Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 01:50 am BST

PDB ID	:	5NNR
Title	:	Structure of Naa15/Naa10 bound to HypK-THB
Authors	:	Weyer, F.A.; Gumiero, A.; Kopp, J.; Sinning, I.
Deposited on	:	2017-04-10
Resolution	:	3.10 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 following versions of software and data (see references (1)) were used in the production of this report:

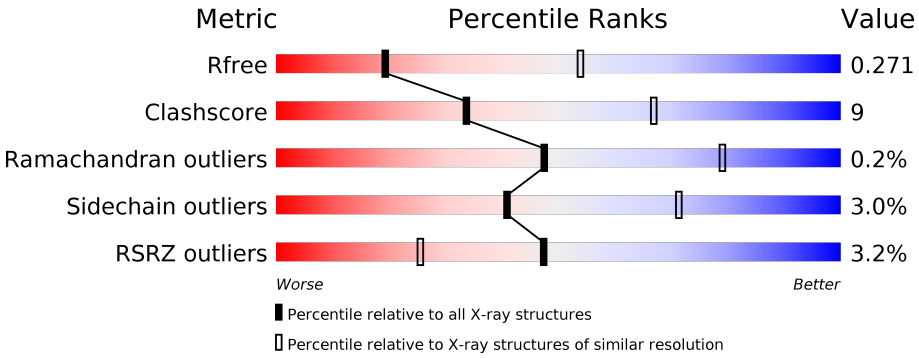
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 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	751	3% 73% 15% • 11%
1	D	751	2% 71% 16% • 11%
2	B	195	4% 67% 23% 10%
2	E	195	2% 72% 16% • • 8%
3	C	133	2% 40% 16% •• 43%
3	F	133	4% 41% 8% • 49%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14719 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 N-terminal acetyltransferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5391	3430	941	998	22			
1	D	665	Total	C	N	O	S	0	0	0
			5390	3429	940	999	22			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP G0S4M4
A	-5	GLY	-	expression tag	UNP G0S4M4
A	-4	HIS	-	expression tag	UNP G0S4M4
A	-3	HIS	-	expression tag	UNP G0S4M4
A	-2	HIS	-	expression tag	UNP G0S4M4
A	-1	HIS	-	expression tag	UNP G0S4M4
A	0	HIS	-	expression tag	UNP G0S4M4
A	1	HIS	-	expression tag	UNP G0S4M4
A	707	LYS	ASN	conflict	UNP G0S4M4
A	724	ASP	GLY	conflict	UNP G0S4M4
D	-6	MET	-	initiating methionine	UNP G0S4M4
D	-5	GLY	-	expression tag	UNP G0S4M4
D	-4	HIS	-	expression tag	UNP G0S4M4
D	-3	HIS	-	expression tag	UNP G0S4M4
D	-2	HIS	-	expression tag	UNP G0S4M4
D	-1	HIS	-	expression tag	UNP G0S4M4
D	0	HIS	-	expression tag	UNP G0S4M4
D	1	HIS	-	expression tag	UNP G0S4M4
D	707	LYS	ASN	conflict	UNP G0S4M4
D	724	ASP	GLY	conflict	UNP G0S4M4

- Molecule 2 is a protein called Naa10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1424	910	247	260	7			
2	E	179	Total	C	N	O	S	0	0	0
			1451	927	251	266	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	190	HIS	-	expression tag	UNP G0SEE8
B	191	HIS	-	expression tag	UNP G0SEE8
B	192	HIS	-	expression tag	UNP G0SEE8
B	193	HIS	-	expression tag	UNP G0SEE8
B	194	HIS	-	expression tag	UNP G0SEE8
B	195	HIS	-	expression tag	UNP G0SEE8
E	190	HIS	-	expression tag	UNP G0SEE8
E	191	HIS	-	expression tag	UNP G0SEE8
E	192	HIS	-	expression tag	UNP G0SEE8
E	193	HIS	-	expression tag	UNP G0SEE8
E	194	HIS	-	expression tag	UNP G0SEE8
E	195	HIS	-	expression tag	UNP G0SEE8

- Molecule 3 is a protein called HypK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	76	Total	C	N	O	Se	0	0	0
			558	349	96	111	2			
3	F	68	Total	C	N	O	Se	0	0	0
			505	315	86	102	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	MSE	-	initiating methionine	UNP G0SCY6
C	-5	GLY	-	expression tag	UNP G0SCY6
C	-4	HIS	-	expression tag	UNP G0SCY6
C	-3	HIS	-	expression tag	UNP G0SCY6
C	-2	HIS	-	expression tag	UNP G0SCY6
C	-1	HIS	-	expression tag	UNP G0SCY6
C	0	HIS	-	expression tag	UNP G0SCY6
C	1	HIS	-	expression tag	UNP G0SCY6
F	-6	MSE	-	initiating methionine	UNP G0SCY6
F	-5	GLY	-	expression tag	UNP G0SCY6
F	-4	HIS	-	expression tag	UNP G0SCY6

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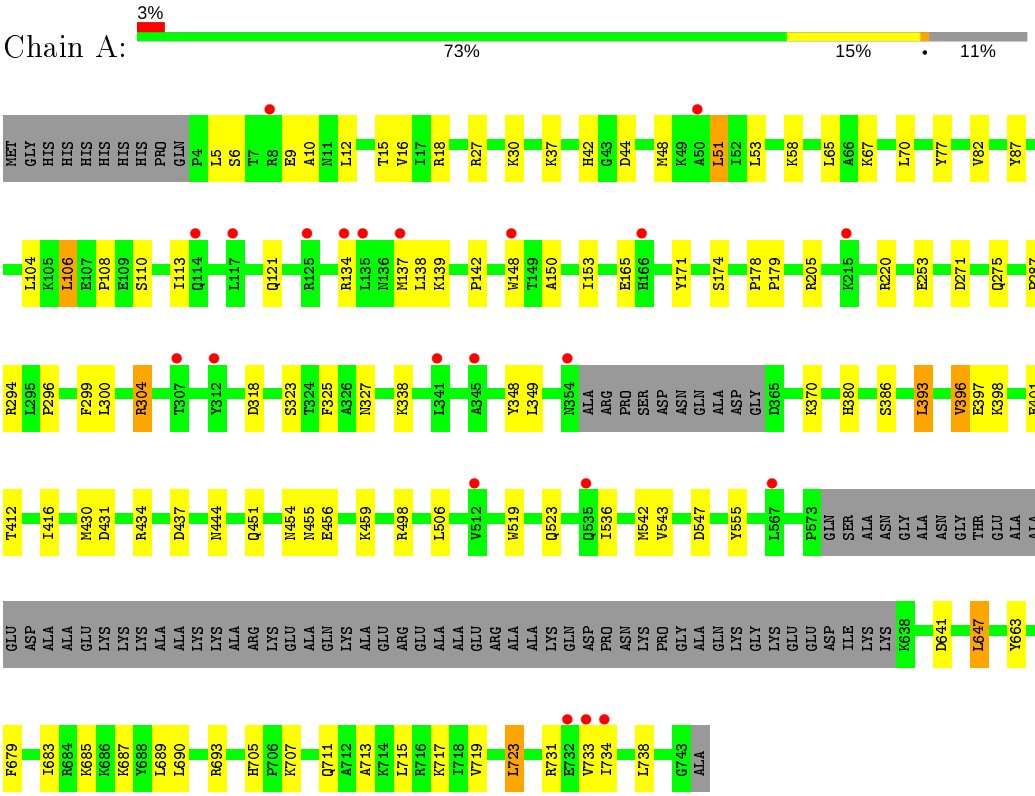
Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	HIS	-	expression tag	UNP G0SCY6
F	-2	HIS	-	expression tag	UNP G0SCY6
F	-1	HIS	-	expression tag	UNP G0SCY6
F	0	HIS	-	expression tag	UNP G0SCY6
F	1	HIS	-	expression tag	UNP G0SCY6

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.

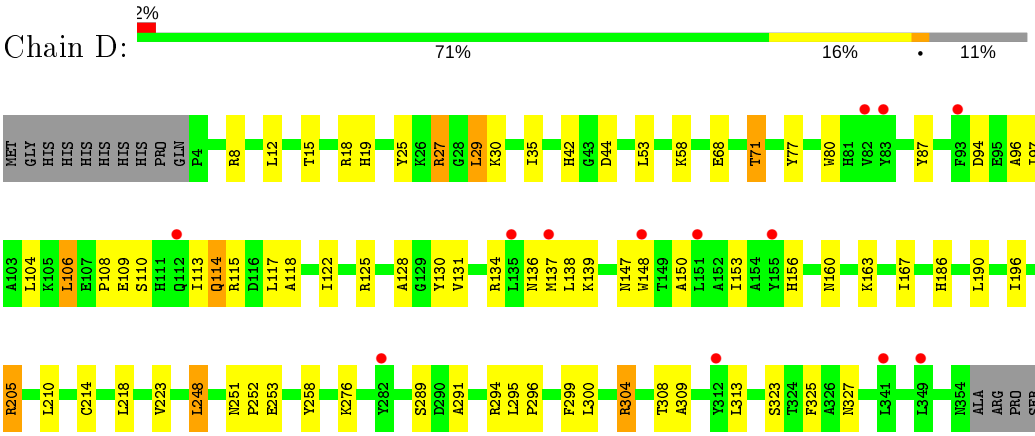
- Molecule 1: N-terminal acetyltransferase-like protein

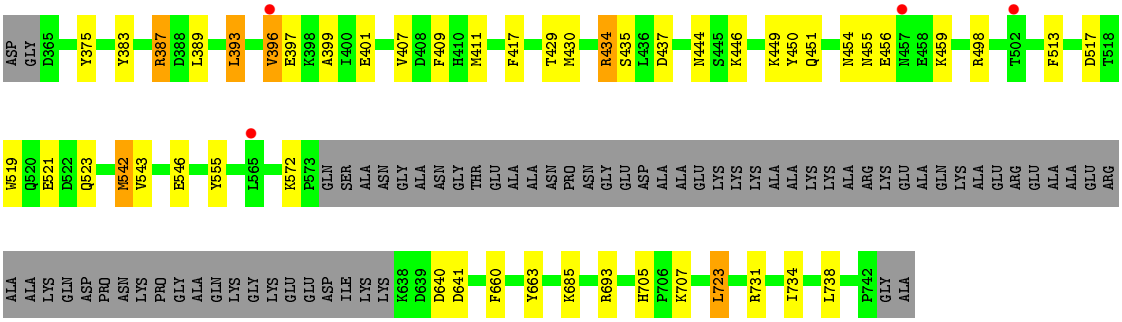
Chain A:



- Molecule 1: N-terminal acetyltransferase-like protein

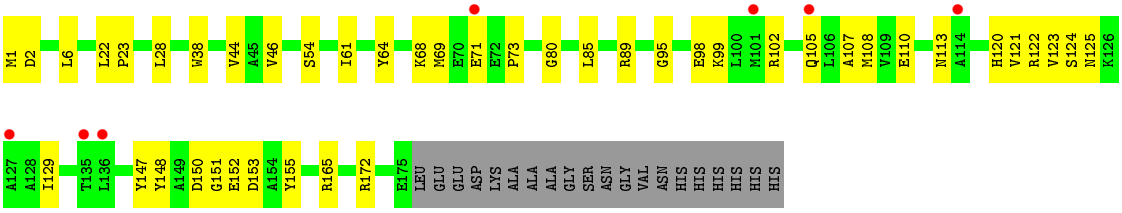
Chain D:





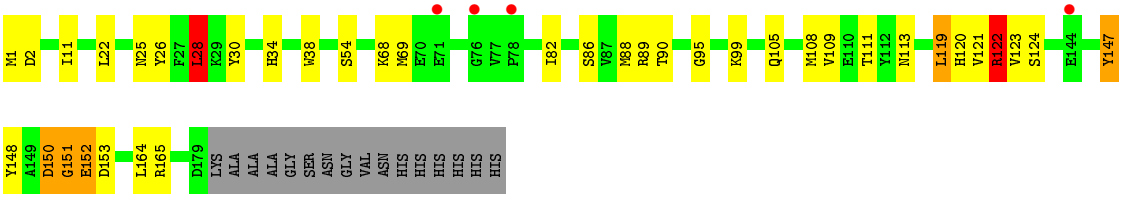
• Molecule 2: Naa10

Chain B:



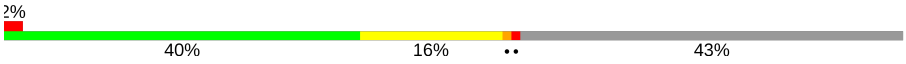
• Molecule 2: Naa10

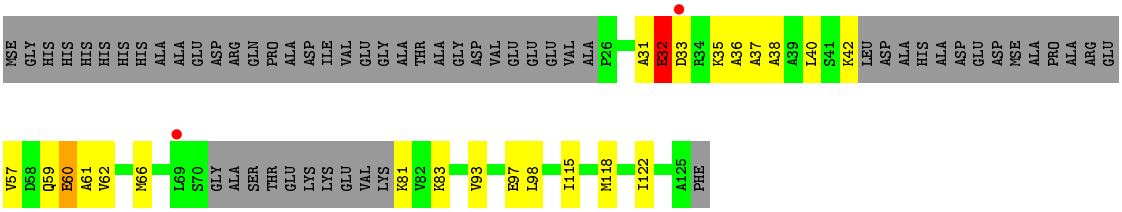
Chain E:



• Molecule 3: HypK

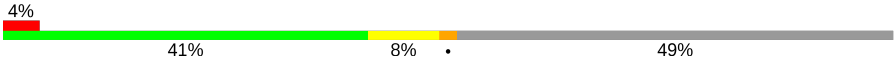
Chain C:

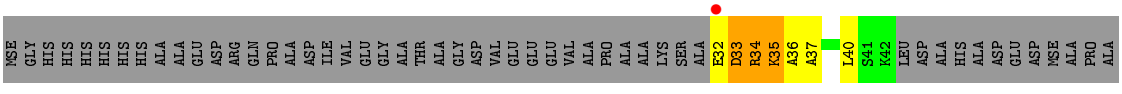


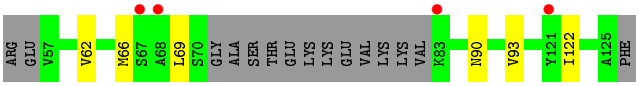


• Molecule 3: HypK

Chain F:






ARG
GLU
V57
V62
M66
S67
A68
L69
S70
GLY
ALA
SER
THR
GLU
LYS
LYS
GLU
VAL
LYS
LYS
VAL
K83
N90
V93
Y121
I122
A125
PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	85.35Å 85.35Å 319.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.30 – 3.10 48.35 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.30-3.10) 93.7 (48.35-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.230 , 0.272 0.233 , 0.271	Depositor DCC
R_{free} test set	2381 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	88.8	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 91.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l 0.469 for h,-h-k,-l 0.037 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14719	wwPDB-VP
Average B, all atoms (Å^2)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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

5.1 Standard geometry

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

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	0.42	0/5502	0.68	0/7414
1	D	0.42	0/5501	0.70	0/7413
2	B	0.48	0/1448	0.82	2/1962 (0.1%)
2	E	0.52	0/1475	0.94	5/1999 (0.3%)
3	C	0.30	0/558	0.57	0/743
3	F	0.29	0/504	0.54	0/671
All	All	0.43	0/14988	0.72	7/20202 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	151	GLY	N-CA-C	-8.51	91.82	113.10
2	E	119	LEU	CB-CG-CD1	6.69	122.37	111.00
2	E	28	LEU	CB-CG-CD1	6.52	122.08	111.00
2	E	28	LEU	CA-CB-CG	5.44	127.81	115.30
2	B	151	GLY	N-CA-C	5.18	126.04	113.10
2	E	122	ARG	NE-CZ-NH1	5.07	122.84	120.30
2	B	6	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	5391	0	5390	85	0
1	D	5390	0	5389	93	0
2	B	1424	0	1422	38	0
2	E	1451	0	1443	33	0
3	C	558	0	586	21	0
3	F	505	0	523	13	0
All	All	14719	0	14753	251	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 9.

All (251) 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)
2:E:124:SER:N	2:E:152:GLU:OE1	1.90	1.03
1:D:118:ALA:HB1	1:D:134:ARG:HH12	1.31	0.95
1:A:437:ASP:OD2	2:B:89:ARG:NH2	2.07	0.87
2:B:44:VAL:HG11	2:B:61:ILE:HD12	1.58	0.85
2:B:123:VAL:HG23	2:B:153:ASP:O	1.78	0.83
1:A:95:GLU:HA	1:A:98:LYS:HE2	1.62	0.82
1:D:118:ALA:HB1	1:D:134:ARG:NH1	1.95	0.81
1:D:723:LEU:HB2	1:D:731:ARG:HE	1.47	0.79
1:A:51:LEU:HD23	1:A:82:VAL:HG13	1.67	0.76
2:B:107:ALA:HA	2:B:110:GLU:HG2	1.69	0.75
2:E:122:ARG:NH1	2:E:147:TYR:HB3	2.01	0.75
2:B:124:SER:N	2:B:152:GLU:OE1	2.20	0.75
2:E:122:ARG:HB3	2:E:152:GLU:HG2	1.70	0.73
2:E:120:HIS:CE1	2:E:147:TYR:HH	2.06	0.72
2:E:148:TYR:HH	3:F:32:GLU:N	1.86	0.72
1:D:150:ALA:HA	1:D:153:ILE:HD12	1.75	0.69
1:D:519:TRP:CD2	2:E:28:LEU:HD23	2.27	0.69
1:A:134:ARG:NH1	1:A:137:MET:SD	2.67	0.68
1:A:455:ASN:OD1	1:A:498:ARG:NH1	2.26	0.68
1:D:542:MET:HG3	1:D:543:VAL:N	2.09	0.68
1:A:689:LEU:HD22	3:C:118:MSE:HE2	1.76	0.67
1:D:114:GLN:HE22	1:D:137:MET:HG2	1.59	0.67
1:A:542:MET:HG3	1:A:543:VAL:N	2.10	0.67
1:A:431:ASP:OD1	1:A:434:ARG:NH1	2.27	0.67
2:B:148:TYR:CZ	3:C:31:ALA:HA	2.29	0.67
1:A:220:ARG:HH21	2:B:172:ARG:HE	1.42	0.67
3:F:33:ASP:OD1	3:F:33:ASP:N	2.28	0.67
1:D:101:LYS:HA	1:D:117:LEU:HD11	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:TYR:CE2	2:B:148:TYR:CE2	2.84	0.66
1:D:387:ARG:HD2	1:D:389:LEU:HD11	1.76	0.66
2:E:124:SER:OG	2:E:152:GLU:OE2	2.13	0.66
2:B:113:ASN:OD1	2:B:165:ARG:NH1	2.24	0.66
1:D:136:ASN:O	1:D:139:LYS:HG2	1.96	0.66
2:E:113:ASN:OD1	2:E:165:ARG:NH1	2.29	0.65
1:A:42:HIS:CE1	1:A:44:ASP:HB2	2.31	0.65
1:A:165:GLU:OE2	1:A:205:ARG:NH2	2.29	0.65
2:B:121:VAL:HG12	2:B:122:ARG:O	1.97	0.65
2:B:148:TYR:CE1	3:C:31:ALA:HA	2.32	0.64
2:E:122:ARG:HH12	2:E:147:TYR:HB3	1.64	0.63
1:A:407:VAL:HG21	2:B:89:ARG:CZ	2.28	0.63
1:D:77:TYR:HB3	1:D:106:LEU:HD12	1.81	0.63
1:D:519:TRP:CE2	2:E:28:LEU:HD23	2.34	0.63
1:D:42:HIS:HE1	1:D:44:ASP:HB2	1.64	0.62
1:A:705:HIS:CE1	1:A:707:LYS:HB2	2.34	0.62
1:A:451:GLN:NE2	1:A:459:LYS:HE2	2.15	0.61
2:E:123:VAL:HG23	2:E:152:GLU:OE1	2.00	0.61
2:E:123:VAL:HG13	2:E:153:ASP:O	2.00	0.61
1:D:640:ASP:OD1	1:D:641:ASP:N	2.33	0.61
2:B:125:ASN:O	2:B:129:ILE:HD12	2.01	0.60
1:D:114:GLN:NE2	1:D:137:MET:HG2	2.15	0.60
1:A:397:GLU:O	1:A:401:GLU:HG3	2.01	0.60
2:E:11:ILE:HG21	2:E:28:LEU:HD13	1.83	0.60
1:A:287:PRO:O	1:A:293:LYS:NZ	2.34	0.59
1:A:15:THR:HG22	1:A:18:ARG:HH21	1.68	0.59
1:A:220:ARG:HG3	2:B:172:ARG:HH11	1.68	0.59
1:D:42:HIS:CE1	1:D:44:ASP:HB2	2.38	0.58
2:E:120:HIS:ND1	2:E:147:TYR:OH	2.18	0.58
2:B:147:TYR:CE2	2:B:148:TYR:HE2	2.21	0.57
2:E:105:GLN:HA	2:E:108:MET:HE2	1.85	0.57
2:B:105:GLN:HA	2:B:108:MET:HE2	1.85	0.57
1:D:389:LEU:HD12	1:D:389:LEU:H	1.69	0.57
1:A:171:TYR:O	1:A:174:SER:OG	2.20	0.57
1:A:506:LEU:HB3	1:A:647:LEU:HD23	1.85	0.57
1:D:434:ARG:HG3	1:D:444:ASN:HA	1.87	0.57
1:A:723:LEU:O	1:A:731:ARG:HD2	2.05	0.57
1:A:87:TYR:HB3	1:A:96:ALA:HB2	1.87	0.57
1:D:411:MET:HG3	1:D:430:MET:SD	2.45	0.57
1:D:80:TRP:CD2	1:D:102:PHE:HZ	2.22	0.57
2:E:95:GLY:O	2:E:99:LYS:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:693:ARG:HB2	3:F:122:ILE:HG22	1.88	0.56
1:A:693:ARG:HB2	3:C:122:ILE:HG22	1.87	0.56
3:C:60:GLU:HG2	3:C:61:ALA:N	2.20	0.56
1:D:455:ASN:OD1	1:D:498:ARG:HD2	2.04	0.56
1:A:411:MET:HG3	1:A:430:MET:SD	2.47	0.55
3:C:83:LYS:HD2	3:C:83:LYS:H	1.70	0.55
1:D:104:LEU:HD23	1:D:113:ILE:HG23	1.89	0.55
3:F:90:ASN:HA	3:F:93:VAL:HG22	1.88	0.55
1:A:77:TYR:HB3	1:A:106:LEU:HB3	1.87	0.55
1:D:417:PHE:HE2	1:D:429:THR:HG21	1.72	0.54
2:E:22:LEU:HD11	2:E:86:SER:HB3	1.89	0.54
1:A:42:HIS:HE1	1:A:44:ASP:HB2	1.70	0.54
1:A:723:LEU:HD11	1:D:204:GLU:OE1	2.07	0.54
1:A:253:GLU:O	2:B:2:ASP:HA	2.08	0.54
1:D:294:ARG:HD2	1:D:327:ASN:HB3	1.89	0.54
1:A:454:ASN:ND2	1:A:456:GLU:OE2	2.39	0.54
2:E:124:SER:H	2:E:152:GLU:CD	2.05	0.54
1:A:687:LYS:HB3	1:A:690:LEU:HD12	1.90	0.54
1:D:19:HIS:CE1	1:D:27:ARG:HG2	2.43	0.54
1:D:407:VAL:HG21	1:D:437:ASP:HB2	1.90	0.54
1:A:300:LEU:HD22	1:A:304:ARG:HB3	1.89	0.54
1:A:323:SER:O	1:A:327:ASN:HB2	2.07	0.54
1:D:102:PHE:O	1:D:106:LEU:N	2.41	0.54
1:D:705:HIS:CE1	1:D:707:LYS:HB2	2.43	0.53
1:D:397:GLU:O	1:D:401:GLU:HG3	2.08	0.53
1:D:399:ALA:HB1	1:D:409:PHE:CE2	2.44	0.53
1:D:201:GLY:O	1:D:203:ILE:HD12	2.09	0.53
3:F:32:GLU:HA	3:F:35:LYS:HD3	1.91	0.52
2:B:122:ARG:HH22	2:B:150:ASP:HB3	1.74	0.52
1:D:122:ILE:HB	1:D:130:TYR:CE2	2.44	0.52
1:A:349:LEU:HD12	1:A:370:LYS:HG3	1.90	0.52
1:D:87:TYR:HB3	1:D:96:ALA:HB2	1.91	0.52
1:A:434:ARG:HG3	1:A:444:ASN:HA	1.92	0.52
2:B:71:GLU:O	2:B:73:PRO:HD3	2.09	0.52
1:D:723:LEU:HB2	1:D:731:ARG:NE	2.19	0.52
1:D:12:LEU:HD12	1:D:35:ILE:HG13	1.92	0.52
1:D:542:MET:HG3	1:D:543:VAL:H	1.74	0.51
1:A:523:GLN:CB	1:A:542:MET:HE1	2.41	0.51
2:B:123:VAL:HG21	2:B:153:ASP:HB2	1.92	0.51
1:D:519:TRP:CG	2:E:28:LEU:HD23	2.43	0.51
1:A:523:GLN:HB3	1:A:542:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:PHE:CE1	1:A:683:ILE:HD13	2.45	0.51
1:D:210:LEU:HD21	1:D:223:VAL:HG13	1.92	0.51
1:D:296:PRO:HA	1:D:299:PHE:CE2	2.45	0.51
1:D:134:ARG:HE	1:D:150:ALA:HB1	1.75	0.51
1:D:451:GLN:NE2	1:D:459:LYS:HE2	2.26	0.51
1:A:138:LEU:HD11	1:A:148:TRP:CE2	2.46	0.51
2:E:25:ASN:O	3:F:34:ARG:NH2	2.44	0.51
1:A:139:LYS:HA	3:C:66:MSE:SE	2.60	0.51
1:A:142:PRO:HB2	3:C:62:VAL:HG11	1.93	0.50
2:B:68:LYS:NZ	3:C:33:ASP:OD2	2.24	0.50
1:A:672:ILE:H	1:A:672:ILE:HD12	1.75	0.50
1:A:519:TRP:CD2	2:B:28:LEU:HD13	2.47	0.50
2:B:38:TRP:CZ3	2:B:68:LYS:HB2	2.47	0.50
2:E:122:ARG:HB3	2:E:152:GLU:CG	2.38	0.50
1:A:5:LEU:HB2	1:A:9:GLU:HB2	1.94	0.49
1:A:296:PRO:HA	1:A:299:PHE:CE2	2.48	0.49
1:A:542:MET:HG3	1:A:543:VAL:H	1.76	0.49
1:A:6:SER:O	1:A:10:ALA:HB2	2.12	0.49
1:D:323:SER:HB3	2:E:90:THR:O	2.13	0.49
2:B:122:ARG:NH2	2:B:150:ASP:HB3	2.28	0.49
1:A:679:PHE:CE1	1:A:711:GLN:HB3	2.48	0.48
1:D:128:ALA:O	1:D:131:VAL:HG22	2.14	0.48
1:D:291:ALA:HB1	1:D:295:LEU:HD12	1.96	0.48
3:C:57:VAL:HG12	3:C:59:GLN:HG3	1.95	0.48
1:D:523:GLN:NE2	1:D:546:GLU:HG2	2.29	0.47
1:A:689:LEU:CD2	3:C:118:MSE:HE2	2.44	0.47
1:D:252:PRO:HB2	1:D:289:SER:HB2	1.96	0.47
1:D:454:ASN:ND2	1:D:456:GLU:OE2	2.47	0.47
2:E:38:TRP:CZ3	2:E:68:LYS:HB2	2.49	0.47
1:D:523:GLN:CD	1:D:546:GLU:HG2	2.35	0.47
3:C:31:ALA:O	3:C:33:ASP:N	2.38	0.47
1:D:138:LEU:HD11	1:D:148:TRP:CE2	2.49	0.47
3:F:35:LYS:H	3:F:35:LYS:HD2	1.79	0.47
2:B:1:FME:HG2	2:B:46:VAL:O	2.14	0.47
1:A:338:LYS:HE3	1:A:386:SER:HB3	1.97	0.47
1:A:97:ILE:HD11	1:A:121:GLN:HG3	1.97	0.47
1:D:375:TYR:HB2	1:D:409:PHE:CE2	2.50	0.47
2:E:121:VAL:HG22	2:E:122:ARG:O	2.14	0.47
1:D:167:ILE:HD11	3:F:69:LEU:HD22	1.96	0.46
1:D:101:LYS:HG3	1:D:117:LEU:CD2	2.45	0.46
1:A:641:ASP:OD2	1:A:647:LEU:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:ILE:O	1:A:738:LEU:HB2	2.15	0.46
1:D:15:THR:HG22	1:D:18:ARG:NH2	2.30	0.46
1:A:398:LYS:O	1:A:401:GLU:HB2	2.16	0.46
1:A:434:ARG:HD2	1:A:444:ASN:HD22	1.81	0.46
1:A:153:ILE:HD11	1:A:536:ILE:HD12	1.98	0.46
3:C:93:VAL:HG23	3:C:98:LEU:O	2.15	0.46
1:D:437:ASP:OD2	2:E:89:ARG:NH2	2.47	0.46
1:A:705:HIS:HE1	1:A:707:LYS:HB2	1.78	0.46
1:A:715:LEU:O	1:A:719:VAL:HG23	2.16	0.46
2:B:110:GLU:CB	2:B:172:ARG:HH12	2.28	0.46
1:A:12:LEU:O	1:A:16:VAL:HG23	2.16	0.46
1:D:430:MET:HG2	1:D:450:TYR:HD2	1.80	0.46
3:C:81:LYS:HE3	3:C:81:LYS:HB2	1.68	0.45
1:A:685:LYS:NZ	3:C:97:GLU:OE1	2.50	0.45
1:D:555:TYR:OH	1:D:663:TYR:HB2	2.16	0.45
1:D:125:ARG:CZ	1:D:543:VAL:HG13	2.46	0.45
1:A:67:LYS:O	1:A:70:LEU:HG	2.17	0.45
1:A:393:LEU:O	1:A:396:VAL:HG12	2.16	0.45
3:F:62:VAL:O	3:F:66:MSE:HG2	2.16	0.45
1:A:519:TRP:CE2	2:B:28:LEU:HD13	2.52	0.45
3:F:34:ARG:HG3	3:F:35:LYS:HD2	1.99	0.45
1:A:294:ARG:HD3	1:A:327:ASN:ND2	2.32	0.44
1:A:271:ASP:O	1:A:275:GLN:HG3	2.17	0.44
1:A:434:ARG:HD2	1:A:444:ASN:ND2	2.33	0.44
1:D:53:LEU:HB3	1:D:58:LYS:HB2	1.99	0.44
1:A:407:VAL:HG21	2:B:89:ARG:NH1	2.33	0.44
2:B:22:LEU:HA	2:B:23:PRO:HD3	1.90	0.44
2:B:64:TYR:O	2:B:85:LEU:HD12	2.18	0.44
1:A:27:ARG:HA	1:A:30:LYS:HE2	1.98	0.44
2:B:69:MET:HG2	2:B:80:GLY:HA2	1.99	0.44
1:D:190:LEU:HB3	1:D:214:CYS:SG	2.57	0.44
1:D:430:MET:CE	1:D:450:TYR:HE2	2.30	0.44
1:A:253:GLU:OE2	1:A:289:SER:HA	2.18	0.44
1:A:150:ALA:HA	1:A:153:ILE:HD12	2.00	0.44
1:D:101:LYS:HG3	1:D:117:LEU:HD22	2.00	0.44
1:D:202:ASP:OD2	1:D:205:ARG:HB3	2.18	0.44
1:D:309:ALA:O	1:D:313:LEU:HD13	2.17	0.44
1:D:389:LEU:N	1:D:389:LEU:HD12	2.32	0.44
2:E:82:ILE:HB	2:E:119:LEU:HB3	1.99	0.44
3:C:38:ALA:O	3:C:42:LYS:N	2.50	0.44
1:D:186:HIS:CE1	1:D:190:LEU:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:123:VAL:CG2	2:E:152:GLU:OE1	2.65	0.44
2:B:95:GLY:O	2:B:99:LYS:HG2	2.17	0.43
1:A:220:ARG:NH2	2:B:172:ARG:HE	2.11	0.43
1:D:542:MET:HE3	1:D:542:MET:HB2	1.87	0.43
1:A:555:TYR:OH	1:A:663:TYR:HB2	2.18	0.43
1:D:734:ILE:O	1:D:738:LEU:HB2	2.18	0.43
1:A:110:SER:OG	1:A:113:ILE:HB	2.19	0.43
1:D:276:LYS:HE2	1:D:308:THR:HG22	1.99	0.43
1:D:300:LEU:HD22	1:D:304:ARG:HB3	2.00	0.43
1:D:134:ARG:HA	1:D:134:ARG:HD3	1.60	0.43
1:D:160:ASN:ND2	1:D:163:LYS:HD2	2.33	0.43
1:A:37:LYS:HA	1:A:37:LYS:HD2	1.87	0.43
2:B:110:GLU:HB2	2:B:172:ARG:HH12	1.83	0.43
1:D:291:ALA:HB1	1:D:295:LEU:CD1	2.49	0.43
1:D:393:LEU:O	1:D:396:VAL:HG12	2.19	0.43
2:B:147:TYR:CD2	2:B:148:TYR:CD2	3.06	0.43
2:B:98:GLU:OE2	2:B:102:ARG:NH1	2.51	0.43
1:D:104:LEU:CD2	1:D:113:ILE:HG23	2.48	0.43
1:D:104:LEU:HD21	1:D:114:GLN:HB2	2.01	0.42
2:B:123:VAL:HG13	2:B:155:TYR:HE2	1.84	0.42
1:D:248:LEU:HD21	1:D:258:TYR:CD1	2.54	0.42
1:A:104:LEU:HD13	1:A:104:LEU:O	2.18	0.42
1:D:519:TRP:CD1	2:E:28:LEU:HD23	2.55	0.42
1:A:178:PRO:HA	1:A:179:PRO:HD2	1.89	0.42
1:D:134:ARG:NE	1:D:150:ALA:HB1	2.34	0.42
3:F:33:ASP:O	3:F:37:ALA:N	2.47	0.42
3:F:36:ALA:O	3:F:40:LEU:HG	2.20	0.42
1:A:30:LYS:HB2	1:A:30:LYS:HE3	1.66	0.42
1:D:253:GLU:HG3	2:E:1:FME:HCN	2.01	0.42
1:D:513:PHE:HB2	1:D:660:PHE:HE1	1.85	0.42
1:A:325:PHE:CE2	1:A:380:HIS:HA	2.55	0.41
1:A:53:LEU:HB3	1:A:58:LYS:HB2	2.02	0.41
2:E:150:ASP:HB2	2:E:151:GLY:H	1.61	0.41
1:A:542:MET:HB2	1:A:542:MET:HE3	1.89	0.41
1:D:138:LEU:HA	1:D:147:ASN:HB3	2.02	0.41
1:D:30:LYS:HB2	1:D:30:LYS:HE3	1.82	0.41
1:D:218:LEU:HB3	2:E:111:THR:HA	2.01	0.41
2:B:120:HIS:CD2	2:B:147:TYR:CE1	3.08	0.41
1:D:251:ASN:HA	1:D:252:PRO:HD2	1.85	0.41
1:D:25:TYR:O	1:D:29:LEU:HD22	2.21	0.41
3:F:35:LYS:CD	3:F:35:LYS:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:ASP:HA	3:C:36:ALA:HB3	2.01	0.41
3:C:66:MSE:HB3	3:C:66:MSE:HE2	1.88	0.41
1:A:713:ALA:O	1:A:717:LYS:HG3	2.20	0.41
3:C:33:ASP:O	3:C:37:ALA:N	2.45	0.41
1:D:446:LYS:O	1:D:449:LYS:HB3	2.20	0.41
1:D:97:ILE:HG23	1:D:98:LYS:HG3	2.02	0.41
3:C:32:GLU:O	3:C:35:LYS:HE2	2.20	0.41
1:D:325:PHE:HZ	1:D:383:TYR:HB2	1.86	0.41
2:E:109:VAL:HG21	2:E:164:LEU:HD23	2.02	0.41
2:E:30:TYR:CZ	2:E:34:HIS:HE1	2.39	0.41
1:A:412:THR:O	1:A:416:ILE:HG13	2.21	0.40
1:A:547:ASP:O	1:A:667:PHE:HE1	2.03	0.40
1:D:68:GLU:O	1:D:71:THR:HG22	2.21	0.40
1:A:318:ASP:OD1	1:A:348:TYR:OH	2.36	0.40
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.90	0.40
1:A:733:VAL:HG22	3:C:115:ILE:HG23	2.03	0.40
1:D:156:HIS:CE1	1:D:196:ILE:HG12	2.55	0.40
1:D:517:ASP:O	1:D:521:GLU:HG3	2.21	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	660/751 (88%)	647 (98%)	12 (2%)	1 (0%)	47 79
1	D	659/751 (88%)	647 (98%)	11 (2%)	1 (0%)	47 79
2	B	173/195 (89%)	170 (98%)	3 (2%)	0	100 100
2	E	177/195 (91%)	173 (98%)	3 (2%)	1 (1%)	25 59
3	C	70/133 (53%)	67 (96%)	2 (3%)	1 (1%)	11 40
3	F	62/133 (47%)	61 (98%)	1 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1801/2158 (84%)	1765 (98%)	32 (2%)	4 (0%)	47 79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	150	ASP
3	C	32	GLU
1	D	108	PRO
1	A	108	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	560/620 (90%)	552 (99%)	8 (1%)	67 86
1	D	561/620 (90%)	539 (96%)	22 (4%)	32 65
2	B	151/166 (91%)	150 (99%)	1 (1%)	84 93
2	E	153/166 (92%)	144 (94%)	9 (6%)	19 50
3	C	57/95 (60%)	54 (95%)	3 (5%)	22 54
3	F	52/95 (55%)	49 (94%)	3 (6%)	20 51
All	All	1534/1762 (87%)	1488 (97%)	46 (3%)	41 71

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	MET
1	A	51	LEU
1	A	106	LEU
1	A	304	ARG
1	A	393	LEU
1	A	396	VAL
1	A	647	LEU
1	A	723	LEU

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Mol	Chain	Res	Type
2	B	54	SER
3	C	32	GLU
3	C	40	LEU
3	C	60	GLU
1	D	8	ARG
1	D	27	ARG
1	D	29	LEU
1	D	71	THR
1	D	94	ASP
1	D	106	LEU
1	D	109	GLU
1	D	110	SER
1	D	114	GLN
1	D	115	ARG
1	D	205	ARG
1	D	248	LEU
1	D	304	ARG
1	D	387	ARG
1	D	393	LEU
1	D	396	VAL
1	D	434	ARG
1	D	435	SER
1	D	542	MET
1	D	572	LYS
1	D	685	LYS
1	D	723	LEU
2	E	2	ASP
2	E	26	TYR
2	E	28	LEU
2	E	54	SER
2	E	69	MET
2	E	88	MET
2	E	122	ARG
2	E	147	TYR
2	E	152	GLU
3	F	33	ASP
3	F	34	ARG
3	F	35	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	ASN
1	A	444	ASN
1	D	19	HIS
1	D	114	GLN
1	D	186	HIS
2	E	105	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FME	E	1	2	8,9,10	0.81	0	7,9,11	1.12	1 (14%)
2	FME	B	1	2	8,9,10	0.83	0	7,9,11	1.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	E	1	2	-	5/7/9/11	-
2	FME	B	1	2	-	5/7/9/11	-

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	E	1	FME	CA-N-CN	2.39	126.49	122.82

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	FME	O1-CN-N-CA
2	E	1	FME	N-CA-CB-CG
2	B	1	FME	CB-CA-N-CN
2	B	1	FME	N-CA-CB-CG
2	B	1	FME	O-C-CA-CB
2	B	1	FME	CA-CB-CG-SD
2	E	1	FME	C-CA-CB-CG
2	B	1	FME	C-CA-CB-CG
2	E	1	FME	CB-CG-SD-CE
2	E	1	FME	CB-CA-N-CN

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	FME	1	0
2	B	1	FME	1	0

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^{th} 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	666/751 (88%)	0.25	22 (3%)	46	24	75, 137, 189, 233	0
1	D	665/751 (88%)	0.17	18 (2%)	54	31	78, 132, 189, 248	0
2	B	174/195 (89%)	0.26	7 (4%)	38	19	76, 125, 218, 299	0
2	E	178/195 (91%)	0.20	4 (2%)	62	41	73, 125, 238, 269	0
3	C	74/133 (55%)	0.01	2 (2%)	54	31	143, 189, 279, 340	0
3	F	66/133 (49%)	0.18	5 (7%)	13	5	138, 190, 301, 355	0
All	All	1823/2158 (84%)	0.21	58 (3%)	47	25	73, 137, 214, 355	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	67	SER	6.2
1	A	341	LEU	5.1
2	E	71	GLU	4.7
1	D	148	TRP	4.0
1	D	349	LEU	3.9
3	F	32	GLU	3.8
3	F	121	TYR	3.7
1	D	112	GLN	3.6
1	A	135	LEU	3.3
3	C	33	ASP	3.3
1	A	354	ASN	3.3
2	B	105	GLN	3.2
1	D	151	LEU	3.1
1	A	137	MET	3.0
2	B	135	THR	3.0
1	D	135	LEU	2.9
1	D	137	MET	2.9
3	C	69	LEU	2.9
2	B	127	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	134	ARG	2.7
1	D	282	TYR	2.6
1	D	101	LYS	2.6
1	A	148	TRP	2.6
2	B	114	ALA	2.6
2	E	78	PRO	2.5
3	F	83	LYS	2.5
1	D	83	TYR	2.4
1	D	565	LEU	2.4
1	A	215	LYS	2.4
1	A	733	VAL	2.3
1	A	50	ALA	2.3
1	D	155	TYR	2.3
2	B	136	LEU	2.3
2	B	71	GLU	2.3
1	A	567	LEU	2.3
1	D	396	VAL	2.2
3	F	68	ALA	2.2
1	A	345	ALA	2.2
1	A	114	GLN	2.2
1	D	93	PHE	2.2
2	B	101	MET	2.2
1	A	8	ARG	2.1
2	E	76	GLY	2.1
1	A	307	THR	2.1
1	A	125	ARG	2.1
1	A	512	VAL	2.1
1	A	166	HIS	2.1
1	D	502	THR	2.1
1	D	457	ASN	2.1
2	E	144	GLU	2.1
1	D	82	VAL	2.1
1	D	341	LEU	2.1
1	A	117	LEU	2.0
1	A	535	GLN	2.0
1	A	312	TYR	2.0
1	D	312	TYR	2.0
1	A	734	ILE	2.0
1	A	732	GLU	2.0

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

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. The B-factors column lists the minimum, median, 95^{th} 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	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FME	B	1	10/11	0.89	0.36	34,130,158,293	0
2	FME	E	1	10/11	0.91	0.30	88,100,144,205	0

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.