



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2023 – 02:32 am GMT

PDB ID : 2XQW
Title : Structure of Factor H domains 19-20 in complex with complement C3d
Authors : Kajander, T.; Lehtinen, M.J.; Hyvarinen, S.; Bhattacharjee, A.; Leung, E.; Isenman, D.E.; Meri, S.; Jokiranta, T.S.; Goldman, A.
Deposited on : 2010-09-07
Resolution : 2.31 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
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

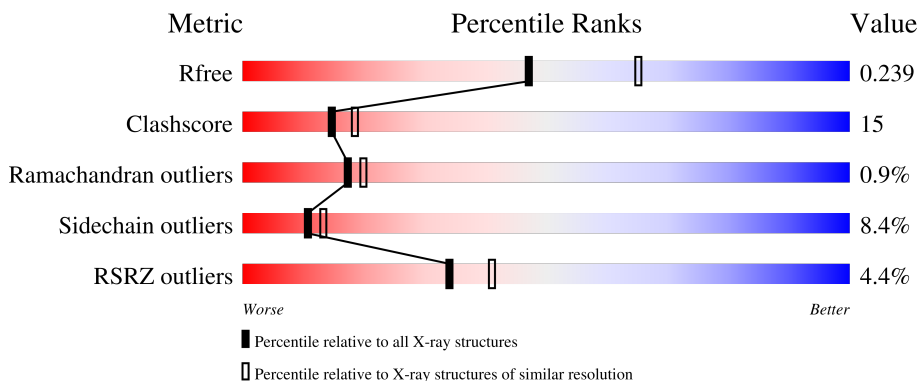
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 $\leq 5\%$. 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	A	294	 70% 27% .
1	B	294	 69% 29% .
2	C	133	 56% 31% 6% 8%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5700 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
			Total	C	N	O	S			
1	A	294	2290	1472	382	426	10	0	0	0
1	B	294	2290	1476	379	425	10	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P01024
A	2	LEU	-	expression tag	UNP P01024
A	17	ALA	CYS	engineered mutation	UNP P01024
B	1	MET	-	expression tag	UNP P01024
B	2	LEU	-	expression tag	UNP P01024
B	17	ALA	CYS	engineered mutation	UNP P01024

- Molecule 2 is a protein called COMPLEMENT FACTOR H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	123	927	583	161	174	9	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1099	ALA	-	expression tag	UNP P08603
C	1100	GLY	-	expression tag	UNP P08603
C	1101	ILE	-	expression tag	UNP P08603
C	1102	GLN	-	expression tag	UNP P08603
C	1119	GLY	ASP	engineered mutation	UNP P08603
C	1139	ALA	GLN	engineered mutation	UNP P08603

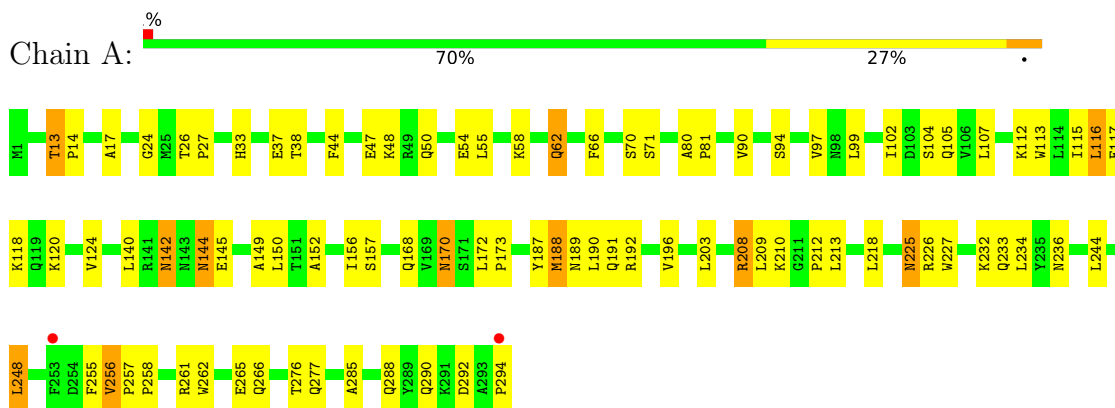
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total 102	O 102	0	0
3	B	48	Total 48	O 48	0	0
3	C	43	Total 43	O 43	0	0

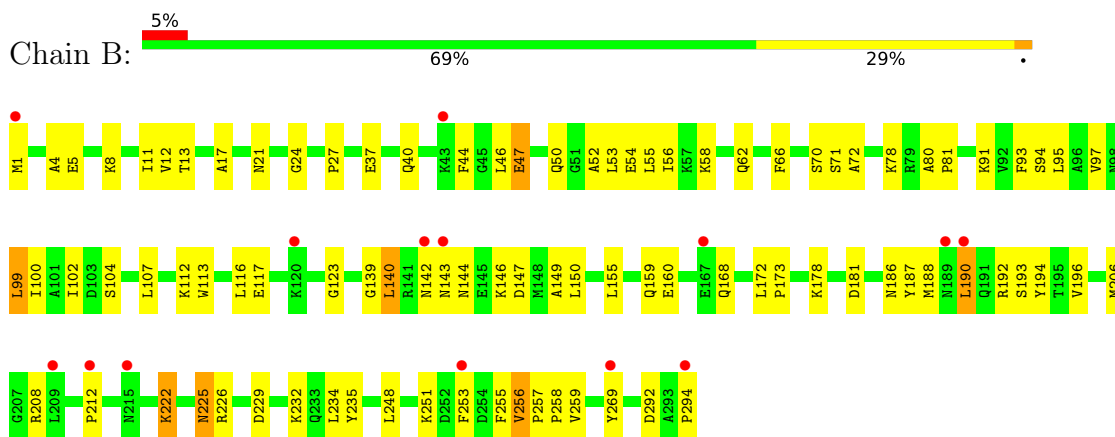
3 Residue-property plots [i](#)

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.

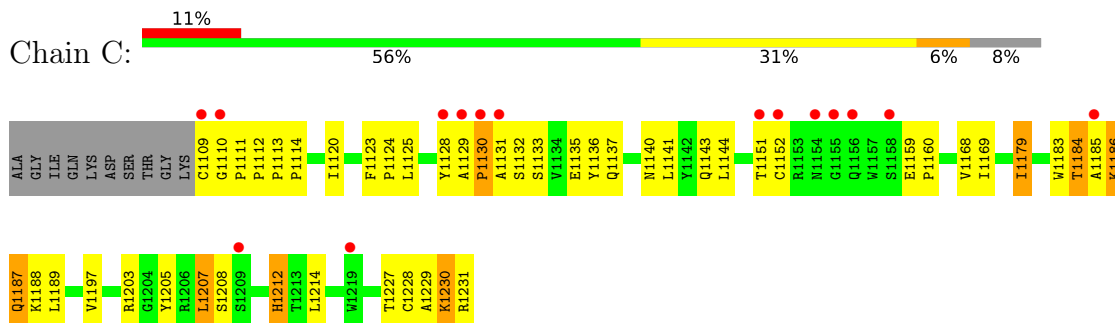
- Molecule 1: COMPLEMENT C3



- Molecule 1: COMPLEMENT C3



- Molecule 2: COMPLEMENT FACTOR H



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	103.55Å 103.55Å 141.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.75 – 2.31 41.75 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.4 (41.75-2.31) 99.7 (41.75-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.32Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.201 , 0.242 0.198 , 0.239	Depositor DCC
R_{free} test set	1884 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtrriage
Anisotropy	0.331	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.056 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5700	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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](#)

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	0.35	0/2339	0.50	0/3175
1	B	0.31	0/2339	0.45	0/3172
2	C	0.37	0/952	0.58	0/1298
All	All	0.34	0/5630	0.49	0/7645

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	1183	TRP	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	A	2290	0	2266	64	0
1	B	2290	0	2282	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	927	0	863	45	0
3	A	102	0	0	2	0
3	B	48	0	0	0	0
3	C	43	0	0	0	0
All	All	5700	0	5411	167	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 15.

All (167) 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:C:1229:ALA:O	2:C:1230:LYS:HB3	1.48	1.06
2:C:1186:LYS:CB	2:C:1188:LYS:H	1.80	0.94
1:B:97:VAL:HA	1:B:102:ILE:HD12	1.50	0.93
2:C:1186:LYS:HB3	2:C:1188:LYS:H	1.35	0.89
1:A:104:SER:HB3	1:A:168:GLN:HE22	1.35	0.88
2:C:1109:CYS:N	2:C:1129:ALA:HB2	1.90	0.86
1:A:58:LYS:O	1:A:62:GLN:HG2	1.77	0.83
1:B:225:ASN:HD21	1:B:226:ARG:HH11	1.21	0.83
1:A:170:ASN:OD1	2:C:1114:PRO:HB3	1.79	0.83
1:A:233:GLN:NE2	1:A:236:ASN:HD22	1.76	0.83
1:A:292:ASP:O	1:A:294:PRO:HD3	1.79	0.82
1:B:56:ILE:HG22	1:B:100:ILE:HD13	1.63	0.81
2:C:1186:LYS:HB3	2:C:1187:GLN:CB	2.13	0.79
2:C:1186:LYS:CB	2:C:1187:GLN:HB2	2.13	0.79
2:C:1186:LYS:HB3	2:C:1187:GLN:HB2	1.63	0.78
2:C:1186:LYS:HB3	2:C:1188:LYS:N	1.98	0.77
1:A:97:VAL:HG12	1:A:102:ILE:HB	1.68	0.74
1:A:170:ASN:HD22	1:A:170:ASN:H	1.36	0.72
1:A:170:ASN:HD22	1:A:170:ASN:N	1.87	0.72
1:B:256:VAL:HG22	1:B:257:PRO:HD3	1.72	0.72
2:C:1212:HIS:H	2:C:1212:HIS:CD2	2.08	0.71
1:A:70:SER:O	1:A:71:SER:HB2	1.90	0.71
2:C:1113:PRO:HG2	2:C:1160:PRO:HG3	1.72	0.71
2:C:1207:LEU:O	2:C:1208:SER:HB3	1.91	0.70
2:C:1229:ALA:O	2:C:1230:LYS:CB	2.29	0.69
2:C:1186:LYS:HB2	2:C:1188:LYS:H	1.56	0.68
1:A:233:GLN:HE21	1:A:236:ASN:HD22	1.40	0.68
1:A:26:THR:HB	1:A:27:PRO:HD3	1.74	0.67
1:A:172:LEU:HB3	1:A:173:PRO:HD3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:GLY:HA2	1:B:178:LYS:HG2	1.78	0.65
2:C:1186:LYS:CA	2:C:1187:GLN:HB2	2.25	0.65
1:B:112:LYS:HG2	1:B:116:LEU:HD23	1.79	0.64
1:B:172:LEU:HB3	1:B:173:PRO:HD3	1.80	0.63
1:B:58:LYS:O	1:B:62:GLN:HG2	1.99	0.63
1:B:140:LEU:HD22	1:B:149:ALA:HB1	1.81	0.62
1:B:139:GLY:HA3	1:B:194:TYR:CE1	2.35	0.62
1:B:225:ASN:HD22	1:B:226:ARG:N	1.98	0.61
1:B:94:SER:OG	1:B:160:GLU:HG3	2.01	0.60
2:C:1129:ALA:HA	2:C:1152:CYS:SG	2.42	0.60
2:C:1184:THR:HG22	2:C:1184:THR:O	2.01	0.60
1:B:140:LEU:CD2	1:B:149:ALA:HB1	2.32	0.60
1:A:255:PHE:O	1:A:258:PRO:HD2	2.03	0.59
1:A:256:VAL:HG22	1:A:257:PRO:HD3	1.84	0.58
1:A:115:ILE:HG22	1:A:116:LEU:HD13	1.85	0.58
1:B:5:GLU:HG3	1:B:8:LYS:HE3	1.86	0.58
1:A:189:ASN:HD21	1:B:46:LEU:HD23	1.68	0.57
1:B:123:GLY:CA	1:B:178:LYS:HG2	2.34	0.57
1:A:191:GLN:OE1	1:B:47:GLU:HG2	2.04	0.57
1:A:188:MET:SD	1:A:213:LEU:HD12	2.45	0.57
2:C:1212:HIS:CD2	2:C:1212:HIS:N	2.72	0.57
1:B:253:PHE:CE2	1:B:294:PRO:HG2	2.39	0.57
1:B:253:PHE:HE2	1:B:294:PRO:HG2	1.70	0.56
2:C:1186:LYS:HB3	2:C:1187:GLN:CA	2.35	0.55
1:A:187:TYR:CD2	1:A:213:LEU:HG	2.42	0.55
2:C:1186:LYS:HA	2:C:1187:GLN:HB2	1.86	0.55
1:B:225:ASN:HD21	1:B:226:ARG:NH1	1.99	0.55
1:B:190:LEU:HB3	1:B:196:VAL:HG12	1.89	0.55
1:A:226:ARG:HD3	1:A:262:TRP:NE1	2.22	0.55
1:A:292:ASP:C	1:A:294:PRO:HD3	2.27	0.55
2:C:1207:LEU:O	2:C:1227:THR:O	2.25	0.55
1:A:266:GLN:NE2	1:A:266:GLN:HA	2.23	0.54
1:A:112:LYS:HG3	1:A:116:LEU:HD22	1.90	0.54
2:C:1130:PRO:HA	2:C:1152:CYS:SG	2.48	0.54
1:A:115:ILE:HD11	1:A:172:LEU:HD13	1.89	0.53
1:A:113:TRP:CD1	1:A:117:GLU:HG3	2.43	0.53
1:A:227:TRP:HA	3:A:2084:HOH:O	2.08	0.52
2:C:1179:ILE:HD11	2:C:1214:LEU:CD2	2.39	0.52
1:A:261:ARG:O	1:A:265:GLU:HG3	2.10	0.52
1:A:225:ASN:HD21	1:A:226:ARG:HH11	1.57	0.52
2:C:1130:PRO:O	2:C:1131:ALA:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1120:ILE:HD11	2:C:1124:PRO:HG3	1.91	0.51
1:A:244:LEU:HD23	1:A:285:ALA:HB1	1.92	0.51
1:B:269:TYR:CD2	1:B:269:TYR:N	2.78	0.51
1:B:155:LEU:O	1:B:159:GLN:HG3	2.11	0.51
1:A:104:SER:HB3	1:A:168:GLN:NE2	2.15	0.50
1:B:187:TYR:HA	1:B:190:LEU:HD22	1.94	0.49
1:B:251:LYS:HA	1:B:253:PHE:CE1	2.46	0.49
2:C:1112:PRO:HD3	2:C:1128:TYR:CE2	2.46	0.49
1:A:17:ALA:HA	1:A:66:PHE:CZ	2.47	0.49
1:A:170:ASN:H	1:A:170:ASN:ND2	2.08	0.49
1:A:33:HIS:O	1:A:37:GLU:HG2	2.13	0.49
1:A:170:ASN:N	1:A:170:ASN:ND2	2.59	0.49
1:B:4:ALA:HB1	1:B:44:PHE:HB2	1.95	0.49
1:A:142:ASN:HD22	1:A:192:ARG:CZ	2.26	0.49
1:A:142:ASN:ND2	1:A:192:ARG:CZ	2.76	0.49
1:B:72:ALA:HB2	1:B:113:TRP:CD2	2.48	0.49
1:B:70:SER:O	1:B:71:SER:HB3	2.13	0.48
1:A:44:PHE:CE2	1:A:48:LYS:HD2	2.48	0.48
1:A:203:LEU:HD22	1:A:208:ARG:HB2	1.94	0.48
2:C:1184:THR:O	2:C:1186:LYS:N	2.47	0.48
1:A:144:ASN:O	1:A:145:GLU:HB2	2.14	0.48
1:A:276:THR:HG22	1:A:277:GLN:NE2	2.29	0.48
1:A:218:LEU:HD22	1:A:255:PHE:CE2	2.49	0.47
2:C:1159:GLU:HA	2:C:1160:PRO:HD3	1.78	0.47
1:B:104:SER:HB3	1:B:168:GLN:HE22	1.78	0.47
1:B:21:ASN:OD1	1:B:62:GLN:HG3	2.15	0.47
1:B:113:TRP:O	1:B:117:GLU:HB2	2.15	0.47
1:B:193:SER:HB2	1:B:229:ASP:OD2	2.14	0.47
2:C:1205:TYR:CE2	2:C:1230:LYS:HB2	2.49	0.47
1:A:257:PRO:HB2	1:A:258:PRO:HD3	1.96	0.47
1:B:140:LEU:HD23	1:B:194:TYR:HE2	1.80	0.47
1:A:225:ASN:H	1:A:225:ASN:HD22	1.62	0.46
1:A:152:ALA:O	1:A:156:ILE:HD12	2.15	0.46
2:C:1112:PRO:HD3	2:C:1128:TYR:HE2	1.81	0.46
2:C:1140:ASN:O	2:C:1141:LEU:HB2	2.16	0.46
1:A:120:LYS:NZ	2:C:1140:ASN:HD21	2.14	0.46
1:B:255:PHE:CD1	1:B:255:PHE:O	2.69	0.46
1:B:256:VAL:O	1:B:259:VAL:N	2.49	0.46
1:B:24:GLY:O	1:B:27:PRO:HD2	2.16	0.45
1:B:188:MET:HE1	1:B:212:PRO:O	2.16	0.45
1:B:256:VAL:HG22	1:B:257:PRO:CD	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:CD2	1:A:149:ALA:HB1	2.46	0.45
2:C:1111:PRO:HA	2:C:1112:PRO:HD3	1.86	0.45
1:A:232:LYS:HE2	1:A:234:LEU:HD12	1.99	0.45
1:B:292:ASP:C	1:B:294:PRO:HD3	2.37	0.45
2:C:1179:ILE:HD12	2:C:1228:CYS:SG	2.57	0.44
2:C:1110:GLY:O	2:C:1128:TYR:HD2	2.00	0.44
1:A:24:GLY:O	1:A:27:PRO:HD2	2.18	0.44
2:C:1169:ILE:HD11	2:C:1197:VAL:HG21	2.00	0.44
1:B:222:LYS:HG2	1:B:226:ARG:NH2	2.33	0.44
2:C:1129:ALA:HA	2:C:1130:PRO:HA	1.78	0.44
1:A:80:ALA:HA	1:A:81:PRO:HD3	1.80	0.44
1:A:192:ARG:O	1:A:196:VAL:HG13	2.18	0.44
1:A:248:LEU:HD23	1:A:288:GLN:CG	2.48	0.44
1:B:255:PHE:O	1:B:255:PHE:HD1	2.00	0.44
1:B:257:PRO:HB2	1:B:258:PRO:HD3	1.99	0.44
1:A:113:TRP:CZ2	1:A:118:LYS:HE3	2.53	0.43
1:B:50:GLN:O	1:B:54:GLU:HG3	2.17	0.43
1:B:155:LEU:HD11	1:B:206:MET:HE3	2.00	0.43
1:B:188:MET:HE2	1:B:212:PRO:HB2	2.00	0.43
1:B:95:LEU:HD23	1:B:95:LEU:O	2.18	0.43
1:B:192:ARG:O	1:B:196:VAL:HG13	2.18	0.43
1:A:256:VAL:N	1:A:257:PRO:CD	2.81	0.43
1:A:113:TRP:O	1:A:117:GLU:HB2	2.19	0.43
1:A:225:ASN:HD22	1:A:225:ASN:N	2.17	0.43
2:C:1130:PRO:C	2:C:1132:SER:H	2.22	0.43
2:C:1123:PHE:HA	2:C:1124:PRO:HD3	1.93	0.43
1:A:38:THR:HG22	1:A:290:GLN:HG3	2.01	0.43
1:A:187:TYR:HD2	1:A:213:LEU:HG	1.81	0.43
1:B:1:MET:HG3	1:B:40:GLN:NE2	2.33	0.43
1:B:17:ALA:HA	1:B:66:PHE:CZ	2.54	0.43
1:A:112:LYS:CG	1:A:116:LEU:HD22	2.48	0.43
2:C:1120:ILE:HA	2:C:1135:GLU:O	2.18	0.42
1:A:209:LEU:O	1:A:210:LYS:HG3	2.19	0.42
1:B:70:SER:O	1:B:71:SER:CB	2.67	0.42
1:B:251:LYS:HA	1:B:253:PHE:HE1	1.83	0.42
1:B:99:LEU:HD12	1:B:99:LEU:HA	1.92	0.42
1:A:90:VAL:O	1:A:94:SER:HB3	2.20	0.42
1:B:253:PHE:CD1	1:B:253:PHE:N	2.85	0.42
2:C:1125:LEU:HG	2:C:1128:TYR:CZ	2.54	0.42
2:C:1207:LEU:O	2:C:1207:LEU:HD23	2.18	0.42
1:B:181:ASP:HA	1:B:208:ARG:HH22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:PHE:O	1:B:102:ILE:HD13	2.19	0.42
2:C:1133:SER:HB3	2:C:1151:THR:HG22	2.02	0.42
1:B:146:LYS:HG3	1:B:147:ASP:N	2.35	0.41
1:A:140:LEU:HD12	3:A:2043:HOH:O	2.19	0.41
1:B:37:GLU:HA	1:B:37:GLU:OE1	2.20	0.41
1:B:11:ILE:HD13	1:B:52:ALA:HB2	2.03	0.41
1:B:232:LYS:HE2	1:B:235:TYR:OH	2.20	0.41
1:B:142:ASN:OD1	1:B:144:ASN:HB2	2.21	0.41
2:C:1113:PRO:HD2	2:C:1136:TYR:OH	2.20	0.41
1:A:188:MET:HE1	1:A:212:PRO:O	2.21	0.40
1:A:50:GLN:O	1:A:54:GLU:HG2	2.20	0.40
1:B:160:GLU:OE2	2:C:1203:ARG:HD2	2.21	0.40
1:B:255:PHE:O	1:B:258:PRO:HD2	2.21	0.40
1:A:13:THR:HA	1:A:14:PRO:HD3	1.78	0.40
1:B:80:ALA:HA	1:B:81:PRO:HD3	1.92	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	292/294 (99%)	283 (97%)	8 (3%)	1 (0%)	41	50
1	B	292/294 (99%)	281 (96%)	11 (4%)	0	100	100
2	C	121/133 (91%)	109 (90%)	7 (6%)	5 (4%)	3	1
All	All	705/721 (98%)	673 (96%)	26 (4%)	6 (1%)	17	20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1130	PRO
2	C	1184	THR

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Mol	Chain	Res	Type
2	C	1185	ALA
2	C	1230	LYS
2	C	1187	GLN
1	A	142	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	236/243 (97%)	217 (92%)	19 (8%)	11	15
1	B	237/243 (98%)	218 (92%)	19 (8%)	12	15
2	C	97/116 (84%)	87 (90%)	10 (10%)	7	8
All	All	570/602 (95%)	522 (92%)	48 (8%)	11	13

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	47	GLU
1	A	55	LEU
1	A	62	GLN
1	A	99	LEU
1	A	105	GLN
1	A	107	LEU
1	A	116	LEU
1	A	124	VAL
1	A	144	ASN
1	A	150	LEU
1	A	157	SER
1	A	170	ASN
1	A	188	MET
1	A	190	LEU
1	A	208	ARG
1	A	225	ASN
1	A	248	LEU

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Mol	Chain	Res	Type
1	A	256	VAL
1	B	12	VAL
1	B	13	THR
1	B	47	GLU
1	B	53	LEU
1	B	55	LEU
1	B	78	LYS
1	B	91	LYS
1	B	99	LEU
1	B	107	LEU
1	B	140	LEU
1	B	143	ASN
1	B	150	LEU
1	B	186	ASN
1	B	190	LEU
1	B	222	LYS
1	B	225	ASN
1	B	234	LEU
1	B	248	LEU
1	B	256	VAL
2	C	1137	GLN
2	C	1143	GLN
2	C	1144	LEU
2	C	1168	VAL
2	C	1179	ILE
2	C	1186	LYS
2	C	1189	LEU
2	C	1207	LEU
2	C	1212	HIS
2	C	1231	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	168	GLN
1	A	170	ASN
1	A	189	ASN
1	A	225	ASN
1	A	233	GLN
1	A	266	GLN
1	B	40	GLN

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Mol	Chain	Res	Type
1	B	168	GLN
1	B	170	ASN
1	B	186	ASN
1	B	225	ASN
2	C	1140	ASN
2	C	1212	HIS

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](#)

There are no ligands in this entry.

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, 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	A	294/294 (100%)	-0.08	2 (0%) 87 91	29, 44, 67, 95	0
1	B	294/294 (100%)	0.15	14 (4%) 30 37	35, 58, 80, 102	0
2	C	123/133 (92%)	0.34	15 (12%) 4 6	36, 52, 85, 95	0
All	All	711/721 (98%)	0.09	31 (4%) 34 41	29, 51, 78, 102	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1185	ALA	6.1
2	C	1129	ALA	4.9
1	A	294	PRO	4.8
2	C	1158	SER	4.7
2	C	1130	PRO	4.2
2	C	1152	CYS	3.9
2	C	1151	THR	3.8
1	B	143	ASN	3.7
1	B	212	PRO	3.3
1	B	120	LYS	3.3
1	B	1	MET	3.1
1	B	253	PHE	2.9
2	C	1110	GLY	2.9
2	C	1156	GLN	2.9
2	C	1131	ALA	2.7
1	B	215	ASN	2.7
1	B	294	PRO	2.7
1	B	43	LYS	2.6
2	C	1154	ASN	2.6
1	B	209	LEU	2.5
1	B	167	GLU	2.4
2	C	1128	TYR	2.4
2	C	1155	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	1219	TRP	2.3
1	B	269	TYR	2.2
2	C	1209	SER	2.2
1	B	189	ASN	2.2
1	A	253	PHE	2.1
1	B	142	ASN	2.1
2	C	1109	CYS	2.1
1	B	190	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.