Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 10:35 AM EDT

PDB ID	:	4XMM
Title	:	Structure of the yeast coat nucleoporin complex, space group C2
Authors	:	Stuwe, T.; Correia, A.R.; Lin, D.H.; Paduch, M.; Lu, V.T.; Kossiakoff, A.A.; Hoelz, A.
Deposited on	:	2015-01-14
Resolution	:	7.38 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:

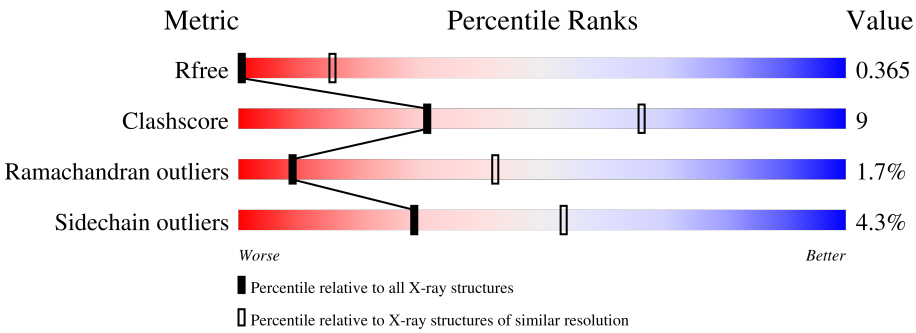
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 7.38 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	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)

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%

Mol	Chain	Length	Quality of chain
1	A	297	64% 25% • 8%
2	B	652	56% 19% • 22%
3	C	349	61% 26% • 12%
4	D	715	66% 19% • 13%
5	E	1045	71% 14% • 14%
6	F	454	68% 21% • 8%
7	H	271	71% 8% 20%

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Mol	Chain	Length	Quality of chain
8	L	217	86% 10%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 26139 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 Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	274	2160	1379	369	409	3	0	0	0

- Molecule 2 is a protein called Nucleoporin NUP145.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	511	3805	2417	648	730	10	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	61	MET	-	initiating methionine	UNP P49687
B	62	GLY	-	expression tag	UNP P49687
B	63	SER	-	expression tag	UNP P49687
B	64	SER	-	expression tag	UNP P49687
B	65	HIS	-	expression tag	UNP P49687
B	66	HIS	-	expression tag	UNP P49687
B	67	HIS	-	expression tag	UNP P49687
B	68	HIS	-	expression tag	UNP P49687
B	69	HIS	-	expression tag	UNP P49687
B	70	HIS	-	expression tag	UNP P49687
B	71	SER	-	expression tag	UNP P49687
B	72	ASP	-	expression tag	UNP P49687
B	73	GLN	-	expression tag	UNP P49687
B	74	PRO	-	expression tag	UNP P49687

- Molecule 3 is a protein called Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	307	2438	1543	422	462	11	0	0	0

- Molecule 4 is a protein called Nucleoporin NUP85.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	620	4535	2884	753	877	21	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	30	MET	-	initiating methionine	UNP P46673
D	31	GLY	-	expression tag	UNP P46673
D	32	SER	-	expression tag	UNP P46673
D	33	SER	-	expression tag	UNP P46673
D	34	HIS	-	expression tag	UNP P46673
D	35	HIS	-	expression tag	UNP P46673
D	36	HIS	-	expression tag	UNP P46673
D	37	HIS	-	expression tag	UNP P46673
D	38	HIS	-	expression tag	UNP P46673
D	39	HIS	-	expression tag	UNP P46673
D	40	SER	-	expression tag	UNP P46673
D	41	ASP	-	expression tag	UNP P46673
D	42	GLN	-	expression tag	UNP P46673
D	43	PRO	-	expression tag	UNP P46673

- Molecule 5 is a protein called Nucleoporin NUP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	896	6622	4232	1099	1275	16	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	MET	-	initiating methionine	UNP P35729
E	-6	HIS	-	expression tag	UNP P35729
E	-5	HIS	-	expression tag	UNP P35729
E	-4	HIS	-	expression tag	UNP P35729
E	-3	HIS	-	expression tag	UNP P35729
E	-2	HIS	-	expression tag	UNP P35729
E	-1	HIS	-	expression tag	UNP P35729
E	0	SER	-	expression tag	UNP P35729
E	1	THR	-	expression tag	UNP P35729

- Molecule 6 is a protein called Nucleoporin NUP84.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	419	3404	2178	557	657	12	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P52891
F	-1	PRO	-	expression tag	UNP P52891
F	0	HIS	-	expression tag	UNP P52891

- Molecule 7 is a protein called Antibody 57 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	H	217	1576	988	267	315	6	0	0	0

- Molecule 8 is a protein called Antibody 57 light chain.

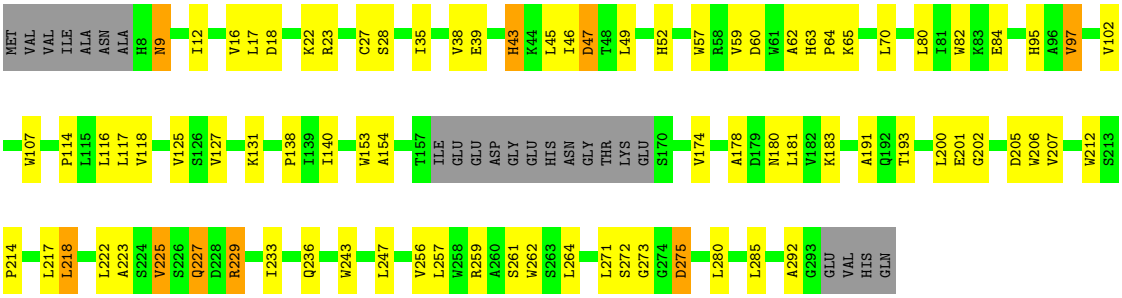
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	L	210	1599	996	270	327	6	0	0	0

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. 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. 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.

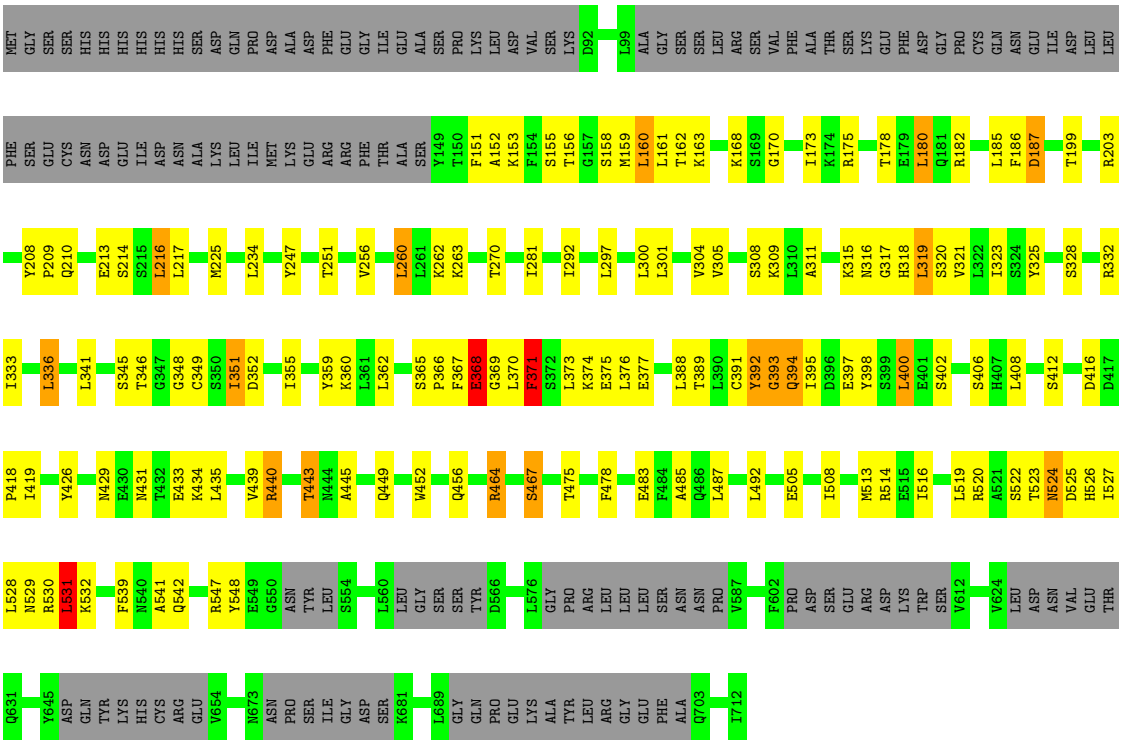
- Molecule 1: Protein transport protein SEC13

Chain A:



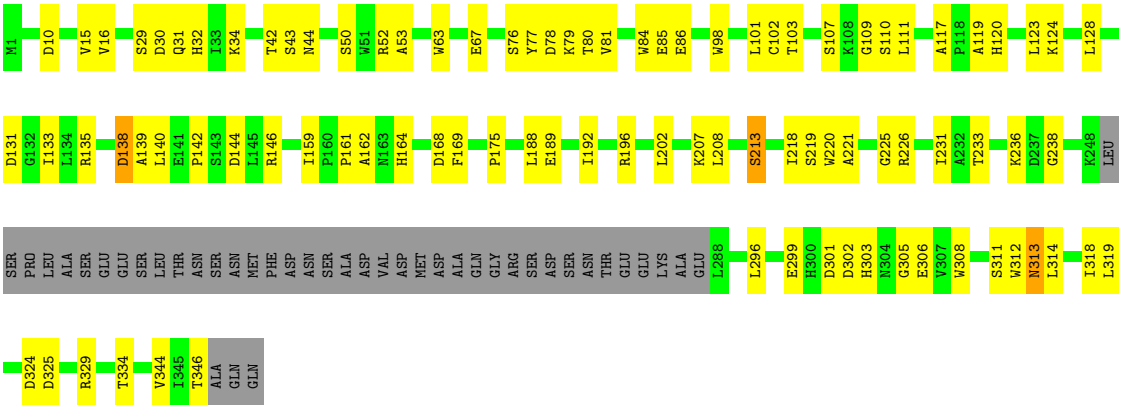
- Molecule 2: Nucleoporin NUP145

Chain B:



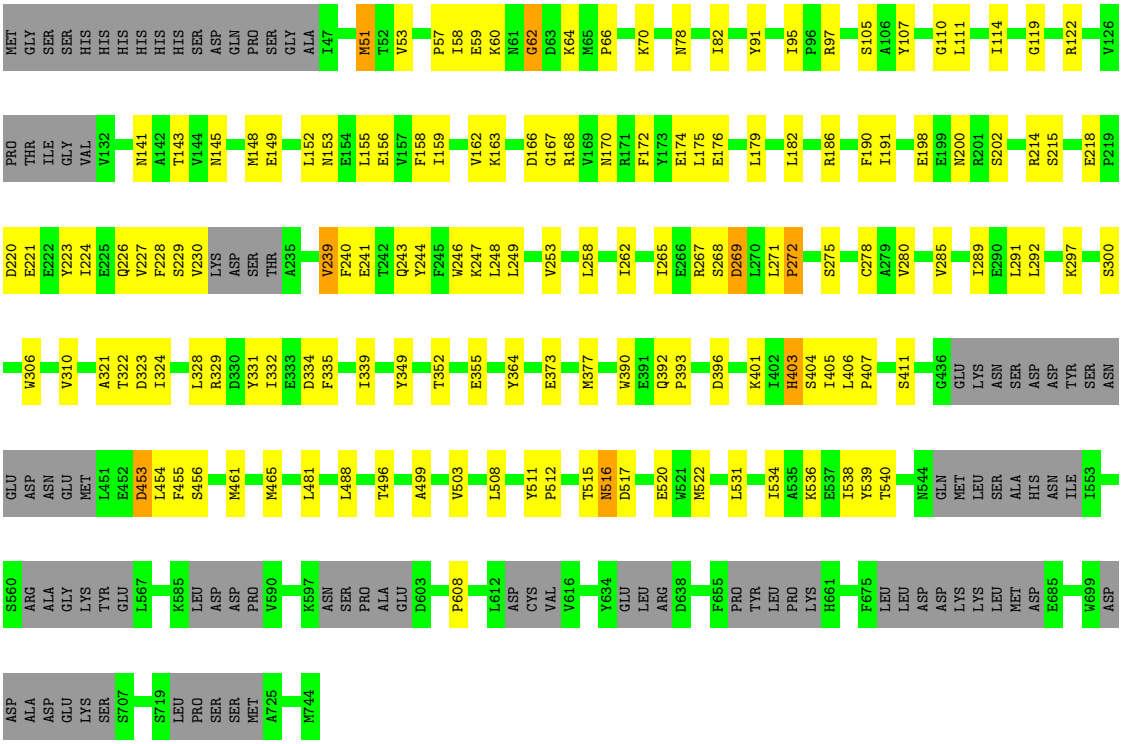
- Molecule 3: Nucleoporin SEH1

Chain C:



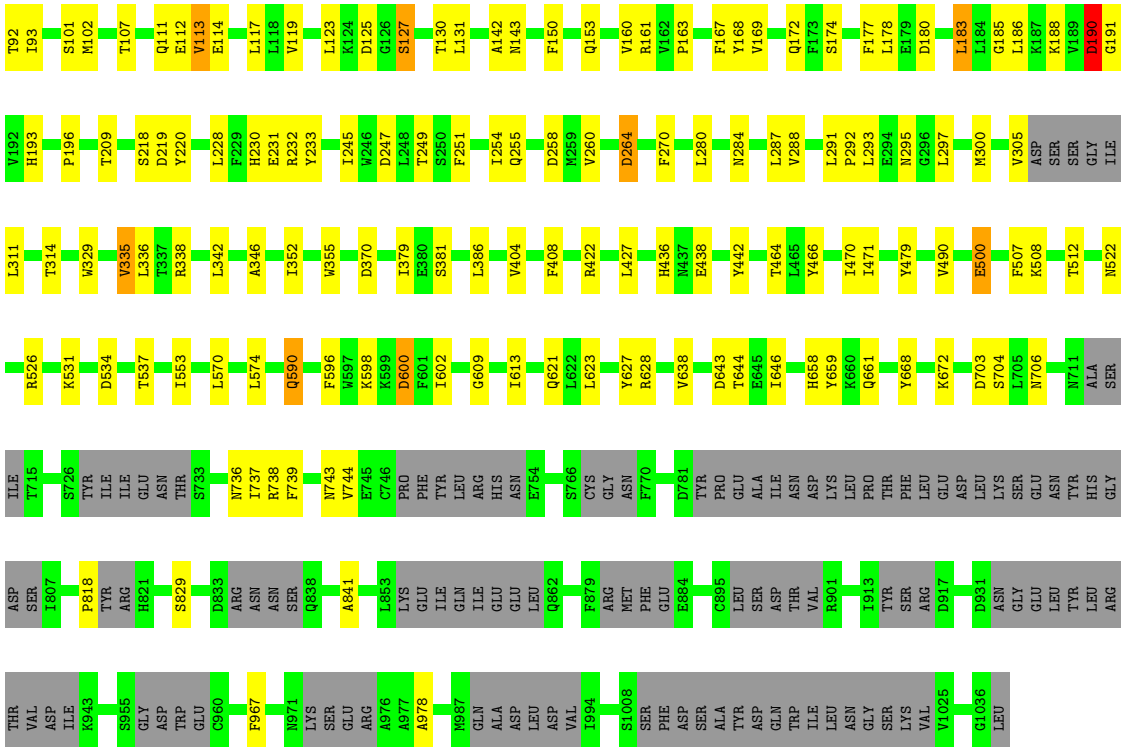
- Molecule 4: Nucleoporin NUP85

Chain D:



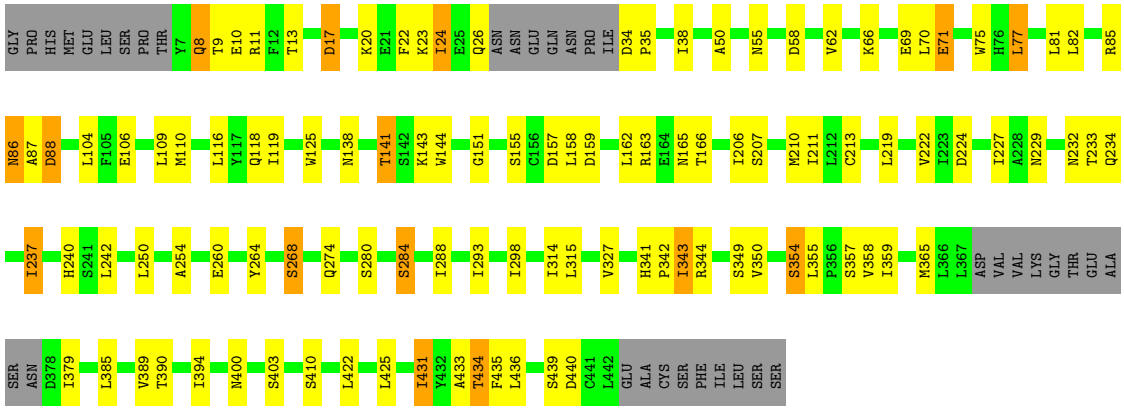
- Molecule 5: Nucleoporin NUP120

Chain E:



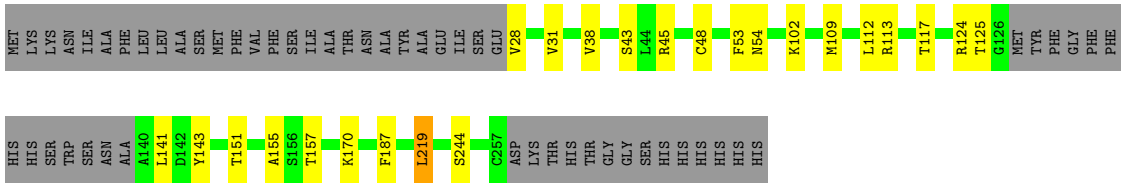
- Molecule 6: Nucleoporin NUP84

Chain F:



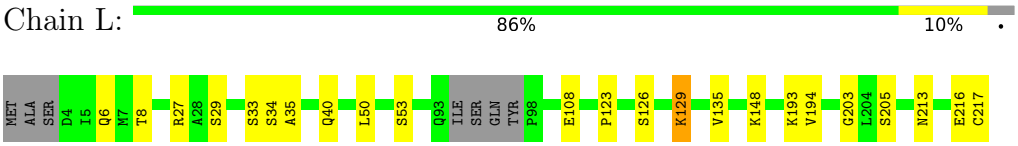
- Molecule 7: Antibody 57 heavy chain

Chain H:



- Molecule 8: Antibody 57 light chain

Chain L:


86%
10%
MET
ALA
SER
D4
I5
Q6
M7
T8
R27
A28
S29
S33
S34
A35
Q40
L50
S53
Q93
ILE
SER
GLN
TYR
P98
E108
P123
S126
K129
V135
K148
K193
V194
G203
L204
S205
N213
E216
C217

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	210.65Å 186.30Å 199.57Å 90.00° 100.85° 90.00°	Depositor
Resolution (Å)	67.52 – 7.38 68.01 – 7.38	Depositor EDS
% Data completeness (in resolution range)	99.5 (67.52-7.38) 99.7 (68.01-7.38)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 7.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1809)	Depositor
R, R_{free}	0.330 , 0.353 0.339 , 0.365	Depositor DCC
R_{free} test set	1025 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	734.6	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.48 , -10.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.75	EDS
Total number of atoms	26139	wwPDB-VP
Average B, all atoms (Å^2)	716.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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	0.32	0/2220	0.62	0/3028
2	B	0.37	0/3860	0.66	2/5224 (0.0%)
3	C	0.28	0/2499	0.64	0/3388
4	D	0.30	0/4602	0.58	2/6246 (0.0%)
5	E	0.33	0/6730	0.55	1/9158 (0.0%)
6	F	0.35	0/3472	0.64	2/4714 (0.0%)
7	H	0.31	0/1610	0.62	1/2194 (0.0%)
8	L	0.29	0/1631	0.60	0/2210
All	All	0.32	0/26624	0.60	8/36162 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
5	E	0	2
6	F	0	1
All	All	0	5

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	167	GLY	N-CA-C	-6.40	97.09	113.10
4	D	608	PRO	N-CA-CB	6.10	110.62	103.30
2	B	187	ASP	CB-CG-OD2	6.04	123.73	118.30
7	H	219	LEU	CA-CB-CG	6.04	129.19	115.30
5	E	818	PRO	N-CA-CB	5.78	110.23	103.30
2	B	260	LEU	CB-CG-CD2	-5.54	101.58	111.00
6	F	24	ILE	N-CA-C	5.49	125.83	111.00
6	F	24	ILE	CG1-CB-CG2	5.04	122.48	111.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	371	PHE	Peptide
2	B	392	TYR	Peptide
5	E	190	ASP	Mainchain
5	E	264	ASP	Sidechain
6	F	151	GLY	Mainchain

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	2160	0	2096	60	0
2	B	3805	0	3499	106	0
3	C	2438	0	2378	56	0
4	D	4535	0	4073	104	0
5	E	6622	0	5907	80	0
6	F	3404	0	3378	77	2
7	H	1576	0	1532	13	0
8	L	1599	0	1554	9	2
All	All	26139	0	24417	462	2

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 (462) 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)
5:E:537:THR:HG22	5:E:743:ASN:HA	1.54	0.86
5:E:293:LEU:HD13	5:E:297:LEU:HD12	1.59	0.85
4:D:517:ASP:OD1	7:H:54:ASN:N	2.10	0.85
4:D:159:ILE:HG12	4:D:175:LEU:HB3	1.59	0.84
4:D:156:GLU:OE2	4:D:214:ARG:NH1	2.13	0.81
6:F:314:ILE:HG22	6:F:315:LEU:HG	1.64	0.80
4:D:155:LEU:O	4:D:159:ILE:HG13	1.82	0.80
1:A:18:ASP:OD2	2:B:548:TYR:OH	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:113:VAL:HG23	5:E:114:GLU:H	1.49	0.77
4:D:141:ASN:O	4:D:145:ASN:ND2	2.18	0.76
2:B:416:ASP:HA	2:B:443:THR:HG21	1.66	0.76
2:B:292:ILE:HD12	2:B:292:ILE:H	1.52	0.75
2:B:317:GLY:HA3	6:F:250:LEU:HD13	1.70	0.74
6:F:70:LEU:HD22	6:F:343:ILE:HD11	1.68	0.74
3:C:329:ARG:HG2	3:C:344:VAL:HG22	1.70	0.73
4:D:152:LEU:HD21	4:D:182:LEU:HB3	1.70	0.72
4:D:241:GLU:HG2	4:D:328:LEU:HD13	1.71	0.71
1:A:12:ILE:HD12	2:B:170:GLY:HA3	1.73	0.71
6:F:62:VAL:HG12	6:F:66:LYS:HE3	1.73	0.71
8:L:126:SER:O	8:L:129:LYS:HB3	1.91	0.70
5:E:404:VAL:HG11	5:E:438:GLU:HA	1.74	0.70
2:B:315:LYS:HG3	6:F:162:LEU:HB3	1.74	0.70
2:B:367:PHE:O	2:B:369:GLY:N	2.26	0.69
4:D:454:LEU:O	4:D:456:SER:N	2.26	0.69
2:B:483:GLU:CD	2:B:514:ARG:HH22	1.96	0.69
4:D:163:LYS:HB2	4:D:172:PHE:CD1	2.29	0.68
3:C:220:TRP:HA	3:C:231:ILE:HG22	1.76	0.67
3:C:102:CYS:SG	3:C:103:THR:N	2.67	0.67
3:C:161:PRO:HB2	3:C:164:HIS:CD2	2.30	0.67
8:L:193:LYS:HE3	8:L:213:ASN:HB3	1.76	0.67
3:C:306:GLU:N	3:C:324:ASP:OD2	2.27	0.66
2:B:152:ALA:HB1	2:B:160:LEU:HD11	1.78	0.66
5:E:335:VAL:HG13	5:E:352:ILE:HB	1.77	0.66
2:B:209:PRO:HB3	2:B:532:LYS:HB2	1.78	0.66
8:L:33:SER:O	8:L:35:ALA:N	2.29	0.65
4:D:119:GLY:O	4:D:122:ARG:HG2	1.97	0.65
2:B:305:VAL:HG22	6:F:242:LEU:HD22	1.78	0.65
3:C:221:ALA:HB2	3:C:312:TRP:CE2	2.31	0.65
5:E:63:SER:OG	5:E:112:GLU:OE1	2.15	0.64
6:F:8:GLN:C	6:F:10:GLU:H	1.99	0.64
6:F:13:THR:O	6:F:17:ASP:N	2.24	0.64
6:F:20:LYS:O	6:F:24:ILE:HG12	1.97	0.64
5:E:55:GLU:HB2	5:E:74:SER:HA	1.78	0.64
1:A:227:GLN:HA	1:A:256:VAL:HG13	1.79	0.63
1:A:180:ASN:HA	1:A:207:VAL:HG23	1.79	0.63
7:H:109:MET:HB3	7:H:112:LEU:HD21	1.79	0.63
3:C:85:GLU:HB2	3:C:101:LEU:HD11	1.80	0.63
2:B:318:HIS:NE2	6:F:260:GLU:OE2	2.29	0.63
3:C:313:ASN:HB2	3:C:318:ILE:H	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:829:SER:HA	5:E:841:ALA:HB1	1.81	0.62
3:C:81:VAL:HG23	3:C:111:LEU:HD13	1.81	0.62
8:L:216:GLU:O	8:L:217:CYS:HB2	1.98	0.62
4:D:265:ILE:HG21	4:D:289:ILE:HD11	1.81	0.61
2:B:300:LEU:HD23	2:B:388:LEU:HD21	1.82	0.61
4:D:170:ASN:O	4:D:174:GLU:HG3	2.00	0.61
2:B:332:ARG:NH1	6:F:213:CYS:SG	2.73	0.61
3:C:42:THR:O	3:C:44:ASN:N	2.31	0.61
5:E:119:VAL:HB	5:E:131:LEU:HB2	1.82	0.61
4:D:515:THR:HG22	4:D:516:ASN:H	1.65	0.61
4:D:148:MET:HE3	4:D:152:LEU:HG	1.83	0.60
4:D:240:PHE:O	4:D:241:GLU:HG3	2.01	0.60
2:B:297:LEU:HD23	2:B:300:LEU:HD12	1.84	0.60
2:B:519:LEU:O	2:B:529:ASN:ND2	2.34	0.60
4:D:244:TYR:O	4:D:248:LEU:HG	2.02	0.59
6:F:207:SER:HA	6:F:210:MET:HE3	1.83	0.59
2:B:525:ASP:O	2:B:528:LEU:HB2	2.02	0.59
5:E:609:GLY:O	5:E:613:ILE:HG22	2.02	0.59
2:B:426:TYR:O	2:B:464:ARG:NH2	2.36	0.59
5:E:596:PHE:CZ	5:E:704:SER:HA	2.38	0.59
5:E:91:LYS:NZ	5:E:142:ALA:O	2.30	0.59
4:D:162:VAL:O	4:D:166:ASP:HB3	2.03	0.59
2:B:152:ALA:HB1	2:B:160:LEU:CD1	2.32	0.59
1:A:217:LEU:HD22	1:A:218:LEU:H	1.69	0.58
4:D:258:LEU:HD22	4:D:292:LEU:HD22	1.85	0.58
4:D:534:ILE:O	4:D:538:ILE:HG12	2.02	0.58
3:C:123:LEU:HB2	3:C:139:ALA:HB3	1.86	0.58
4:D:163:LYS:HD2	4:D:172:PHE:CZ	2.39	0.58
2:B:321:VAL:HG11	6:F:211:ILE:HG23	1.85	0.58
4:D:520:GLU:OE2	7:H:54:ASN:ND2	2.37	0.58
5:E:185:GLY:O	5:E:196:PRO:HA	2.04	0.58
1:A:205:ASP:HB3	1:A:227:GLN:HB3	1.85	0.57
2:B:180:LEU:HD21	2:B:185:LEU:HD13	1.85	0.57
5:E:245:ILE:HB	5:E:255:GLN:HB2	1.84	0.57
6:F:280:SER:HB2	6:F:284:SER:HB3	1.86	0.57
3:C:225:GLY:O	4:D:453:ASP:HB3	2.04	0.57
6:F:433:ALA:HB1	6:F:439:SER:OG	2.05	0.57
5:E:329:TRP:HB3	5:E:355:TRP:HB3	1.85	0.57
3:C:238:GLY:HA2	3:C:305:GLY:O	2.05	0.57
5:E:342:LEU:HD13	5:E:379:ILE:HD12	1.86	0.57
5:E:101:SER:HA	5:E:123:LEU:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:71:GLU:OE1	6:F:75:TRP:NE1	2.36	0.57
6:F:343:ILE:HD13	6:F:344:ARG:N	2.19	0.57
1:A:117:LEU:HB2	1:A:153:TRP:NE1	2.20	0.56
2:B:199:THR:HB	2:B:213:GLU:HB2	1.87	0.56
4:D:145:ASN:OD1	4:D:190:PHE:HA	2.04	0.56
4:D:159:ILE:HG22	4:D:172:PHE:CE1	2.39	0.56
4:D:271:LEU:O	4:D:275:SER:HB3	2.04	0.56
5:E:659:TYR:OH	5:E:744:VAL:HA	2.05	0.56
4:D:508:LEU:HG	4:D:522:MET:HE3	1.87	0.56
5:E:288:VAL:HG12	5:E:300:MET:HB3	1.88	0.56
2:B:156:THR:HG22	2:B:514:ARG:HD2	1.88	0.56
5:E:537:THR:CG2	5:E:743:ASN:HA	2.31	0.56
4:D:536:LYS:O	4:D:540:THR:OG1	2.20	0.56
7:H:157:THR:HG22	7:H:244:SER:HB3	1.87	0.56
1:A:49:LEU:HB3	1:A:82:TRP:CZ3	2.42	0.56
6:F:34:ASP:HB3	6:F:35:PRO:HD3	1.88	0.55
2:B:256:VAL:HA	6:F:222:VAL:CG1	2.36	0.55
4:D:159:ILE:HG21	4:D:176:GLU:HG2	1.87	0.55
2:B:359:TYR:HA	2:B:362:LEU:HD12	1.86	0.55
6:F:237:ILE:HD11	6:F:240:HIS:HA	1.87	0.55
6:F:410:SER:HA	6:F:436:LEU:HD11	1.88	0.55
2:B:433:GLU:OE1	2:B:467:SER:OG	2.20	0.55
1:A:200:LEU:HD11	1:A:243:TRP:CD1	2.41	0.55
2:B:180:LEU:HD11	2:B:478:PHE:HE1	1.71	0.55
2:B:292:ILE:HD11	6:F:163:ARG:HD3	1.88	0.55
5:E:245:ILE:HG21	5:E:311:LEU:HD23	1.88	0.55
8:L:33:SER:C	8:L:35:ALA:H	2.09	0.55
1:A:95:HIS:CE1	1:A:97:VAL:HG22	2.42	0.55
3:C:15:VAL:O	4:D:70:LYS:HD2	2.07	0.55
4:D:163:LYS:HB2	4:D:172:PHE:CE1	2.41	0.55
1:A:236:GLN:HB2	1:A:243:TRP:CE3	2.42	0.55
4:D:461:MET:O	4:D:465:MET:HG3	2.07	0.55
6:F:350:VAL:HG22	6:F:355:LEU:HD22	1.90	0.54
4:D:328:LEU:O	4:D:332:ILE:HG13	2.08	0.54
1:A:9:ASN:OD1	1:A:12:ILE:HD11	2.08	0.54
1:A:212:TRP:HA	1:A:222:LEU:HD23	1.90	0.54
2:B:351:ILE:HA	6:F:155:SER:HA	1.88	0.54
2:B:525:ASP:HA	2:B:528:LEU:HD12	1.90	0.54
4:D:186:ARG:HA	4:D:190:PHE:HB2	1.90	0.54
4:D:280:VAL:HG21	4:D:321:ALA:HB3	1.89	0.54
2:B:520:ARG:NH2	2:B:542:GLN:HE21	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:102:MET:HB3	5:E:107:THR:HG21	1.89	0.54
1:A:64:PRO:HB3	2:B:548:TYR:HB2	1.90	0.54
1:A:275:ASP:OD1	1:A:275:ASP:N	2.41	0.53
6:F:341:HIS:CE1	6:F:343:ILE:HD12	2.43	0.53
4:D:265:ILE:C	4:D:267:ARG:H	2.12	0.53
2:B:186:PHE:HD1	2:B:487:LEU:HD11	1.74	0.53
3:C:128:LEU:HD23	3:C:169:PHE:HB3	1.89	0.53
3:C:53:ALA:HB1	3:C:84:TRP:CZ2	2.44	0.52
2:B:336:LEU:HB3	6:F:206:ILE:HG23	1.91	0.52
2:B:345:SER:HB3	2:B:371:PHE:CE2	2.43	0.52
2:B:520:ARG:HH21	2:B:542:GLN:HE21	1.58	0.52
2:B:256:VAL:HA	6:F:222:VAL:HG12	1.90	0.52
5:E:232:ARG:NE	5:E:249:THR:OG1	2.39	0.52
3:C:324:ASP:HB3	4:D:64:LYS:HB3	1.90	0.52
4:D:227:VAL:C	4:D:229:SER:H	2.12	0.52
1:A:154:ALA:HB2	1:A:212:TRP:CE3	2.44	0.52
1:A:178:ALA:HB1	1:A:206:TRP:CE2	2.44	0.52
6:F:431:ILE:HD12	6:F:431:ILE:H	1.74	0.52
2:B:355:ILE:HG21	6:F:157:ASP:HB3	1.92	0.52
2:B:524:ASN:O	2:B:528:LEU:HG	2.10	0.52
4:D:517:ASP:CG	7:H:53:PHE:HA	2.31	0.52
2:B:178:THR:HG21	2:B:485:ALA:HB2	1.91	0.51
5:E:739:PHE:O	5:E:743:ASN:N	2.36	0.51
1:A:117:LEU:HB2	1:A:153:TRP:HE1	1.75	0.51
1:A:214:PRO:HG2	1:A:264:LEU:HA	1.93	0.51
3:C:29:SER:C	3:C:31:GLN:H	2.13	0.51
1:A:261:SER:CB	2:B:153:LYS:HA	2.41	0.51
5:E:258:ASP:OD1	5:E:260:VAL:HG22	2.11	0.51
5:E:500:GLU:HB2	5:E:507:PHE:CZ	2.45	0.51
5:E:531:LYS:HB3	5:E:553:ILE:HG12	1.93	0.51
1:A:62:ALA:HB2	1:A:107:TRP:CE2	2.46	0.51
2:B:315:LYS:NZ	6:F:254:ALA:O	2.40	0.51
5:E:58:ASN:HB3	5:E:70:TYR:CZ	2.46	0.51
4:D:152:LEU:O	4:D:156:GLU:HG3	2.11	0.51
1:A:259:ARG:HB2	1:A:272:SER:HB2	1.93	0.51
2:B:281:ILE:HB	2:B:301:LEU:HD21	1.93	0.51
2:B:435:LEU:O	2:B:439:VAL:HG23	2.11	0.51
5:E:70:TYR:HA	5:E:80:THR:O	2.10	0.51
3:C:308:TRP:CD1	4:D:66:PRO:HA	2.46	0.51
5:E:190:ASP:OD2	5:E:191:GLY:N	2.44	0.51
2:B:186:PHE:CD1	2:B:487:LEU:HD11	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:156:GLU:HG2	4:D:179:LEU:CD2	2.41	0.50
6:F:50:ALA:HB1	6:F:69:GLU:HG3	1.93	0.50
2:B:397:GLU:OE1	2:B:397:GLU:N	2.40	0.50
3:C:117:ALA:HB3	3:C:124:LYS:HB3	1.93	0.50
4:D:107:TYR:CZ	4:D:111:LEU:HD11	2.47	0.50
5:E:288:VAL:HG13	5:E:336:LEU:HD22	1.94	0.50
2:B:374:LYS:O	2:B:377:GLU:HB2	2.11	0.50
6:F:354:SER:O	6:F:358:VAL:HG23	2.11	0.50
2:B:389:THR:O	2:B:393:GLY:HA3	2.10	0.50
3:C:10:ASP:HB3	3:C:29:SER:HB2	1.92	0.50
3:C:218:ILE:HG22	3:C:233:THR:HG22	1.94	0.50
4:D:218:GLU:HA	4:D:220:ASP:N	2.27	0.50
4:D:306:TRP:O	4:D:310:VAL:HG23	2.12	0.50
5:E:466:TYR:HB3	5:E:470:ILE:HB	1.92	0.50
1:A:57:TRP:HD1	1:A:102:VAL:O	1.94	0.50
5:E:125:ASP:OD1	5:E:127:SER:OG	2.17	0.50
3:C:67:GLU:OE1	3:C:119:ALA:HB1	2.12	0.49
4:D:110:GLY:O	4:D:114:ILE:HG13	2.12	0.49
4:D:158:PHE:O	4:D:162:VAL:HG23	2.12	0.49
6:F:233:THR:HG22	6:F:234:GLN:O	2.12	0.49
8:L:40:GLN:HB2	8:L:50:LEU:HD11	1.93	0.49
1:A:138:PRO:HB2	1:A:140:ILE:HD11	1.93	0.49
6:F:379:ILE:HG13	6:F:385:LEU:HD23	1.94	0.49
2:B:523:THR:HA	2:B:526:HIS:HB2	1.95	0.49
4:D:60:LYS:C	4:D:62:GLY:H	2.14	0.49
1:A:174:VAL:HA	1:A:183:LYS:O	2.13	0.49
4:D:278:CYS:SG	4:D:323:ASP:HB2	2.53	0.49
5:E:53:GLY:HA2	5:E:73:SER:HA	1.94	0.49
1:A:181:LEU:HD23	1:A:201:GLU:HG2	1.95	0.49
2:B:317:GLY:O	2:B:320:SER:HB3	2.13	0.49
2:B:483:GLU:OE2	2:B:514:ARG:NH2	2.35	0.49
1:A:229:ARG:HH11	1:A:229:ARG:HB2	1.78	0.48
1:A:272:SER:OG	2:B:152:ALA:HB3	2.13	0.48
3:C:77:TYR:HA	3:C:110:SER:HB3	1.95	0.48
1:A:118:VAL:O	1:A:125:VAL:HA	2.14	0.48
2:B:182:ARG:HD2	2:B:449:GLN:OE1	2.13	0.48
5:E:160:VAL:HG23	5:E:161:ARG:N	2.28	0.48
5:E:522:ASN:O	5:E:526:ARG:HG3	2.12	0.48
2:B:173:ILE:HD12	2:B:173:ILE:H	1.78	0.48
5:E:967:PHE:HA	5:E:978:ALA:HB2	1.95	0.48
6:F:349:SER:OG	6:F:358:VAL:HG21	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:ASP:OD1	3:C:32:HIS:HB2	2.13	0.48
4:D:228:PHE:HE2	4:D:267:ARG:HB3	1.77	0.48
3:C:311:SER:O	3:C:319:LEU:HD12	2.13	0.48
3:C:312:TRP:CZ3	3:C:319:LEU:HB2	2.48	0.48
1:A:38:VAL:O	1:A:39:GLU:HG3	2.14	0.48
4:D:262:ILE:HG12	4:D:289:ILE:HG23	1.96	0.48
5:E:24:VAL:HG11	5:E:143:ASN:HA	1.95	0.48
5:E:233:TYR:CG	5:E:311:LEU:HD22	2.49	0.47
2:B:262:LYS:NZ	2:B:398:TYR:O	2.36	0.47
5:E:188:LYS:HE2	5:E:191:GLY:HA2	1.95	0.47
5:E:247:ASP:O	5:E:251:PHE:N	2.47	0.47
3:C:324:ASP:HB3	4:D:64:LYS:HD3	1.95	0.47
1:A:43:HIS:CD2	2:B:173:ILE:HD11	2.50	0.47
3:C:34:LYS:HG2	3:C:50:SER:HB2	1.95	0.47
4:D:152:LEU:HD22	4:D:179:LEU:HD12	1.97	0.47
3:C:159:ILE:O	3:C:161:PRO:HD3	2.15	0.47
5:E:24:VAL:HG23	5:E:93:ILE:HG23	1.95	0.47
5:E:160:VAL:HG23	5:E:161:ARG:H	1.79	0.47
6:F:431:ILE:HD12	6:F:431:ILE:N	2.30	0.47
3:C:312:TRP:CE2	3:C:319:LEU:HD13	2.50	0.47
4:D:186:ARG:HG3	4:D:190:PHE:HB2	1.97	0.47
4:D:392:GLN:HB3	4:D:393:PRO:HD3	1.96	0.47
5:E:163:PRO:HA	5:E:178:LEU:HA	1.95	0.47
6:F:293:ILE:HD11	6:F:327:VAL:HG21	1.97	0.47
7:H:31:VAL:O	7:H:48:CYS:HA	2.14	0.47
2:B:270:THR:OG1	2:B:391:CYS:SG	2.72	0.47
6:F:157:ASP:OD1	6:F:163:ARG:NH2	2.46	0.47
4:D:249:LEU:O	4:D:253:VAL:HG23	2.15	0.47
6:F:86:ASN:OD1	6:F:400:ASN:ND2	2.48	0.47
2:B:304:VAL:HG13	2:B:323:ILE:HG22	1.97	0.47
3:C:219:SER:HG	3:C:312:TRP:HD1	1.61	0.47
5:E:570:LEU:O	5:E:574:LEU:HB2	2.15	0.47
6:F:207:SER:O	6:F:211:ILE:HG13	2.15	0.47
6:F:431:ILE:H	6:F:431:ILE:CD1	2.28	0.47
3:C:140:LEU:O	3:C:142:PRO:HD3	2.15	0.46
1:A:227:GLN:OE1	1:A:256:VAL:HG11	2.15	0.46
2:B:256:VAL:HG13	6:F:222:VAL:O	2.15	0.46
2:B:309:LYS:HE3	6:F:314:ILE:HD12	1.98	0.46
3:C:236:LYS:HG3	3:C:306:GLU:OE1	2.15	0.46
1:A:12:ILE:HA	1:A:28:SER:HA	1.96	0.46
2:B:319:LEU:HB2	6:F:159:ASP:OD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:VAL:HG12	3:C:63:TRP:HD1	1.81	0.46
3:C:196:ARG:HH11	3:C:202:LEU:HD21	1.78	0.46
2:B:431:ASN:HB2	2:B:434:LYS:HB3	1.96	0.46
4:D:226:GLN:O	4:D:230:VAL:HG23	2.15	0.46
1:A:12:ILE:HG23	1:A:27:CYS:O	2.15	0.46
4:D:223:TYR:HA	4:D:226:GLN:HB2	1.96	0.46
6:F:8:GLN:O	6:F:10:GLU:N	2.48	0.46
2:B:156:THR:HG22	2:B:514:ARG:CD	2.45	0.46
5:E:490:VAL:HG22	5:E:590:GLN:HG3	1.97	0.46
1:A:16:VAL:HG21	1:A:59:VAL:O	2.16	0.46
1:A:259:ARG:NH1	2:B:151:PHE:HB2	2.30	0.46
5:E:177:PHE:CD1	5:E:183:LEU:HD22	2.51	0.46
2:B:526:HIS:C	2:B:528:LEU:N	2.68	0.46
1:A:95:HIS:NE2	1:A:138:PRO:HB3	2.31	0.46
1:A:116:LEU:O	1:A:127:VAL:HA	2.16	0.46
2:B:360:LYS:HG3	2:B:366:PRO:HA	1.97	0.46
2:B:526:HIS:C	2:B:530:ARG:HD2	2.36	0.46
3:C:208:LEU:HD11	3:C:231:ILE:CD1	2.46	0.46
2:B:325:TYR:OH	6:F:210:MET:O	2.21	0.45
4:D:97:ARG:HB3	4:D:97:ARG:NH1	2.32	0.45
4:D:268:SER:HB2	4:D:269:ASP:OD1	2.17	0.45
6:F:433:ALA:O	6:F:435:PHE:N	2.44	0.45
6:F:219:LEU:HD22	6:F:227:ILE:HG12	1.98	0.45
4:D:97:ARG:NH2	4:D:411:SER:O	2.50	0.45
8:L:123:PRO:HD3	8:L:135:VAL:HG22	1.98	0.45
2:B:492:LEU:HD12	2:B:508:ILE:HD13	1.96	0.45
4:D:152:LEU:CD2	4:D:182:LEU:HB3	2.44	0.45
4:D:453:ASP:OD1	4:D:499:ALA:HB1	2.17	0.45
7:H:43:SER:HA	7:H:109:MET:O	2.16	0.45
2:B:178:THR:HG22	2:B:180:LEU:H	1.81	0.45
2:B:352:ASP:HB3	2:B:355:ILE:HD13	1.98	0.45
3:C:124:LYS:HG3	3:C:138:ASP:OD1	2.17	0.45
5:E:291:LEU:HA	5:E:292:PRO:HD3	1.76	0.45
5:E:643:ASP:OD2	5:E:646:ILE:HG13	2.17	0.45
6:F:144:TRP:CH2	6:F:158:LEU:HA	2.51	0.45
1:A:16:VAL:HG23	1:A:59:VAL:HG23	1.98	0.45
4:D:153:ASN:HA	4:D:156:GLU:OE1	2.16	0.45
5:E:4:LEU:HB2	5:E:381:SER:HB2	1.96	0.45
2:B:393:GLY:O	2:B:394:GLN:HB2	2.17	0.45
3:C:208:LEU:HD11	3:C:231:ILE:HD11	1.97	0.45
6:F:284:SER:O	6:F:288:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:513:MET:HG2	2:B:541:ALA:HB2	1.99	0.45
4:D:198:GLU:HG2	4:D:300:SER:CB	2.47	0.45
4:D:268:SER:O	4:D:272:PRO:HG2	2.16	0.45
5:E:436:HIS:NE2	5:E:438:GLU:HB2	2.31	0.45
1:A:18:ASP:OD1	1:A:18:ASP:N	2.46	0.45
5:E:130:THR:O	5:E:150:PHE:HA	2.17	0.45
6:F:143:LYS:HG3	6:F:144:TRP:N	2.32	0.45
4:D:322:THR:HG23	4:D:329:ARG:HD3	1.97	0.44
1:A:43:HIS:HD2	2:B:173:ILE:HD11	1.82	0.44
3:C:296:LEU:HD21	3:C:299:GLU:HG3	1.98	0.44
7:H:155:ALA:HB3	7:H:187:PHE:CE1	2.52	0.44
5:E:623:LEU:HD23	5:E:623:LEU:HA	1.74	0.44
6:F:81:LEU:HD13	6:F:85:ARG:NH2	2.32	0.44
6:F:116:LEU:O	6:F:119:ILE:HB	2.17	0.44
6:F:264:TYR:O	6:F:268:SER:OG	2.34	0.44
4:D:285:VAL:O	4:D:289:ILE:HG13	2.18	0.44
4:D:406:LEU:HB2	4:D:407:PRO:HD3	1.98	0.44
6:F:8:GLN:C	6:F:10:GLU:N	2.68	0.44
7:H:28:VAL:HG11	7:H:143:TYR:CE1	2.53	0.44
3:C:31:GLN:OE1	3:C:52:ARG:NH1	2.50	0.44
4:D:202:SER:HA	4:D:297:LYS:O	2.18	0.44
5:E:247:ASP:HB2	5:E:254:ILE:HG13	1.98	0.44
1:A:257:LEU:HA	1:A:273:GLY:HA2	1.98	0.44
5:E:352:ILE:HD13	5:E:471:ILE:HG12	1.99	0.44
5:E:658:HIS:HA	5:E:661:GLN:OE1	2.18	0.44
1:A:35:ILE:HB	1:A:47:ASP:HB2	2.00	0.44
2:B:391:CYS:O	2:B:395:ILE:HD11	2.17	0.44
5:E:534:ASP:HA	5:E:537:THR:OG1	2.18	0.44
4:D:141:ASN:N	4:D:141:ASN:HD22	2.16	0.44
5:E:668:TYR:CZ	5:E:672:LYS:HE3	2.53	0.44
7:H:125:THR:HG23	7:H:141:LEU:HD23	1.99	0.44
2:B:256:VAL:HG22	6:F:222:VAL:O	2.18	0.44
2:B:392:TYR:O	2:B:394:GLN:N	2.44	0.44
3:C:107:SER:HA	3:C:135:ARG:HH21	1.83	0.44
5:E:218:SER:OG	5:E:219:ASP:N	2.50	0.44
5:E:427:LEU:HD13	5:E:442:TYR:CE1	2.53	0.44
2:B:311:ALA:HB1	2:B:316:ASN:O	2.18	0.43
4:D:328:LEU:HA	4:D:331:TYR:HB2	2.00	0.43
6:F:106:GLU:O	6:F:110:MET:HG2	2.18	0.43
2:B:394:GLN:HG2	2:B:397:GLU:HB2	2.00	0.43
6:F:385:LEU:O	6:F:389:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:ILE:HG23	6:F:210:MET:SD	2.59	0.43
5:E:297:LEU:HD23	5:E:297:LEU:HA	1.88	0.43
1:A:52:HIS:CE1	1:A:80:LEU:HD12	2.53	0.43
2:B:319:LEU:N	6:F:159:ASP:OD2	2.29	0.43
6:F:390:THR:O	6:F:394:ILE:HG12	2.19	0.43
2:B:309:LYS:CE	6:F:314:ILE:HD12	2.48	0.43
4:D:58:ILE:HG22	4:D:59:GLU:N	2.33	0.43
4:D:221:GLU:HA	4:D:224:ILE:HG13	2.00	0.43
5:E:736:ASN:C	5:E:738:ARG:H	2.21	0.43
8:L:6:GLN:HB2	8:L:29:SER:HB3	2.01	0.43
1:A:63:HIS:CD2	1:A:64:PRO:HD2	2.53	0.43
2:B:400:LEU:HB3	2:B:426:TYR:OH	2.18	0.43
3:C:303:HIS:HA	3:C:325:ASP:OD2	2.19	0.43
5:E:508:LYS:O	5:E:512:THR:HG23	2.19	0.43
6:F:109:LEU:HD23	6:F:298:ILE:HG13	2.00	0.43
4:D:243:GLN:O	4:D:247:LYS:HG3	2.19	0.43
4:D:390:TRP:C	4:D:393:PRO:HD2	2.39	0.43
6:F:82:LEU:HD23	6:F:82:LEU:HA	1.87	0.43
8:L:194:VAL:HG22	8:L:213:ASN:ND2	2.34	0.43
3:C:131:ASP:OD2	3:C:135:ARG:NH2	2.51	0.43
4:D:511:TYR:HA	4:D:512:PRO:HD3	1.73	0.43
6:F:77:LEU:HG	6:F:125:TRP:CD2	2.54	0.43
7:H:117:THR:HG23	7:H:151:THR:HA	2.01	0.43
4:D:215:SER:HB2	4:D:390:TRP:CH2	2.54	0.43
4:D:215:SER:HB2	4:D:390:TRP:CZ2	2.53	0.43
4:D:335:PHE:O	4:D:339:ILE:HG13	2.19	0.43
5:E:627:TYR:HA	5:E:661:GLN:OE1	2.19	0.43
1:A:45:LEU:HB2	2:B:168:LYS:HE2	2.01	0.42
1:A:261:SER:HB2	2:B:153:LYS:HA	2.01	0.42
1:A:280:LEU:HB2	1:A:292:ALA:O	2.19	0.42
2:B:345:SER:HB3	2:B:371:PHE:HE2	1.84	0.42
2:B:531:LEU:O	2:B:532:LYS:HG2	2.19	0.42
6:F:86:ASN:C	6:F:88:ASP:H	2.23	0.42
6:F:227:ILE:C	6:F:229:ASN:H	2.22	0.42
6:F:293:ILE:HD11	6:F:327:VAL:CG2	2.49	0.42
2:B:208:TYR:CE2	2:B:505:GLU:HG3	2.54	0.42
2:B:247:TYR:CE2	2:B:260:LEU:HD13	2.54	0.42
2:B:513:MET:HA	2:B:541:ALA:HB1	2.02	0.42
3:C:313:ASN:HD22	3:C:313:ASN:HA	1.61	0.42
4:D:454:LEU:HD21	4:D:503:VAL:HG21	2.01	0.42
2:B:418:PRO:HB3	2:B:445:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:295:ASN:ND2	5:E:329:TRP:O	2.52	0.42
6:F:341:HIS:HA	6:F:342:PRO:HD3	1.89	0.42
5:E:177:PHE:HD1	5:E:183:LEU:HD22	1.84	0.42
5:E:180:ASP:HA	5:E:220:TYR:CD1	2.55	0.42
2:B:203:ARG:NE	2:B:210:GLN:HB2	2.34	0.42
4:D:168:ARG:HD3	4:D:170:ASN:HB3	2.02	0.42
5:E:53:GLY:HA3	5:E:71:HIS:HB3	2.02	0.42
5:E:92:THR:HG21	5:E:479:TYR:OH	2.19	0.42
3:C:76:SER:HB3	3:C:78:ASP:OD1	2.19	0.42
4:D:149:GLU:HG3	4:D:186:ARG:NE	2.34	0.42
4:D:159:ILE:HD13	4:D:176:GLU:HA	2.01	0.42
5:E:386:LEU:HD23	5:E:621:GLN:HA	2.01	0.42
2:B:365:SER:HB3	2:B:368:GLU:HB2	2.01	0.42
2:B:452:TRP:CD1	2:B:475:THR:HA	2.54	0.42
3:C:189:GLU:HA	3:C:213:SER:O	2.20	0.42
4:D:57:PRO:HB3	4:D:91:TYR:OH	2.19	0.42
5:E:111:GLN:HG3	5:E:168:TYR:CG	2.55	0.42
1:A:222:LEU:O	1:A:233:ILE:HA	2.20	0.42
3:C:192:ILE:HG22	3:C:207:LYS:HG2	2.02	0.42
5:E:436:HIS:CD2	5:E:438:GLU:H	2.37	0.42
6:F:23:LYS:HD2	6:F:434:THR:HG21	2.01	0.42
1:A:60:ASP:H	1:A:70:LEU:CD1	2.33	0.42
5:E:59:CYS:HB2	5:E:464:THR:OG1	2.19	0.42
5:E:153:GLN:OE1	5:E:193:HIS:HA	2.20	0.42
5:E:287:LEU:O	5:E:300:MET:HA	2.20	0.41
6:F:22:PHE:CG	6:F:38:ILE:HD11	2.54	0.41
4:D:78:ASN:HD21	4:D:95:ILE:HG13	1.85	0.41
4:D:269:ASP:OD1	4:D:269:ASP:N	2.53	0.41
6:F:104:LEU:HG	6:F:224:ASP:HB3	2.02	0.41
6:F:359:ILE:HD13	6:F:389:VAL:HG13	2.02	0.41
7:H:102:LYS:HE2	7:H:102:LYS:HB3	1.87	0.41
2:B:216:LEU:O	2:B:217:LEU:HD23	2.19	0.41
3:C:77:TYR:HD1	3:C:110:SER:HB3	1.86	0.41
3:C:131:ASP:O	3:C:133:ILE:HG13	2.20	0.41
3:C:175:PRO:HD3	3:C:220:TRP:HB3	2.02	0.41
5:E:117:LEU:HD23	5:E:117:LEU:HA	1.90	0.41
7:H:38:VAL:HG11	7:H:112:LEU:HD13	2.02	0.41
1:A:191:ALA:C	1:A:193:THR:H	2.23	0.41
2:B:162:THR:HG22	2:B:163:LYS:N	2.35	0.41
2:B:373:LEU:HB3	2:B:376:LEU:HD12	2.02	0.41
3:C:79:LYS:HG2	3:C:109:GLY:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LEU:HD22	2:B:440:ARG:HB3	2.02	0.41
2:B:155:SER:HB3	2:B:159:MET:H	1.85	0.41
3:C:346:THR:C	4:D:51:MET:HB3	2.41	0.41
4:D:152:LEU:HD23	4:D:152:LEU:HA	1.85	0.41
5:E:186:LEU:HD12	5:E:186:LEU:HA	1.91	0.41
6:F:81:LEU:HD12	6:F:350:VAL:HG12	2.00	0.41
4:D:141:ASN:C	4:D:145:ASN:HD22	2.24	0.41
4:D:396:ASP:OD1	4:D:401:LYS:HE3	2.20	0.41
2:B:263:LYS:HD3	2:B:263:LYS:HA	1.75	0.41
3:C:144:ASP:C	3:C:146:ARG:H	2.24	0.41
4:D:57:PRO:HB2	4:D:82:ILE:HD11	2.03	0.41
4:D:141:ASN:C	4:D:145:ASN:ND2	2.74	0.41
4:D:373:GLU:O	4:D:377:MET:HG3	2.21	0.41
5:E:167:PHE:O	5:E:174:SER:HB2	2.21	0.41
1:A:223:ALA:HB2	1:A:262:TRP:CZ2	2.55	0.41
2:B:247:TYR:CZ	2:B:260:LEU:HD13	2.56	0.41
2:B:375:GLU:C	2:B:377:GLU:H	2.24	0.41
4:D:403:HIS:O	4:D:405:ILE:HG23	2.20	0.41
1:A:63:HIS:HD2	1:A:65:LYS:H	1.68	0.41
4:D:240:PHE:CD1	4:D:268:SER:HB3	2.56	0.41
5:E:169:VAL:HG13	5:E:228:LEU:HD22	2.03	0.41
1:A:261:SER:HB2	2:B:153:LYS:HG2	2.03	0.40
3:C:86:GLU:HB2	3:C:98:TRP:CZ2	2.56	0.40
4:D:145:ASN:OD1	4:D:190:PHE:CA	2.69	0.40
4:D:159:ILE:HG12	4:D:175:LEU:CB	2.40	0.40
4:D:531:LEU:HB3	4:D:534:ILE:CG1	2.51	0.40
6:F:13:THR:O	6:F:17:ASP:HB2	2.21	0.40
1:A:217:LEU:HD13	1:A:218:LEU:N	2.36	0.40
1:A:225:VAL:CG2	1:A:271:LEU:HD22	2.51	0.40
4:D:246:TRP:CD1	4:D:331:TYR:CD2	3.09	0.40
4:D:291:LEU:HD13	4:D:310:VAL:HG22	2.03	0.40
6:F:425:LEU:HD23	6:F:425:LEU:HA	1.90	0.40
1:A:17:LEU:HG	2:B:161:LEU:HD11	2.03	0.40
3:C:16:VAL:HG12	3:C:63:TRP:CD1	2.55	0.40
4:D:97:ARG:HB3	4:D:97:ARG:HH11	1.86	0.40
4:D:105:SER:HB2	4:D:481:LEU:HD21	2.03	0.40
5:E:19:GLU:HA	5:E:20:PRO:HD3	1.99	0.40
1:A:23:ARG:NH1	1:A:84:GLU:OE1	2.54	0.40
1:A:59:VAL:HB	1:A:70:LEU:HD11	2.03	0.40
2:B:187:ASP:C	2:B:187:ASP:OD1	2.60	0.40
4:D:352:THR:OG1	4:D:355:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:492:LEU:HD11	2:B:508:ILE:HG23	2.04	0.40
4:D:334:ASP:HB3	4:D:349:TYR:HE2	1.86	0.40
6:F:343:ILE:HD13	6:F:344:ARG:H	1.85	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:233:THR:OG1	8:L:203:GLY:O[4_455]	2.05	0.15
6:F:232:ASN:O	8:L:205:SER:N[4_455]	2.08	0.12

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	270/297 (91%)	228 (84%)	36 (13%)	6 (2%)	6	35
2	B	491/652 (75%)	451 (92%)	30 (6%)	10 (2%)	7	38
3	C	303/349 (87%)	266 (88%)	31 (10%)	6 (2%)	7	38
4	D	592/715 (83%)	532 (90%)	50 (8%)	10 (2%)	9	42
5	E	858/1045 (82%)	798 (93%)	49 (6%)	11 (1%)	12	48
6	F	413/454 (91%)	368 (89%)	34 (8%)	11 (3%)	5	31
7	H	213/271 (79%)	206 (97%)	7 (3%)	0	100	100
8	L	206/217 (95%)	198 (96%)	6 (3%)	2 (1%)	15	54
All	All	3346/4000 (84%)	3047 (91%)	243 (7%)	56 (2%)	9	42

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	158	SER

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Mol	Chain	Res	Type
2	B	368	GLU
2	B	371	PHE
2	B	394	GLN
3	C	43	SER
4	D	272	PRO
4	D	403	HIS
4	D	455	PHE
6	F	9	THR
6	F	11	ARG
6	F	138	ASN
6	F	165	ASN
8	L	34	SER
1	A	218	LEU
2	B	180	LEU
2	B	348	GLY
2	B	429	ASN
2	B	527	ILE
3	C	162	ALA
3	C	302	ASP
4	D	62	GLY
4	D	239	VAL
5	E	113	VAL
5	E	598	LYS
5	E	602	ILE
6	F	8	GLN
6	F	55	ASN
6	F	141	THR
6	F	354	SER
8	L	129	LYS
3	C	120	HIS
4	D	404	SER
5	E	264	ASP
6	F	434	THR
6	F	440	ASP
2	B	531	LEU
3	C	213	SER
5	E	284	ASN
5	E	346	ALA
6	F	87	ALA
1	A	114	PRO
1	A	131	LYS
4	D	53	VAL

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Mol	Chain	Res	Type
4	D	200	ASN
4	D	364	TYR
5	E	190	ASP
5	E	600	ASP
1	A	247	LEU
3	C	188	LEU
5	E	231	GLU
5	E	500	GLU
2	B	393	GLY
5	E	737	ILE
1	A	202	GLY
4	D	191	ILE
1	A	97	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	233/252 (92%)	224 (96%)	9 (4%)	32	56
2	B	367/594 (62%)	332 (90%)	35 (10%)	8	27
3	C	269/305 (88%)	261 (97%)	8 (3%)	41	63
4	D	424/642 (66%)	414 (98%)	10 (2%)	49	69
5	E	639/980 (65%)	616 (96%)	23 (4%)	35	59
6	F	387/418 (93%)	367 (95%)	20 (5%)	23	48
7	H	175/224 (78%)	170 (97%)	5 (3%)	42	64
8	L	184/191 (96%)	179 (97%)	5 (3%)	44	65
All	All	2678/3606 (74%)	2563 (96%)	115 (4%)	29	53

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	22	LYS

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Mol	Chain	Res	Type
1	A	43	HIS
1	A	46	ILE
1	A	47	ASP
1	A	225	VAL
1	A	227	GLN
1	A	229	ARG
1	A	275	ASP
2	B	160	LEU
2	B	175	ARG
2	B	214	SER
2	B	216	LEU
2	B	225	MET
2	B	234	LEU
2	B	251	THR
2	B	308	SER
2	B	319	LEU
2	B	328	SER
2	B	336	LEU
2	B	341	LEU
2	B	346	THR
2	B	349	CYS
2	B	351	ILE
2	B	368	GLU
2	B	370	LEU
2	B	371	PHE
2	B	400	LEU
2	B	402	SER
2	B	406	SER
2	B	408	LEU
2	B	412	SER
2	B	419	ILE
2	B	440	ARG
2	B	443	THR
2	B	456	GLN
2	B	464	ARG
2	B	467	SER
2	B	516	ILE
2	B	522	SER
2	B	524	ASN
2	B	531	LEU
2	B	539	PHE
2	B	547	ARG

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Mol	Chain	Res	Type
3	C	80	THR
3	C	138	ASP
3	C	168	ASP
3	C	226	ARG
3	C	301	ASP
3	C	313	ASN
3	C	314	LEU
3	C	334	THR
4	D	51	MET
4	D	143	THR
4	D	239	VAL
4	D	269	ASP
4	D	324	ILE
4	D	453	ASP
4	D	488	LEU
4	D	496	THR
4	D	516	ASN
4	D	539	TYR
5	E	63	SER
5	E	72	PHE
5	E	127	SER
5	E	172	GLN
5	E	183	LEU
5	E	209	THR
5	E	230	HIS
5	E	270	PHE
5	E	280	LEU
5	E	305	VAL
5	E	314	THR
5	E	335	VAL
5	E	338	ARG
5	E	370	ASP
5	E	408	PHE
5	E	422	ARG
5	E	590	GLN
5	E	600	ASP
5	E	628	ARG
5	E	638	VAL
5	E	644	THR
5	E	703	ASP
5	E	706	ASN
6	F	17	ASP

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Mol	Chain	Res	Type
6	F	26	GLN
6	F	58	ASP
6	F	71	GLU
6	F	77	LEU
6	F	86	ASN
6	F	88	ASP
6	F	118	GLN
6	F	141	THR
6	F	166	THR
6	F	237	ILE
6	F	268	SER
6	F	274	GLN
6	F	284	SER
6	F	343	ILE
6	F	357	SER
6	F	365	MET
6	F	403	SER
6	F	422	LEU
6	F	431	ILE
7	H	45	ARG
7	H	113	ARG
7	H	124	ARG
7	H	170	LYS
7	H	219	LEU
8	L	8	THR
8	L	27	ARG
8	L	53	SER
8	L	108	GLU
8	L	148	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	43	HIS
1	A	63	HIS
2	B	210	GLN
2	B	329	ASN
2	B	536	GLN
2	B	542	GLN
3	C	313	ASN
4	D	467	ASN

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Mol	Chain	Res	Type
5	E	255	GLN
5	E	284	ASN
5	E	295	ASN
5	E	350	ASN
5	E	575	ASN
5	E	588	ASN
6	F	97	HIS
8	L	213	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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.