



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:49 AM GMT

PDB ID : 3E41
Title : Q138F HincII bound to GTCGAC and 5 mM Ca²⁺
Authors : Horton, N.C.; Babic, A.C.; Little, E.J.; Manohar, V.M.
Deposited on : 2008-08-08
Resolution : 2.73 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

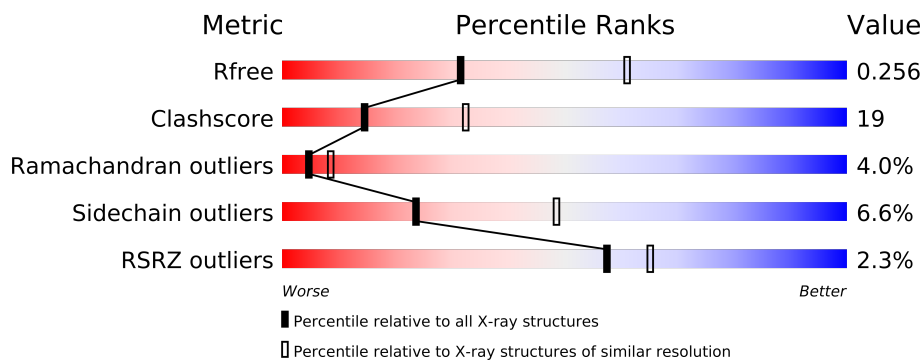
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.73 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}	66092	2164 (2.78-2.70)
Clashscore	79885	2639 (2.78-2.70)
Ramachandran outliers	78287	2594 (2.78-2.70)
Sidechain outliers	78261	2595 (2.78-2.70)
RSRZ outliers	66119	2166 (2.78-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	257	
1	B	257	
2	E	14	
2	F	14	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	NA	B	260	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4533 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Type-2 restriction enzyme HindII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1951	1272	311	362	6			
1	B	243	Total	C	N	O	S	0	0	0
			1883	1233	298	346	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ASN	LYS	CONFLICT	UNP P44413
A	138	PHE	GLN	ENGINEERED	UNP P44413
B	67	ASN	LYS	CONFLICT	UNP P44413
B	138	PHE	GLN	ENGINEERED	UNP P44413

- Molecule 2 is a DNA chain called 5'-D(*DGP*DCP*DCP*DGP*DGP*DTP*DCP*DGP*DAP*DCP*DCP*DGP*DGP*DC)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	P	0	0	0
			284	134	55	82	13			
2	F	14	Total	C	N	O	P	0	0	0
			284	134	55	82	13			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

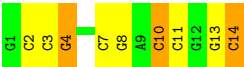
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Na 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	74	Total 74	O 74	0	0
5	B	26	Total 26	O 26	0	0
5	E	17	Total 17	O 17	0	0
5	F	11	Total 11	O 11	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.06Å 90.14Å 66.33Å 90.00° 104.55° 90.00°	Depositor
Resolution (Å)	44.41 – 2.73 44.41 – 2.73	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.41-2.73) 100.0 (44.41-2.73)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.184 , 0.266 0.176 , 0.256	Depositor DCC
R_{free} test set	754 reflections (4.95%)	DCC
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 15259 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4533	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA

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	0.46	0/1997	0.62	0/2713
1	B	0.41	0/1928	0.58	1/2625 (0.0%)
2	E	0.97	1/318 (0.3%)	1.88	11/489 (2.2%)
2	F	1.04	0/318	1.78	7/489 (1.4%)
All	All	0.56	1/4561 (0.0%)	0.91	19/6316 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	DC	C3'-O3'	-5.83	1.36	1.44

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	9	DA	O4'-C1'-C2'	-10.00	97.90	105.90
2	F	7	DC	O4'-C4'-C3'	-9.55	100.27	106.00
2	E	13	DG	P-O3'-C3'	-9.19	108.67	119.70
2	E	9	DA	C1'-O4'-C4'	-8.51	101.59	110.10
2	F	10	DC	O4'-C1'-N1	7.46	113.22	108.00
2	E	6	DT	N3-C4-O4	7.32	124.29	119.90
2	E	10	DC	O4'-C1'-N1	6.66	112.66	108.00
1	B	36	PRO	N-CA-CB	6.55	111.16	103.30
2	E	6	DT	C5-C4-O4	-6.54	120.32	124.90
2	E	8	DG	O4'-C1'-N9	6.46	112.52	108.00
2	F	8	DG	O4'-C1'-N9	6.02	112.22	108.00
2	F	14	DC	O4'-C1'-N1	5.56	111.89	108.00
2	F	10	DC	C1'-O4'-C4'	-5.54	104.56	110.10
2	E	12	DG	O4'-C1'-N9	5.36	111.75	108.00
2	F	4	DG	C5-C6-O6	-5.30	125.42	128.60
2	E	13	DG	O4'-C1'-N9	5.28	111.69	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	4	DG	N1-C6-O6	5.24	123.04	119.90
2	E	3	DC	C1'-O4'-C4'	-5.21	104.89	110.10
2	E	10	DC	O4'-C1'-C2'	5.08	109.96	105.90

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1951	0	1840	65	0
1	B	1883	0	1732	83	0
2	E	284	0	157	15	0
2	F	284	0	157	11	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	1	0	0	0	0
5	A	74	0	0	3	0
5	B	26	0	0	1	0
5	E	17	0	0	0	0
5	F	11	0	0	0	0
All	All	4533	0	3886	160	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (160) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:4:DG:H1	2:F:11:DC:H42	1.06	0.99
1:B:37:PHE:HA	1:B:40:LEU:HD23	1.43	0.97
2:E:11:DC:N4	2:F:4:DG:H1	1.63	0.97
2:E:11:DC:H42	2:F:4:DG:H1	0.91	0.90
2:E:7:DC:H2''	2:E:8:DG:H5'	1.55	0.88
1:B:70:ILE:HG12	1:B:79:LEU:HD21	1.57	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:4:DG:H1	2:F:11:DC:N4	1.73	0.85
1:B:70:ILE:HD12	1:B:70:ILE:O	1.77	0.84
1:B:3:PHE:CZ	1:B:122:PHE:HD2	1.96	0.84
2:E:11:DC:N3	2:F:4:DG:N2	2.25	0.84
1:B:52:LEU:O	1:B:117:LEU:HA	1.77	0.83
2:F:2:DC:H2''	2:F:3:DC:H5''	1.59	0.82
1:B:15:LEU:HD13	1:B:185:THR:HG21	1.62	0.79
2:E:9:DA:H2''	2:E:10:DC:H5''	1.63	0.79
1:A:140:PRO:HG3	5:A:281:HOH:O	1.82	0.79
1:B:70:ILE:CD1	1:B:79:LEU:HD11	2.16	0.76
1:A:107:GLU:HG2	1:A:108:LYS:H	1.52	0.74
1:A:235:VAL:HG13	1:B:250:VAL:HG13	1.69	0.73
1:A:250:VAL:HG13	1:B:235:VAL:HG13	1.69	0.73
2:E:5:DG:H2''	2:E:6:DT:H5'	1.70	0.73
2:F:13:DG:H2''	2:F:14:DC:H5'	1.71	0.73
1:B:169:LEU:HD12	1:B:186:SER:O	1.88	0.72
2:E:4:DG:N2	2:F:11:DC:N3	2.36	0.71
1:B:70:ILE:HD11	1:B:79:LEU:HD11	1.76	0.66
2:E:7:DC:C2'	2:E:8:DG:H5'	2.26	0.66
1:A:107:GLU:HG2	1:A:108:LYS:N	2.11	0.66
1:A:22:ARG:HG2	1:A:23:PRO:HD2	1.77	0.65
1:B:49:LEU:HB3	1:B:52:LEU:HD11	1.76	0.64
1:A:247:ASP:O	1:A:252:PRO:HD3	1.97	0.64
1:A:12:ASN:O	1:A:16:ILE:HG13	1.97	0.64
1:B:217:GLN:HA	1:B:217:GLN:HE21	1.63	0.63
1:B:170:GLU:HB2	1:B:212:VAL:HB	1.80	0.63
1:A:15:LEU:HA	1:A:18:GLN:HG3	1.80	0.62
1:A:193:SER:O	1:A:195:PRO:HD3	1.99	0.62
1:B:3:PHE:CZ	1:B:122:PHE:CD2	2.85	0.62
1:A:76:ARG:O	1:A:79:LEU:HB2	2.01	0.61
1:A:22:ARG:HB2	1:A:180:LEU:HD13	1.83	0.61
1:A:222:THR:OG1	1:A:225:GLU:HG3	2.01	0.60
1:A:52:LEU:O	1:A:117:LEU:HA	2.01	0.60
1:B:14:ILE:HD12	1:B:15:LEU:N	2.17	0.59
1:A:248:LYS:O	1:A:252:PRO:HG2	2.02	0.59
1:A:210:PHE:HB3	5:A:277:HOH:O	2.03	0.58
1:A:171:VAL:HG23	1:A:171:VAL:O	2.02	0.58
1:B:152:CYS:O	1:B:156:ILE:HG12	2.03	0.58
1:A:16:ILE:HD13	1:A:184:SER:HA	1.87	0.57
1:B:155:MET:HE1	1:B:223:ARG:HG3	1.87	0.57
1:B:63:LEU:HD11	1:B:79:LEU:HB3	1.87	0.56
1:B:217:GLN:HA	1:B:217:GLN:NE2	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:142:ILE:O	1:B:143:ILE:HB	2.05	0.56
1:A:155:MET:HE1	5:A:307:HOH:O	2.06	0.56
1:B:189:GLU:OE1	1:B:192:LYS:NZ	2.38	0.56
1:B:251:LYS:N	1:B:252:PRO:CD	2.70	0.55
1:B:49:LEU:HB3	1:B:52:LEU:CD1	2.36	0.55
1:A:205:ALA:HA	1:B:203:ALA:O	2.06	0.55
1:B:20:VAL:HG12	1:B:40:LEU:HD21	1.88	0.55
1:B:211:HIS:HA	5:B:270:HOH:O	2.07	0.55
1:B:11:ILE:O	1:B:14:ILE:HG13	2.06	0.54
1:A:71:ILE:HG22	1:A:72:GLY:N	2.23	0.53
1:A:199:TYR:OH	2:E:4:DG:H8	1.92	0.53
1:B:49:LEU:O	1:B:51:ASP:N	2.41	0.53
1:A:108:LYS:HD3	1:A:110:ASN:HD21	1.74	0.52
1:B:195:PRO:O	1:B:197:GLU:N	2.42	0.52
1:B:50:SER:O	1:B:51:ASP:HB2	2.09	0.52
1:A:175:LEU:HD12	1:A:176:ASN:N	2.24	0.52
1:A:52:LEU:N	1:A:52:LEU:HD12	2.25	0.51
1:A:5:LYS:N	1:A:6:PRO:HD2	2.25	0.51
2:F:2:DC:C2'	2:F:3:DC:H5''	2.38	0.51
1:A:158:ASN:HB2	1:A:160:GLU:HG3	1.92	0.50
1:B:195:PRO:C	1:B:197:GLU:H	2.14	0.50
1:A:73:HIS:HA	1:A:96:THR:HG22	1.93	0.50
1:A:138:PHE:HB3	2:F:10:DC:C6	2.47	0.50
1:B:132:ASN:HB3	1:B:135:LYS:CG	2.42	0.50
1:A:63:LEU:O	1:A:67:ASN:ND2	2.45	0.49
1:A:159:LYS:HA	1:A:161:PHE:CE2	2.47	0.49
1:A:80:PHE:CD1	1:A:86:LEU:HD23	2.48	0.49
1:B:161:PHE:HB3	1:B:223:ARG:HB3	1.95	0.49
1:B:4:ILE:HD11	1:B:45:LEU:HD21	1.94	0.49
1:A:192:LYS:O	1:A:217:GLN:HA	2.13	0.49
1:A:189:GLU:H	1:A:217:GLN:HE22	1.59	0.49
1:B:148:LEU:O	1:B:151:THR:HB	2.14	0.48
1:A:156:ILE:HD13	1:A:161:PHE:HE1	1.79	0.48
1:B:73:HIS:CD2	1:B:97:GLU:OE1	2.67	0.48
1:B:126:LEU:HD12	1:B:127:ASP:H	1.77	0.48
1:B:83:PRO:HB2	1:B:158:ASN:ND2	2.28	0.48
1:B:254:LYS:O	1:B:257:ILE:HG12	2.14	0.48
1:B:175:LEU:O	1:B:177:GLY:N	2.46	0.48
1:B:117:LEU:N	1:B:117:LEU:HD22	2.29	0.48
1:A:234:PHE:CE1	1:B:249:PHE:HB3	2.49	0.48
1:B:61:ASN:O	1:B:65:MET:HG3	2.14	0.47
1:A:188:ALA:HB3	1:A:212:VAL:HG13	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:255:LYS:HG3	1:B:256:TYR:CD2	2.49	0.47
1:B:40:LEU:HD22	1:B:40:LEU:H	1.80	0.47
2:E:9:DA:C2'	2:E:10:DC:H5''	2.41	0.47
1:B:37:PHE:O	1:B:40:LEU:HB2	2.15	0.47
1:A:203:ALA:O	1:B:205:ALA:HA	2.15	0.47
1:B:140:PRO:HD2	1:B:210:PHE:O	2.15	0.47
1:A:65:MET:O	1:A:68:PRO:HD3	2.15	0.46
1:A:22:ARG:HG3	1:A:180:LEU:HD11	1.97	0.46
1:A:108:LYS:HD3	1:A:110:ASN:ND2	2.31	0.46
1:A:54:PHE:HE2	1:A:118:VAL:HG13	1.81	0.46
1:B:70:ILE:HD13	1:B:76:ARG:HG2	1.97	0.46
1:B:161:PHE:CE1	1:B:224:GLU:HA	2.50	0.45
1:A:55:LYS:HE3	1:A:55:LYS:HB3	1.57	0.45
1:B:18:GLN:HA	1:B:18:GLN:OE1	2.15	0.45
2:E:5:DG:H2''	2:E:6:DT:C5'	2.45	0.45
1:B:41:VAL:HG21	1:B:128:VAL:HG11	1.98	0.45
1:B:174:GLU:O	1:B:181:VAL:HG12	2.17	0.45
1:B:45:LEU:HD23	1:B:49:LEU:HD12	1.99	0.44
1:B:210:PHE:CZ	1:B:215:LEU:HD22	2.52	0.44
2:E:9:DA:H2''	2:E:10:DC:C5'	2.40	0.44
1:B:72:GLY:HA2	1:B:97:GLU:CD	2.38	0.44
1:B:73:HIS:O	1:B:74:GLU:C	2.54	0.44
1:A:94:ALA:O	1:A:97:GLU:HB3	2.16	0.44
1:A:114:ASP:C	1:A:115:ILE:HG12	2.38	0.44
1:B:193:SER:HA	1:B:216:ASP:O	2.18	0.44
1:A:80:PHE:O	1:A:81:ASN:HB2	2.18	0.43
1:A:148:LEU:O	1:A:151:THR:HB	2.17	0.43
1:A:5:LYS:N	1:A:6:PRO:CD	2.81	0.43
1:B:135:LYS:CG	1:B:136:SER:H	2.31	0.43
1:B:45:LEU:O	1:B:49:LEU:HB2	2.18	0.43
1:B:4:ILE:CD1	1:B:45:LEU:HD21	2.48	0.43
1:B:193:SER:CB	1:B:215:LEU:HD11	2.48	0.43
1:B:199:TYR:O	1:B:208:ILE:HA	2.19	0.43
1:B:16:ILE:H	1:B:16:ILE:HG13	1.62	0.43
1:B:3:PHE:HZ	1:B:122:PHE:HD2	1.58	0.43
1:B:123:TYR:O	1:B:164:PHE:HA	2.18	0.43
1:B:73:HIS:ND1	1:B:74:GLU:N	2.66	0.42
1:B:83:PRO:HG2	1:B:158:ASN:CG	2.40	0.42
1:A:169:LEU:HD12	1:A:186:SER:O	2.18	0.42
1:B:40:LEU:CD2	1:B:40:LEU:H	2.32	0.42
1:B:180:LEU:O	1:B:181:VAL:HB	2.19	0.42
1:B:143:ILE:O	1:B:143:ILE:HG23	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:129:LYS:HD2	1:A:142:ILE:HD13	2.01	0.42
1:B:195:PRO:C	1:B:197:GLU:N	2.73	0.42
1:A:188:ALA:CB	1:A:212:VAL:HG13	2.49	0.42
1:B:49:LEU:O	1:B:50:SER:C	2.58	0.42
1:A:156:ILE:HD11	1:A:227:ALA:HB3	2.02	0.42
1:A:108:LYS:O	1:A:109:GLN:C	2.58	0.42
1:A:166:ILE:HD13	1:A:166:ILE:N	2.35	0.42
1:B:35:GLU:O	1:B:36:PRO:CB	2.68	0.42
1:A:41:VAL:HG12	1:A:45:LEU:HD12	2.02	0.41
1:A:71:ILE:CG2	1:A:72:GLY:N	2.83	0.41
1:B:139:ALA:HA	1:B:140:PRO:HD3	1.83	0.41
1:B:53:THR:HA	1:B:117:LEU:HD13	2.01	0.41
1:A:99:TRP:CD2	1:A:100:SER:N	2.88	0.41
1:B:39:LYS:O	1:B:40:LEU:C	2.58	0.41
1:B:196:SER:HA	1:B:233:HIS:CG	2.56	0.41
1:B:50:SER:O	1:B:51:ASP:CB	2.69	0.41
1:A:85:LEU:HA	1:A:85:LEU:HD12	1.86	0.41
1:B:37:PHE:CA	1:B:40:LEU:HD23	2.32	0.41
2:E:11:DC:C2	2:F:4:DG:N2	2.77	0.41
1:B:223:ARG:HH11	1:B:223:ARG:HG2	1.86	0.40
1:A:54:PHE:CE2	1:A:118:VAL:HG13	2.56	0.40
1:A:172:ASP:O	1:A:182:CYS:HA	2.20	0.40
1:A:70:ILE:HG22	1:A:70:ILE:O	2.20	0.40
1:B:116:LEU:HA	1:B:116:LEU:HD12	1.97	0.40
1:A:256:TYR:C	1:A:257:ILE:HG13	2.41	0.40
1:A:81:ASN:O	1:A:82:SER:HB2	2.22	0.40
1:A:125:LEU:HD22	1:A:166:ILE:HD12	2.04	0.40
1:A:35:GLU:N	1:A:36:PRO:CD	2.84	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	240/257 (93%)	214 (89%)	21 (9%)	5 (2%)	11 25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	239/257 (93%)	204 (85%)	21 (9%)	14 (6%)	2	3
All	All	479/514 (93%)	418 (87%)	42 (9%)	19 (4%)	5	8

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	B	36	PRO
1	B	51	ASP
1	B	143	ILE
1	B	156	ILE
1	B	181	VAL
1	A	136	SER
1	B	11	ILE
1	B	35	GLU
1	B	50	SER
1	B	157	ASP
1	A	135	LYS
1	B	196	SER
1	B	12	ASN
1	B	180	LEU
1	A	50	SER
1	B	176	ASN
1	A	82	SER
1	B	195	PRO

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	199/229 (87%)	182 (92%)	17 (8%)	15	33
1	B	182/229 (80%)	174 (96%)	8 (4%)	39	70
All	All	381/458 (83%)	356 (93%)	25 (7%)	24	48

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	16	ILE
1	A	20	VAL
1	A	22	ARG
1	A	54	PHE
1	A	67	ASN
1	A	85	LEU
1	A	100	SER
1	A	106	GLU
1	A	110	ASN
1	A	115	ILE
1	A	118	VAL
1	A	138	PHE
1	A	181	VAL
1	A	198	LEU
1	A	214	ASP
1	A	244	SER
1	B	41	VAL
1	B	52	LEU
1	B	85	LEU
1	B	138	PHE
1	B	144	SER
1	B	213	ARG
1	B	231	LEU
1	B	240	GLN

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	12	ASN
1	A	67	ASN
1	A	110	ASN
1	A	217	GLN
1	A	237	GLN
1	B	67	ASN
1	B	150	GLN
1	B	158	ASN
1	B	220	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	246/257 (95%)	-0.18	3 (1%) 75 82	30, 47, 68, 90	0
1	B	243/257 (94%)	0.04	9 (3%) 39 46	28, 57, 85, 94	0
2	E	14/14 (100%)	-0.46	0 100 100	33, 44, 52, 55	0
2	F	14/14 (100%)	-0.55	0 100 100	27, 41, 48, 54	0
All	All	517/542 (95%)	-0.10	12 (2%) 57 65	27, 51, 81, 94	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	ASN	3.4
1	B	183	VAL	3.2
1	B	257	ILE	3.1
1	B	181	VAL	3.1
1	B	182	CYS	2.9
1	B	15	LEU	2.9
1	A	20	VAL	2.5
1	B	175	LEU	2.3
1	B	19	LYS	2.2
1	B	220	ASN	2.2
1	B	180	LEU	2.2
1	A	180	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NA	B	260	1/1	0.20	2.54	58,58,58,58	0
3	CA	B	259	1/1	0.10	-1.65	67,67,67,67	0
3	CA	A	259	1/1	0.10	-1.83	42,42,42,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.