0.26	-	75,85,92,92	0
7	GAL	A	1341	11/12	0.81	0.44	-	124,133,137,139	0
5	BMA	C	1333	11/12	0.91	0.16	-	81,85,88,89	0
5	BMA	A	1331	11/12	0.87	0.13	-	75,78,80,80	0
6	NAG	E	1332	14/15	0.82	0.34	-	82,94,102,103	0
7	BGC	A	1337	12/12	0.81	0.39	-	122,130,135,137	0
9	GAL	C	1337	11/12	0.90	0.28	-	101,130,138,141	0
6	NAG	B	1175	14/15	0.89	0.30	-	85,98,101,101	0
7	BGC	E	1340	12/12	0.74	0.34	-	142,152,158,159	0
6	NAG	C	1330	14/15	0.75	0.35	-	109,116,121,122	0
9	NAG	C	1341	14/15	0.81	0.54	-	139,149,153,153	0
4	NAG	A	1328	14/15	0.75	0.33	-	92,104,114,116	0
7	NAG	E	1338	14/15	0.85	0.37	-	98,108,117,122	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	FLC	E	1336	13/13	0.66	0.50	8.36	82,96,107,108	0
8	FLC	D	1174	13/13	0.86	0.48	7.24	53,58,67,68	0
8	FLC	E	1337	13/13	0.79	0.52	7.20	94,100,104,110	0
8	FLC	C	1339	13/13	0.82	0.45	4.83	60,76,83,84	0
8	FLC	B	1177	13/13	0.77	0.45	4.56	60,68,74,75	0
8	FLC	B	1176	13/13	0.79	0.45	4.43	48,60,69,70	0
3	NAG	C	1328	14/15	0.81	0.30	1.46	68,75,80,82	0
8	FLC	F	1175	13/13	0.93	0.28	1.38	77,81,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	FLC	A	1338	13/13	0.82	0.34	1.37	75,99,105,105	0
3	NAG	A	1326	14/15	0.71	0.31	1.22	70,84,89,91	0
8	FLC	C	1338	13/13	0.90	0.26	0.79	60,76,88,90	0
8	FLC	E	1335	13/13	0.80	0.25	0.34	71,100,107,107	0
3	NAG	E	1327	14/15	0.91	0.15	-2.56	46,53,56,56	0
8	FLC	B	1178	13/13	0.81	0.52	-	71,82,92,94	0
8	FLC	A	1339	13/13	0.56	0.54	-	101,112,118,126	0
3	NAG	F	1174	14/15	0.86	0.29	-	58,65,69,69	0
3	NAG	D	1173	14/15	0.94	0.25	-	71,84,87,89	0
8	FLC	C	1340	13/13	0.83	0.44	-	84,91,96,99	0

6.5 Other polymers (i)

There are no such residues in this entry.