Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 02:01 PM EST

PDB ID	:	1RP3
Title	:	Cocrystal structure of the flagellar sigma/anti-sigma complex, Sigma-28/FlgM
Authors	:	Sorenson, M.K.; Ray, S.S.; Darst, S.A.
Deposited on	:	2003-12-02
Resolution	:	2.30 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 (i) 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 (1)) were used in the production of this report:

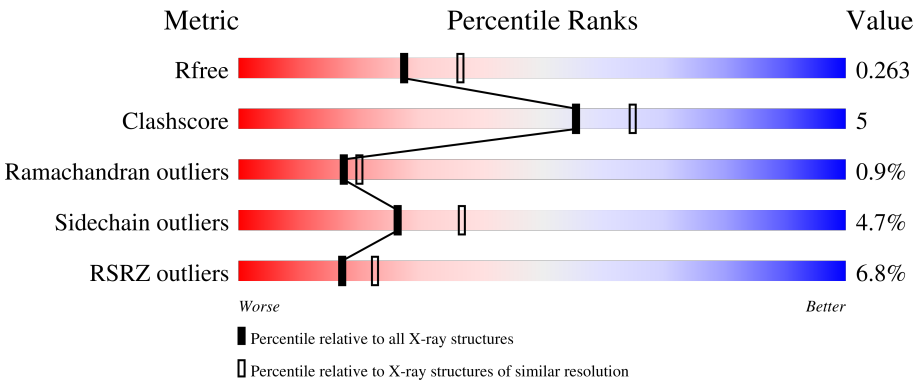
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.30 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 <=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	239	5%, 82%, 15%, • •
1	C	239	7%, 87%, 10%, •
1	E	239	7%, 83%, 13%, • •
1	G	239	2%, 80%, 13%, • 5%
2	B	88	16%, 70%, 15%, • 13%

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Mol	Chain	Length	Quality of chain
2	D	88	8% 72% 7% 20%
2	F	88	3% 66% 7% 27%
2	H	88	10% 70% 9% 20%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9110 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 RNA polymerase sigma factor SIGMA-28 (FliA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	235	1807	1160	303	343	1	0	0	0
1	C	234	1789	1140	306	342	1	0	0	0
1	E	235	1788	1144	299	344	1	0	0	0
1	G	226	1749	1121	298	329	1	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP O67268
A	-1	SER	-	cloning artifact	UNP O67268
A	0	HIS	-	cloning artifact	UNP O67268
C	-2	GLY	-	cloning artifact	UNP O67268
C	-1	SER	-	cloning artifact	UNP O67268
C	0	HIS	-	cloning artifact	UNP O67268
E	-2	GLY	-	cloning artifact	UNP O67268
E	-1	SER	-	cloning artifact	UNP O67268
E	0	HIS	-	cloning artifact	UNP O67268
G	-2	GLY	-	cloning artifact	UNP O67268
G	-1	SER	-	cloning artifact	UNP O67268
G	0	HIS	-	cloning artifact	UNP O67268

- Molecule 2 is a protein called anti sigma factor FlgM.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	77	531	337	86	108	0	0	0
2	D	70	466	299	77	90	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	F	64	428	274	69	85	0	0	0
			Total	C	N	O			
2	H	70	479	306	82	91	0	0	0

- Molecule 3 is water.

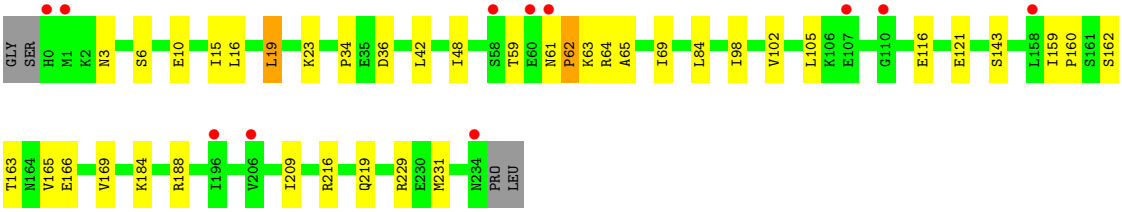
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	21	21	21	0	0
			Total	O		
3	B	4	4	4	0	0
			Total	O		
3	C	17	17	17	0	0
			Total	O		
3	E	16	16	16	0	0
			Total	O		
3	G	14	14	14	0	0
			Total	O		
3	H	1	1	1	0	0

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.

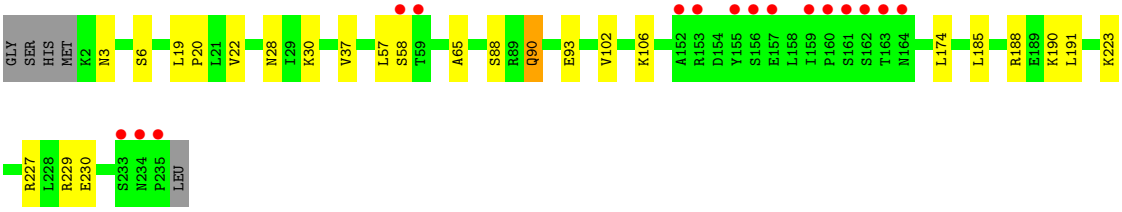
• Molecule 1: RNA polymerase sigma factor SIGMA-28 (FliA)

Chain A:



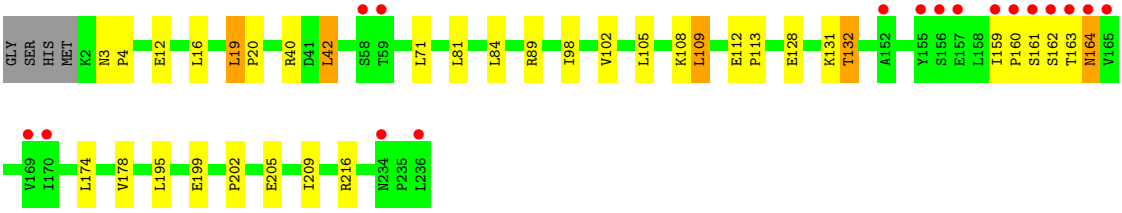
• Molecule 1: RNA polymerase sigma factor SIGMA-28 (FliA)

Chain C:



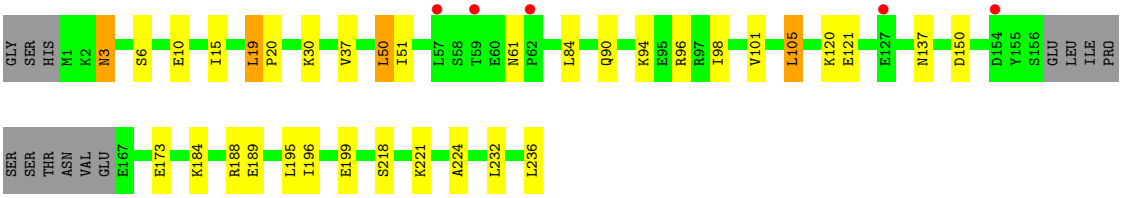
• Molecule 1: RNA polymerase sigma factor SIGMA-28 (FliA)

Chain E:



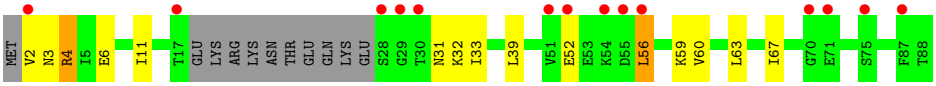
• Molecule 1: RNA polymerase sigma factor SIGMA-28 (FliA)

Chain G:



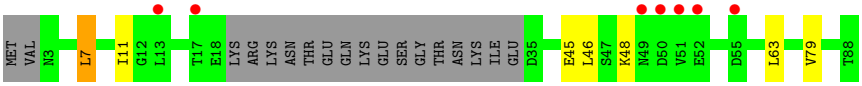
• Molecule 2: anti sigma factor FlgM

Chain B:



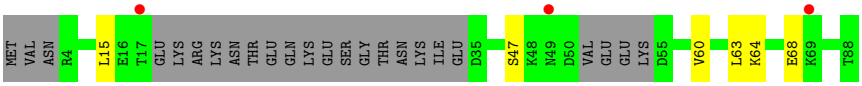
• Molecule 2: anti sigma factor FlgM

Chain D:



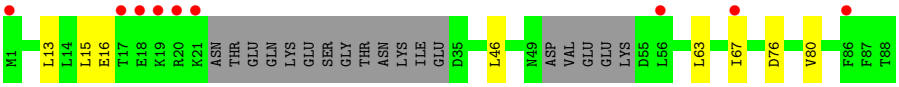
• Molecule 2: anti sigma factor FlgM

Chain F:



• Molecule 2: anti sigma factor FlgM

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.39Å 119.67Å 100.06Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	29.92 – 2.30 29.92 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.5 (29.92-2.30) 90.0 (29.92-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1, REFMAC 5.1.24	Depositor
R, R_{free}	0.242 , 0.262 0.243 , 0.263	Depositor DCC
R_{free} test set	4095 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9110	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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 (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	0.38	0/1830	0.54	0/2478
1	C	0.39	0/1811	0.54	0/2453
1	E	0.40	0/1811	0.55	0/2454
1	G	0.38	0/1769	0.56	0/2386
2	B	0.35	0/532	0.55	0/721
2	D	0.36	0/467	0.49	0/633
2	F	0.36	0/428	0.49	0/577
2	H	0.51	0/479	0.63	1/645 (0.2%)
All	All	0.39	0/9127	0.55	1/12347 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	16	GLU	N-CA-C	-5.60	95.87	111.00

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	1807	0	1817	25	0
1	C	1789	0	1772	17	0
1	E	1788	0	1748	21	0
1	G	1749	0	1771	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	531	0	477	12	0
2	D	466	0	395	6	0
2	F	428	0	371	4	0
2	H	479	0	429	3	0
3	A	21	0	0	2	0
3	B	4	0	0	0	0
3	C	17	0	0	1	0
3	E	16	0	0	0	0
3	G	14	0	0	0	0
3	H	1	0	0	0	0
All	All	9110	0	8780	91	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 (91) 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:C:223:LYS:HE2	1:C:227:ARG:HH22	1.39	0.87
1:C:223:LYS:HE2	1:C:227:ARG:NH2	1.92	0.84
1:A:105:LEU:HD11	1:A:121:GLU:HG3	1.62	0.81
1:C:88:SER:HB2	1:C:90:GLN:HE21	1.47	0.80
1:E:128:GLU:O	1:E:132:THR:HG22	1.85	0.77
1:A:65:ALA:O	1:A:69:ILE:HG12	1.90	0.71
1:G:196:ILE:HD13	1:G:221:LYS:HD2	1.73	0.70
1:C:185:LEU:HD23	1:C:227:ARG:HD2	1.73	0.70
1:A:16:LEU:HD13	2:B:11:ILE:HD12	1.78	0.66
1:A:61:ASN:ND2	3:A:251:HOH:O	2.32	0.62
1:A:98:ILE:O	1:A:102:VAL:HG23	2.01	0.61
1:E:112:GLU:OE2	1:E:216:ARG:HD3	2.02	0.60
2:B:2:VAL:HA	2:B:6:GLU:HB2	1.84	0.59
2:B:63:LEU:O	2:B:67:ILE:HG13	2.03	0.57
1:A:6:SER:O	1:A:10:GLU:HG2	2.05	0.56
1:G:15:ILE:HG23	1:G:50:LEU:HD13	1.87	0.56
1:C:30:LYS:HE2	1:C:37:VAL:O	2.05	0.56
1:A:216:ARG:HH11	1:A:219:GLN:NE2	2.03	0.56
1:C:3:ASN:HD22	1:C:6:SER:H	1.53	0.56
1:E:216:ARG:HG2	1:E:216:ARG:HH11	1.69	0.56
1:A:61:ASN:O	1:A:63:LYS:N	2.38	0.55
1:C:190:LYS:HG2	2:D:79:VAL:HG21	1.87	0.55
1:A:16:LEU:HA	1:A:19:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:VAL:HA	2:B:6:GLU:CB	2.36	0.55
1:C:191:LEU:HD13	1:G:184:LYS:HD3	1.89	0.54
1:G:19:LEU:HG	2:H:46:LEU:HD11	1.88	0.54
1:C:90:GLN:H	1:C:90:GLN:CD	2.10	0.54
1:A:209:ILE:CG2	2:B:67:ILE:HD12	2.38	0.53
1:E:174:LEU:O	1:E:178:VAL:HG23	2.09	0.53
1:C:19:LEU:HG	2:D:46:LEU:HD21	1.90	0.53
1:A:48:ILE:HD11	2:B:39:LEU:HD11	1.90	0.53
1:A:59:THR:HG23	3:A:251:HOH:O	2.08	0.53
1:C:19:LEU:HD23	2:D:7:LEU:HG	1.90	0.52
1:C:57:LEU:HD21	1:C:65:ALA:HB1	1.92	0.52
2:H:76:ASP:O	2:H:80:VAL:HG23	2.10	0.52
1:E:12:GLU:HG2	2:F:15:LEU:HD12	1.93	0.51
1:A:159:ILE:HA	1:A:162:SER:OG	2.11	0.51
1:G:3:ASN:ND2	1:G:6:SER:H	2.08	0.50
1:G:30:LYS:HE2	1:G:37:VAL:O	2.11	0.50
1:A:143:SER:HB3	1:A:229:ARG:HD3	1.93	0.50
1:A:61:ASN:HB2	1:A:64:ARG:HB2	1.94	0.49
1:A:34:PRO:HB2	1:A:36:ASP:OD1	2.12	0.48
1:A:184:LYS:HD2	1:A:231:MET:CE	2.44	0.48
2:B:2:VAL:C	2:B:4:ARG:H	2.16	0.48
1:G:105:LEU:HD21	1:G:121:GLU:HG3	1.93	0.48
1:A:16:LEU:HA	1:A:19:LEU:CD2	2.44	0.48
1:A:159:ILE:N	1:A:160:PRO:HD2	2.29	0.48
2:B:56:LEU:O	2:B:60:VAL:HG23	2.14	0.47
1:A:163:THR:OG1	1:A:166:GLU:HG3	2.13	0.47
1:E:162:SER:C	1:E:164:ASN:H	2.16	0.47
2:H:63:LEU:O	2:H:67:ILE:HG13	2.14	0.47
1:G:137:ASN:HD21	1:G:218:SER:HB3	1.79	0.47
1:C:30:LYS:NZ	3:C:245:HOH:O	2.25	0.46
1:A:184:LYS:HD2	1:A:231:MET:HE1	1.97	0.46
1:C:19:LEU:N	1:C:20:PRO:CD	2.78	0.46
1:E:202:PRO:HG2	1:E:205:GLU:HG2	1.98	0.46
1:C:102:VAL:O	1:C:106:LYS:HB2	2.16	0.46
1:G:189:GLU:HB3	1:G:224:ALA:HB2	1.97	0.46
1:G:101:VAL:O	1:G:105:LEU:HD22	2.16	0.45
1:E:195:LEU:HD23	1:E:199:GLU:HG3	1.98	0.45
1:E:89:ARG:HH11	1:E:89:ARG:HG2	1.82	0.45
1:E:209:ILE:HG13	2:F:60:VAL:HG13	1.98	0.45
1:E:71:LEU:HD23	1:E:71:LEU:HA	1.87	0.45
1:G:120:LYS:HE3	1:G:120:LYS:HB2	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:LEU:HD13	2:D:45:GLU:HG2	2.00	0.44
1:C:229:ARG:HG3	1:C:230:GLU:N	2.32	0.44
1:E:159:ILE:O	1:E:161:SER:N	2.51	0.44
1:E:98:ILE:O	1:E:102:VAL:HG23	2.19	0.43
1:E:195:LEU:O	1:E:199:GLU:HB2	2.18	0.43
2:B:2:VAL:O	2:B:6:GLU:HB3	2.18	0.43
2:F:64:LYS:O	2:F:68:GLU:HG3	2.18	0.43
1:E:3:ASN:HA	1:E:4:PRO:HD2	1.89	0.43
1:A:231:MET:HB3	1:A:231:MET:HE3	1.85	0.43
1:G:15:ILE:HD13	1:G:51:ILE:HG12	2.01	0.42
1:G:195:LEU:O	1:G:199:GLU:HB2	2.19	0.42
1:G:19:LEU:N	1:G:20:PRO:CD	2.82	0.42
1:G:105:LEU:HD11	1:G:121:GLU:HG3	2.00	0.42
1:E:42:LEU:HD11	1:E:81:LEU:HD21	2.01	0.42
1:A:19:LEU:HD21	2:B:11:ILE:HD11	2.02	0.42
2:D:7:LEU:HD12	2:D:7:LEU:HA	1.93	0.41
1:E:163:THR:O	1:E:164:ASN:CB	2.68	0.41
1:G:94:LYS:O	1:G:98:ILE:HG13	2.20	0.41
1:A:15:ILE:O	1:A:19:LEU:HD22	2.20	0.41
1:E:40:ARG:HG2	2:F:47:SER:HB3	2.03	0.41
1:E:112:GLU:HA	1:E:113:PRO:HD3	1.94	0.41
1:A:165:VAL:O	1:A:169:VAL:HG23	2.21	0.40
1:E:19:LEU:N	1:E:20:PRO:CD	2.84	0.40
1:E:108:LYS:HG2	1:E:109:LEU:HD13	2.03	0.40
1:C:19:LEU:HD22	2:D:11:ILE:HD11	2.02	0.40
2:B:2:VAL:O	2:B:4:ARG:N	2.45	0.40
2:B:59:LYS:O	2:B:63:LEU:HB2	2.22	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	233/239 (98%)	227 (97%)	5 (2%)	1 (0%)	34	42
1	C	232/239 (97%)	225 (97%)	6 (3%)	1 (0%)	34	42
1	E	233/239 (98%)	226 (97%)	5 (2%)	2 (1%)	17	20
1	G	222/239 (93%)	219 (99%)	2 (1%)	1 (0%)	29	35
2	B	73/88 (83%)	62 (85%)	6 (8%)	5 (7%)	1	0
2	D	66/88 (75%)	65 (98%)	0	1 (2%)	10	10
2	F	58/88 (66%)	56 (97%)	2 (3%)	0	100	100
2	H	64/88 (73%)	61 (95%)	3 (5%)	0	100	100
All	All	1181/1308 (90%)	1141 (97%)	29 (2%)	11 (1%)	17	20

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	PRO
2	B	31	ASN
1	E	164	ASN
2	B	4	ARG
2	B	52	GLU
2	B	3	ASN
1	C	58	SER
1	E	160	PRO
2	B	32	LYS
2	D	48	LYS
1	G	61	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	188/219 (86%)	180 (96%)	8 (4%)	29	40
1	C	183/219 (84%)	177 (97%)	6 (3%)	38	53
1	E	179/219 (82%)	171 (96%)	8 (4%)	27	39
1	G	180/219 (82%)	167 (93%)	13 (7%)	14	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	48/83 (58%)	46 (96%)	2 (4%)	30	42
2	D	35/83 (42%)	33 (94%)	2 (6%)	20	28
2	F	35/83 (42%)	34 (97%)	1 (3%)	42	58
2	H	39/83 (47%)	37 (95%)	2 (5%)	24	33
All	All	887/1208 (73%)	845 (95%)	42 (5%)	26	37

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	19	LEU
1	A	23	LYS
1	A	42	LEU
1	A	62	PRO
1	A	84	LEU
1	A	116	GLU
1	A	188	ARG
2	B	33	ILE
2	B	56	LEU
1	C	22	VAL
1	C	28	ASN
1	C	90	GLN
1	C	93	GLU
1	C	174	LEU
1	C	188	ARG
2	D	7	LEU
2	D	63	LEU
1	E	16	LEU
1	E	19	LEU
1	E	42	LEU
1	E	84	LEU
1	E	105	LEU
1	E	109	LEU
1	E	131	LYS
1	E	132	THR
2	F	63	LEU
1	G	3	ASN
1	G	10	GLU
1	G	19	LEU
1	G	50	LEU
1	G	84	LEU

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Mol	Chain	Res	Type
1	G	90	GLN
1	G	96	ARG
1	G	105	LEU
1	G	150	ASP
1	G	173	GLU
1	G	188	ARG
1	G	232	LEU
1	G	236	LEU
2	H	13	LEU
2	H	15	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	GLN
1	C	3	ASN
1	C	28	ASN
1	C	61	ASN
1	C	90	GLN
1	C	137	ASN
1	C	234	ASN
1	E	28	ASN
1	E	56	ASN
1	G	3	ASN
1	G	28	ASN
1	G	137	ASN

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 (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	235/239 (98%)	0.08	11 (4%)	31	38	23, 47, 73, 91	0
1	C	234/239 (97%)	0.34	16 (6%)	17	22	26, 44, 90, 116	0
1	E	235/239 (98%)	0.26	17 (7%)	15	20	25, 43, 103, 119	0
1	G	226/239 (94%)	0.07	5 (2%)	62	69	26, 43, 88, 100	0
2	B	77/88 (87%)	0.76	14 (18%)	1	1	28, 67, 102, 108	0
2	D	70/88 (79%)	0.40	7 (10%)	7	10	32, 65, 101, 104	0
2	F	64/88 (72%)	0.19	3 (4%)	31	38	33, 68, 82, 89	0
2	H	70/88 (79%)	0.53	9 (12%)	3	5	35, 62, 107, 130	0
All	All	1211/1308 (92%)	0.26	82 (6%)	17	22	23, 47, 92, 130	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	155	TYR	11.7
1	E	236	LEU	9.9
1	E	162	SER	8.1
1	C	156	SER	8.0
1	C	161	SER	6.2
2	B	52	GLU	6.1
2	B	51	VAL	5.6
1	E	163	THR	5.4
1	E	160	PRO	5.3
2	H	18	GLU	5.2
1	C	235	PRO	5.2
1	A	60	GLU	4.8
2	H	1	MET	4.5
2	H	17	THR	4.5
2	D	52	GLU	4.4
1	A	0	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	59	THR	4.3
2	D	50	ASP	4.2
1	E	161	SER	4.2
1	G	59	THR	4.0
1	C	58	SER	4.0
1	E	159	ILE	4.0
2	D	49	ASN	4.0
2	B	71	GLU	3.9
1	C	59	THR	3.9
2	F	49	ASN	3.8
2	D	51	VAL	3.8
2	F	17	THR	3.7
1	C	162	SER	3.7
1	E	234	ASN	3.5
2	B	56	LEU	3.5
1	E	155	TYR	3.4
2	B	70	GLY	3.4
2	B	29	GLY	3.3
1	E	169	VAL	3.3
2	B	28	SER	3.2
1	C	160	PRO	3.2
1	E	157	GLU	3.1
2	H	21	LYS	3.1
1	E	152	ALA	3.0
1	C	152	ALA	2.9
1	E	164	ASN	2.9
1	E	156	SER	2.9
1	C	234	ASN	2.8
1	A	1	MET	2.8
1	C	153	ARG	2.8
1	C	157	GLU	2.7
1	A	58	SER	2.7
1	E	165	VAL	2.7
1	C	164	ASN	2.6
1	A	107	GLU	2.6
2	H	56	LEU	2.6
1	A	234	ASN	2.6
1	A	158	LEU	2.6
2	B	75	SER	2.5
1	C	163	THR	2.5
1	G	57	LEU	2.5
2	F	69	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	2	VAL	2.4
2	D	55	ASP	2.4
1	G	62	PRO	2.4
1	A	206	VAL	2.4
2	D	17	THR	2.4
1	A	196	ILE	2.3
2	H	19	LYS	2.3
2	B	17	THR	2.3
1	E	58	SER	2.3
1	G	154	ASP	2.3
2	B	55	ASP	2.3
2	D	13	LEU	2.3
2	B	87	PHE	2.3
1	E	170	ILE	2.2
1	G	127	GLU	2.2
2	H	20	ARG	2.2
2	B	54	LYS	2.2
1	C	159	ILE	2.2
2	H	67	ILE	2.1
1	A	110	GLY	2.1
2	H	86	PHE	2.1
1	C	233	SER	2.0
1	A	61	ASN	2.0
2	B	30	THR	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.