Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2023 – 07:38 PM EDT

PDB ID	:	3RJ3
Title	:	Complement components factor H CCP19-20 (S1191L mutant) and C3D in complex
Authors	:	Morgan, H.P.; Hannan, J.P.
Deposited on	:	2011-04-15
Resolution	:	2.35 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 ⓘ 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 ⓘ) were used in the production of this report:

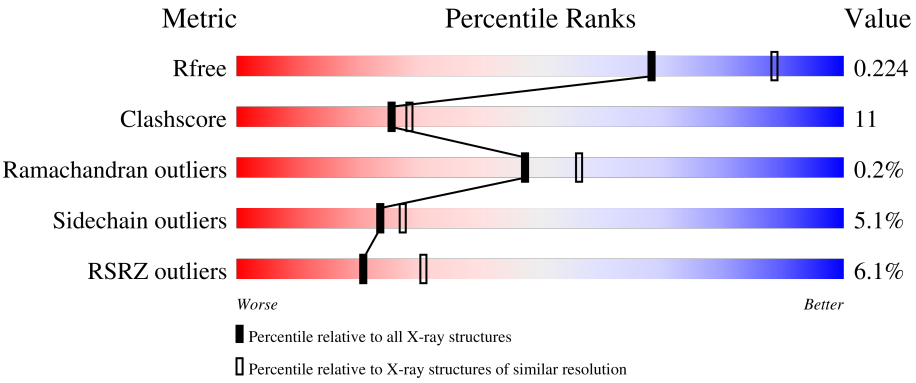
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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



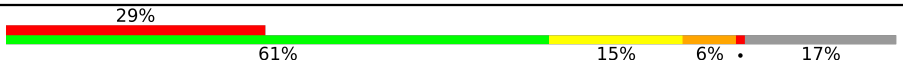
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	76% 15% • 8%
1	B	317	5% 76% 17% • 5%
1	C	317	5% 69% 22% • 8%
2	D	129	2% 69% 25%
2	E	129	2% 73% 19% • 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	129	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10236 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 C3d fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	4	0
			2328	1497	391	431	9			
1	B	300	Total	C	N	O	S	0	3	0
			2376	1526	395	446	9			
1	C	292	Total	C	N	O	S	0	1	0
			2306	1484	387	426	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	conflict	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	conflict	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	conflict	UNP P01024

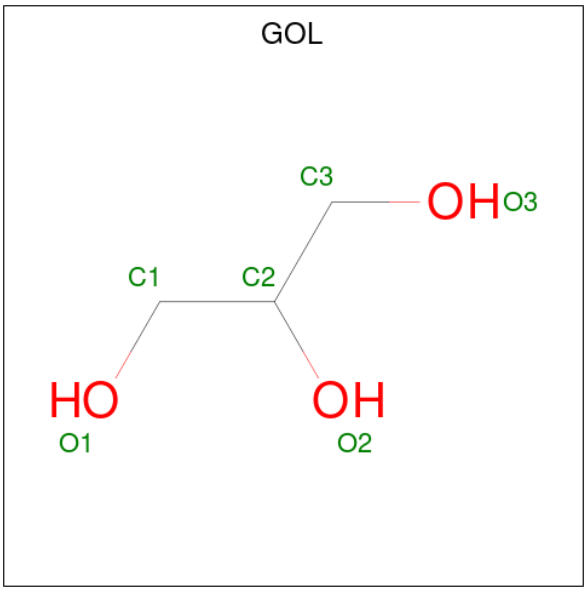
- Molecule 2 is a protein called Complement Factor H-related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	125	Total	C	N	O	S	0	1	0
			1005	632	181	183	9			
2	E	121	Total	C	N	O	S	0	2	0
			980	613	178	180	9			
2	F	107	Total	C	N	O	S	0	0	0
			845	535	145	156	9			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1103	GLU	-	expression tag	UNP Q03591
D	1104	ALA	-	expression tag	UNP Q03591
D	1105	GLU	-	expression tag	UNP Q03591
D	1106	PHE	-	expression tag	UNP Q03591
D	1197	VAL	ALA	SEE REMARK 999	UNP Q03591
E	1103	GLU	-	expression tag	UNP Q03591
E	1104	ALA	-	expression tag	UNP Q03591
E	1105	GLU	-	expression tag	UNP Q03591
E	1106	PHE	-	expression tag	UNP Q03591
E	1197	VAL	ALA	SEE REMARK 999	UNP Q03591
F	1103	GLU	-	expression tag	UNP Q03591
F	1104	ALA	-	expression tag	UNP Q03591
F	1105	GLU	-	expression tag	UNP Q03591
F	1106	PHE	-	expression tag	UNP Q03591
F	1197	VAL	ALA	SEE REMARK 999	UNP Q03591

- 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	C	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

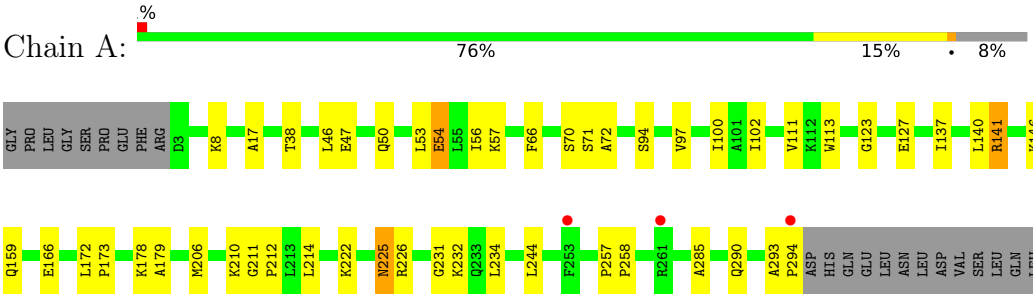
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	112	Total O 112 112	0	0
4	B	97	Total O 97 97	0	0
4	C	42	Total O 42 42	0	0
4	D	59	Total O 59 59	0	0
4	E	45	Total O 45 45	0	0
4	F	17	Total O 17 17	0	0

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.

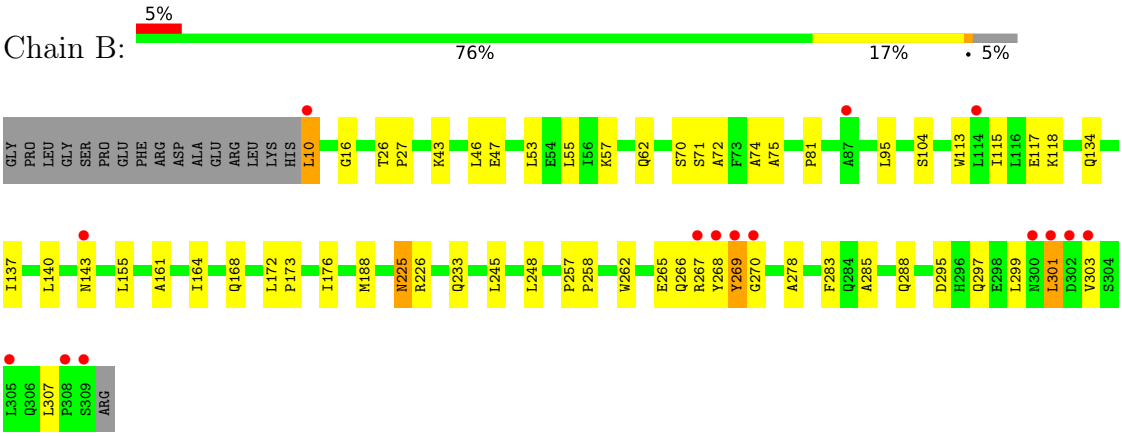
• Molecule 1: Complement C3d fragment

Chain A:



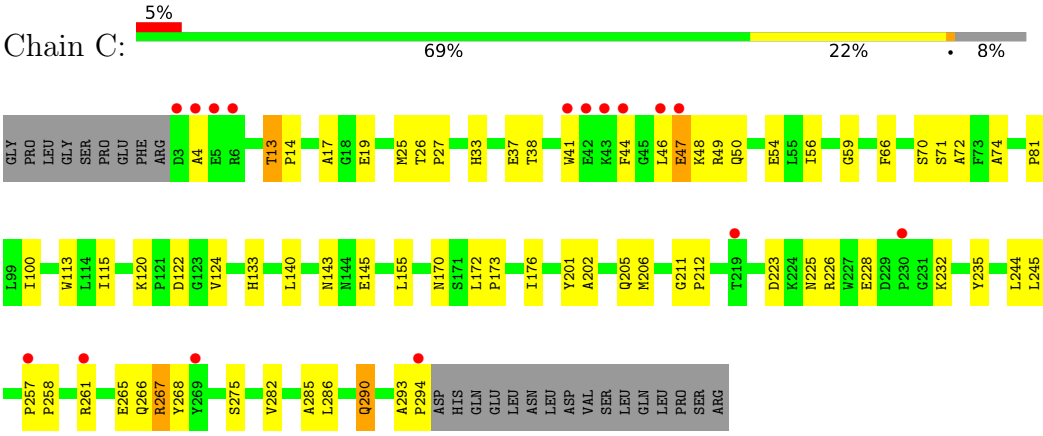
• Molecule 1: Complement C3d fragment

Chain B:



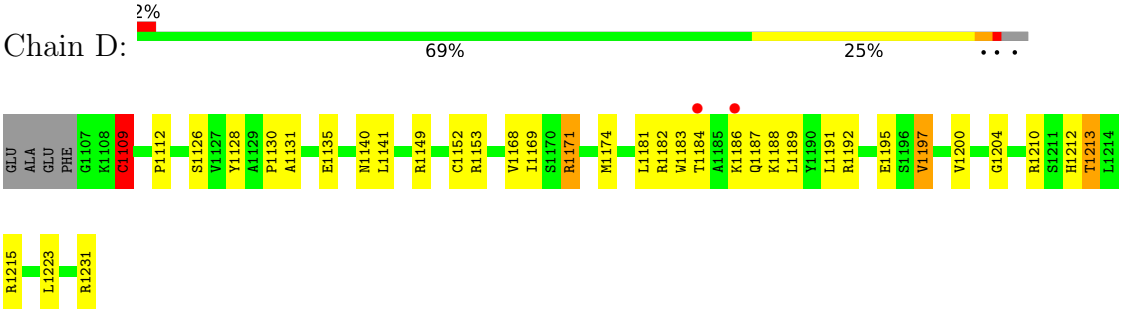
• Molecule 1: Complement C3d fragment

Chain C:



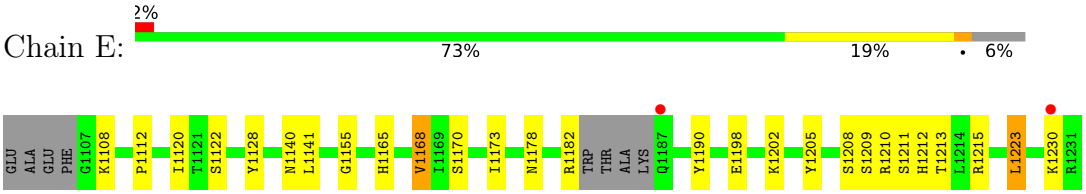
• Molecule 2: Complement Factor H-related protein 1

Chain D:



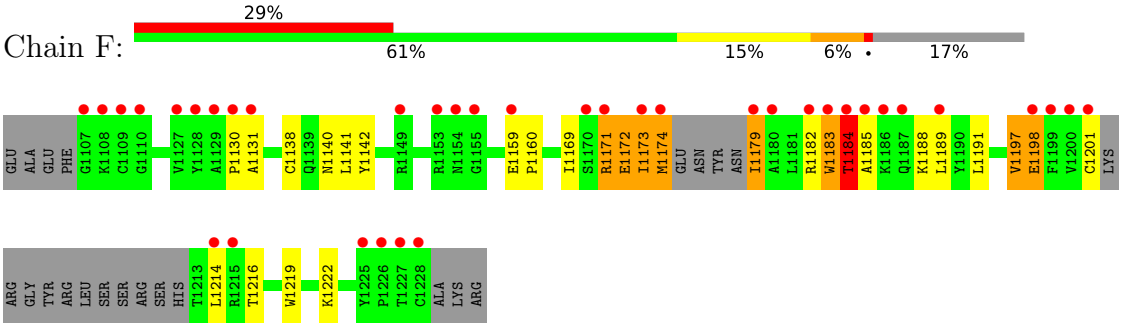
• Molecule 2: Complement Factor H-related protein 1

Chain E:



• Molecule 2: Complement Factor H-related protein 1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	74.75Å 82.62Å 85.40Å 112.61° 110.26° 99.84°	Depositor
Resolution (Å)	41.60 – 2.35 41.60 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.3 (41.60-2.35) 96.3 (41.60-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.191 , 0.232 0.185 , 0.224	Depositor DCC
R_{free} test set	3357 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	42.6	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10236	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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	0.29	0/2383	0.40	0/3228
1	B	0.26	0/2432	0.42	0/3299
1	C	0.27	0/2358	0.40	0/3194
2	D	0.39	0/1034	0.51	1/1402 (0.1%)
2	E	0.23	0/1009	0.39	0/1364
2	F	0.35	0/866	0.51	1/1176 (0.1%)
All	All	0.29	0/10082	0.43	2/13663 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1184	THR	CB-CA-C	-5.41	96.99	111.60
2	D	1109	CYS	CA-CB-SG	5.35	123.64	114.00

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	2328	0	2339	30	0
1	B	2376	0	2376	42	0
1	C	2306	0	2319	41	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1005	0	992	29	0
2	E	980	0	964	20	0
2	F	845	0	824	51	0
3	A	6	0	8	1	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	E	6	0	8	0	0
4	A	112	0	0	2	0
4	B	97	0	0	1	0
4	C	42	0	0	0	0
4	D	59	0	0	0	0
4	E	45	0	0	0	0
4	F	17	0	0	0	0
All	All	10236	0	9846	208	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 11.

All (208) 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:1184:THR:CG2	2:F:1185:ALA:HB2	1.14	1.59
2:F:1184:THR:HG23	2:F:1185:ALA:CB	1.26	1.57
2:F:1184:THR:HG23	2:F:1185:ALA:CA	1.52	1.36
2:F:1184:THR:CG2	2:F:1185:ALA:CB	1.90	1.32
2:F:1172:GLU:CB	2:F:1173:ILE:HG13	1.70	1.20
2:D:1109:CYS:SG	2:D:1152:CYS:CB	2.39	1.09
2:F:1172:GLU:HB3	2:F:1173:ILE:HG13	1.30	1.06
2:D:1109:CYS:SG	2:D:1152:CYS:SG	1.06	1.06
2:F:1173:ILE:CA	2:F:1174:MET:C	2.30	1.00
2:F:1173:ILE:HA	2:F:1174:MET:C	1.82	0.99
2:F:1172:GLU:CA	2:F:1173:ILE:HG13	1.91	0.98
2:F:1184:THR:HG21	2:F:1185:ALA:HB2	0.98	0.96
1:B:269:TYR:HB3	1:B:270:GLY:HA2	1.48	0.95
2:F:1184:THR:CG2	2:F:1185:ALA:CA	2.34	0.93
2:F:1173:ILE:O	2:F:1173:ILE:HG22	1.69	0.92
2:F:1184:THR:HG23	2:F:1185:ALA:N	1.63	0.90
2:F:1172:GLU:HB3	2:F:1173:ILE:CG1	2.01	0.90
2:F:1172:GLU:CB	2:F:1173:ILE:CG1	2.52	0.88
2:F:1172:GLU:HA	2:F:1173:ILE:HG13	1.59	0.84
2:F:1184:THR:CG2	2:F:1185:ALA:N	2.32	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ILE:HD12	1:B:164:ILE:H	1.42	0.82
2:D:1109:CYS:CB	2:D:1152:CYS:HG	1.92	0.82
1:C:38:THR:HG22	1:C:290:GLN:HG2	1.62	0.80
2:F:1173:ILE:O	2:F:1173:ILE:CG2	2.29	0.79
2:F:1173:ILE:N	2:F:1174:MET:C	2.36	0.78
1:B:283:PHE:HE1	1:B:303:VAL:HG12	1.50	0.76
2:F:1184:THR:CB	2:F:1185:ALA:HB2	2.13	0.76
1:A:137:ILE:HD11	1:A:141:ARG:HA	1.67	0.76
1:B:269:TYR:HB3	1:B:270:GLY:CA	2.17	0.73
2:D:1183:TRP:HB3	2:D:1186:LYS:HD3	1.70	0.73
2:F:1184:THR:CB	2:F:1185:ALA:CA	2.65	0.73
1:C:70:SER:O	1:C:71:SER:HB2	1.89	0.72
2:F:1184:THR:OG1	2:F:1185:ALA:HA	1.90	0.72
1:A:70:SER:O	1:A:71:SER:HB2	1.90	0.70
1:C:205:GLN:HA	1:C:249:GLN:HG2	1.74	0.70
2:F:1184:THR:CB	2:F:1185:ALA:HA	2.22	0.68
1:B:16:GLY:HA3	1:B:75:ALA:HB1	1.75	0.67
1:C:17:ALA:HA	1:C:66:PHE:CZ	2.29	0.67
2:D:1213:THR:HG22	2:D:1215:ARG:O	1.95	0.67
2:F:1172:GLU:HB3	2:F:1173:ILE:CD1	2.24	0.66
1:B:164:ILE:HD12	1:B:164:ILE:N	2.11	0.66
2:D:1135:GLU:HG2	2:D:1149:ARG:HG3	1.78	0.66
2:F:1184:THR:HG23	2:F:1185:ALA:HB3	1.66	0.65
1:C:4:ALA:HB1	1:C:44:PHE:HD1	1.62	0.64
2:D:1213:THR:HG23	2:D:1215:ARG:H	1.61	0.64
1:A:8:LYS:HE2	2:D:1168:VAL:HG11	1.79	0.64
1:B:269:TYR:CB	1:B:270:GLY:HA2	2.17	0.63
2:F:1191:LEU:HD21	2:F:1197:VAL:HG13	1.82	0.62
1:B:283:PHE:CE1	1:B:303:VAL:HG12	2.33	0.61
1:B:299:LEU:O	1:B:301:LEU:HA	1.99	0.61
1:C:155:LEU:HD21	1:C:206:MET:HE1	1.83	0.61
2:F:1171:ARG:O	2:F:1174:MET:C	2.40	0.60
1:A:38:THR:HG22	1:A:290:GLN:HG3	1.84	0.60
1:C:115:ILE:HD11	1:C:172:LEU:HD13	1.84	0.59
1:A:53:LEU:O	1:A:57[B]:LYS:HG3	2.02	0.59
1:B:172:LEU:HB3	1:B:173:PRO:HD3	1.84	0.59
1:A:94:SER:O	1:A:97:VAL:HG22	2.03	0.59
1:B:70:SER:O	1:B:71:SER:HB2	2.01	0.59
1:C:155:LEU:HD11	1:C:176:ILE:HG23	1.85	0.59
1:A:50:GLN:O	1:A:54:GLU:HG2	2.03	0.58
1:C:232:LYS:HG3	1:C:235:TYR:CZ	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1169:ILE:HD11	2:D:1191:LEU:CD1	2.34	0.58
2:F:1173:ILE:HA	2:F:1174:MET:O	2.04	0.58
2:E:1178:ASN:HA	2:E:1202:LYS:NZ	2.18	0.58
2:E:1112:PRO:HD3	2:E:1128:TYR:CE1	2.39	0.57
2:F:1184:THR:HG21	2:F:1185:ALA:CB	1.93	0.57
1:B:74:ALA:HB2	1:B:81:PRO:HA	1.86	0.56
1:C:268:TYR:OH	1:C:275:SER:HB2	2.05	0.56
1:A:123:GLY:HA2	1:A:178:LYS:HG2	1.88	0.56
1:B:262:TRP:O	1:B:266:GLN:HG2	2.06	0.56
2:E:1182:ARG:HD2	2:E:1198:GLU:HB3	1.87	0.56
1:B:164:ILE:H	1:B:164:ILE:CD1	2.15	0.55
1:C:282:VAL:O	1:C:286:LEU:HG	2.07	0.55
1:A:127:GLU:HG2	3:A:311:GOL:H2	1.88	0.54
1:C:47:GLU:OE1	1:C:48:LYS:HG2	2.08	0.54
1:A:257:PRO:HB2	1:A:258:PRO:HD3	1.89	0.53
2:F:1184:THR:CB	2:F:1185:ALA:CB	2.76	0.53
1:C:253:PHE:O	1:C:257:PRO:HD3	2.08	0.53
2:D:1169:ILE:HB	2:D:1171:ARG:NH1	2.24	0.53
1:A:97:VAL:HG12	1:A:102:ILE:HB	1.90	0.53
1:C:170:ASN:O	1:C:173:PRO:HD2	2.10	0.52
2:D:1169:ILE:HD11	2:D:1191:LEU:HD11	1.91	0.52
2:F:1172:GLU:CB	2:F:1173:ILE:CD1	2.86	0.52
1:A:166:GLU:HG2	4:A:422:HOH:O	2.09	0.52
1:C:293:ALA:N	1:C:294:PRO:HD2	2.25	0.52
2:E:1212:HIS:HD2	2:E:1213:THR:O	1.92	0.52
2:E:1140:ASN:ND2	2:E:1141:LEU:HG	2.25	0.52
1:B:257:PRO:HB2	1:B:258:PRO:HD3	1.92	0.51
2:E:1178:ASN:HA	2:E:1202:LYS:HZ1	1.74	0.51
1:C:4:ALA:HB1	1:C:44:PHE:CD1	2.44	0.51
2:F:1159:GLU:HG3	2:F:1160:PRO:HD2	1.92	0.51
2:D:1213:THR:CG2	2:D:1215:ARG:H	2.24	0.51
2:F:1130:PRO:O	2:F:1131:ALA:HB3	2.11	0.51
2:D:1140:ASN:O	2:D:1141:LEU:HB2	2.11	0.51
2:D:1212:HIS:CD2	2:D:1213:THR:N	2.80	0.50
1:C:266:GLN:C	1:C:268:TYR:H	2.15	0.50
1:C:56:ILE:HG22	1:C:100:ILE:HD13	1.93	0.50
2:E:1213:THR:HG23	2:E:1215:ARG:O	2.12	0.50
2:F:1182:ARG:O	2:F:1183:TRP:CB	2.59	0.50
1:C:261:ARG:O	1:C:265:GLU:HG3	2.12	0.49
1:A:225:ASN:HD21	1:A:226:ARG:HH11	1.60	0.49
2:D:1182:ARG:CZ	2:D:1200:VAL:HG12	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1171:ARG:O	2:F:1174:MET:O	2.30	0.49
2:F:1184:THR:OG1	2:F:1185:ALA:CA	2.60	0.49
1:A:231:GLY:N	1:B:43:LYS:HE2	2.27	0.49
1:C:120:LYS:HD3	2:D:1140:ASN:ND2	2.28	0.49
1:B:46:LEU:HD23	1:B:46:LEU:O	2.13	0.49
2:F:1179:ILE:O	2:F:1179:ILE:HG12	2.12	0.49
1:B:268:TYR:OH	1:B:278:ALA:HB3	2.13	0.48
2:D:1184:THR:O	2:D:1187:GLN:HG2	2.13	0.48
2:F:1173:ILE:H	2:F:1174:MET:HB3	1.77	0.48
2:E:1205:TYR:OH	2:E:1230:LYS:HE2	2.13	0.48
1:C:26:THR:HB	1:C:27:PRO:HD3	1.94	0.48
1:B:26:THR:N	1:B:27:PRO:HD2	2.28	0.48
1:C:33:HIS:O	1:C:37:GLU:HG2	2.14	0.48
2:D:1204:GLY:O	2:D:1231:ARG:HG2	2.14	0.48
1:B:134:GLN:O	1:B:137:ILE:HG12	2.14	0.48
1:B:267:ARG:NH1	1:B:267:ARG:HB3	2.29	0.48
1:C:257:PRO:N	1:C:258:PRO:HD2	2.29	0.48
1:A:56:ILE:HG22	1:A:100:ILE:HD13	1.96	0.47
2:F:1174:MET:HB2	2:F:1179:ILE:HG12	1.96	0.47
1:C:201:TYR:CE1	1:C:245:LEU:HB3	2.49	0.47
2:E:1208:SER:OG	2:E:1211:SER:HB2	2.14	0.47
1:C:13:THR:HA	1:C:14:PRO:HD3	1.71	0.47
2:D:1192:ARG:HB2	2:D:1195:GLU:HG3	1.97	0.47
2:F:1140:ASN:ND2	2:F:1141:LEU:HG	2.30	0.47
2:F:1188:LYS:HG2	2:F:1189:LEU:N	2.29	0.47
2:F:1219:TRP:O	2:F:1222:LYS:HD2	2.15	0.47
1:A:159:GLN:OE1	1:A:206:MET:HG3	2.15	0.46
2:F:1173:ILE:N	2:F:1174:MET:CA	2.77	0.46
1:C:74:ALA:HB2	1:C:81:PRO:HA	1.97	0.46
2:D:1169:ILE:HB	2:D:1171:ARG:HH11	1.79	0.46
1:B:268:TYR:CG	1:B:269:TYR:N	2.83	0.46
2:F:1140:ASN:O	2:F:1141:LEU:HB2	2.15	0.46
1:B:16:GLY:CA	1:B:75:ALA:HB1	2.46	0.46
1:A:111:VAL:HG13	1:A:158:LEU:HD22	1.97	0.46
2:D:1191:LEU:HD11	2:D:1197[A]:VAL:HG22	1.98	0.46
2:D:1187:GLN:NE2	2:D:1187:GLN:HA	2.31	0.46
1:C:155:LEU:HD21	1:C:206:MET:CE	2.46	0.45
1:C:122:ASP:OD1	1:C:124:VAL:HG23	2.16	0.45
1:A:155:LEU:HD21	1:A:206:MET:CE	2.46	0.45
1:C:226:ARG:HE	1:C:228:GLU:CD	2.20	0.45
2:D:1212:HIS:HD2	2:D:1213:THR:O	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1140:ASN:ND2	2:D:1141:LEU:HG	2.32	0.45
1:C:19:GLU:OE1	1:C:133:HIS:HD2	2.00	0.44
2:D:1171:ARG:HA	2:D:1171:ARG:HD3	1.74	0.44
2:E:1182:ARG:HG3	2:E:1198:GLU:O	2.17	0.44
1:A:17:ALA:HA	1:A:66:PHE:CZ	2.51	0.44
1:C:223:ASP:HB2	1:C:225:ASN:ND2	2.33	0.44
1:A:234:LEU:HD11	4:A:378:HOH:O	2.18	0.44
1:B:248:LEU:HD13	1:B:288:GLN:HG3	2.00	0.44
1:C:232:LYS:HG3	1:C:235:TYR:CE1	2.52	0.44
1:C:223:ASP:HB2	1:C:225:ASN:HD21	1.82	0.44
1:B:113:TRP:CD1	1:B:117:GLU:HG3	2.53	0.44
2:D:1188:LYS:HD3	2:D:1191:LEU:HD21	2.00	0.44
1:B:225:ASN:N	1:B:225:ASN:HD22	2.15	0.44
2:D:1112:PRO:HD3	2:D:1128:TYR:CE1	2.52	0.44
2:E:1213:THR:CG2	2:E:1215:ARG:O	2.66	0.44
1:B:155:LEU:HD11	1:B:176:ILE:HG23	2.00	0.43
1:A:293:ALA:HA	1:A:294:PRO:HA	1.73	0.43
2:E:1108:LYS:O	2:E:1155:GLY:HA2	2.18	0.43
1:A:231:GLY:H	1:B:43:LYS:HE2	1.83	0.43
1:B:161:ALA:HA	1:B:164:ILE:HD13	2.00	0.43
2:D:1130:PRO:O	2:D:1131:ALA:HB3	2.18	0.43
1:B:265:GLU:C	1:B:267:ARG:N	2.71	0.43
1:A:172:LEU:N	1:A:173:PRO:HD2	2.34	0.43
1:B:62:GLN:HG2	2:E:1212:HIS:CE1	2.53	0.43
1:A:72:ALA:HB2	1:A:113:TRP:CD2	2.54	0.42
1:B:10:LEU:HD12	1:B:10:LEU:HA	1.77	0.42
2:F:1184:THR:OG1	2:F:1185:ALA:CB	2.67	0.42
1:A:155:LEU:HD21	1:A:206:MET:HE1	2.01	0.42
2:E:1140:ASN:O	2:E:1141:LEU:HB2	2.19	0.42
1:B:115:ILE:HD11	1:B:172:LEU:HD13	2.01	0.42
1:B:225:ASN:HD21	1:B:226:ARG:NH1	2.17	0.42
2:E:1168:VAL:HG23	2:E:1190:TYR:CE2	2.53	0.42
2:F:1172:GLU:H	2:F:1172:GLU:HG2	1.21	0.42
2:F:1138:CYS:HB3	2:F:1142:TYR:HB2	2.02	0.42
1:B:265:GLU:C	1:B:267:ARG:H	2.22	0.42
1:B:72:ALA:HB2	1:B:113:TRP:CD2	2.55	0.42
1:C:244:LEU:HD23	1:C:285:ALA:HB1	2.01	0.42
2:E:1209:SER:O	2:E:1210:ARG:HB2	2.20	0.42
2:F:1172:GLU:HA	2:F:1173:ILE:CG1	2.40	0.42
2:E:1120:ILE:HG13	2:E:1122:SER:O	2.19	0.42
1:C:72:ALA:HB2	1:C:113:TRP:CD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1182:ARG:HG2	2:F:1198:GLU:HB3	2.01	0.41
1:B:57:LYS:HG3	4:B:355:HOH:O	2.20	0.41
1:B:104[B]:SER:HB3	1:B:168:GLN:HE22	1.85	0.41
1:C:202:ALA:O	1:C:206:MET:HE2	2.19	0.41
1:A:244:LEU:HD23	1:A:285:ALA:HB1	2.01	0.41
2:D:1174:MET:HE1	2:D:1181:LEU:HG	2.02	0.41
2:E:1170:SER:OG	2:E:1173:ILE:HG13	2.21	0.41
1:A:155:LEU:HD13	1:A:179:ALA:HB3	2.03	0.41
1:B:233:GLN:HE21	1:B:233:GLN:HB3	1.63	0.41
2:F:1172:GLU:CA	2:F:1173:ILE:CG1	2.82	0.41
1:C:25:MET:HG2	1:C:59:GLY:HA3	2.02	0.41
1:A:54:GLU:HG2	1:A:54:GLU:H	1.60	0.41
1:B:245:LEU:HD21	1:B:285:ALA:HA	2.03	0.41
1:C:41:TRP:CE3	1:C:49:ARG:HB2	2.55	0.41
2:F:1169:ILE:HD11	2:F:1191:LEU:HD11	2.02	0.41
1:C:41:TRP:O	1:C:46:LEU:N	2.54	0.41
1:C:50:GLN:O	1:C:54:GLU:HG2	2.21	0.41
1:C:211:GLY:HA3	1:C:212:PRO:HD2	1.93	0.41
2:E:1223:LEU:HD23	2:E:1223:LEU:HA	1.84	0.41
1:A:211:GLY:HA3	1:A:212:PRO:HD2	1.97	0.40
1:B:43:LYS:HD3	1:B:43:LYS:HA	1.79	0.40
1:A:210:LYS:HA	1:A:214:LEU:HB2	2.03	0.40
1:B:118:LYS:HA	1:B:118:LYS:HD3	1.89	0.40
2:E:1168:VAL:HG23	2:E:1190:TYR:CD2	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	293/317 (92%)	285 (97%)	7 (2%)	1 (0%)	41 47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	301/317 (95%)	286 (95%)	15 (5%)	0	100 100
1	C	291/317 (92%)	277 (95%)	13 (4%)	1 (0%)	41 47
2	D	124/129 (96%)	122 (98%)	2 (2%)	0	100 100
2	E	119/129 (92%)	119 (100%)	0	0	100 100
2	F	101/129 (78%)	96 (95%)	4 (4%)	1 (1%)	15 15
All	All	1229/1338 (92%)	1185 (96%)	41 (3%)	3 (0%)	47 56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	1173	ILE
1	A	141	ARG
1	C	267	ARG

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	245/264 (93%)	237 (97%)	8 (3%)	38 46
1	B	253/264 (96%)	239 (94%)	14 (6%)	21 24
1	C	242/264 (92%)	233 (96%)	9 (4%)	34 42
2	D	113/115 (98%)	103 (91%)	10 (9%)	10 8
2	E	111/115 (96%)	108 (97%)	3 (3%)	44 55
2	F	96/115 (84%)	85 (88%)	11 (12%)	5 5
All	All	1060/1137 (93%)	1005 (95%)	55 (5%)	24 27

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	47	GLU
1	A	54	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	140	LEU
1	A	146	LYS
1	A	222	LYS
1	A	225	ASN
1	A	232	LYS
1	B	10	LEU
1	B	47	GLU
1	B	53	LEU
1	B	55	LEU
1	B	95	LEU
1	B	140	LEU
1	B	143	ASN
1	B	188	MET
1	B	225	ASN
1	B	269	TYR
1	B	295	ASP
1	B	297	GLN
1	B	301	LEU
1	B	307	LEU
1	C	13	THR
1	C	47	GLU
1	C	95	LEU
1	C	98	ASN
1	C	140	LEU
1	C	143	ASN
1	C	145	GLU
1	C	267	ARG
1	C	290	GLN
2	D	1109	CYS
2	D	1126	SER
2	D	1153	ARG
2	D	1171	ARG
2	D	1189	LEU
2	D	1197[A]	VAL
2	D	1197[B]	VAL
2	D	1210	ARG
2	D	1213	THR
2	D	1223	LEU
2	E	1165	HIS
2	E	1168	VAL
2	E	1223	LEU
2	F	1171	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	1172	GLU
2	F	1174	MET
2	F	1179	ILE
2	F	1183	TRP
2	F	1184	THR
2	F	1197	VAL
2	F	1198	GLU
2	F	1201	CYS
2	F	1214	LEU
2	F	1216	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	170	ASN
1	A	189	ASN
1	A	191	GLN
1	A	225	ASN
1	B	105	GLN
1	B	159	GLN
1	B	168	GLN
1	B	225	ASN
1	B	233	GLN
1	B	266	GLN
1	C	105	GLN
1	C	133	HIS
1	C	159	GLN
1	C	170	ASN
1	C	225	ASN
1	C	290	GLN
2	D	1140	ASN
2	D	1165	HIS
2	D	1187	GLN
2	D	1212	HIS
2	E	1137	GLN
2	E	1140	ASN
2	E	1187	GLN
2	E	1212	HIS
2	F	1140	ASN
2	F	1143	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	C	311	-	5,5,5	0.49	0	5,5,5	0.24	0
3	GOL	E	1	-	5,5,5	0.34	0	5,5,5	0.29	0
3	GOL	B	311	-	5,5,5	0.49	0	5,5,5	0.70	0
3	GOL	A	311	-	5,5,5	0.40	0	5,5,5	0.28	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	311	-	-	2/4/4/4	-
3	GOL	E	1	-	-	2/4/4/4	-
3	GOL	B	311	-	-	2/4/4/4	-
3	GOL	A	311	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	311	GOL	C1-C2-C3-O3
3	C	311	GOL	O1-C1-C2-C3
3	A	311	GOL	O1-C1-C2-C3
3	A	311	GOL	C1-C2-C3-O3
3	A	311	GOL	O1-C1-C2-O2
3	B	311	GOL	O2-C2-C3-O3
3	C	311	GOL	O1-C1-C2-O2
3	A	311	GOL	O2-C2-C3-O3
3	E	1	GOL	O1-C1-C2-O2
3	E	1	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	311	GOL	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	292/317 (92%)	-0.26	3 (1%) 82 88	21, 38, 74, 115	0
1	B	300/317 (94%)	0.20	15 (5%) 28 41	21, 45, 88, 177	0
1	C	292/317 (92%)	0.14	17 (5%) 23 33	28, 59, 113, 174	0
2	D	125/129 (96%)	-0.14	2 (1%) 72 80	28, 44, 76, 135	0
2	E	121/129 (93%)	-0.12	2 (1%) 70 78	32, 50, 82, 102	0
2	F	107/129 (82%)	1.25	37 (34%) 0 0	35, 77, 129, 184	0
All	All	1237/1338 (92%)	0.10	76 (6%) 21 31	21, 49, 103, 184	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	270	GLY	9.4
2	F	1183	TRP	7.0
1	B	300	ASN	6.7
1	B	269	TYR	6.5
1	B	301	LEU	6.4
2	F	1108	LYS	6.0
1	B	302	ASP	5.7
1	C	41	TRP	5.6
1	B	309	SER	5.5
2	F	1201	CYS	5.5
1	C	4	ALA	5.5
1	B	268	TYR	4.8
1	B	267	ARG	4.8
1	C	42	GLU	4.7
2	F	1130	PRO	4.4
2	F	1200	VAL	4.3
2	F	1153	ARG	4.2
2	F	1199	PHE	4.1
2	F	1185	ALA	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	1227	THR	4.1
1	C	253	PHE	4.1
2	F	1154	ASN	3.9
1	A	294	PRO	3.8
1	C	46	LEU	3.7
2	F	1179	ILE	3.7
1	B	10	LEU	3.6
2	F	1173	ILE	3.6
1	C	261	ARG	3.6
2	F	1110	GLY	3.5
2	F	1149	ARG	3.5
2	F	1214	LEU	3.5
2	F	1107	GLY	3.4
2	F	1128	TYR	3.4
1	C	5	GLU	3.3
2	F	1226	PRO	3.2
2	F	1127	VAL	3.2
2	F	1180	ALA	3.1
1	C	44	PHE	3.1
2	F	1155	GLY	3.1
2	F	1182	ARG	3.1
2	F	1131	ALA	3.0
2	F	1187	GLN	2.9
2	F	1228	CYS	2.9
1	C	230	PRO	2.8
2	D	1184	THR	2.8
2	D	1186	LYS	2.8
1	C	6	ARG	2.8
1	C	219	THR	2.8
2	F	1171	ARG	2.8
1	C	47	GLU	2.7
1	C	294	PRO	2.7
1	C	43	LYS	2.6
2	F	1225	TYR	2.6
2	F	1184	THR	2.6
2	E	1187	GLN	2.6
1	A	253	PHE	2.5
2	F	1129	ALA	2.5
2	F	1174	MET	2.5
1	B	143	ASN	2.4
1	C	269	TYR	2.4
1	B	114	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	305	LEU	2.4
2	F	1215	ARG	2.4
2	F	1198	GLU	2.4
2	F	1186	LYS	2.3
2	E	1230	LYS	2.2
1	B	303	VAL	2.2
2	F	1170	SER	2.2
1	C	3	ASP	2.2
1	B	308	PRO	2.1
1	B	87	ALA	2.1
1	A	261	ARG	2.1
2	F	1189	LEU	2.1
2	F	1159	GLU	2.1
1	C	257	PRO	2.1
2	F	1109	CYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	C	311	6/6	0.84	0.17	62,64,67,79	0
3	GOL	B	311	6/6	0.85	0.17	61,67,68,68	0
3	GOL	E	1	6/6	0.88	0.19	51,58,67,68	0
3	GOL	A	311	6/6	0.98	0.13	29,39,43,45	0

6.5 Other polymers (i)

There are no such residues in this entry.