



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2017 – 09:03 PM EST

PDB ID : 5NBQ  
Title : The structure of the tripartite complex between OspE, the C-terminal domains of factor H and C3dg  
Authors : Kolodziejczyk, R.; Mikula, K.M.; Kotila, T.M.; Postis, V.L.G.; Sakari, J.T.; Meri, T.  
Deposited on : unknown  
Resolution : 3.18 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
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)	:	rb-20030345

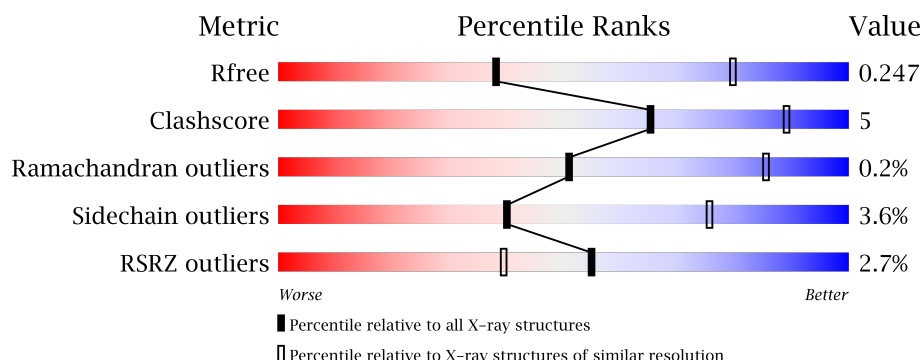
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.18 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	1123 (3.20-3.16)
Clashscore	112137	1255 (3.20-3.16)
Ramachandran outliers	110173	1233 (3.20-3.16)
Sidechain outliers	110143	1232 (3.20-3.16)
RSRZ outliers	101464	1128 (3.20-3.16)

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  $\geq 3$ , 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	A	294	
1	B	294	
1	C	294	
2	D	127	
2	E	127	

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Mol	Chain	Length	Quality of chain
2	F	127	<div><div></div><div>4%</div><div>81%</div><div>13%</div><div>6%</div></div>
3	G	129	<div><div></div><div>8%</div><div>89%</div><div>10%</div><div></div></div>
3	I	129	<div><div></div><div>8%</div><div>87%</div><div>10%</div><div></div></div>
4	H	134	<div><div></div><div></div><div>96%</div><div></div><div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11754 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	290	Total	C	N	O	S	0	0	0
			2246	1445	377	415	9			
1	B	293	Total	C	N	O	S	0	0	0
			2307	1484	387	427	9			
1	C	293	Total	C	N	O	S	0	0	0
			2300	1479	386	426	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1010	ALA	CYS	engineered mutation	UNP P01024
B	1010	ALA	CYS	engineered mutation	UNP P01024
C	1010	ALA	CYS	engineered mutation	UNP P01024

- Molecule 2 is a protein called Complement factor H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	127	Total	C	N	O	S	0	0	0
			1009	630	180	190	9			
2	E	122	Total	C	N	O	S	0	0	0
			947	597	162	179	9			
2	F	120	Total	C	N	O	S	0	0	0
			954	599	167	179	9			

- Molecule 3 is a protein called Outer surface protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	129	Total	C	N	O	S	0	0	0
			989	622	159	207	1			
3	I	125	Total	C	N	O	S	0	0	0
			975	619	158	197	1			

- Molecule 4 is a protein called Outer surface protein E,Outer surface protein E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	5	Total	C	N	O	0	0	0
			25	15	5	5			

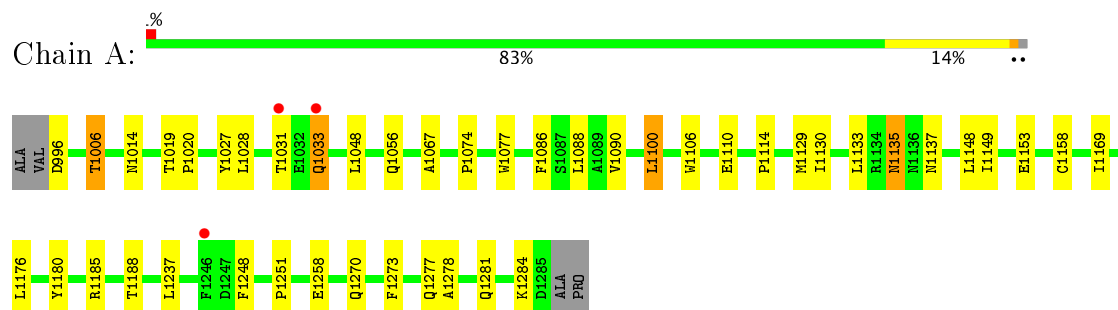
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	O	0	0
			1	1		
5	I	1	Total	O	0	0
			1	1		

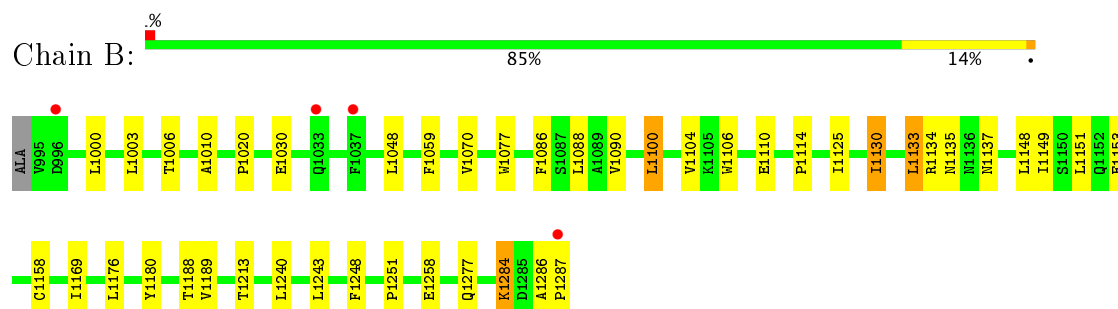
### 3 Residue-property plots [i](#)

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

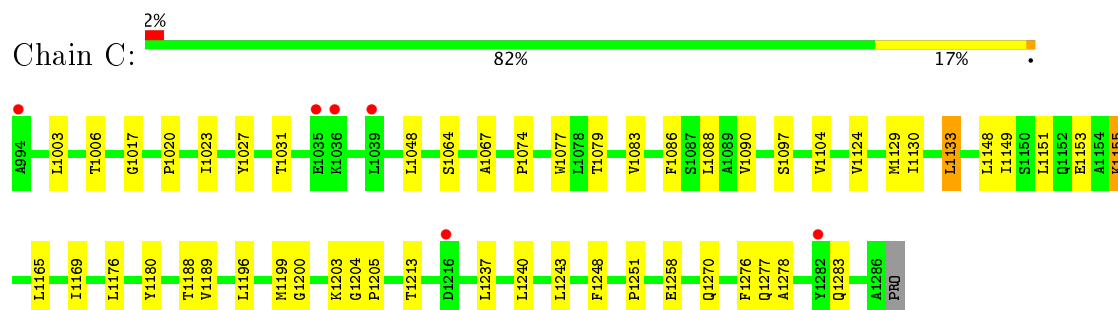
- Molecule 1: Complement C3



- Molecule 1: Complement C3

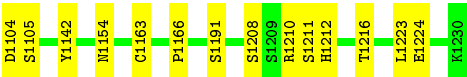


- Molecule 1: Complement C3

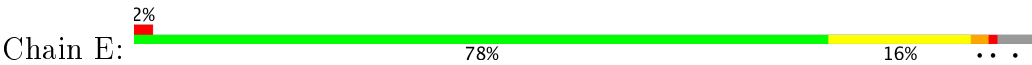


- Molecule 2: Complement factor H

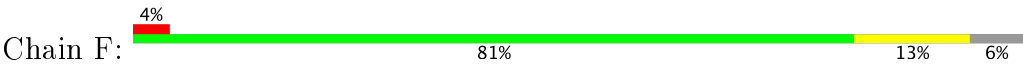




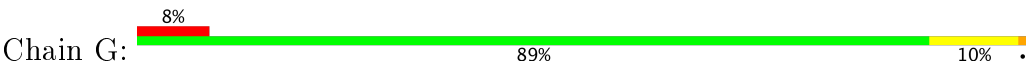
• Molecule 2: Complement factor H



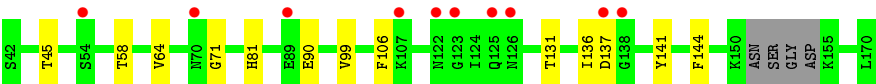
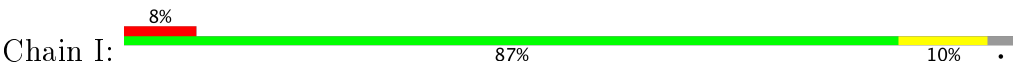
• Molecule 2: Complement factor H



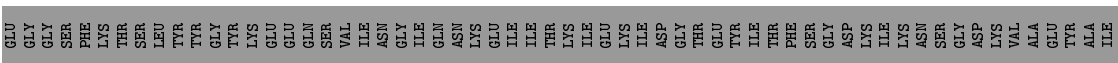
• Molecule 3: Outer surface protein E



• Molecule 3: Outer surface protein E



• Molecule 4: Outer surface protein E,Outer surface protein E



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.91Å 165.06Å 84.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 – 3.18 29.47 – 3.18	Depositor EDS
% Data completeness (in resolution range)	97.1 (29.60-3.18) 97.1 (29.47-3.18)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 3.18Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.233 , 0.261 0.252 , 0.247	Depositor DCC
$R_{free}$ test set	1418 reflections (5.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	84.3	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 60.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11754	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.47	0/2294	0.65	0/3114
1	B	0.48	0/2356	0.66	0/3191
1	C	0.46	0/2348	0.65	0/3182
2	D	0.43	0/1035	0.67	0/1404
2	E	0.48	0/972	0.70	0/1323
2	F	0.44	0/978	0.69	0/1327
3	G	0.45	0/1002	0.66	0/1349
3	I	0.45	0/987	0.71	0/1322
All	All	0.46	0/11972	0.67	0/16212

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 [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	2246	0	2218	22	0
1	B	2307	0	2314	26	0
1	C	2300	0	2301	27	0
2	D	1009	0	978	7	0
2	E	947	0	900	12	0
2	F	954	0	925	10	0
3	G	989	0	944	9	0
3	I	975	0	965	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	25	0	10	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
All	All	11754	0	11555	110	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 5.

All (110) 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)
3:G:131:THR:HG22	3:G:144:PHE:HB3	1.54	0.89
1:A:1031:THR:HG23	1:A:1033:GLN:HB2	1.65	0.79
2:F:1170:SER:OG	2:F:1173:ILE:HG13	1.88	0.74
1:A:1014:ASN:HD22	1:A:1056:GLN:HE21	1.37	0.73
1:C:1189:VAL:HG21	1:C:1213:THR:HG21	1.74	0.69
1:B:1189:VAL:HG21	1:B:1213:THR:HG21	1.74	0.69
2:E:1181:LEU:HD22	2:E:1184:THR:HG22	1.76	0.66
3:G:74:THR:HG23	3:G:85:PHE:HB3	1.77	0.66
1:C:1031:THR:HG22	1:C:1283:GLN:OE1	1.98	0.64
1:B:1137:ASN:HA	1:C:1203:LYS:HD2	1.78	0.64
1:B:1130:ILE:HG23	1:B:1133:LEU:HB2	1.79	0.63
3:G:148:LYS:HE2	3:G:154:ASP:HA	1.80	0.63
2:F:1214:LEU:HA	2:F:1226:PRO:HG3	1.82	0.61
2:D:1191:SER:HA	3:G:80:GLY:HA3	1.83	0.61
2:F:1196:SER:HB2	3:I:81:HIS:CE1	2.36	0.59
1:B:1114:PRO:HG3	2:E:1166:PRO:HG2	1.86	0.57
1:B:1088:LEU:HD11	1:B:1277:GLN:HG3	1.88	0.56
2:F:1183:TRP:CD1	3:I:64:VAL:HB	2.42	0.55
1:B:1149:ILE:O	1:B:1153:GLU:HG2	2.06	0.55
1:B:1135:ASN:OD1	1:B:1137:ASN:HB3	2.06	0.55
2:E:1181:LEU:HD11	2:E:1189:LEU:HD22	1.89	0.55
1:A:1149:ILE:O	1:A:1153:GLU:HG2	2.07	0.54
1:A:1100:LEU:HD23	1:A:1158:CYS:SG	2.48	0.54
2:D:1104:ASP:HB2	2:D:1154:ASN:HB2	1.90	0.54
1:A:1086:PHE:O	1:A:1090:VAL:HG13	2.08	0.53
1:A:1281:GLN:HA	1:A:1284:LYS:HE3	1.90	0.53
1:B:1086:PHE:O	1:B:1090:VAL:HG13	2.09	0.53
1:B:1030:GLU:HG2	1:B:1284:LYS:HG3	1.90	0.53
1:C:1149:ILE:O	1:C:1153:GLU:HG2	2.09	0.52
1:B:1077:TRP:HE1	1:B:1133:LEU:HD13	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1086:PHE:O	1:C:1090:VAL:HG13	2.09	0.52
3:I:71:GLY:H	3:I:90:GLU:HG2	1.75	0.52
1:A:1067:ALA:HB2	1:A:1074:PRO:HA	1.91	0.51
1:B:1137:ASN:HB2	1:C:1200:GLY:O	2.10	0.51
1:A:1114:PRO:HG3	2:D:1166:PRO:HG2	1.93	0.51
1:B:1000:LEU:HB3	1:B:1003:LEU:HD12	1.92	0.50
2:D:1210:ARG:HD2	2:D:1212:HIS:HE1	1.76	0.50
2:E:1150:ILE:HG13	2:E:1157:TRP:CE3	2.47	0.50
1:C:1088:LEU:HD11	1:C:1277:GLN:HG3	1.94	0.50
2:E:1179:ILE:HG22	2:E:1201:CYS:HA	1.94	0.49
1:A:1027:TYR:O	1:A:1031:THR:HG22	2.13	0.49
3:I:131:THR:HG22	3:I:144:PHE:HB3	1.94	0.49
2:E:1136:TYR:HE2	2:E:1150:ILE:HD13	1.76	0.49
1:C:1067:ALA:HB2	1:C:1074:PRO:HA	1.93	0.49
1:B:1130:ILE:HG23	1:B:1133:LEU:CB	2.43	0.48
3:G:100:MET:CE	3:G:131:THR:HG21	2.44	0.48
1:B:1010:ALA:HA	1:B:1059:PHE:CZ	2.49	0.48
1:C:1077:TRP:HE1	1:C:1133:LEU:HD13	1.79	0.48
1:C:1027:TYR:CZ	1:C:1031:THR:HG21	2.49	0.48
1:C:1196:LEU:HD23	1:C:1199:MET:CE	2.44	0.47
1:C:1104:VAL:HG13	1:C:1151:LEU:HD22	1.95	0.47
2:D:1142:TYR:HB3	2:D:1163:CYS:HB3	1.95	0.47
1:A:1088:LEU:HD11	1:A:1277:GLN:HG3	1.95	0.47
1:A:1019:THR:HB	1:A:1020:PRO:HD3	1.95	0.47
1:A:1006:THR:HA	1:A:1048:LEU:HD22	1.96	0.47
2:F:1182:ARG:HG3	2:F:1200:VAL:HB	1.97	0.47
1:C:1017:GLY:O	1:C:1020:PRO:HD2	2.15	0.47
3:I:99:VAL:HG11	3:I:106:PHE:HD1	1.81	0.47
1:B:1006:THR:HA	1:B:1048:LEU:HD22	1.97	0.46
1:A:1077:TRP:CZ2	1:A:1130:ILE:HA	2.51	0.46
1:B:1125:ILE:CD1	2:F:1176:ASN:HB3	2.46	0.46
1:A:1135:ASN:HD21	1:A:1137:ASN:HB3	1.80	0.45
3:G:117:GLU:HB3	3:G:147:ASP:HB3	1.98	0.45
1:A:1106:TRP:CD1	1:A:1110:GLU:HG3	2.51	0.45
1:B:1148:LEU:HD11	1:B:1169:ILE:HG23	1.98	0.45
1:B:1100:LEU:HD23	1:B:1158:CYS:SG	2.56	0.45
1:C:1155:LYS:HA	1:C:1165:LEU:HD21	1.97	0.45
2:E:1216:THR:HG21	2:E:1224:GLU:O	2.17	0.45
1:B:1176:LEU:O	1:B:1180:TYR:HB2	2.17	0.44
2:F:1178:ASN:HA	2:F:1202:LYS:HD3	1.99	0.44
1:C:1129:MET:O	1:C:1270:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:117:GLU:OE2	3:G:157:ALA:HB3	2.18	0.44
1:A:1148:LEU:HD11	1:A:1169:ILE:HG23	2.00	0.44
1:C:1124:VAL:HG21	1:C:1130:ILE:HG23	2.00	0.44
1:C:1006:THR:HA	1:C:1048:LEU:HD22	1.99	0.43
1:C:1176:LEU:O	1:C:1180:TYR:HB2	2.18	0.43
1:B:1003:LEU:O	1:B:1020:PRO:HB2	2.19	0.43
1:B:1286:ALA:HB1	1:B:1287:PRO:HD2	2.00	0.43
1:A:1129:MET:O	1:A:1270:GLN:HG2	2.18	0.43
1:B:1248:PHE:O	1:B:1251:PRO:HD2	2.18	0.43
1:A:1176:LEU:O	1:A:1180:TYR:HB2	2.18	0.43
1:B:1104:VAL:HG13	1:B:1151:LEU:HD22	2.00	0.43
3:I:136:ILE:HB	3:I:141:TYR:CE1	2.54	0.43
1:C:1023:ILE:HG13	1:C:1276:PHE:HB2	2.01	0.43
2:E:1181:LEU:CD2	2:E:1184:THR:HG22	2.46	0.43
1:C:1003:LEU:O	1:C:1020:PRO:HB2	2.18	0.42
1:B:1240:LEU:HA	1:B:1243:LEU:HD12	2.01	0.42
1:B:1106:TRP:CD1	1:B:1110:GLU:HG3	2.55	0.42
1:C:1240:LEU:HA	1:C:1243:LEU:HD12	2.02	0.42
2:E:1142:TYR:HB3	2:E:1163:CYS:HB3	2.00	0.42
3:G:113:GLY:HA3	3:G:117:GLU:OE1	2.20	0.42
2:E:1174:MET:O	2:E:1179:ILE:HG13	2.20	0.42
1:A:1088:LEU:HD12	1:A:1273:PHE:CZ	2.55	0.42
1:C:1148:LEU:HD11	1:C:1169:ILE:HG23	2.01	0.42
1:A:1028:LEU:HA	1:A:1031:THR:HG22	2.01	0.42
2:F:1183:TRP:HD1	3:I:64:VAL:HB	1.84	0.41
1:C:1248:PHE:O	1:C:1251:PRO:HD2	2.20	0.41
2:D:1104:ASP:CB	2:D:1154:ASN:HB2	2.50	0.41
2:F:1196:SER:HB2	3:I:81:HIS:HE1	1.81	0.41
1:C:1079:THR:O	1:C:1083:VAL:HG23	2.20	0.41
1:C:1196:LEU:HA	1:C:1199:MET:HE3	2.03	0.41
1:A:1237:LEU:HD23	1:A:1278:ALA:HB1	2.03	0.41
1:B:1125:ILE:HD13	2:F:1176:ASN:HB3	2.02	0.40
2:D:1216:THR:HG21	2:D:1224:GLU:N	2.35	0.40
3:G:149:ILE:HD11	3:G:157:ALA:HB2	2.03	0.40
1:A:1248:PHE:O	1:A:1251:PRO:HD2	2.21	0.40
1:C:1204:GLY:HA3	1:C:1205:PRO:HD3	1.98	0.40
1:C:1237:LEU:HD23	1:C:1278:ALA:HB1	2.03	0.40
2:E:1153:ARG:HG3	2:E:1153:ARG:HH11	1.87	0.40
2:E:1171:ARG:HB2	2:E:1187:GLN:HB3	2.04	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	A	288/294 (98%)	283 (98%)	5 (2%)	0	100	100
1	B	291/294 (99%)	285 (98%)	6 (2%)	0	100	100
1	C	291/294 (99%)	285 (98%)	5 (2%)	1 (0%)	44	81
2	D	125/127 (98%)	121 (97%)	4 (3%)	0	100	100
2	E	118/127 (93%)	112 (95%)	5 (4%)	1 (1%)	22	64
2	F	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
3	G	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	22	64
3	I	121/129 (94%)	117 (97%)	4 (3%)	0	100	100
All	All	1477/1521 (97%)	1430 (97%)	44 (3%)	3 (0%)	51	85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	154	ASP
1	C	1155	LYS
2	E	1184	THR

### 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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	230/242 (95%)	221 (96%)	9 (4%)	37	73
1	B	242/242 (100%)	234 (97%)	8 (3%)	43	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	240/242 (99%)	235 (98%)	5 (2%)	59	85
2	D	114/114 (100%)	110 (96%)	4 (4%)	41	76
2	E	105/114 (92%)	96 (91%)	9 (9%)	12	42
2	F	108/114 (95%)	102 (94%)	6 (6%)	25	62
3	G	106/112 (95%)	105 (99%)	1 (1%)	82	94
3	I	106/112 (95%)	103 (97%)	3 (3%)	49	81
All	All	1251/1292 (97%)	1206 (96%)	45 (4%)	40	75

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	996	ASP
1	A	1006	THR
1	A	1033	GLN
1	A	1100	LEU
1	A	1133	LEU
1	A	1135	ASN
1	A	1185	ARG
1	A	1188	THR
1	A	1258	GLU
1	B	1070	VAL
1	B	1100	LEU
1	B	1130	ILE
1	B	1133	LEU
1	B	1134	ARG
1	B	1188	THR
1	B	1258	GLU
1	B	1284	LYS
1	C	1064	SER
1	C	1097	SER
1	C	1133	LEU
1	C	1188	THR
1	C	1258	GLU
2	D	1105	SER
2	D	1208	SER
2	D	1211	SER
2	D	1223	LEU
2	E	1105	SER
2	E	1106	THR
2	E	1151	THR

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Mol	Chain	Res	Type
2	E	1152	CYS
2	E	1159	GLU
2	E	1179	ILE
2	E	1184	THR
2	E	1216	THR
2	E	1228	CYS
2	F	1122	SER
2	F	1127	VAL
2	F	1172	GLU
2	F	1207	LEU
2	F	1216	THR
2	F	1228	CYS
3	G	118	GLN
3	I	45	THR
3	I	58	THR
3	I	137	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1055	GLN
1	A	1056	GLN
1	A	1135	ASN
1	B	1014	ASN
1	B	1055	GLN
1	C	1055	GLN
2	D	1212	HIS
2	F	1137	GLN
2	F	1178	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 [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	290/294 (98%)	-0.02	3 (1%) 82 70	53, 81, 120, 244	0
1	B	293/294 (99%)	-0.05	4 (1%) 75 62	49, 75, 104, 159	0
1	C	293/294 (99%)	-0.10	6 (2%) 65 50	58, 82, 110, 155	0
2	D	127/127 (100%)	-0.11	0 100 100	55, 82, 98, 114	0
2	E	122/127 (96%)	0.04	3 (2%) 58 43	50, 75, 128, 145	0
2	F	120/127 (94%)	0.21	5 (4%) 37 23	77, 97, 115, 130	0
3	G	129/129 (100%)	0.47	10 (7%) 14 7	84, 131, 155, 165	0
3	I	125/129 (96%)	0.49	10 (8%) 13 7	79, 111, 143, 161	0
4	H	0/134	-	-	-	-
All	All	1499/1655 (90%)	0.06	41 (2%) 55 39	49, 85, 137, 244	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	70	ASN	4.5
3	G	165	GLU	4.3
3	G	138	GLY	4.1
3	G	130	ILE	3.9
3	I	126	ASN	3.8
2	F	1107	GLY	3.6
3	I	89	GLU	3.5
3	I	125	GLN	3.4
1	B	996	ASP	3.2
3	G	154	ASP	3.0
2	E	1105	SER	2.9
2	F	1204	GLY	2.8
2	E	1207	LEU	2.8
1	A	1033	GLN	2.7
2	F	1205	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
3	I	54	SER	2.6
1	C	1036	LYS	2.6
1	B	1287	PRO	2.6
3	I	122	ASN	2.6
1	C	1282	TYR	2.5
1	C	1216	ASP	2.4
1	C	994	ALA	2.4
1	B	1033	GLN	2.4
2	F	1106	THR	2.4
3	G	70	ASN	2.4
3	I	123	GLY	2.4
1	A	1246	PHE	2.3
3	G	140	GLU	2.2
1	C	1039	LEU	2.2
1	B	1037	PHE	2.2
1	A	1031	THR	2.2
1	C	1035	GLU	2.1
2	F	1178	ASN	2.1
2	E	1193	THR	2.1
3	I	107	LYS	2.1
3	G	153	GLY	2.1
3	G	169	ASN	2.1
3	I	137	ASP	2.1
3	G	168	LYS	2.0
3	G	93	VAL	2.0
3	I	138	GLY	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.