Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:02 PM GMT

PDB ID	:	3SOH
Title	:	Architecture of the Flagellar Rotor
Authors	:	Koushik, P.; Gonzalez-Bonet, G.; Bilwes, A.M.; Crane, B.R.; Blair, D.
Deposited on	:	2011-06-30
Resolution	:	3.50 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

http://wwpdb.org/validation/2016/XrayValidationReportHelp

with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	trunk26865

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 3.50 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	Percentile Ranks	Value
Rfree		0.298
Clashscore		24
Ramachandran outliers		3.8%
Sidechain outliers		11.1%
RSRZ outliers		4.1%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
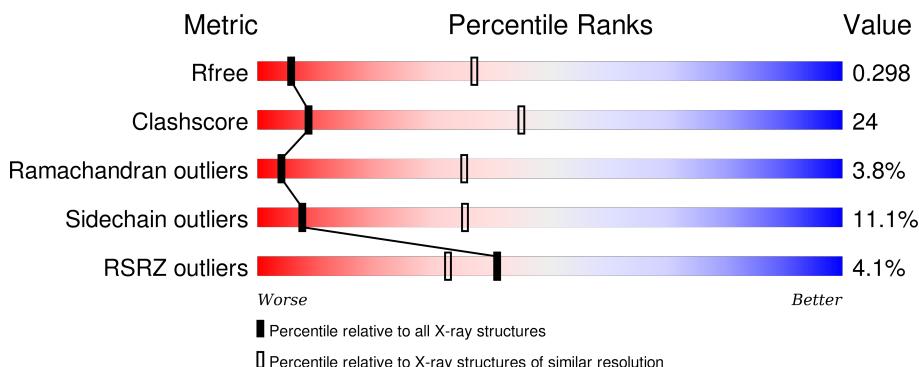
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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. 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	188	4% / 50% 44% 6%
1	C	188	3% / 55% 37% 7% ·
2	B	80	5% / 48% 48% · ·
2	D	80	6% / 46% 46% 8%
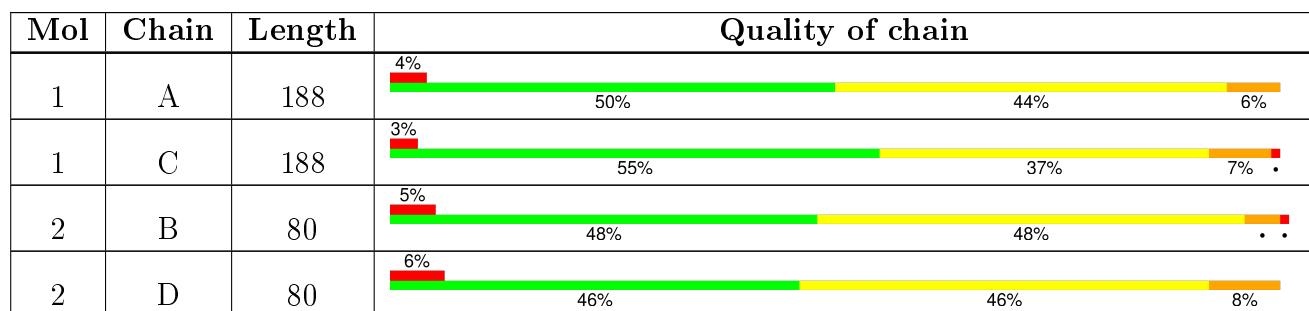
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4285 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 Flagellar motor switch protein FliM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total 1535	C 1003	N 240	O 283	S 9	0	0	0
1	C	188	Total 1535	C 1003	N 240	O 283	S 9	0	0	0

- Molecule 2 is a protein called Flagellar motor switch protein FliG.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	80	Total 607	C 387	N 101	O 119	0	0	0
2	D	80	Total 607	C 387	N 101	O 119	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	113	GLY	-	CLONING ARTIFACT	UNP Q9WY63
B	114	SER	-	CLONING ARTIFACT	UNP Q9WY63
B	115	HIS	-	CLONING ARTIFACT	UNP Q9WY63
B	116	MET	-	CLONING ARTIFACT	UNP Q9WY63
B	?	-	VAL	DELETION	UNP Q9WY63
D	113	GLY	-	CLONING ARTIFACT	UNP Q9WY63
D	114	SER	-	CLONING ARTIFACT	UNP Q9WY63
D	115	HIS	-	CLONING ARTIFACT	UNP Q9WY63
D	116	MET	-	CLONING ARTIFACT	UNP Q9WY63
D	?	-	VAL	DELETION	UNP Q9WY63

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Flagellar motor switch protein FliM
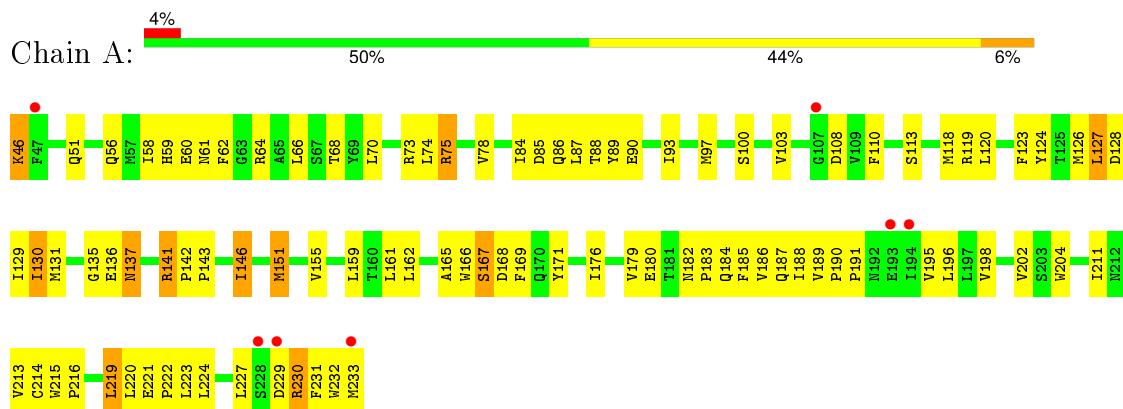
Chain A:

- Molecule 1: Flagellar motor switch protein FliM

Chain C:

- Molecule 2: Flagellar motor switch protein FliG

Chain B:

• **Molecule 2: Flagellar motor switch protein FliG**

Chain D:
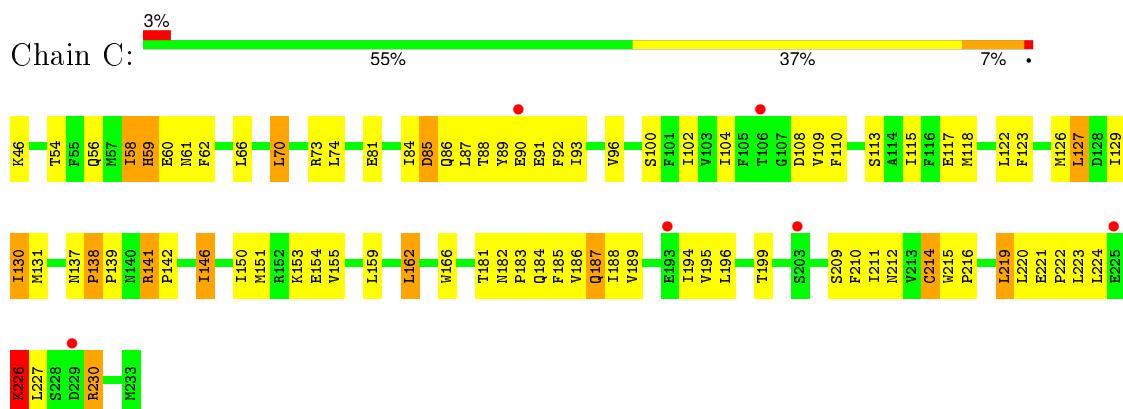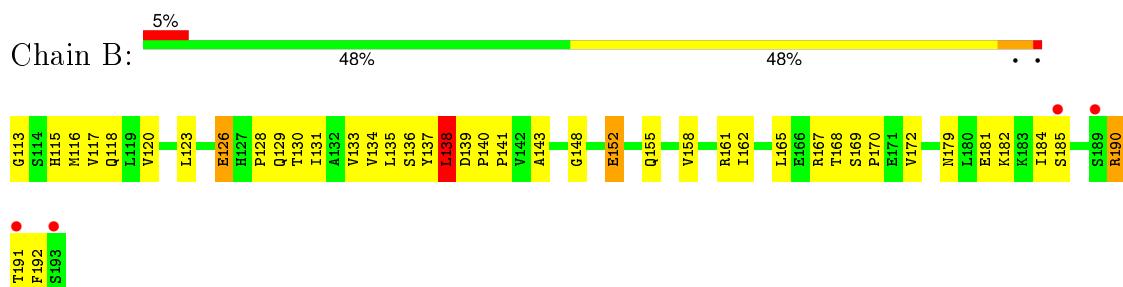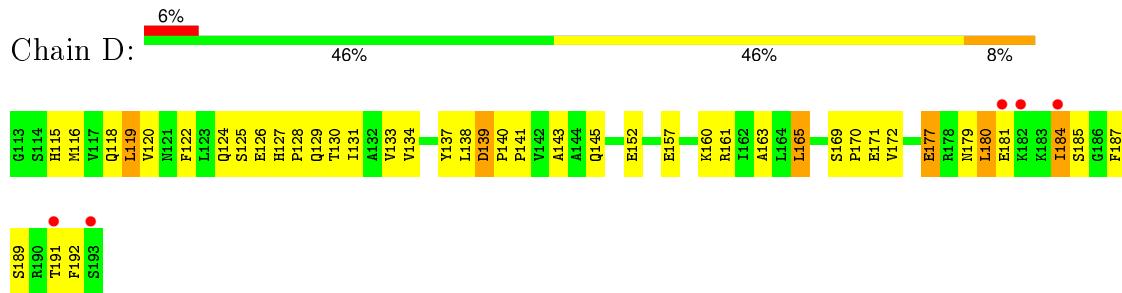
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	91.39Å 91.39Å 226.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.21 – 3.50 37.36 – 3.31	Depositor EDS
% Data completeness (in resolution range)	87.2 (26.21-3.50) 83.5 (37.36-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 3.32Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.253 , 0.301 0.258 , 0.298	Depositor DCC
R_{free} test set	1275 reflections (10.14%)	DCC
Wilson B-factor (Å^2)	88.3	Xtriage
Anisotropy	0.737	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 96.5	EDS
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	1 of 15965 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4285	wwPDB-VP
Average B, all atoms (Å^2)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.50	1/1576 (0.1%)	0.77	2/2143 (0.1%)
1	C	0.44	0/1576	0.70	0/2143
2	B	0.57	0/616	0.89	1/838 (0.1%)
2	D	0.51	0/616	0.78	0/838
All	All	0.49	1/4384 (0.0%)	0.77	3/5962 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	ASP	C-O	5.31	1.33	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ASP	CA-C-N	5.90	130.17	117.20
2	B	190	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	229	ASP	CB-CA-C	5.32	121.04	110.40

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	1535	0	1516	75	0
1	C	1535	0	1516	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	607	0	615	32	0
2	D	607	0	615	34	0
3	B	1	0	0	0	0
All	All	4285	0	4262	202	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 24.

All (202) 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)
1:A:195:VAL:HG11	1:A:214:CYS:SG	2.01	1.01
1:A:113:SER:HB2	1:A:188:ILE:HD11	1.46	0.96
1:C:113:SER:HB2	1:C:188:ILE:HD11	1.57	0.87
2:D:134:VAL:HA	2:D:192:PHE:HZ	1.39	0.85
2:D:138:LEU:HD22	2:D:191:THR:HG21	1.58	0.85
1:C:59:HIS:CE1	1:C:166:TRP:HE1	1.96	0.83
1:A:227:LEU:HD22	2:D:170:PRO:HB3	1.62	0.81
1:C:146:ILE:HD13	1:C:146:ILE:H	1.47	0.77
1:A:59:HIS:HE1	1:A:215:TRP:HE1	1.31	0.77
1:C:122:LEU:HD23	1:C:211:ILE:HD11	1.65	0.77
1:C:188:ILE:HG23	1:C:189:VAL:HG22	1.67	0.76
1:A:84:ILE:HD11	1:A:196:LEU:HD11	1.67	0.75
1:A:220:LEU:O	1:A:224:LEU:HB2	1.87	0.74
1:C:93:ILE:HD11	1:C:186:VAL:HG23	1.68	0.74
2:D:118:GLN:NE2	2:D:184:ILE:HA	2.05	0.72
1:A:89:TYR:CZ	1:A:188:ILE:HG22	2.25	0.71
1:C:220:LEU:O	1:C:224:LEU:HB2	1.91	0.70
2:B:167:ARG:O	2:B:168:THR:HG23	1.92	0.70
1:C:113:SER:HB2	1:C:188:ILE:CD1	2.23	0.68
1:C:122:LEU:CD2	1:C:211:ILE:HD11	2.22	0.68
2:B:137:TYR:HD1	2:B:192:PHE:HE1	1.41	0.68
1:C:199:THR:HG23	1:C:212:ASN:HD21	1.58	0.68
1:A:155:VAL:O	1:A:159:LEU:HB2	1.94	0.68
1:A:146:ILE:H	1:A:146:ILE:HD13	1.57	0.67
1:C:195:VAL:HG11	1:C:214:CYS:SG	2.35	0.67
2:B:138:LEU:HA	2:B:191:THR:HG21	1.76	0.67
2:D:134:VAL:HA	2:D:192:PHE:CZ	2.26	0.67
1:C:86:GLN:O	1:C:87:LEU:HD12	1.95	0.67
1:C:84:ILE:HD11	1:C:196:LEU:HD11	1.77	0.66
1:A:186:VAL:HG23	1:A:187:GLN:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LEU:HB3	1:C:215:TRP:HB2	1.79	0.65
2:B:128:PRO:HB2	2:B:161:ARG:HE	1.62	0.65
1:C:66:LEU:HG	1:C:70:LEU:CD2	2.28	0.64
1:A:100:SER:HA	1:A:120:LEU:HG	1.79	0.64
1:C:127:LEU:CD2	1:C:131:MET:SD	2.86	0.64
1:C:56:GLN:O	1:C:60:GLU:HB2	1.98	0.64
1:C:141:ARG:HB2	1:C:142:PRO:HD2	1.80	0.64
1:C:59:HIS:CE1	1:C:215:TRP:HE1	2.17	0.63
1:A:186:VAL:HG23	1:A:187:GLN:N	2.14	0.63
2:B:137:TYR:HD1	2:B:192:PHE:CE1	2.17	0.63
1:C:199:THR:HG23	1:C:212:ASN:ND2	2.13	0.62
2:D:129:GLN:HE21	2:D:161:ARG:HH11	1.46	0.62
2:B:131:ILE:HG22	2:B:135:LEU:HD12	1.82	0.62
1:C:155:VAL:O	1:C:159:LEU:HB2	2.01	0.61
2:D:122:PHE:HE2	2:D:180:LEU:CD1	2.15	0.60
1:C:89:TYR:CZ	1:C:188:ILE:HG22	2.36	0.60
1:C:104:ILE:HG22	1:C:115:ILE:HG12	1.84	0.60
2:B:140:PRO:HB2	2:B:141:PRO:HD3	1.83	0.60
1:A:56:GLN:O	1:A:60:GLU:HB2	2.02	0.60
1:C:166:TRP:HZ3	1:C:223:LEU:HD11	1.67	0.60
2:B:133:VAL:O	2:B:136:SER:HB2	2.01	0.60
2:D:141:PRO:O	2:D:145:GLN:HG3	2.02	0.60
1:C:127:LEU:HD22	1:C:131:MET:SD	2.42	0.60
1:A:128:ASP:OD1	1:A:135:GLY:HA2	2.01	0.60
1:A:59:HIS:CE1	1:A:215:TRP:HE1	2.15	0.59
1:C:96:VAL:HG11	1:C:102:ILE:HD11	1.84	0.59
1:A:123:PHE:CE1	1:A:151:MET:HG2	2.38	0.59
2:B:129:GLN:HE21	2:B:161:ARG:NH1	2.01	0.58
1:C:216:PRO:HG2	1:C:219:LEU:HB2	1.86	0.57
2:B:129:GLN:HE21	2:B:161:ARG:HH11	1.51	0.57
1:A:221:GLU:HG3	1:A:222:PRO:HD3	1.87	0.57
1:A:188:ILE:HG23	1:A:189:VAL:HG22	1.86	0.56
2:D:137:TYR:HB2	2:D:192:PHE:CE1	2.41	0.56
1:A:90:GLU:HG2	1:A:191:PRO:HB2	1.88	0.56
1:A:189:VAL:HB	1:A:190:PRO:HD2	1.87	0.56
1:A:216:PRO:HG2	1:A:219:LEU:HB2	1.87	0.56
2:D:181:GLU:HG3	2:D:187:PHE:CB	2.36	0.56
2:D:184:ILE:HG22	2:D:184:ILE:O	2.06	0.56
1:C:87:LEU:O	1:C:194:ILE:HD12	2.07	0.55
1:A:74:LEU:HD21	1:A:126:MET:HG2	1.87	0.55
1:A:223:LEU:H	1:A:223:LEU:HD23	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:HG2	1:A:191:PRO:CB	2.37	0.54
1:A:59:HIS:HE1	1:A:215:TRP:NE1	2.04	0.54
1:C:183:PRO:C	1:C:185:PHE:H	2.10	0.54
1:C:150:ILE:O	1:C:153:LYS:HG2	2.07	0.54
2:B:134:VAL:HA	2:B:192:PHE:HZ	1.72	0.54
1:A:103:VAL:CG2	1:A:179:VAL:HG13	2.36	0.54
2:B:136:SER:OG	2:B:165:LEU:HD13	2.07	0.54
2:D:160:LYS:O	2:D:163:ALA:HB3	2.08	0.54
2:D:127:HIS:ND1	2:D:128:PRO:HD2	2.22	0.54
1:A:183:PRO:C	1:A:185:PHE:H	2.09	0.53
1:C:90:GLU:HG3	1:C:91:GLU:N	2.23	0.53
1:A:113:SER:HB2	1:A:188:ILE:CD1	2.30	0.53
1:A:62:PHE:O	1:A:66:LEU:HB2	2.08	0.53
2:B:116:MET:O	2:B:120:VAL:HG23	2.09	0.52
2:B:170:PRO:HB3	1:C:227:LEU:HD22	1.92	0.52
2:B:148:GLY:HA2	2:B:155:GLN:NE2	2.24	0.52
1:A:74:LEU:HD12	1:A:78:VAL:HG21	1.91	0.52
1:C:62:PHE:CD1	1:C:162:LEU:HA	2.45	0.52
1:C:92:PHE:O	1:C:96:VAL:HG23	2.09	0.52
1:A:182:ASN:HB3	1:A:185:PHE:CD2	2.44	0.52
1:C:58:ILE:HG21	1:C:166:TRP:CD1	2.45	0.51
2:B:169:SER:CB	2:B:172:VAL:HG12	2.41	0.51
2:B:129:GLN:NE2	2:B:161:ARG:HH11	2.08	0.50
1:A:97:MET:O	1:A:100:SER:HB2	2.12	0.50
2:D:115:HIS:O	2:D:119:LEU:HB2	2.11	0.50
2:B:169:SER:HB3	2:B:172:VAL:HG12	1.93	0.50
2:D:116:MET:O	2:D:120:VAL:HG23	2.12	0.50
1:A:166:TRP:HZ3	1:A:223:LEU:HD11	1.76	0.50
1:A:131:MET:HG2	2:B:172:VAL:HG21	1.94	0.50
1:A:120:LEU:HD22	1:A:124:TYR:CE1	2.47	0.49
2:B:169:SER:HB3	2:B:172:VAL:CG1	2.42	0.49
2:B:113:GLY:O	2:B:117:VAL:HG23	2.13	0.49
1:A:230:ARG:NH1	1:A:231:PHE:HD2	2.10	0.49
1:C:186:VAL:HG23	1:C:187:GLN:H	1.78	0.49
1:A:61:ASN:HA	1:A:64:ARG:HG3	1.93	0.49
1:A:93:ILE:HD11	1:A:186:VAL:CG2	2.43	0.49
1:A:84:ILE:HD11	1:A:196:LEU:CD1	2.40	0.49
2:D:122:PHE:HE2	2:D:180:LEU:HD12	1.78	0.49
1:C:56:GLN:HE21	1:C:84:ILE:HG22	1.78	0.48
2:B:169:SER:OG	2:B:172:VAL:HG12	2.13	0.48
2:D:137:TYR:HB2	2:D:192:PHE:HE1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:MET:HG3	1:C:211:ILE:CD1	2.43	0.48
1:A:59:HIS:CE1	1:A:215:TRP:NE1	2.80	0.48
2:B:182:LYS:HB3	2:B:182:LYS:NZ	2.29	0.48
2:D:152:GLU:CD	2:D:152:GLU:H	2.17	0.48
1:C:74:LEU:HD21	1:C:126:MET:HG2	1.96	0.48
2:B:158:VAL:O	2:B:162:ILE:HG13	2.14	0.48
2:D:130:THR:O	2:D:134:VAL:HG23	2.14	0.47
2:D:129:GLN:NE2	2:D:161:ARG:HD3	2.28	0.47
2:D:129:GLN:O	2:D:133:VAL:HG23	2.13	0.47
1:A:141:ARG:HB2	1:A:142:PRO:HD2	1.96	0.47
1:A:120:LEU:HD22	1:A:124:TYR:HE1	1.80	0.47
2:D:140:PRO:HB2	2:D:141:PRO:HD3	1.96	0.47
2:B:128:PRO:HB2	2:B:161:ARG:NE	2.28	0.47
1:C:183:PRO:O	1:C:186:VAL:HG22	2.14	0.47
1:A:196:LEU:HB3	1:A:215:TRP:HB2	1.95	0.47
1:A:51:GLN:HE22	1:A:224:LEU:HD11	1.78	0.47
2:D:137:TYR:HD1	2:D:192:PHE:HE1	1.63	0.46
1:A:190:PRO:HA	1:A:191:PRO:HD2	1.61	0.46
1:A:128:ASP:CG	1:A:135:GLY:HA2	2.36	0.46
1:C:73:ARG:HA	1:C:73:ARG:HE	1.81	0.46
1:A:232:TRP:HE3	1:A:233:MET:HB2	1.81	0.46
2:B:152:GLU:CD	2:B:152:GLU:H	2.19	0.46
1:A:232:TRP:CE3	1:A:233:MET:HB2	2.50	0.46
2:D:127:HIS:O	2:D:131:ILE:HG13	2.16	0.45
1:A:182:ASN:O	1:A:185:PHE:HB2	2.17	0.45
1:C:66:LEU:O	1:C:70:LEU:HD22	2.16	0.45
2:B:136:SER:OG	2:B:165:LEU:CD1	2.64	0.45
1:C:182:ASN:O	1:C:185:PHE:HB2	2.16	0.45
1:C:58:ILE:O	1:C:61:ASN:N	2.45	0.45
1:C:74:LEU:HA	1:C:129:ILE:HG21	1.98	0.45
1:C:123:PHE:CZ	1:C:151:MET:HG3	2.50	0.45
1:C:221:GLU:HG3	1:C:222:PRO:HD3	1.98	0.45
2:D:129:GLN:HE21	2:D:161:ARG:HD3	1.81	0.45
1:C:151:MET:HA	1:C:154:GLU:HB2	1.99	0.45
1:A:58:ILE:HG21	1:A:166:TRP:CD1	2.53	0.44
2:D:177:GLU:C	2:D:179:ASN:H	2.18	0.44
1:C:146:ILE:N	1:C:146:ILE:HD13	2.24	0.44
1:A:74:LEU:O	1:A:75:ARG:HB2	2.16	0.44
1:C:84:ILE:HG12	1:C:85:ASP:N	2.33	0.44
2:B:140:PRO:O	2:B:143:ALA:HB3	2.18	0.44
1:C:89:TYR:CZ	1:C:93:ILE:HD12	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HG23	1:A:189:VAL:N	2.33	0.44
2:D:157:GLU:O	2:D:161:ARG:HG3	2.18	0.43
1:A:103:VAL:HG22	1:A:179:VAL:HG13	2.00	0.43
1:A:119:ARG:HH11	1:A:119:ARG:HG3	1.83	0.43
1:C:146:ILE:HD11	2:D:126:GLU:OE1	2.18	0.43
1:A:141:ARG:CB	1:A:142:PRO:HD2	2.48	0.43
1:A:161:LEU:HG	1:A:161:LEU:H	1.54	0.43
2:B:118:GLN:HB3	2:B:184:ILE:HG13	2.00	0.43
1:A:169:PHE:N	1:A:169:PHE:CD1	2.87	0.43
2:D:169:SER:OG	2:D:172:VAL:HG13	2.19	0.43
1:A:127:LEU:HD22	1:A:131:MET:SD	2.58	0.43
1:C:138:PRO:HA	1:C:139:PRO:HD2	1.72	0.43
1:A:58:ILE:HG23	1:A:165:ALA:O	2.18	0.42
1:A:221:GLU:HG3	1:A:222:PRO:CD	2.49	0.42
1:C:102:ILE:HG12	1:C:117:GLU:HG3	2.00	0.42
1:A:221:GLU:N	1:A:222:PRO:HD2	2.34	0.42
1:A:198:VAL:HB	1:A:213:VAL:HB	2.01	0.42
1:C:100:SER:O	1:C:181:THR:HA	2.19	0.42
1:C:183:PRO:O	1:C:185:PHE:N	2.52	0.42
1:C:222:PRO:O	1:C:226:LYS:HE2	2.20	0.42
1:A:103:VAL:HG23	1:A:179:VAL:HG13	2.00	0.42
1:C:129:ILE:O	1:C:131:MET:N	2.53	0.42
1:A:129:ILE:C	1:A:131:MET:H	2.22	0.42
1:C:54:THR:O	1:C:58:ILE:HG13	2.20	0.42
1:C:141:ARG:CB	1:C:142:PRO:HD2	2.46	0.42
1:A:230:ARG:HH12	1:A:231:PHE:HD2	1.66	0.42
1:A:142:PRO:HA	1:A:143:PRO:HD2	1.82	0.42
1:C:151:MET:O	1:C:155:VAL:HG13	2.19	0.42
1:A:118:MET:HG3	1:A:211:ILE:CD1	2.50	0.42
1:A:129:ILE:O	1:A:131:MET:N	2.53	0.41
1:A:137:ASN:ND2	1:A:137:ASN:O	2.53	0.41
2:D:177:GLU:O	2:D:179:ASN:N	2.53	0.41
1:C:209:SER:OG	1:C:210:PHE:N	2.53	0.41
2:D:137:TYR:CD1	2:D:192:PHE:HE1	2.38	0.41
1:A:46:LYS:HD3	1:A:46:LYS:N	2.34	0.41
1:A:167:SER:O	2:D:171:GLU:HG3	2.21	0.41
1:C:59:HIS:HE1	1:C:166:TRP:HE1	1.62	0.41
1:A:86:GLN:C	1:A:87:LEU:HD12	2.40	0.41
1:A:90:GLU:CG	1:A:191:PRO:HB2	2.51	0.41
1:C:127:LEU:HA	1:C:130:ILE:HG12	2.02	0.41
2:B:137:TYR:CD1	2:B:192:PHE:HE1	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:ARG:HA	1:C:73:ARG:NE	2.36	0.41
2:B:126:GLU:HB3	2:B:130:THR:HB	2.03	0.41
2:B:123:LEU:HA	2:B:123:LEU:HD23	1.86	0.41
1:A:59:HIS:CE1	1:A:166:TRP:HE1	2.39	0.41
2:D:177:GLU:C	2:D:179:ASN:N	2.73	0.41
1:C:129:ILE:C	1:C:131:MET:H	2.23	0.40
2:D:139:ASP:O	2:D:143:ALA:N	2.52	0.40
1:A:123:PHE:CD2	1:A:123:PHE:C	2.95	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	186/188 (99%)	164 (88%)	19 (10%)	3 (2%)	12	55
1	C	186/188 (99%)	165 (89%)	13 (7%)	8 (4%)	3	31
2	B	78/80 (98%)	57 (73%)	15 (19%)	6 (8%)	1	14
2	D	78/80 (98%)	63 (81%)	12 (15%)	3 (4%)	4	35
All	All	528/536 (98%)	449 (85%)	59 (11%)	20 (4%)	4	35

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	185	SER
1	A	130	ILE
2	B	126	GLU
2	B	190	ARG
1	C	184	GLN
1	C	230	ARG
1	A	167	SER

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Mol	Chain	Res	Type
2	B	138	LEU
2	B	185	SER
1	C	58	ILE
1	C	130	ILE
2	B	115	HIS
1	C	226	LYS
2	D	124	GLN
2	D	165	LEU
1	A	184	GLN
2	B	181	GLU
1	C	138	PRO
1	C	59	HIS
1	C	109	VAL

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	175/175 (100%)	150 (86%)	25 (14%)	4	24
1	C	175/175 (100%)	158 (90%)	17 (10%)	10	42
2	B	68/72 (94%)	64 (94%)	4 (6%)	24	65
2	D	68/72 (94%)	60 (88%)	8 (12%)	6	31
All	All	486/494 (98%)	432 (89%)	54 (11%)	8	35

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LYS
1	A	68	THR
1	A	70	LEU
1	A	73	ARG
1	A	75	ARG
1	A	85	ASP
1	A	88	THR
1	A	108	ASP

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Mol	Chain	Res	Type
1	A	110	PHE
1	A	127	LEU
1	A	130	ILE
1	A	136	GLU
1	A	137	ASN
1	A	141	ARG
1	A	146	ILE
1	A	151	MET
1	A	162	LEU
1	A	168	ASP
1	A	171	TYR
1	A	176	ILE
1	A	180	GLU
1	A	202	VAL
1	A	204	TRP
1	A	219	LEU
1	A	230	ARG
2	B	138	LEU
2	B	139	ASP
2	B	152	GLU
2	B	179	ASN
1	C	46	LYS
1	C	70	LEU
1	C	81	GLU
1	C	85	ASP
1	C	88	THR
1	C	108	ASP
1	C	110	PHE
1	C	127	LEU
1	C	137	ASN
1	C	141	ARG
1	C	146	ILE
1	C	162	LEU
1	C	187	GLN
1	C	214	CYS
1	C	219	LEU
1	C	226	LYS
1	C	230	ARG
2	D	119	LEU
2	D	125	SER
2	D	139	ASP
2	D	165	LEU

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Mol	Chain	Res	Type
2	D	177	GLU
2	D	180	LEU
2	D	184	ILE
2	D	189	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	59	HIS
1	A	86	GLN
1	A	137	ASN
1	A	140	ASN
1	A	187	GLN
1	A	212	ASN
2	B	129	GLN
2	B	179	ASN
1	C	51	GLN
1	C	56	GLN
1	C	59	HIS
1	C	137	ASN
1	C	157	ASN
1	C	170	GLN
1	C	212	ASN
2	D	118	GLN
2	D	129	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 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	188/188 (100%)	-0.03	7 (3%)	45	36	67, 111, 204, 263	0
1	C	188/188 (100%)	0.04	6 (3%)	51	42	71, 125, 209, 233	0
2	B	80/80 (100%)	0.02	4 (5%)	32	25	54, 108, 224, 255	0
2	D	80/80 (100%)	-0.02	5 (6%)	23	18	59, 113, 221, 266	0
All	All	536/536 (100%)	0.00	22 (4%)	41	32	54, 116, 215, 266	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	ASP	5.1
2	D	193	SER	3.4
1	C	229	ASP	3.3
2	D	191	THR	3.3
1	A	228	SER	3.1
1	C	90	GLU	3.1
2	D	182	LYS	3.0
2	B	189	SER	2.9
2	D	181	GLU	2.8
1	C	193	GLU	2.7
1	A	194	ILE	2.7
1	A	193	GLU	2.6
1	C	106	THR	2.5
1	C	225	GLU	2.4
2	B	193	SER	2.3
2	D	184	ILE	2.3
2	B	191	THR	2.2
1	A	233	MET	2.2
1	A	107	GLY	2.1
1	C	203	SER	2.1
1	A	47	PHE	2.1
2	B	185	SER	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 carbohydrates 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.