Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 11:11 AM EDT

PDB ID	:	3OXU
Title	:	Complement components factor H CCP19-20 and C3d in complex
Authors	:	Morgan, H.P.; Schmidt, C.Q.; Guariento, M.; Gillespie, D.; Herbert, A.P.; Mertens, H.; Blaum, B.S.; Svergun, D.; Johansson, C.M.; Uhrin, D.; Barlow, P.N.; Hannan, J.P.
Deposited on	:	2010-09-22
Resolution	:	2.10 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

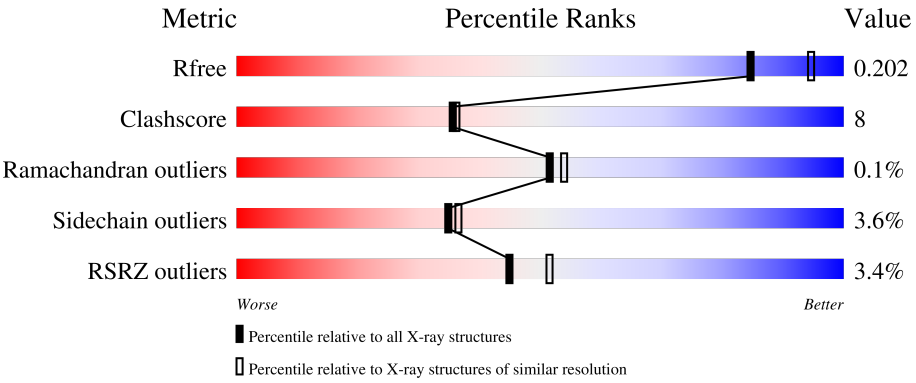
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	317	80% 11% • 7%
1	B	317	78% 14% • 7%
1	C	317	5% 72% 19% • 7%
2	D	129	2% 86% 9% • •
2	E	129	2% 82% 12% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	129	13% 67% 24% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	C	312	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10982 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 C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	2	0
			2348	1508	394	437	9			
1	B	295	Total	C	N	O	S	0	4	0
			2337	1501	388	439	9			
1	C	294	Total	C	N	O	S	0	2	0
			2335	1502	393	431	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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

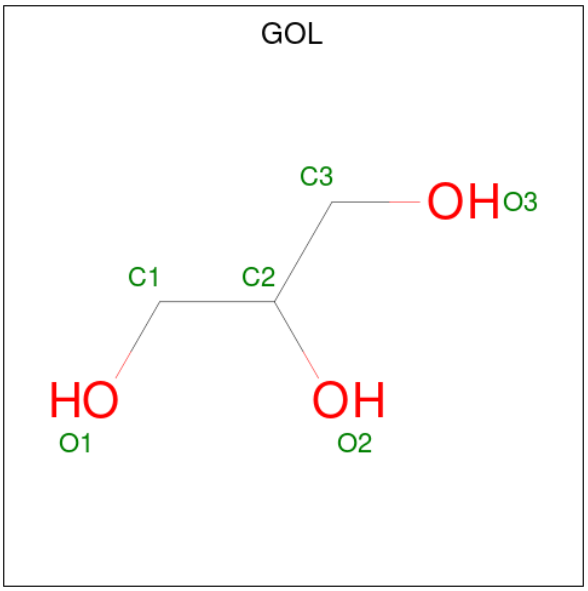
- Molecule 2 is a protein called HF protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	125	Total	C	N	O	S	0	1	0
			1006	630	182	185	9			
2	E	121	Total	C	N	O	S	0	2	0
			976	611	177	179	9			
2	F	122	Total	C	N	O	S	0	1	0
			984	614	179	182	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1103	GLU	-	expression tag	UNP Q14006
D	1104	ALA	-	expression tag	UNP Q14006
D	1105	GLU	-	expression tag	UNP Q14006
D	1106	PHE	-	expression tag	UNP Q14006
E	1103	GLU	-	expression tag	UNP Q14006
E	1104	ALA	-	expression tag	UNP Q14006
E	1105	GLU	-	expression tag	UNP Q14006
E	1106	PHE	-	expression tag	UNP Q14006
F	1103	GLU	-	expression tag	UNP Q14006
F	1104	ALA	-	expression tag	UNP Q14006
F	1105	GLU	-	expression tag	UNP Q14006
F	1106	PHE	-	expression tag	UNP Q14006

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	240	Total O 240 240	0	0
4	B	228	Total O 228 228	0	0
4	C	155	Total O 155 155	0	0
4	D	141	Total O 141 141	0	0

Continued on next page...

Continued from previous page...

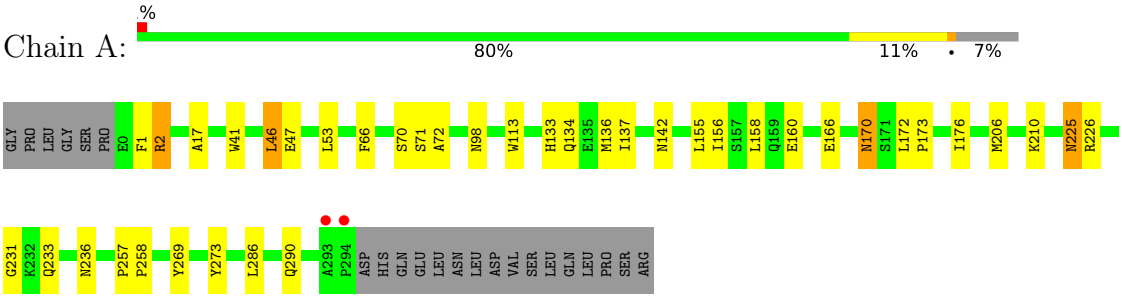
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	125	Total O 125 125	0	0
4	F	59	Total O 59 59	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

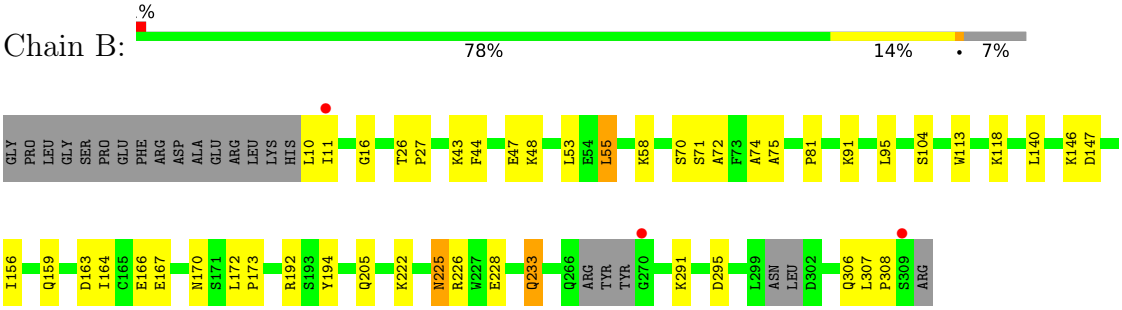
• Molecule 1: Complement C3

Chain A:



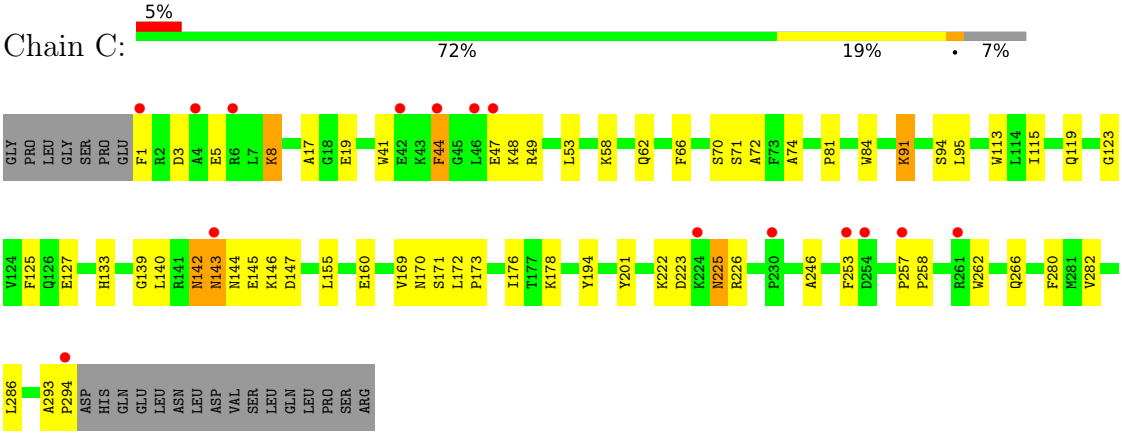
• Molecule 1: Complement C3

Chain B:



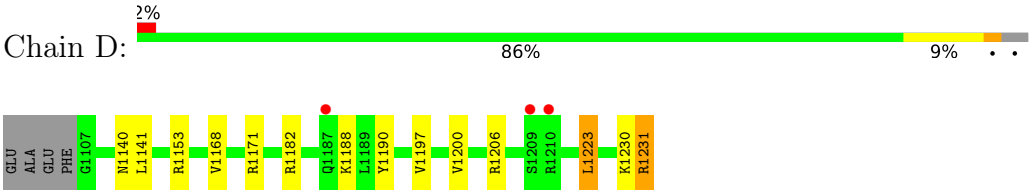
• Molecule 1: Complement C3

Chain C:



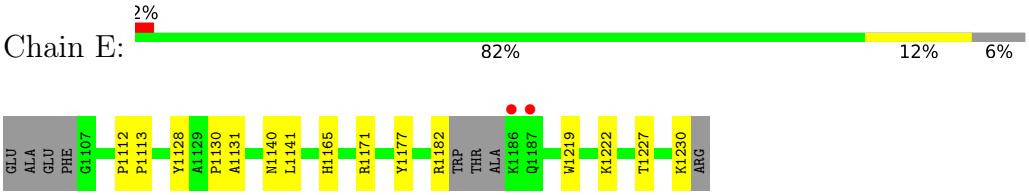
• Molecule 2: HF protein

Chain D:



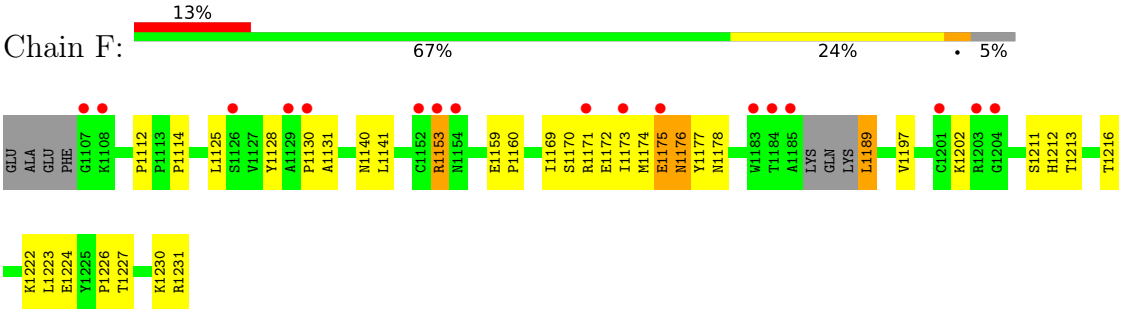
• Molecule 2: HF protein

Chain E:



• Molecule 2: HF protein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	74.67Å 82.99Å 85.61Å 112.75° 110.14° 99.96°	Depositor
Resolution (Å)	40.48 – 2.10 40.48 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.9 (40.48-2.10) 95.8 (40.48-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	4.11 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.171 , 0.206 0.167 , 0.202	Depositor DCC
R_{free} test set	4681 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10982	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL

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	0.41	0/2398	0.52	0/3248
1	B	0.41	0/2386	0.53	0/3234
1	C	0.34	0/2388	0.48	0/3235
2	D	0.39	0/1032	0.52	0/1399
2	E	0.37	0/1004	0.50	0/1354
2	F	0.30	0/1009	0.52	0/1366
All	All	0.38	0/10217	0.51	0/13836

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2348	0	2345	27	0
1	B	2337	0	2339	40	0
1	C	2335	0	2345	46	0
2	D	1006	0	983	12	0
2	E	976	0	965	10	0
2	F	984	0	952	32	0
3	A	6	0	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	16	0	0
3	C	12	0	16	4	0
3	D	12	0	16	2	0
3	E	6	0	8	3	0
4	A	240	0	0	2	0
4	B	228	0	0	8	0
4	C	155	0	0	3	0
4	D	141	0	0	2	0
4	E	125	0	0	2	0
4	F	59	0	0	2	0
All	All	10982	0	9993	163	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 8.

All (163) 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)
2:F:1172:GLU:HG2	2:F:1174:MET:HB2	1.41	1.00
1:B:55:LEU:HA	1:B:58:LYS:HE2	1.54	0.87
1:B:164:ILE:HD12	4:B:1004:HOH:O	1.74	0.86
2:F:1171:ARG:HA	2:F:1172:GLU:HG3	1.62	0.81
1:C:155:LEU:HD11	1:C:176:ILE:HG23	1.71	0.73
1:C:8:LYS:O	1:C:8:LYS:HE3	1.89	0.71
2:F:1171:ARG:HA	2:F:1172:GLU:CG	2.20	0.71
2:F:1178:ASN:HA	2:F:1202:LYS:HE3	1.72	0.71
1:B:159:GLN:HG2	4:B:1055:HOH:O	1.90	0.70
1:B:225:ASN:HD21	1:B:226:ARG:HH11	1.40	0.70
2:F:1172:GLU:HB3	2:F:1175:GLU:HB2	1.73	0.69
2:D:1206:ARG:NH2	2:D:1231:ARG:HA	2.08	0.67
1:A:225:ASN:HD21	1:A:226:ARG:HH11	1.42	0.66
1:A:233:GLN:NE2	1:A:236:ASN:HD22	1.94	0.65
1:C:84:TRP:CB	3:C:312:GOL:H12	2.27	0.65
2:F:1170:SER:HB3	2:F:1173:ILE:HG22	1.78	0.65
2:F:1173:ILE:HA	2:F:1176:ASN:HD21	1.62	0.64
1:C:282:VAL:O	1:C:286:LEU:HG	1.98	0.64
1:C:70:SER:O	1:C:71:SER:HB2	1.97	0.64
1:C:169:VAL:HG12	4:C:995:HOH:O	1.97	0.64
1:A:98:ASN:HB2	4:A:772:HOH:O	1.98	0.63
1:C:142:ASN:HD22	1:C:142:ASN:C	2.01	0.63
2:F:1176:ASN:ND2	2:F:1176:ASN:H	1.97	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:SER:O	1:B:71:SER:HB2	2.00	0.61
1:A:70:SER:O	1:A:71:SER:HB2	1.99	0.61
2:F:1172:GLU:HB3	2:F:1175:GLU:H	1.65	0.60
1:B:159:GLN:NE2	1:B:205:GLN:OE1	2.35	0.60
2:F:1153:ARG:HB3	2:F:1153:ARG:NH1	2.17	0.59
1:B:10:LEU:HG	1:B:11:ILE:H	1.66	0.59
2:D:1182:ARG:NH1	2:D:1200:VAL:HG12	2.17	0.59
1:C:139:GLY:HA3	1:C:194:TYR:CE1	2.38	0.59
1:A:156:ILE:O	1:A:160:GLU:HG3	2.02	0.59
2:F:1171:ARG:HG2	2:F:1172:GLU:HG3	1.83	0.59
1:A:257:PRO:HB2	1:A:258:PRO:HD3	1.84	0.58
1:B:170[B]:ASN:OD1	2:F:1114:PRO:HB3	2.03	0.58
1:C:74:ALA:HB2	1:C:81:PRO:HA	1.85	0.58
1:B:91:LYS:HD2	4:B:363:HOH:O	2.04	0.58
1:B:16:GLY:HA3	1:B:75:ALA:HB1	1.86	0.57
1:A:170:ASN:HD22	1:A:170:ASN:C	2.08	0.57
1:C:293:ALA:HB3	1:C:294:PRO:HD3	1.85	0.57
1:A:166[A]:GLU:HG2	4:A:395:HOH:O	2.05	0.56
1:C:58:LYS:HE2	1:C:62:GLN:OE1	2.06	0.56
2:F:1212:HIS:CD2	2:F:1212:HIS:H	2.24	0.56
1:B:91:LYS:CE	4:B:816:HOH:O	2.53	0.56
2:D:1182:ARG:CZ	2:D:1200:VAL:HG12	2.35	0.56
1:C:123:GLY:CA	1:C:178:LYS:HG3	2.36	0.56
1:A:273:TYR:CE2	3:D:6:GOL:H31	2.42	0.55
1:C:115:ILE:HD11	1:C:172:LEU:HD13	1.89	0.55
1:A:142:ASN:ND2	1:B:295:ASP:H	2.05	0.55
1:B:166[B]:GLU:HG2	1:B:166[B]:GLU:O	2.07	0.55
1:C:201:TYR:HA	1:C:246:ALA:HB2	1.90	0.54
1:B:222:LYS:HD2	1:B:228:GLU:HG2	1.90	0.54
1:B:91:LYS:HE3	4:B:816:HOH:O	2.07	0.54
2:F:1176:ASN:H	2:F:1176:ASN:HD22	1.54	0.54
1:C:19:GLU:OE1	1:C:133:HIS:HD2	1.91	0.53
1:C:95:LEU:HD22	1:C:280:PHE:CZ	2.43	0.53
2:E:1219:TRP:CG	3:E:2:GOL:H12	2.44	0.53
1:A:155:LEU:HD21	1:A:206:MET:HE1	1.91	0.52
1:B:164:ILE:HD12	1:B:164:ILE:H	1.73	0.52
2:F:1211:SER:HB2	4:F:930:HOH:O	2.10	0.52
1:B:146:LYS:HG3	1:B:147:ASP:N	2.26	0.51
1:C:84:TRP:CG	3:C:312:GOL:H12	2.45	0.51
1:B:72:ALA:HB2	1:B:113:TRP:CD2	2.46	0.51
1:C:17:ALA:HA	1:C:66:PHE:CZ	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1112:PRO:HD3	2:F:1128:TYR:CE1	2.46	0.50
1:A:2:ARG:HG3	1:A:269:TYR:HE1	1.75	0.50
1:A:155:LEU:HD21	1:A:206:MET:CE	2.41	0.50
2:D:1197[A]:VAL:HG21	2:D:1223:LEU:HD11	1.94	0.50
1:C:253:PHE:O	1:C:257:PRO:HD3	2.12	0.50
2:F:1216:THR:HG23	2:F:1223:LEU:HD11	1.93	0.50
1:C:172:LEU:N	4:C:995:HOH:O	2.45	0.50
2:F:1222:LYS:HD3	4:F:411:HOH:O	2.11	0.49
1:B:74:ALA:HB2	1:B:81:PRO:HA	1.94	0.49
1:C:127:GLU:HG2	3:C:312:GOL:H31	1.93	0.49
1:C:72:ALA:HB2	1:C:113:TRP:CD2	2.48	0.49
1:B:44:PHE:CE2	1:B:48:LYS:HD2	2.48	0.49
1:B:225:ASN:HD21	1:B:226:ARG:NH1	2.09	0.49
1:B:55:LEU:HA	1:B:58:LYS:CE	2.35	0.49
1:C:91:LYS:HD3	1:C:280:PHE:CE1	2.47	0.49
1:C:146:LYS:HG3	1:C:147:ASP:N	2.27	0.49
2:D:1206:ARG:CZ	2:D:1231:ARG:HA	2.41	0.49
1:B:113:TRP:CZ2	1:B:118:LYS:HE3	2.48	0.49
1:A:233:GLN:NE2	1:A:233:GLN:HA	2.27	0.49
2:F:1177:TYR:CD1	2:F:1227:THR:HG22	2.48	0.48
2:D:1230:LYS:O	2:D:1231:ARG:CB	2.60	0.48
1:C:142:ASN:C	1:C:142:ASN:ND2	2.65	0.48
1:C:47:GLU:OE1	1:C:48:LYS:HG3	2.13	0.48
1:C:94:SER:HB3	1:C:160:GLU:HG3	1.96	0.48
2:F:1159:GLU:HG3	2:F:1160:PRO:HD2	1.95	0.48
1:C:226:ARG:HD3	1:C:262:TRP:NE1	2.28	0.47
2:E:1112:PRO:HD3	2:E:1128:TYR:CE1	2.49	0.47
2:D:1230:LYS:O	2:D:1231:ARG:CG	2.62	0.47
2:F:1230:LYS:HE3	2:F:1230:LYS:HB2	1.55	0.47
1:B:291:LYS:HE2	3:D:6:GOL:O3	2.15	0.47
1:A:233:GLN:HE22	1:A:236:ASN:HD22	1.60	0.47
1:B:306:GLN:C	1:B:308:PRO:HD3	2.35	0.47
1:C:223:ASP:HB2	1:C:225:ASN:ND2	2.30	0.47
1:B:172:LEU:HB3	1:B:173:PRO:HD3	1.97	0.46
2:F:1170:SER:O	2:F:1172:GLU:HA	2.15	0.46
1:C:119:GLN:HB2	1:C:125:PHE:CE1	2.51	0.46
2:D:1140:ASN:O	2:D:1141:LEU:HB2	2.16	0.46
2:E:1140:ASN:O	2:E:1141:LEU:HB2	2.15	0.46
2:E:1219:TRP:CD2	3:E:2:GOL:H12	2.51	0.46
1:B:140[B]:LEU:HD12	1:B:194:TYR:HE2	1.81	0.45
1:C:127:GLU:HG2	3:C:312:GOL:C3	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1140:ASN:ND2	2:F:1141:LEU:HG	2.30	0.45
2:F:1125:LEU:HD12	2:F:1128:TYR:CE2	2.52	0.45
2:F:1153:ARG:HB3	2:F:1153:ARG:HH11	1.81	0.45
1:C:144:ASN:O	1:C:145:GLU:HB2	2.17	0.45
2:D:1141:LEU:HD23	2:D:1141:LEU:HA	1.83	0.45
2:D:1230:LYS:O	2:D:1231:ARG:HG2	2.17	0.45
2:E:1171:ARG:HD3	4:E:1032:HOH:O	2.16	0.45
1:A:17:ALA:HA	1:A:66:PHE:CZ	2.52	0.45
1:A:286:LEU:O	1:A:290:GLN:HG2	2.17	0.45
1:C:123:GLY:HA3	1:C:178:LYS:HG3	1.99	0.45
1:B:233:GLN:HG2	4:B:351:HOH:O	2.16	0.44
1:C:257:PRO:N	1:C:258:PRO:HD2	2.32	0.44
1:B:170[B]:ASN:CG	2:F:1114:PRO:HB3	2.37	0.44
2:E:1177:TYR:CD2	2:E:1227:THR:HG22	2.53	0.44
1:B:192:ARG:NE	4:B:681:HOH:O	2.32	0.44
1:A:172:LEU:HB3	1:A:173:PRO:HD3	2.00	0.44
1:B:225:ASN:ND2	1:B:226:ARG:HG2	2.33	0.44
2:F:1172:GLU:HB3	2:F:1175:GLU:N	2.31	0.44
1:A:72:ALA:HB2	1:A:113:TRP:CD2	2.52	0.44
1:A:134:GLN:O	1:A:137:ILE:HG12	2.19	0.43
2:E:1222:LYS:HE2	4:E:946:HOH:O	2.17	0.43
1:C:170:ASN:O	1:C:173:PRO:HD2	2.18	0.43
1:B:205:GLN:HG2	4:D:1063:HOH:O	2.18	0.43
1:B:16:GLY:CA	1:B:75:ALA:HB1	2.48	0.43
1:B:307:LEU:N	1:B:308:PRO:HD3	2.33	0.43
2:F:1172:GLU:CB	2:F:1175:GLU:HB2	2.43	0.43
1:C:142:ASN:HD22	1:C:143:ASN:N	2.16	0.42
1:B:163:ASP:HB2	4:B:1004:HOH:O	2.18	0.42
1:A:155:LEU:HD11	1:A:176:ILE:HG23	2.01	0.42
1:B:26:THR:HB	1:B:27:PRO:HD3	2.01	0.42
1:B:140[A]:LEU:HD23	1:B:140[A]:LEU:HA	1.87	0.42
1:C:8:LYS:HZ2	1:C:44:PHE:HZ	1.68	0.42
1:C:225:ASN:HD22	1:C:225:ASN:N	2.18	0.42
1:B:156:ILE:HA	1:B:159:GLN:NE2	2.35	0.42
2:F:1169:ILE:HD12	2:F:1189:LEU:HD23	2.00	0.42
2:E:1219:TRP:CD1	3:E:2:GOL:H12	2.55	0.41
1:A:231:GLY:N	1:B:43:LYS:HE3	2.35	0.41
1:A:41:TRP:HB3	1:A:46:LEU:HD13	2.01	0.41
1:C:41:TRP:CE3	1:C:49:ARG:HB2	2.55	0.41
2:F:1130:PRO:O	2:F:1131:ALA:HB3	2.20	0.41
1:C:171:SER:C	4:C:995:HOH:O	2.58	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1213:THR:O	2:F:1226:PRO:HB3	2.19	0.41
1:C:123:GLY:HA2	1:C:178:LYS:HG3	2.02	0.41
2:F:1177:TYR:CG	2:F:1227:THR:HG22	2.56	0.41
1:C:3:ASP:OD2	1:C:5:GLU:HB2	2.20	0.41
1:A:225:ASN:C	1:A:225:ASN:HD22	2.23	0.41
2:D:1188:LYS:HD3	4:D:976:HOH:O	2.19	0.41
1:C:58:LYS:O	1:C:62:GLN:HG3	2.20	0.41
1:C:223:ASP:HB2	1:C:225:ASN:HD21	1.86	0.41
1:A:225:ASN:HD22	1:A:226:ARG:N	2.19	0.41
1:C:222:LYS:O	1:C:223:ASP:HB2	2.21	0.41
2:E:1112:PRO:HA	2:E:1113:PRO:HD3	1.93	0.41
1:C:262:TRP:CE2	1:C:266:GLN:NE2	2.89	0.40
1:B:118:LYS:HD3	1:B:118:LYS:HA	1.79	0.40
2:E:1130:PRO:O	2:E:1131:ALA:HB3	2.22	0.40
1:A:133:HIS:O	1:A:136:MET:HG2	2.21	0.40
1:A:158:LEU:HB3	1:A:172:LEU:HD11	2.03	0.40
2:D:1168:VAL:HG22	2:D:1190:TYR:CE2	2.56	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	295/317 (93%)	290 (98%)	5 (2%)	0	100	100
1	B	293/317 (92%)	287 (98%)	6 (2%)	0	100	100
1	C	294/317 (93%)	280 (95%)	13 (4%)	1 (0%)	41	41
2	D	124/129 (96%)	119 (96%)	5 (4%)	0	100	100
2	E	118/129 (92%)	117 (99%)	1 (1%)	0	100	100
2	F	119/129 (92%)	115 (97%)	4 (3%)	0	100	100
All	All	1243/1338 (93%)	1208 (97%)	34 (3%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	143	ASN

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	246/264 (93%)	238 (97%)	8 (3%)	38	40
1	B	249/264 (94%)	241 (97%)	8 (3%)	39	41
1	C	245/264 (93%)	237 (97%)	8 (3%)	38	40
2	D	113/115 (98%)	109 (96%)	4 (4%)	36	38
2	E	111/115 (96%)	107 (96%)	4 (4%)	35	36
2	F	110/115 (96%)	103 (94%)	7 (6%)	17	14
All	All	1074/1137 (94%)	1035 (96%)	39 (4%)	35	36

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	PHE
1	A	2	ARG
1	A	46	LEU
1	A	47	GLU
1	A	53	LEU
1	A	170	ASN
1	A	210	LYS
1	A	225	ASN
1	B	47	GLU
1	B	53	LEU
1	B	55	LEU
1	B	95	LEU
1	B	104	SER
1	B	167	GLU
1	B	225	ASN
1	B	233	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1	PHE
1	C	8	LYS
1	C	44	PHE
1	C	53	LEU
1	C	91	LYS
1	C	140	LEU
1	C	142	ASN
1	C	225	ASN
2	D	1153	ARG
2	D	1171	ARG
2	D	1223	LEU
2	D	1231	ARG
2	E	1165	HIS
2	E	1182	ARG
2	E	1230[A]	LYS
2	E	1230[B]	LYS
2	F	1153	ARG
2	F	1175	GLU
2	F	1176	ASN
2	F	1189	LEU
2	F	1197	VAL
2	F	1224	GLU
2	F	1231	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	170	ASN
1	A	225	ASN
1	A	233	GLN
1	B	40	GLN
1	B	105	GLN
1	B	159	GLN
1	B	189	ASN
1	B	205	GLN
1	B	225	ASN
1	B	233	GLN
1	B	264	ASN
1	B	290	GLN
1	C	133	HIS
1	C	142	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	159	GLN
1	C	225	ASN
1	C	264	ASN
1	C	266	GLN
1	C	290	GLN
2	D	1137	GLN
2	D	1140	ASN
2	D	1212	HIS
2	E	1137	GLN
2	E	1187	GLN
2	E	1212	HIS
2	F	1137	GLN
2	F	1140	ASN
2	F	1176	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	C	312	-	5,5,5	0.49	0	5,5,5	0.89	0
3	GOL	B	311	-	5,5,5	0.35	0	5,5,5	0.29	0
3	GOL	C	311	-	5,5,5	0.33	0	5,5,5	0.26	0
3	GOL	A	311	-	5,5,5	0.49	0	5,5,5	0.54	0
3	GOL	B	312	-	5,5,5	0.47	0	5,5,5	0.58	0
3	GOL	E	2	-	5,5,5	0.32	0	5,5,5	0.55	0
3	GOL	D	6	-	5,5,5	0.26	0	5,5,5	0.52	0
3	GOL	D	8	-	5,5,5	0.30	0	5,5,5	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	312	-	-	4/4/4/4	-
3	GOL	B	311	-	-	0/4/4/4	-
3	GOL	C	311	-	-	2/4/4/4	-
3	GOL	A	311	-	-	0/4/4/4	-
3	GOL	B	312	-	-	4/4/4/4	-
3	GOL	E	2	-	-	2/4/4/4	-
3	GOL	D	6	-	-	2/4/4/4	-
3	GOL	D	8	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	312	GOL	C1-C2-C3-O3
3	C	311	GOL	O1-C1-C2-C3
3	C	312	GOL	O1-C1-C2-O2
3	C	312	GOL	O1-C1-C2-C3
3	D	6	GOL	O1-C1-C2-C3
3	E	2	GOL	O1-C1-C2-C3
3	C	311	GOL	O1-C1-C2-O2
3	B	312	GOL	O1-C1-C2-C3
3	C	312	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	8	GOL	O1-C1-C2-C3
3	B	312	GOL	O2-C2-C3-O3
3	D	6	GOL	O1-C1-C2-O2
3	D	8	GOL	O1-C1-C2-O2
3	E	2	GOL	O1-C1-C2-O2
3	C	312	GOL	O2-C2-C3-O3
3	B	312	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	312	GOL	4	0
3	E	2	GOL	3	0
3	D	6	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

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	295/317 (93%)	-0.46	2 (0%) 87 89	14, 24, 47, 84	0
1	B	295/317 (93%)	-0.19	3 (1%) 82 85	12, 27, 53, 77	0
1	C	294/317 (92%)	0.03	15 (5%) 28 33	18, 38, 75, 98	0
2	D	125/129 (96%)	-0.36	3 (2%) 59 64	17, 29, 52, 69	0
2	E	121/129 (93%)	-0.42	2 (1%) 70 74	19, 31, 51, 75	0
2	F	122/129 (94%)	0.50	17 (13%) 2 3	22, 47, 76, 99	0
All	All	1252/1338 (93%)	-0.17	42 (3%) 45 51	12, 31, 66, 99	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	1186	LYS	5.7
1	B	270	GLY	5.4
2	F	1185	ALA	5.0
1	A	294	PRO	4.6
1	B	309	SER	4.5
1	C	253	PHE	4.1
2	D	1209	SER	4.0
1	C	230	PRO	4.0
2	F	1171	ARG	3.9
1	C	46	LEU	3.8
1	C	1	PHE	3.7
2	F	1173	ILE	3.6
2	D	1187	GLN	3.4
2	F	1183	TRP	3.4
2	F	1153	ARG	3.3
1	C	42	GLU	3.2
2	F	1184	THR	3.1
1	C	224	LYS	3.1
2	F	1203	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	1175	GLU	2.9
1	C	294	PRO	2.8
2	F	1154	ASN	2.7
1	C	261	ARG	2.5
2	F	1129	ALA	2.5
1	C	143	ASN	2.5
2	E	1187	GLN	2.5
1	C	44	PHE	2.4
2	F	1107	GLY	2.4
2	F	1130	PRO	2.3
1	C	257	PRO	2.2
2	F	1126	SER	2.2
1	C	4	ALA	2.1
2	D	1210	ARG	2.1
1	C	47	GLU	2.1
2	F	1204	GLY	2.1
1	C	254	ASP	2.1
1	A	293	ALA	2.1
2	F	1201	CYS	2.1
1	B	11	ILE	2.1
1	C	6	ARG	2.1
2	F	1152	CYS	2.1
2	F	1108	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)

There are no monosaccharides in this entry.

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. 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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	D	8	6/6	0.83	0.29	51,54,64,66	0
3	GOL	D	6	6/6	0.86	0.14	45,48,53,59	0
3	GOL	C	311	6/6	0.86	0.17	46,52,54,59	0
3	GOL	E	2	6/6	0.89	0.25	37,44,52,53	0
3	GOL	C	312	6/6	0.93	0.17	26,32,37,49	0
3	GOL	B	312	6/6	0.94	0.15	19,33,43,45	0
3	GOL	B	311	6/6	0.94	0.11	44,50,58,58	0
3	GOL	A	311	6/6	0.97	0.11	17,24,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.