



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 11, 2022 – 12:03 PM JST

PDB ID : 7V1M
Title : Structural basis for the co-chaperone relationship of sNASP and ASF1b
Authors : Bao, H.; Huang, H.
Deposited on : 2021-08-04
Resolution : 2.83 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 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 : 2.27
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) : 2.27

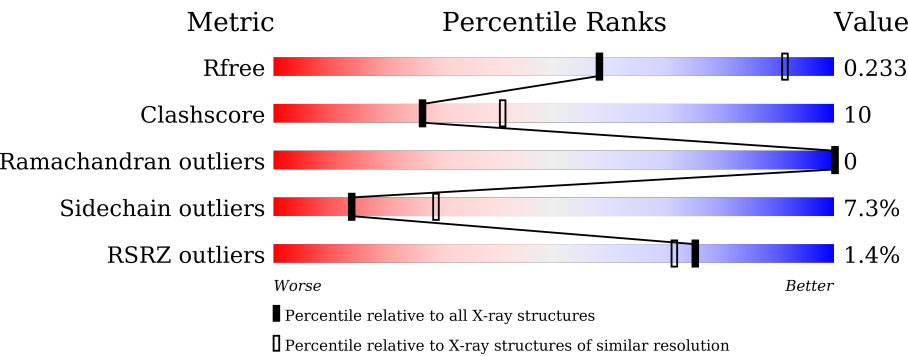
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	135	<div><div></div><div>42%13%•44%</div></div>
1	B	135	<div>%<div><div></div><div>42%21%•36%</div></div></div>
2	C	102	<div><div></div><div>60%19%22%</div></div>
2	E	102	<div>%<div><div></div><div>59%16%•24%</div></div></div>
3	D	158	<div><div></div><div>71%27%•</div></div>
3	F	158	<div><div></div><div>71%24%••</div></div>

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Mol	Chain	Length	Quality of chain
4	G	235	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>57%</div><div>24%</div><div>•</div><div>17%</div></div></div>
4	H	235	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>57%</div><div>27%</div><div>•</div><div>15%</div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7966 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 Histone H3.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	86	Total	C	N	O	S	0	0	0
			679	430	126	121	2			
1	A	75	Total	C	N	O	S	0	0	0
			583	370	110	101	2			

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	80	Total	C	N	O	S	0	0	0
			620	393	118	108	1			
2	E	78	Total	C	N	O	S	0	0	0
			605	383	115	106	1			

- Molecule 3 is a protein called Histone chaperone ASF1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	154	Total	C	N	O	S	0	0	0
			1230	790	203	232	5			
3	F	154	Total	C	N	O	S	0	0	0
			1220	784	201	230	5			

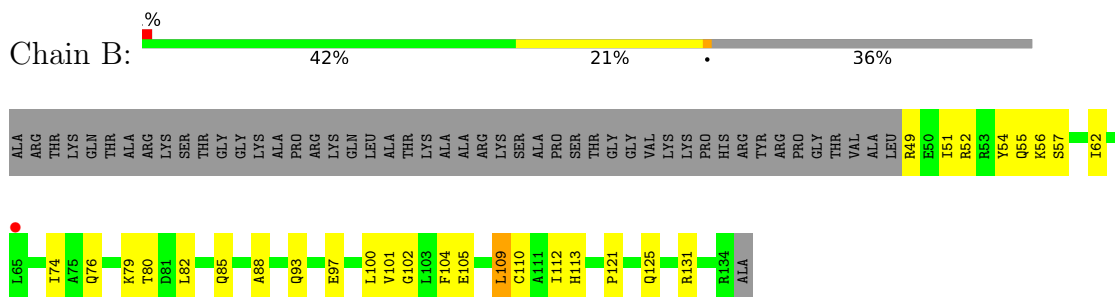
- Molecule 4 is a protein called Isoform 2 of Nuclear autoantigenic sperm protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	195	Total	C	N	O	S	0	0	0
			1480	930	243	303	4			
4	H	200	Total	C	N	O	S	0	0	0
			1549	979	254	311	5			

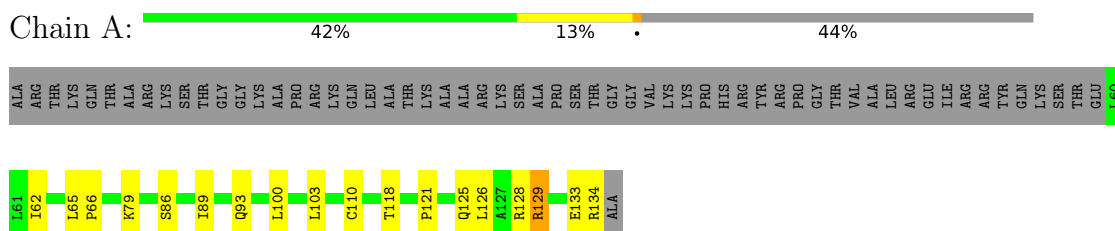
3 Residue-property plots

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.

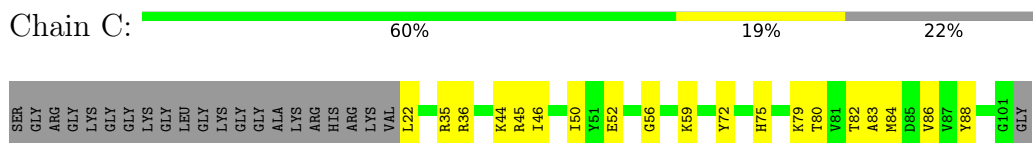
- Molecule 1: Histone H3.3



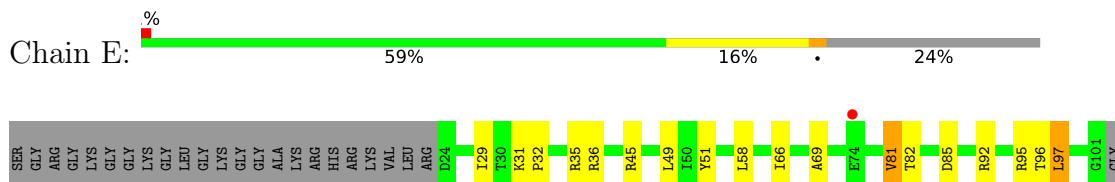
- Molecule 1: Histone H3.3



- Molecule 2: Histone H4

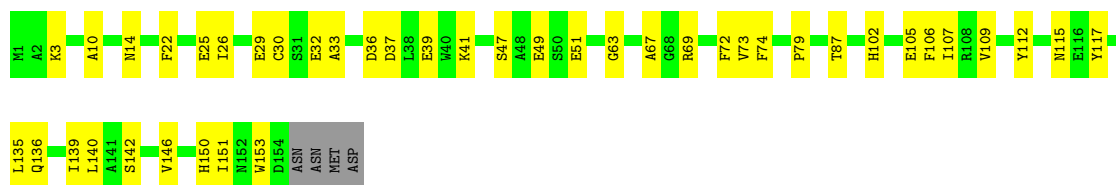


- Molecule 2: Histone H4



- Molecule 3: Histone chaperone ASF1B





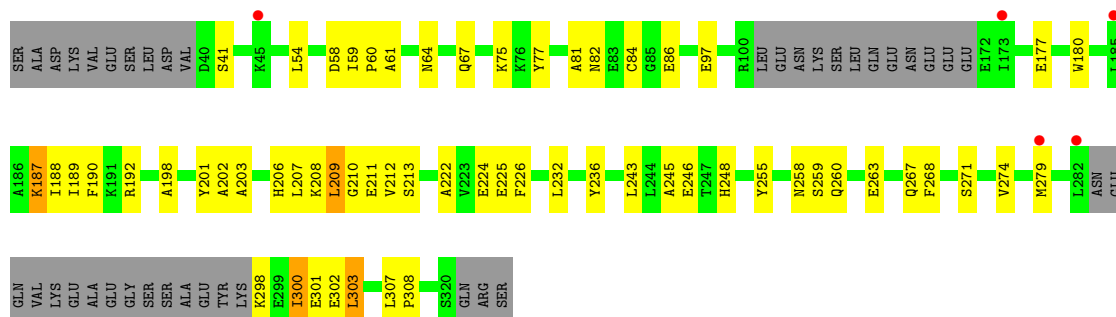
• Molecule 3: Histone chaperone ASF1B

Chain F: 71% 24% . .



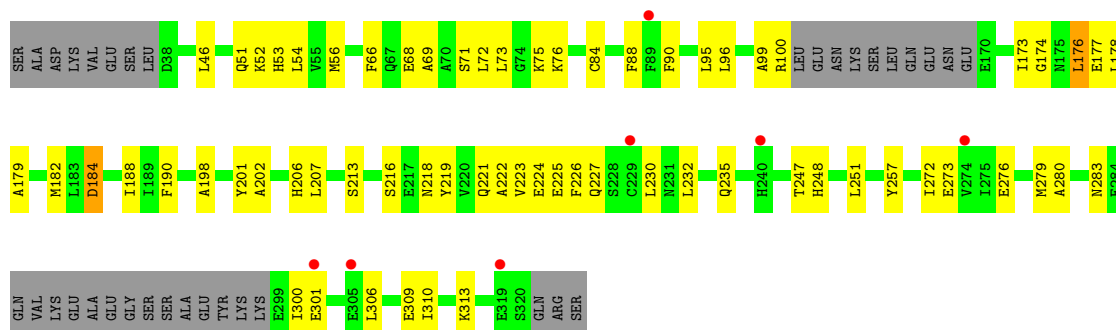
• Molecule 4: Isoform 2 of Nuclear autoantigenic sperm protein

Chain G: 57% 24% 17%



• Molecule 4: Isoform 2 of Nuclear autoantigenic sperm protein

Chain H: 57% 27% 15%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.95Å 71.90Å 93.43Å 70.67° 70.64° 83.61°	Depositor
Resolution (Å)	35.59 – 2.83 35.59 – 2.83	Depositor EDS
% Data completeness (in resolution range)	95.0 (35.59-2.83) 94.8 (35.59-2.83)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.85Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.202 , 0.240 0.199 , 0.233	Depositor DCC
R_{free} test set	1832 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	72.3	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.459 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for -k,-h,-l	Depositor
Outliers	0 of 37598 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7966	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.39% 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	0.64	0/590	0.75	0/790
1	B	0.51	0/687	0.69	0/923
2	C	0.53	0/627	0.72	0/842
2	E	0.58	0/612	0.73	0/820
3	D	0.63	0/1265	0.68	0/1729
3	F	0.61	0/1255	0.70	0/1715
4	G	0.58	0/1500	0.61	0/2019
4	H	0.57	0/1570	0.62	0/2112
All	All	0.59	0/8106	0.67	0/10950

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	583	0	586	16	0
1	B	679	0	686	18	0
2	C	620	0	638	9	0
2	E	605	0	615	12	0
3	D	1230	0	1186	24	0
3	F	1220	0	1157	25	0
4	G	1480	0	1345	30	0
4	H	1549	0	1462	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7966	0	7675	161	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 10.

All (161) 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)
4:H:232:LEU:O	4:H:235:GLN:HB2	1.88	0.74
1:B:51:ILE:HD12	4:H:184:ASP:HB3	1.75	0.68
1:B:113:HIS:NE2	3:D:140:LEU:HD21	2.12	0.64
4:H:84:CYS:HB3	4:H:88:PHE:CE1	2.34	0.63
2:C:72:TYR:HA	2:C:75:HIS:HB3	1.82	0.61
1:A:129:ARG:HG3	1:A:129:ARG:NH2	2.15	0.60
2:C:83:ALA:O	2:C:86:VAL:N	2.35	0.59
2:E:96:THR:C	2:E:97:LEU:HG	2.23	0.59
3:D:106:PHE:HB3	3:D:151:ILE:HD13	1.85	0.58
3:D:30:CYS:HB2	3:D:67:ALA:HA	1.85	0.58
4:G:187:LYS:HG3	4:G:188:ILE:N	2.19	0.57
3:F:99:CYS:SG	3:F:106:PHE:CZ	2.98	0.57
4:H:173:ILE:HA	4:H:176:LEU:HB2	1.86	0.56
4:H:219:TYR:CE1	4:H:257:TYR:HB3	2.39	0.56
4:H:184:ASP:O	4:H:188:ILE:HG23	2.06	0.56
1:A:129:ARG:HG3	1:A:129:ARG:HH21	1.70	0.56
4:H:84:CYS:HB3	4:H:88:PHE:CZ	2.41	0.55
4:G:190:PHE:HB3	4:G:198:ALA:O	2.06	0.55
4:G:210:GLY:HA3	4:G:226:PHE:CE1	2.42	0.55
1:B:110:CYS:HB3	3:D:112:TYR:CE1	2.42	0.55
3:F:55:GLN:NE2	3:F:79:PRO:HB2	2.22	0.54
2:E:31:LYS:HB3	2:E:51:TYR:CE1	2.42	0.54
3:D:37:ASP:OD1	3:D:63:GLY:HA3	2.06	0.54
1:B:52:ARG:NH1	1:B:105:GLU:HG2	2.23	0.54
1:A:62:ILE:HD11	2:E:29:ILE:HD12	1.89	0.54
4:H:69:ALA:O	4:H:73:LEU:HG	2.08	0.53
3:F:81:PRO:HA	3:F:84:ILE:HD12	1.91	0.53
1:B:62:ILE:O	1:B:93:GLN:NE2	2.41	0.53
3:D:33:ALA:N	3:D:67:ALA:HB2	2.24	0.53
3:D:32:GLU:C	3:D:67:ALA:HB2	2.30	0.53
3:F:92:VAL:HA	3:F:113:VAL:O	2.08	0.53
4:H:178:LEU:O	4:H:182:MET:HG2	2.09	0.52
4:G:208:LYS:O	4:G:212:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:31:SER:OG	3:F:32:GLU:N	2.42	0.52
3:D:10:ALA:HB3	3:D:25:GLU:HB3	1.91	0.52
3:F:47:SER:HB2	3:F:85:PRO:HG2	1.91	0.52
1:A:100:LEU:HD11	2:E:58:LEU:HD13	1.92	0.51
3:F:30:CYS:HB3	3:F:67:ALA:HA	1.91	0.51
4:G:232:LEU:O	4:G:236:TYR:HD2	1.93	0.51
1:B:56:LYS:O	1:B:57:SER:HB3	2.10	0.51
4:G:302:GLU:HG3	4:G:302:GLU:O	2.10	0.51
4:H:213:SER:HB2	4:H:222:ALA:HB2	1.93	0.51
3:D:47:SER:OG	3:D:49:GLU:OE2	2.29	0.51
4:G:177:GLU:O	4:G:180:TRP:HB3	2.11	0.50
4:H:190:PHE:HB2	4:H:202:ALA:HB2	1.94	0.50
2:E:66:ILE:HA	2:E:69:ALA:HB3	1.96	0.48
4:H:52:LYS:HB3	4:H:52:LYS:HE2	1.67	0.48
4:G:82:ASN:HA	4:G:189:ILE:HG23	1.96	0.48
4:H:276:GLU:O	4:H:279:MET:CB	2.61	0.47
1:A:110:CYS:HB2	3:F:112:TYR:CZ	2.48	0.47
4:H:100:ARG:N	4:H:100:ARG:HD2	2.30	0.47
3:F:39:GLU:OE1	3:F:59:SER:OG	2.32	0.47
4:G:203:ALA:HB2	4:G:232:LEU:HB3	1.95	0.47
4:H:226:PHE:HB2	4:H:251:LEU:HD13	1.96	0.47
1:A:121:PRO:O	1:A:125:GLN:HG2	2.15	0.47
4:H:272:ILE:HD11	4:H:310:ILE:HB	1.96	0.47
3:D:102:HIS:CG	3:D:102:HIS:O	2.68	0.47
4:H:206:HIS:O	4:H:225:GLU:HB3	2.15	0.47
4:H:66:PHE:CZ	4:H:90:PHE:HB3	2.50	0.46
3:D:25:GLU:HA	3:D:73:VAL:HG22	1.96	0.46
4:G:207:LEU:O	4:G:211:GLU:HG3	2.16	0.46
3:D:115:ASN:HA	3:D:136:GLN:O	2.16	0.46
3:F:104:GLN:HB3	3:F:151:ILE:CG1	2.46	0.46
4:G:300:ILE:HA	4:G:303:LEU:HB2	1.97	0.46
1:A:89:ILE:O	1:A:93:GLN:HG3	2.16	0.46
3:D:117:TYR:CE1	3:D:135:LEU:HD13	2.50	0.46
1:B:100:LEU:O	1:B:104:PHE:CD2	2.68	0.46
4:G:268:PHE:O	4:G:271:SER:HB3	2.16	0.46
3:F:50:SER:HB3	3:F:53:PHE:CE2	2.51	0.45
3:F:115:ASN:HB3	3:F:135:LEU:HD13	1.97	0.45
4:H:306:LEU:HD23	4:H:306:LEU:HA	1.54	0.45
4:H:99:ALA:C	4:H:100:ARG:HD2	2.36	0.45
2:C:46:ILE:HB	2:C:50:ILE:HG13	1.99	0.45
4:G:209:LEU:HB3	4:G:225:GLU:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:258:ASN:HB3	4:G:260:GLN:HG3	1.99	0.45
1:B:79:LYS:HG3	1:B:80:THR:H	1.82	0.44
2:C:79:LYS:HD3	2:C:79:LYS:HA	1.81	0.44
4:H:309:GLU:O	4:H:313:LYS:HG2	2.17	0.44
1:A:65:LEU:N	1:A:66:PRO:HD2	2.32	0.44
2:E:49:LEU:HD12	2:E:49:LEU:H	1.82	0.44
4:G:213:SER:HB2	4:G:222:ALA:HB2	1.99	0.44
4:H:223:VAL:HG13	4:H:251:LEU:HD11	1.99	0.44
3:D:39:GLU:OE2	3:D:41:LYS:NZ	2.49	0.44
4:H:190:PHE:HB3	4:H:198:ALA:O	2.16	0.44
4:G:243:LEU:HA	4:G:246:GLU:OE2	2.17	0.44
4:H:68:GLU:HA	4:H:71:SER:HB3	2.00	0.44
1:B:49:ARG:O	1:B:51:ILE:HG23	2.18	0.44
1:A:110:CYS:HB2	3:F:112:TYR:OH	2.17	0.44
3:F:35:ALA:HA	3:F:64:PRO:HB3	2.00	0.44
3:F:58:ASP:HB3	3:F:74:PHE:HE1	1.82	0.44
4:H:95:LEU:HB2	4:H:179:ALA:HB2	1.98	0.44
2:C:83:ALA:O	2:C:84:MET:C	2.52	0.43
4:H:207:LEU:HD13	4:H:247:THR:HG22	2.00	0.43
3:D:36:ASP:N	3:D:36:ASP:OD1	2.52	0.43
1:A:129:ARG:HH21	1:A:129:ARG:CG	2.28	0.43
2:E:81:VAL:O	2:E:81:VAL:HG22	2.18	0.43
1:B:55:GLN:HG3	1:B:56:LYS:H	1.84	0.43
3:D:14:ASN:HD21	3:D:139:ILE:N	2.16	0.43
1:A:118:THR:HA	2:E:45:ARG:O	2.17	0.43
1:A:100:LEU:O	1:A:103:LEU:HB3	2.18	0.43
1:A:129:ARG:HA	1:A:129:ARG:HD2	1.40	0.43
4:G:232:LEU:O	4:G:236:TYR:CD2	2.71	0.43
3:F:36:ASP:HB2	3:F:101:TYR:CZ	2.53	0.43
3:F:39:GLU:HA	3:F:60:VAL:O	2.19	0.43
1:B:76:GLN:HA	1:B:79:LYS:O	2.19	0.42
4:H:280:ALA:O	4:H:283:ASN:HB3	2.19	0.42
2:C:52:GLU:O	2:C:56:GLY:N	2.48	0.42
4:G:245:ALA:HB2	4:G:274:VAL:HB	2.00	0.42
1:B:88:ALA:HB2	2:C:82:THR:HA	2.00	0.42
1:B:74:ILE:HD11	2:C:59:LYS:HG3	2.01	0.42
3:D:26:ILE:HD12	3:D:72:PHE:CZ	2.54	0.42
4:G:77:TYR:HB3	4:G:81:ALA:HB3	2.01	0.42
1:A:62:ILE:CD1	2:E:29:ILE:HD12	2.49	0.42
3:F:58:ASP:HB3	3:F:74:PHE:CE1	2.55	0.42
4:G:77:TYR:HB3	4:G:81:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:202:ALA:O	4:G:206:HIS:HD2	2.01	0.42
3:F:28:PHE:CE1	3:F:70:HIS:HB2	2.55	0.42
4:G:58:ASP:HB3	4:G:61:ALA:HB3	2.01	0.42
2:E:36:ARG:HD3	4:G:224:GLU:OE2	2.20	0.42
3:F:37:ASP:HA	3:F:62:VAL:O	2.19	0.42
4:H:71:SER:O	4:H:75:LYS:HB3	2.20	0.42
4:H:46:LEU:HD23	4:H:46:LEU:HA	1.79	0.42
3:D:49:GLU:OE2	3:D:49:GLU:N	2.50	0.42
1:A:86:SER:O	1:A:89:ILE:HG22	2.19	0.42
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.86	0.42
4:G:86:GLU:H	4:G:86:GLU:CD	2.23	0.42
2:C:44:LYS:O	2:C:45:ARG:HG3	2.20	0.41
3:F:99:CYS:SG	3:F:106:PHE:HZ	2.41	0.41
3:D:3:LYS:HB2	3:D:153:TRP:CE3	2.55	0.41
3:D:135:LEU:HD12	3:D:135:LEU:HA	1.79	0.41
3:F:100:THR:HA	3:F:105:GLU:HA	2.02	0.41
1:B:100:LEU:HD23	1:B:100:LEU:HA	1.85	0.41
4:H:51:GLN:HA	4:H:54:LEU:HB2	2.02	0.41
4:H:53:HIS:HA	4:H:56:MET:HB2	2.01	0.41
3:F:44:TYR:O	3:F:54:ASP:HA	2.20	0.41
1:B:121:PRO:O	1:B:125:GLN:HG3	2.21	0.41
3:D:22:PHE:HE2	3:D:79:PRO:HD3	1.86	0.41
3:D:14:ASN:ND2	3:D:139:ILE:O	2.54	0.41
1:B:102:GLY:O	1:B:105:GLU:HB2	2.21	0.41
1:B:109:LEU:O	1:B:112:ILE:HB	2.20	0.41
3:D:36:ASP:HB3	3:D:102:HIS:HB3	2.01	0.41
4:H:221:GLN:O	4:H:224:GLU:HB3	2.21	0.41
3:D:29:GLU:HG3	3:D:69:ARG:HA	2.03	0.41
4:G:64:ASN:HA	4:G:67:GLN:HB3	2.03	0.41
4:G:248:HIS:O	4:G:267:GLN:HB3	2.21	0.41
4:G:307:LEU:O	4:G:308:PRO:C	2.59	0.41
4:H:96:LEU:HD11	4:H:100:ARG:HH21	1.86	0.41
4:H:230:LEU:HD21	4:H:248:HIS:CE1	2.56	0.41
1:B:97:GLU:O	1:B:101:VAL:HG23	2.21	0.41
3:F:40:TRP:CZ3	3:F:99:CYS:HB2	2.56	0.41
4:H:221:GLN:HE21	4:H:221:GLN:HB2	1.76	0.41
2:E:95:ARG:CZ	2:E:97:LEU:HD21	2.51	0.40
3:F:91:GLY:O	3:F:114:ASN:HA	2.22	0.40
4:H:68:GLU:O	4:H:72:LEU:N	2.51	0.40
2:E:31:LYS:HB2	2:E:32:PRO:HD3	2.04	0.40
4:G:59:ILE:N	4:G:60:PRO:HD2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:255:TYR:O	4:G:260:GLN:N	2.52	0.40
4:H:227:GLN:OE1	4:H:251:LEU:HD21	2.22	0.40
4:H:176:LEU:HA	4:H:176:LEU:HD12	1.82	0.40
4:G:263:GLU:O	4:G:267:GLN:HG2	2.22	0.40
4:H:174:GLY:HA2	4:H:177:GLU:CD	2.41	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	73/135 (54%)	68 (93%)	5 (7%)	0	100	100
1	B	84/135 (62%)	76 (90%)	8 (10%)	0	100	100
2	C	78/102 (76%)	78 (100%)	0	0	100	100
2	E	76/102 (74%)	73 (96%)	3 (4%)	0	100	100
3	D	152/158 (96%)	146 (96%)	6 (4%)	0	100	100
3	F	152/158 (96%)	144 (95%)	8 (5%)	0	100	100
4	G	189/235 (80%)	182 (96%)	7 (4%)	0	100	100
4	H	194/235 (83%)	185 (95%)	9 (5%)	0	100	100
All	All	998/1260 (79%)	952 (95%)	46 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	56/109 (51%)	51 (91%)	5 (9%)	9	20
1	B	67/109 (62%)	62 (92%)	5 (8%)	13	28
2	C	61/78 (78%)	56 (92%)	5 (8%)	11	24
2	E	58/78 (74%)	52 (90%)	6 (10%)	7	15
3	D	138/142 (97%)	129 (94%)	9 (6%)	17	33
3	F	133/142 (94%)	128 (96%)	5 (4%)	33	59
4	G	138/197 (70%)	123 (89%)	15 (11%)	6	13
4	H	152/197 (77%)	143 (94%)	9 (6%)	19	37
All	All	803/1052 (76%)	744 (93%)	59 (7%)	14	29

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	54	TYR
1	B	82	LEU
1	B	85	GLN
1	B	109	LEU
1	B	131	ARG
2	C	22	LEU
2	C	35	ARG
2	C	36	ARG
2	C	80	THR
2	C	88	TYR
3	D	51	GLU
3	D	74	PHE
3	D	87	THR
3	D	105	GLU
3	D	107	ILE
3	D	109	VAL
3	D	142	SER
3	D	146	VAL
3	D	150	HIS
1	A	79	LYS
1	A	128	ARG
1	A	129	ARG
1	A	133	GLU
1	A	134	ARG

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Mol	Chain	Res	Type
2	E	35	ARG
2	E	81	VAL
2	E	82	THR
2	E	85	ASP
2	E	92	ARG
2	E	97	LEU
3	F	30	CYS
3	F	74	PHE
3	F	105	GLU
3	F	112	TYR
3	F	122	LEU
4	G	41	SER
4	G	54	LEU
4	G	75	LYS
4	G	84	CYS
4	G	97	GLU
4	G	187	LYS
4	G	192	ARG
4	G	201	TYR
4	G	209	LEU
4	G	259	SER
4	G	279	MET
4	G	298	LYS
4	G	300	ILE
4	G	301	GLU
4	G	303	LEU
4	H	76	LYS
4	H	176	LEU
4	H	184	ASP
4	H	201	TYR
4	H	216	SER
4	H	218	ASN
4	H	273	GLU
4	H	300	ILE
4	H	301	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	55	GLN
3	F	134	GLN
3	F	136	GLN

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Mol	Chain	Res	Type
4	H	51	GLN
4	H	175	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

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	75/135 (55%)	0.06	0 100 100	42, 68, 100, 134	0
1	B	86/135 (63%)	0.10	1 (1%) 79 76	44, 71, 100, 120	0
2	C	80/102 (78%)	-0.07	0 100 100	46, 68, 112, 126	0
2	E	78/102 (76%)	0.12	1 (1%) 77 74	45, 66, 118, 124	0
3	D	154/158 (97%)	0.00	0 100 100	41, 60, 87, 103	0
3	F	154/158 (97%)	-0.01	0 100 100	37, 58, 83, 116	0
4	G	195/235 (82%)	0.06	5 (2%) 56 51	55, 88, 119, 141	0
4	H	200/235 (85%)	0.15	7 (3%) 44 36	57, 82, 114, 127	0
All	All	1022/1260 (81%)	0.06	14 (1%) 75 71	37, 73, 111, 141	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	282	LEU	4.5
4	G	185	LEU	4.0
4	H	305	GLU	3.6
4	H	89	PHE	3.5
4	H	240	HIS	3.1
4	G	173	ILE	2.9
2	E	74	GLU	2.8
4	G	45	LYS	2.7
4	G	279	MET	2.7
4	H	229	CYS	2.5
4	H	274	VAL	2.4
4	H	319	GLU	2.2
4	H	301	GLU	2.1
1	B	65	LEU	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 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.