



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:38 pm GMT

PDB ID : 4ONT
Title : Ternary host recognition complex of complement factor H, C3d, and sialic acid
Authors : Blaum, B.S.; Stehle, T.S.
Deposited on : 2014-01-29
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

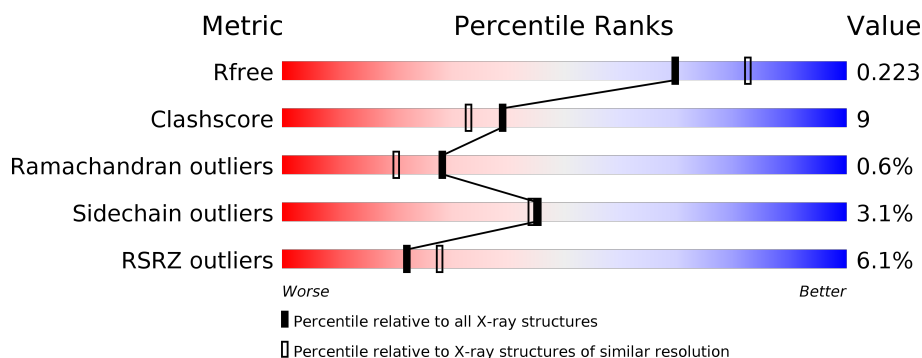
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	100719	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	129	<div> <div>81%</div> <div>17%</div> <div>•</div> </div>
1	E	129	<div> <div>3%</div> <div>82%</div> <div>16%</div> <div>•</div> </div>
1	F	129	<div> <div>41%</div> <div>57%</div> <div>35%</div> <div>• • •</div> </div>
2	A	317	<div> <div>%</div> <div>81%</div> <div>11%</div> <div>• 7%</div> </div>
2	B	317	<div> <div>75%</div> <div>16%</div> <div>• 8%</div> </div>
2	C	317	<div> <div>5%</div> <div>74%</div> <div>16%</div> <div>• 8%</div> </div>

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	SIA	D	1301	-	-	-	X
4	GOL	B	401	-	-	-	X
4	GOL	B	402	-	-	-	X
4	GOL	C	402	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10510 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 Complement factor H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	124	Total	C	N	O	S	0	0	0
			944	595	164	176	9			
1	D	126	Total	C	N	O	S	0	0	0
			997	624	179	185	9			
1	E	126	Total	C	N	O	S	0	2	0
			1004	628	179	188	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1103	GLU	-	EXPRESSION TAG	UNP P08603
D	1104	ALA	-	EXPRESSION TAG	UNP P08603
D	1105	GLU	-	EXPRESSION TAG	UNP P08603
D	1106	PHE	-	EXPRESSION TAG	UNP P08603
E	1103	GLU	-	EXPRESSION TAG	UNP P08603
E	1104	ALA	-	EXPRESSION TAG	UNP P08603
E	1105	GLU	-	EXPRESSION TAG	UNP P08603
E	1106	PHE	-	EXPRESSION TAG	UNP P08603
F	1103	GLU	-	EXPRESSION TAG	UNP P08603
F	1104	ALA	-	EXPRESSION TAG	UNP P08603
F	1105	GLU	-	EXPRESSION TAG	UNP P08603
F	1106	PHE	-	EXPRESSION TAG	UNP P08603

- Molecule 2 is a protein called Complement C3d fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	295	Total	C	N	O	S	0	3	0
			2356	1512	396	439	9			
2	B	292	Total	C	N	O	S	0	0	0
			2287	1468	380	430	9			
2	C	292	Total	C	N	O	S	0	0	0
			2262	1460	374	419	9			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP P01024
A	-5	PRO	-	EXPRESSION TAG	UNP P01024
A	-4	LEU	-	EXPRESSION TAG	UNP P01024
A	-3	GLY	-	EXPRESSION TAG	UNP P01024
A	-2	SER	-	EXPRESSION TAG	UNP P01024
A	-1	PRO	-	EXPRESSION TAG	UNP P01024
A	0	GLU	-	EXPRESSION TAG	UNP P01024
A	1	PHE	-	EXPRESSION TAG	UNP P01024
A	2	ARG	-	EXPRESSION TAG	UNP P01024
A	17	ALA	CYS	ENGINEERED MUTATION	UNP P01024
B	-6	GLY	-	EXPRESSION TAG	UNP P01024
B	-5	PRO	-	EXPRESSION TAG	UNP P01024
B	-4	LEU	-	EXPRESSION TAG	UNP P01024
B	-3	GLY	-	EXPRESSION TAG	UNP P01024
B	-2	SER	-	EXPRESSION TAG	UNP P01024
B	-1	PRO	-	EXPRESSION TAG	UNP P01024
B	0	GLU	-	EXPRESSION TAG	UNP P01024
B	1	PHE	-	EXPRESSION TAG	UNP P01024
B	2	ARG	-	EXPRESSION TAG	UNP P01024
B	17	ALA	CYS	ENGINEERED MUTATION	UNP P01024
C	-6	GLY	-	EXPRESSION TAG	UNP P01024
C	-5	PRO	-	EXPRESSION TAG	UNP P01024
C	-4	LEU	-	EXPRESSION TAG	UNP P01024
C	-3	GLY	-	EXPRESSION TAG	UNP P01024
C	-2	SER	-	EXPRESSION TAG	UNP P01024
C	-1	PRO	-	EXPRESSION TAG	UNP P01024
C	0	GLU	-	EXPRESSION TAG	UNP P01024
C	1	PHE	-	EXPRESSION TAG	UNP P01024
C	2	ARG	-	EXPRESSION TAG	UNP P01024
C	17	ALA	CYS	ENGINEERED MUTATION	UNP P01024

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	3	Total	C	N	O	0	0
			43	23	1	19		
3	E	3	Total	C	N	O	0	0
			43	23	1	19		
3	F	3	Total	C	N	O	0	0
			43	23	1	19		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	5	Total	O	0	0
			5	5		
5	A	133	Total	O	0	0
			133	133		
5	D	85	Total	O	0	0
			85	85		
5	B	127	Total	O	0	0
			127	127		
5	E	59	Total	O	0	0
			59	59		

Continued on next page...

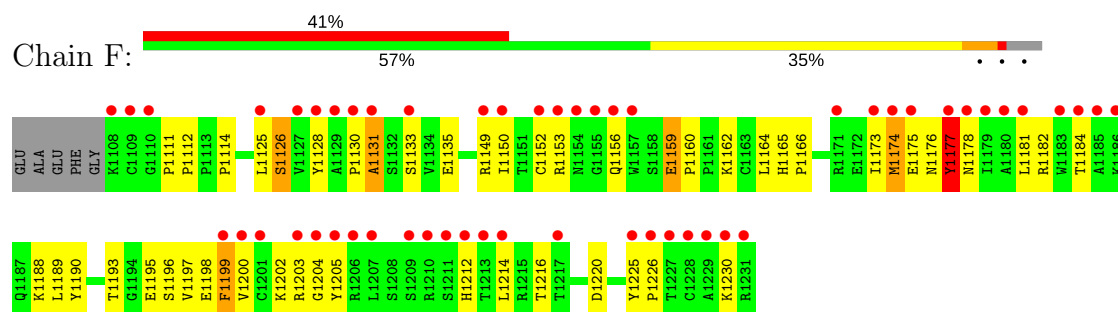
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	80	Total	O	0	0
			80	80		

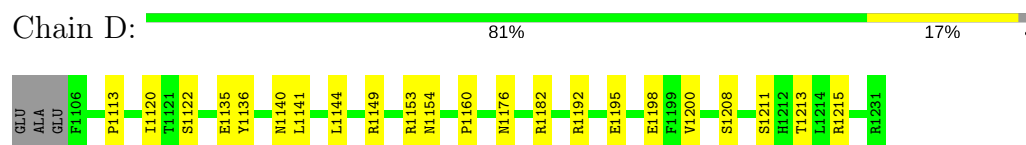
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

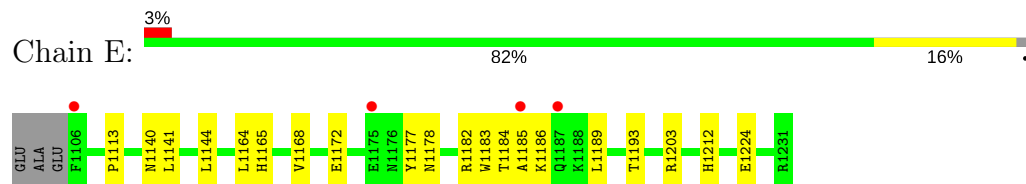
- Molecule 1: Complement factor H



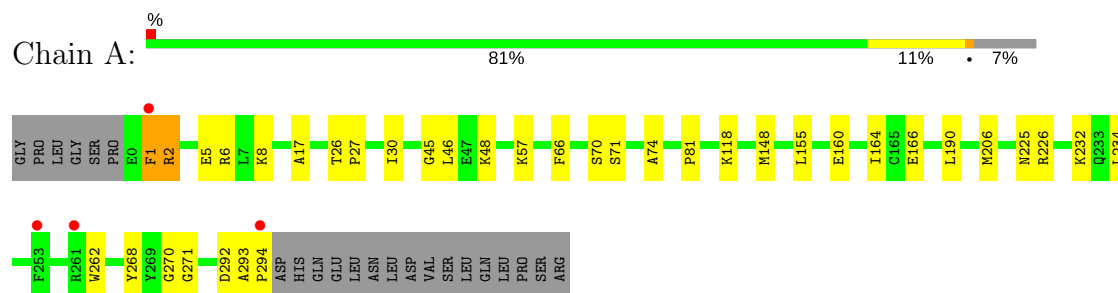
- Molecule 1: Complement factor H



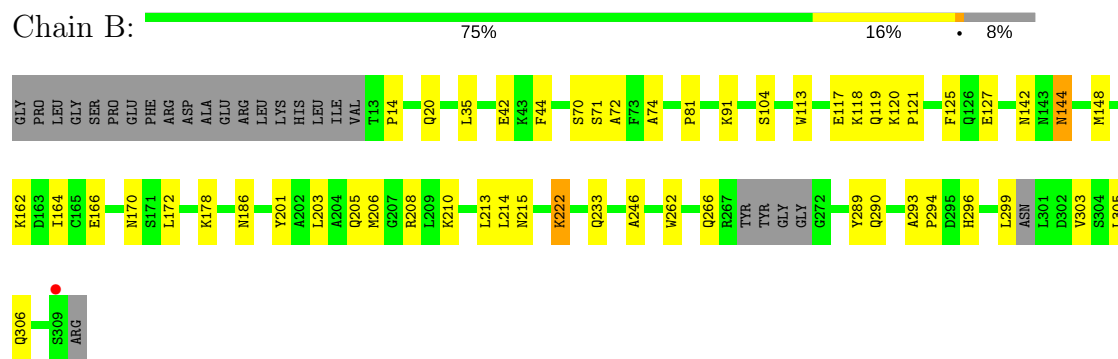
- Molecule 1: Complement factor H



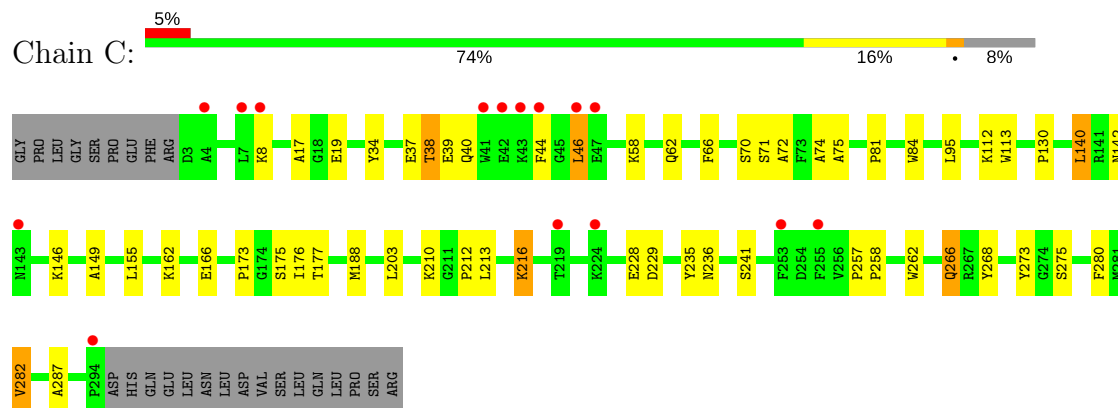
- Molecule 2: Complement C3d fragment



- Molecule 2: Complement C3d fragment



• Molecule 2: Complement C3d fragment



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.46Å 82.54Å 85.75Å 112.50° 110.71° 99.98°	Depositor
Resolution (Å)	46.09 – 2.15 46.08 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.3 (46.09-2.15) 80.3 (46.08-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.172 , 0.223 0.173 , 0.223	Depositor DCC
R_{free} test set	4408 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10510	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SIA, BGC, GAL

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	D	0.63	0/1023	0.75	0/1388
1	E	0.63	0/1030	0.67	0/1400
1	F	0.47	0/970	0.68	0/1325
2	A	0.64	0/2406	0.74	0/3259
2	B	0.64	0/2333	0.75	0/3163
2	C	0.53	0/2311	0.67	0/3138
All	All	0.60	0/10073	0.71	0/13673

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
2	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	229	ASP	Peptide

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	D	997	0	961	15	0
1	E	1004	0	956	17	0
1	F	944	0	870	38	0
2	A	2356	0	2350	27	0
2	B	2287	0	2277	33	0
2	C	2262	0	2241	42	0
3	D	43	0	37	0	0
3	E	43	0	37	0	0
3	F	43	0	37	1	0
4	A	6	0	8	0	0
4	B	18	0	24	1	0
4	C	12	0	16	3	0
4	E	6	0	8	0	0
5	A	133	0	0	5	0
5	B	127	0	0	3	0
5	C	80	0	0	3	0
5	D	85	0	0	3	0
5	E	59	0	0	1	0
5	F	5	0	0	0	0
All	All	10510	0	9822	169	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 9.

All (169) 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:E:1184:THR:HG22	1:E:1186:LYS:H	1.24	1.02
2:A:2:ARG:HG3	2:A:2:ARG:HH11	1.24	1.02
2:C:58:LYS:O	2:C:62:GLN:HG3	1.61	1.00
2:A:166[A]:GLU:HG3	5:A:570:HOH:O	1.73	0.86
2:C:188:MET:HE1	2:C:213:LEU:N	1.90	0.85
2:C:70:SER:O	2:C:71:SER:HB2	1.76	0.84
2:C:188:MET:HE3	2:C:212:PRO:HB2	1.62	0.81
1:D:1213:THR:HG22	5:D:1479:HOH:O	1.79	0.81
2:A:164:ILE:HD12	5:A:591:HOH:O	1.81	0.79
2:B:42:GLU:HG2	5:B:574:HOH:O	1.82	0.77
2:C:95:LEU:HD22	2:C:280:PHE:CZ	2.21	0.74
2:A:1:PHE:O	2:A:1:PHE:HD1	1.70	0.73
1:F:1176:ASN:C	1:F:1178:ASN:H	1.91	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:GLU:CG	5:B:574:HOH:O	2.35	0.71
2:B:44:PHE:CE1	2:B:303:VAL:HG12	2.25	0.70
1:F:1135:GLU:OE2	1:F:1149:ARG:NH2	2.27	0.68
1:F:1130:PRO:O	1:F:1131:ALA:HB3	1.94	0.68
1:F:1176:ASN:O	1:F:1178:ASN:N	2.27	0.67
2:B:70:SER:O	2:B:71:SER:HB2	1.93	0.67
2:B:91:LYS:HE2	5:B:571:HOH:O	1.95	0.66
2:C:95:LEU:HD22	2:C:280:PHE:HZ	1.61	0.66
2:B:127:GLU:HG2	4:B:403:GOL:H2	1.77	0.65
1:F:1195:GLU:OE2	3:F:1301:SIA:H113	1.95	0.65
2:A:155:LEU:HD21	2:A:206:MET:CE	2.25	0.65
1:D:1113:PRO:HG2	1:D:1160:PRO:HG3	1.79	0.64
1:E:1165:HIS:O	1:E:1193[B]:THR:HG22	1.97	0.64
1:F:1130:PRO:HA	1:F:1152:CYS:HB3	1.79	0.64
2:B:262:TRP:O	2:B:266:GLN:HG2	1.97	0.64
2:C:84:TRP:HB2	4:C:402:GOL:H11	1.79	0.63
2:A:155:LEU:HD21	2:A:206:MET:HE1	1.81	0.63
2:C:74:ALA:HB2	2:C:81:PRO:HA	1.79	0.63
1:F:1164:LEU:HB3	1:F:1193:THR:HG21	1.81	0.62
2:C:38:THR:HB	2:C:40:GLN:HG3	1.81	0.62
2:A:2:ARG:HG3	2:A:2:ARG:NH1	2.01	0.61
2:B:162:LYS:O	2:B:166:GLU:HB2	2.00	0.61
2:C:188:MET:CE	2:C:212:PRO:HB2	2.30	0.61
1:F:1204:GLY:C	1:F:1205:TYR:HD1	2.04	0.60
2:C:188:MET:HE1	2:C:213:LEU:CA	2.32	0.60
1:F:1182:ARG:HD3	1:F:1198:GLU:HG2	1.84	0.60
1:F:1177:TYR:H	1:F:1177:TYR:HD1	1.49	0.60
2:B:113:TRP:CZ2	2:B:118:LYS:HE3	2.36	0.59
2:B:14:PRO:O	2:B:20:GLN:HG3	2.03	0.59
2:C:262:TRP:CH2	2:C:266:GLN:NE2	2.70	0.59
1:F:1114:PRO:HB3	2:B:170:ASN:HD22	1.68	0.59
2:A:1:PHE:CD1	2:A:1:PHE:O	2.54	0.58
2:A:5:GLU:OE2	2:A:8:LYS:HD3	2.03	0.58
1:F:1182:ARG:HD2	1:F:1200:VAL:HG13	1.84	0.58
2:A:226:ARG:HD3	2:A:262:TRP:NE1	2.19	0.57
2:C:38:THR:O	2:C:40:GLN:HG3	2.05	0.56
1:D:1140:ASN:O	1:D:1141:LEU:HB2	2.04	0.56
2:C:19:GLU:HG3	2:C:75:ALA:HB2	1.87	0.56
2:C:173:PRO:O	2:C:177:THR:HG23	2.05	0.56
1:F:1176:ASN:C	1:F:1178:ASN:N	2.60	0.56
1:F:1130:PRO:O	1:F:1131:ALA:CB	2.54	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1164:LEU:HB3	1:E:1193[B]:THR:HG21	1.88	0.55
1:D:1198:GLU:CD	1:D:1215:ARG:HH21	2.11	0.54
1:D:1198:GLU:CD	1:D:1215:ARG:NH2	2.60	0.54
1:D:1135:GLU:OE2	1:D:1149:ARG:HB2	2.08	0.54
1:E:1164:LEU:CB	1:E:1193[B]:THR:HG21	2.38	0.54
2:C:112:LYS:CE	5:C:550:HOH:O	2.55	0.54
2:C:262:TRP:CZ2	2:C:266:GLN:NE2	2.76	0.54
1:F:1112:PRO:HD3	1:F:1128:TYR:CE2	2.43	0.54
1:E:1203:ARG:NH1	1:E:1203:ARG:HG2	2.24	0.54
2:A:160:GLU:HG2	5:A:619:HOH:O	2.09	0.52
2:B:290:GLN:OE1	2:B:299:LEU:HD12	2.09	0.52
2:B:35:LEU:HD11	2:B:303:VAL:HG11	1.92	0.52
1:D:1182:ARG:NH2	1:D:1200:VAL:HG12	2.25	0.52
1:F:1164:LEU:CB	1:F:1193:THR:HG21	2.39	0.52
2:B:164:ILE:HD12	2:B:164:ILE:H	1.75	0.52
2:A:74:ALA:HB2	2:A:81:PRO:HA	1.92	0.51
1:E:1193[B]:THR:HG23	5:E:1430:HOH:O	2.09	0.51
2:A:70:SER:O	2:A:71:SER:HB2	2.09	0.51
1:D:1208:SER:OG	1:D:1211:SER:HB2	2.11	0.51
1:F:1214:LEU:HA	1:F:1226:PRO:HG3	1.91	0.51
2:B:113:TRP:CD1	2:B:117:GLU:HG3	2.46	0.51
2:C:34:TYR:HD2	2:C:287:ALA:HB2	1.76	0.51
1:D:1120:ILE:HG13	1:D:1122:SER:O	2.11	0.51
2:A:292:ASP:O	2:A:294:PRO:HD3	2.11	0.51
1:F:1182:ARG:HD3	1:F:1198:GLU:CG	2.41	0.51
1:D:1195:GLU:HB2	5:D:1465:HOH:O	2.11	0.50
2:B:74:ALA:HB2	2:B:81:PRO:HA	1.93	0.50
2:B:206:MET:O	2:B:208:ARG:HG3	2.12	0.50
1:E:1184:THR:HG22	1:E:1186:LYS:N	2.09	0.50
1:F:1205:TYR:CZ	1:F:1230:LYS:HG2	2.47	0.49
1:F:1111:PRO:HD3	1:F:1126:SER:O	2.12	0.49
2:C:8:LYS:HG3	2:C:44:PHE:CZ	2.48	0.49
1:E:1184:THR:CG2	1:E:1185:ALA:N	2.76	0.49
1:E:1168:VAL:O	1:E:1168:VAL:HG23	2.13	0.49
2:A:232:LYS:HG3	5:A:630:HOH:O	2.13	0.48
2:C:188:MET:HE2	2:C:213:LEU:CD1	2.43	0.48
2:A:45:GLY:O	2:A:48:LYS:HB2	2.14	0.48
1:F:1197:VAL:HG22	1:F:1198:GLU:N	2.29	0.48
2:B:210:LYS:HA	2:B:214:LEU:HB2	1.94	0.48
2:C:188:MET:HA	2:C:216:LYS:HE2	1.95	0.47
1:F:1199:PHE:N	1:F:1199:PHE:CD1	2.82	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:112:LYS:HE2	5:C:550:HOH:O	2.14	0.47
1:F:1188:LYS:HG2	1:F:1189:LEU:N	2.30	0.47
2:C:130:PRO:HB3	4:C:402:GOL:H31	1.98	0.46
1:D:1192:ARG:NH1	5:D:1446:HOH:O	2.35	0.46
1:E:1203:ARG:HH11	1:E:1203:ARG:HG2	1.80	0.46
2:C:140:LEU:HD13	2:C:149:ALA:HB1	1.96	0.46
2:C:268:TYR:OH	2:C:275:SER:HB2	2.15	0.45
2:C:155:LEU:HD11	2:C:176:ILE:HG23	1.97	0.45
2:A:271:GLY:O	1:D:1176:ASN:HB2	2.16	0.45
2:B:120:LYS:HA	2:B:120:LYS:HD3	1.87	0.45
2:C:17:ALA:HA	2:C:66:PHE:CZ	2.52	0.45
1:E:1168:VAL:O	1:E:1168:VAL:CG2	2.64	0.45
2:A:225:ASN:OD1	2:A:226:ARG:HG2	2.17	0.45
1:E:1177:TYR:O	1:E:1178:ASN:HB2	2.17	0.45
2:C:188:MET:HE2	2:C:213:LEU:HG	1.99	0.45
2:B:142:ASN:ND2	2:B:144:ASN:OD1	2.48	0.44
1:F:1173:ILE:HG21	1:F:1225:TYR:CE2	2.51	0.44
1:F:1178:ASN:ND2	1:F:1205:TYR:HE2	2.15	0.44
2:C:235:TYR:N	2:C:235:TYR:CD1	2.86	0.44
1:D:1135:GLU:OE2	1:D:1149:ARG:NE	2.40	0.44
2:C:188:MET:CE	2:C:213:LEU:HG	2.47	0.44
1:F:1165:HIS:O	1:F:1193:THR:HG22	2.18	0.44
1:E:1212:HIS:CD2	1:E:1224:GLU:HB3	2.52	0.44
1:F:1197:VAL:CG2	1:F:1198:GLU:N	2.81	0.44
1:E:1182:ARG:HG2	1:E:1183:TRP:CD1	2.53	0.44
2:C:241:SER:OG	2:C:282:VAL:HA	2.17	0.44
2:A:118:LYS:HA	2:A:118:LYS:HD3	1.78	0.43
2:A:17:ALA:HA	2:A:66:PHE:CZ	2.52	0.43
2:C:273:TYR:CE1	4:C:401:GOL:H12	2.52	0.43
2:B:293:ALA:HA	2:B:294:PRO:HD3	1.89	0.43
2:C:112:LYS:NZ	5:C:550:HOH:O	2.50	0.43
2:B:222:LYS:HD3	2:B:222:LYS:HA	1.86	0.43
2:B:72:ALA:HB2	2:B:113:TRP:CD2	2.53	0.43
2:B:121:PRO:O	2:B:178:LYS:HD3	2.19	0.43
2:B:201:TYR:HA	2:B:246:ALA:HB2	2.00	0.42
2:C:203:LEU:HD23	2:C:203:LEU:HA	1.89	0.42
1:F:1165:HIS:O	1:F:1193:THR:CG2	2.67	0.42
1:F:1197:VAL:CG2	1:F:1198:GLU:H	2.32	0.42
1:E:1186:LYS:HD3	1:E:1189:LEU:HD13	2.01	0.42
2:B:148:MET:SD	2:B:186:ASN:HB2	2.60	0.42
2:B:203:LEU:HA	2:B:206:MET:HE2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:6:ARG:HG2	5:A:633:HOH:O	2.19	0.42
2:C:72:ALA:HB2	2:C:113:TRP:CD2	2.55	0.42
1:F:1190:TYR:CE1	2:B:121:PRO:HD2	2.54	0.42
2:C:34:TYR:CD2	2:C:287:ALA:HB2	2.55	0.42
1:D:1153:ARG:O	1:D:1154:ASN:HB2	2.19	0.42
1:F:1193:THR:HG22	1:F:1220:ASP:H	1.84	0.42
2:C:140:LEU:HD13	2:C:149:ALA:CB	2.50	0.42
1:F:1153:ARG:N	1:F:1156:GLN:O	2.49	0.42
2:C:162:LYS:O	2:C:166:GLU:HB2	2.19	0.42
2:C:228:GLU:HA	2:C:236:ASN:OD1	2.20	0.42
1:F:1205:TYR:N	1:F:1205:TYR:CD1	2.88	0.42
2:A:148:MET:HG3	2:A:190:LEU:HD21	2.01	0.42
2:A:293:ALA:HA	2:A:294:PRO:HD2	1.80	0.42
2:B:119:GLN:HB2	2:B:125:PHE:CE1	2.55	0.42
1:D:1113:PRO:HD2	1:D:1136:TYR:OH	2.20	0.41
1:F:1165:HIS:HA	1:F:1166:PRO:HD2	1.90	0.41
1:F:1174:MET:CE	1:F:1181:LEU:HG	2.51	0.41
2:C:210:LYS:HB2	2:C:210:LYS:HE2	1.53	0.41
2:C:257:PRO:N	2:C:258:PRO:HD2	2.35	0.41
2:A:234:LEU:HD23	2:A:234:LEU:HA	1.74	0.41
1:F:1159:GLU:OE2	1:F:1160:PRO:HD2	2.20	0.41
2:B:289:TYR:CE2	2:B:296:HIS:HB2	2.56	0.41
2:A:26:THR:HB	2:A:27:PRO:CD	2.51	0.41
1:F:1177:TYR:CD1	1:F:1177:TYR:N	2.87	0.41
1:E:1140:ASN:O	1:E:1141:LEU:HB2	2.20	0.41
2:B:162:LYS:HA	2:B:172:LEU:HD21	2.03	0.40
2:C:37:GLU:C	2:C:39:GLU:H	2.25	0.40
2:A:30:ILE:HD12	2:A:30:ILE:HA	1.90	0.40
2:A:268:TYR:CZ	2:A:270:GLY:HA2	2.56	0.40
2:B:213:LEU:HD12	2:B:213:LEU:N	2.37	0.40
1:F:1133:SER:HA	1:F:1150:ILE:O	2.21	0.40
2:B:306:GLN:N	2:B:306:GLN:CD	2.75	0.40
1:E:1144:LEU:HD23	1:E:1144:LEU:C	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	D	124/129 (96%)	121 (98%)	3 (2%)	0	100	100
1	E	126/129 (98%)	121 (96%)	5 (4%)	0	100	100
1	F	122/129 (95%)	107 (88%)	9 (7%)	6 (5%)	2	0
2	A	296/317 (93%)	288 (97%)	8 (3%)	0	100	100
2	B	286/317 (90%)	281 (98%)	5 (2%)	0	100	100
2	C	290/317 (92%)	272 (94%)	16 (6%)	2 (1%)	25	17
All	All	1244/1338 (93%)	1190 (96%)	46 (4%)	8 (1%)	28	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	1177	TYR
1	F	1212	HIS
1	F	1175	GLU
1	F	1202	LYS
1	F	1131	ALA
1	F	1203	ARG
2	C	142	ASN
2	C	46	LEU

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	110/115 (96%)	109 (99%)	1 (1%)	82	87
1	E	110/115 (96%)	108 (98%)	2 (2%)	64	68
1	F	99/115 (86%)	89 (90%)	10 (10%)	9	4
2	A	247/264 (94%)	243 (98%)	4 (2%)	68	73
2	B	242/264 (92%)	235 (97%)	7 (3%)	48	46
2	C	232/264 (88%)	224 (97%)	8 (3%)	42	40
All	All	1040/1137 (92%)	1008 (97%)	32 (3%)	45	44

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	1125	LEU
1	F	1126	SER
1	F	1159	GLU
1	F	1162	LYS
1	F	1174	MET
1	F	1177	TYR
1	F	1184	THR
1	F	1196	SER
1	F	1199	PHE
1	F	1216	THR
2	A	1	PHE
2	A	2	ARG
2	A	46	LEU
2	A	57	LYS
1	D	1144	LEU
2	B	104	SER
2	B	144	ASN
2	B	205	GLN
2	B	215	ASN
2	B	222	LYS
2	B	233	GLN
2	B	305	LEU
1	E	1113	PRO
1	E	1172	GLU
2	C	38	THR
2	C	46	LEU
2	C	140	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	146	LYS
2	C	175	SER
2	C	216	LYS
2	C	266	GLN
2	C	282	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	1165	HIS
2	B	170	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 ⓘ

9 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	SIA	D	1301	3	17,20,21	0.66	0	19,28,31	1.50	3 (15%)
3	GAL	D	1302	3	11,11,12	0.53	0	13,15,17	1.27	3 (23%)
3	BGC	D	1303	3	12,12,12	0.52	0	17,17,17	0.50	0
3	SIA	E	1301	3	17,20,21	0.48	0	19,28,31	0.86	0
3	GAL	E	1302	3	11,11,12	0.85	0	13,15,17	1.52	2 (15%)
3	BGC	E	1303	3	12,12,12	0.62	0	17,17,17	0.99	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SIA	F	1301	3	17,20,21	0.34	0	19,28,31	1.11	1 (5%)
3	GAL	F	1302	3	11,11,12	0.55	0	13,15,17	1.22	1 (7%)
3	BGC	F	1303	3	12,12,12	0.47	0	17,17,17	0.88	1 (5%)

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	SIA	D	1301	3	-	0/14/34/38	0/1/1/1
3	GAL	D	1302	3	-	0/2/19/22	0/1/1/1
3	BGC	D	1303	3	-	0/2/22/22	0/1/1/1
3	SIA	E	1301	3	-	0/14/34/38	0/1/1/1
3	GAL	E	1302	3	-	0/2/19/22	0/1/1/1
3	BGC	E	1303	3	-	0/2/22/22	0/1/1/1
3	SIA	F	1301	3	-	0/14/34/38	0/1/1/1
3	GAL	F	1302	3	-	0/2/19/22	0/1/1/1
3	BGC	F	1303	3	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1302	GAL	O3-C3-C2	-2.97	104.61	110.02
3	F	1301	SIA	C4-C5-N5	-2.50	105.25	110.40
3	E	1303	BGC	O3-C3-C2	-2.44	105.05	110.36
3	D	1301	SIA	O4-C4-C3	-2.32	104.41	110.02
3	E	1303	BGC	O5-C1-C2	-2.04	106.66	110.04
3	E	1302	GAL	C1-O5-C5	2.12	115.08	112.17
3	D	1302	GAL	C1-O5-C5	2.16	115.14	112.17
3	F	1303	BGC	O5-C5-C6	2.21	111.70	106.41
3	D	1302	GAL	C1-C2-C3	2.34	112.62	109.65
3	F	1302	GAL	C1-O5-C5	2.71	115.90	112.17
3	D	1302	GAL	C2-C3-C4	2.78	115.73	110.88
3	D	1301	SIA	C4-C3-C2	3.20	115.75	109.75
3	D	1301	SIA	C3-C4-C5	4.13	116.46	111.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1301	SIA	1	0

5.6 Ligand geometry [i](#)

7 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	GOL	A	401	-	5,5,5	0.83	0	5,5,5	1.98	1 (20%)
4	GOL	B	401	-	5,5,5	0.38	0	5,5,5	0.94	0
4	GOL	B	402	-	5,5,5	0.51	0	5,5,5	0.46	0
4	GOL	B	403	-	5,5,5	0.30	0	5,5,5	0.47	0
4	GOL	C	401	-	5,5,5	0.27	0	5,5,5	0.29	0
4	GOL	C	402	-	5,5,5	0.65	0	5,5,5	1.36	1 (20%)
4	GOL	E	1304	-	5,5,5	0.35	0	5,5,5	0.31	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	GOL	A	401	-	-	0/4/4/4	0/0/0/0
4	GOL	B	401	-	-	0/4/4/4	0/0/0/0
4	GOL	B	402	-	-	0/4/4/4	0/0/0/0
4	GOL	B	403	-	-	0/4/4/4	0/0/0/0
4	GOL	C	401	-	-	0/4/4/4	0/0/0/0
4	GOL	C	402	-	-	0/4/4/4	0/0/0/0
4	GOL	E	1304	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	GOL	C3-C2-C1	-4.14	95.07	111.52
4	C	402	GOL	C3-C2-C1	-2.68	100.86	111.52

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
4	B	403	GOL	1	0
4	C	401	GOL	1	0
4	C	402	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	D	126/129 (97%)	-0.20	0	100	100	34, 47, 78, 98	0
1	E	126/129 (97%)	-0.07	4 (3%)	48	56	38, 56, 92, 137	0
1	F	124/129 (96%)	1.65	53 (42%)	0	1	46, 96, 133, 149	0
2	A	295/317 (93%)	-0.12	4 (1%)	75	80	31, 44, 72, 125	0
2	B	292/317 (92%)	-0.12	1 (0%)	93	95	29, 48, 79, 112	0
2	C	292/317 (92%)	0.19	15 (5%)	29	36	37, 61, 106, 133	0
All	All	1255/1338 (93%)	0.12	77 (6%)	22	28	29, 53, 107, 149	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1211	SER	6.8
1	F	1200	VAL	6.7
1	E	1187	GLN	6.1
1	F	1201	CYS	6.1
1	F	1230	LYS	5.9
1	F	1129	ALA	5.2
2	B	309	SER	5.1
1	F	1212	HIS	5.1
1	F	1128	TYR	4.9
1	F	1180	ALA	4.9
1	F	1177	TYR	4.9
1	F	1179	ILE	4.6
1	F	1229	ALA	4.6
1	E	1185	ALA	4.6
2	A	294	PRO	4.3
2	C	41	TRP	4.3
1	E	1106	PHE	4.0
1	F	1184	THR	4.0
1	F	1228	CYS	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	1130	PRO	3.9
1	F	1125	LEU	3.8
2	C	255	PHE	3.7
1	F	1109	CYS	3.7
1	F	1205	TYR	3.5
1	F	1199	PHE	3.5
1	F	1206	ARG	3.5
1	F	1157	TRP	3.4
2	C	44	PHE	3.4
1	F	1227	THR	3.4
2	C	4	ALA	3.3
2	C	294	PRO	3.3
1	F	1207	LEU	3.3
2	C	46	LEU	3.3
1	F	1154	ASN	3.3
1	F	1231	ARG	3.2
2	C	219	THR	3.2
1	F	1210	ARG	3.2
1	F	1185	ALA	3.2
2	A	261	ARG	3.1
1	F	1204	GLY	3.0
1	F	1171	ARG	3.0
1	F	1131	ALA	3.0
2	C	143	ASN	2.9
1	F	1213	THR	2.9
2	C	253	PHE	2.9
1	F	1153	ARG	2.9
1	F	1174	MET	2.9
2	C	7	LEU	2.9
1	F	1226	PRO	2.8
1	F	1110	GLY	2.8
1	F	1156	GLN	2.7
1	F	1214	LEU	2.7
1	F	1152	CYS	2.7
1	F	1133	SER	2.6
1	F	1155	GLY	2.6
1	E	1175	GLU	2.6
1	F	1173	ILE	2.5
1	F	1108	LYS	2.5
2	C	47	GLU	2.5
2	C	8	LYS	2.5
2	C	224	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	1209	SER	2.4
1	F	1181	LEU	2.4
2	C	42	GLU	2.4
1	F	1178	ASN	2.4
1	F	1203	ARG	2.3
2	C	43	LYS	2.3
2	A	1	PHE	2.3
2	A	253	PHE	2.3
1	F	1225	TYR	2.3
1	F	1175	GLU	2.2
1	F	1127	VAL	2.2
1	F	1150	ILE	2.1
1	F	1183	TRP	2.1
1	F	1217	THR	2.1
1	F	1149	ARG	2.0
1	F	1186	LYS	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, 95th 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(\AA^2)	Q<0.9
3	SIA	D	1301	20/21	0.90	0.22	7.67	42,79,98,101	0
3	BGC	D	1303	12/12	0.86	0.23	1.00	94,105,116,125	0
3	BGC	E	1303	12/12	0.92	0.11	-0.13	65,79,88,98	0
3	SIA	F	1301	20/21	0.92	0.16	-0.85	74,89,108,110	0
3	SIA	E	1301	20/21	0.97	0.09	-0.99	44,53,61,67	0
3	GAL	E	1302	11/12	0.96	0.07	-2.97	58,62,65,70	0
3	GAL	D	1302	11/12	0.90	0.17	-	76,85,91,91	0
3	GAL	F	1302	11/12	0.90	0.20	-	100,109,117,120	0
3	BGC	F	1303	12/12	0.80	0.32	-	86,129,135,141	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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
4	GOL	B	402	6/6	0.92	0.19	2.91	64,70,79,90	0
4	GOL	B	401	6/6	0.92	0.19	2.62	67,75,80,81	0
4	GOL	C	402	6/6	0.92	0.15	2.14	45,55,66,70	0
4	GOL	A	401	6/6	0.97	0.17	2.00	33,45,49,74	0
4	GOL	B	403	6/6	0.95	0.12	-0.65	37,47,49,63	0
4	GOL	E	1304	6/6	0.85	0.17	-	64,69,76,77	0
4	GOL	C	401	6/6	0.82	0.25	-	69,90,102,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.