Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 09:39 PM EST

PDB ID	:	4LO8
Title	:	HA70(D3)-HA17
Authors	:	Lee, K.; Gu, S.; Jin, L.; Le, T.T.; Cheng, L.W.; Strotmeier, J.; Kruel, A.M.; Yao, G.; Perry, K.; Rummel, A.; Jin, R.
Deposited on	:	2013-07-12
Resolution	:	2.40 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

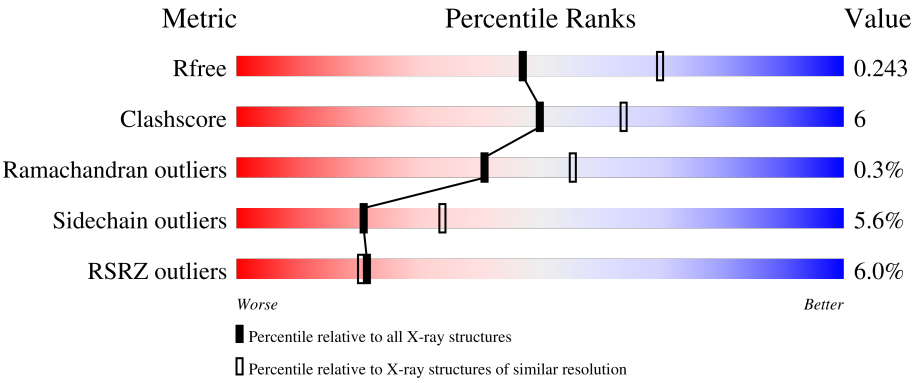
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	254	2% 76% 13% • 8%
1	C	254	11% 73% 16% • 8%
1	E	254	6% 73% 17% • 8%
1	G	254	14% 74% 15% • 8%
2	B	147	% 88% 7% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	147	
2	F	147	
2	H	147	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12680 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 HA-70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	15	0	0
			1889	1195	321	372	1			
1	C	233	Total	C	N	O	S	22	0	0
			1889	1195	321	372	1			
1	E	233	Total	C	N	O	S	22	0	0
			1889	1195	321	372	1			
1	G	233	Total	C	N	O	S	18	0	0
			1889	1195	321	372	1			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	373	GLY	-	expression tag	UNP Q8KHU9
A	374	PRO	-	expression tag	UNP Q8KHU9
A	375	LEU	-	expression tag	UNP Q8KHU9
A	376	GLY	-	expression tag	UNP Q8KHU9
A	377	SER	-	expression tag	UNP Q8KHU9
C	373	GLY	-	expression tag	UNP Q8KHU9
C	374	PRO	-	expression tag	UNP Q8KHU9
C	375	LEU	-	expression tag	UNP Q8KHU9
C	376	GLY	-	expression tag	UNP Q8KHU9
C	377	SER	-	expression tag	UNP Q8KHU9
E	373	GLY	-	expression tag	UNP Q8KHU9
E	374	PRO	-	expression tag	UNP Q8KHU9
E	375	LEU	-	expression tag	UNP Q8KHU9
E	376	GLY	-	expression tag	UNP Q8KHU9
E	377	SER	-	expression tag	UNP Q8KHU9
G	373	GLY	-	expression tag	UNP Q8KHU9
G	374	PRO	-	expression tag	UNP Q8KHU9
G	375	LEU	-	expression tag	UNP Q8KHU9
G	376	GLY	-	expression tag	UNP Q8KHU9
G	377	SER	-	expression tag	UNP Q8KHU9

- Molecule 2 is a protein called HA-17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	143	Total	C	N	O	S	0	0	0
			1180	762	188	225	5			
2	D	143	Total	C	N	O	S	0	0	0
			1180	762	188	225	5			
2	F	142	Total	C	N	O	S	0	0	0
			1171	757	187	222	5			
2	H	143	Total	C	N	O	S	0	0	0
			1180	762	188	225	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP Q45878
B	1	PRO	-	expression tag	UNP Q45878
D	0	GLY	-	expression tag	UNP Q45878
D	1	PRO	-	expression tag	UNP Q45878
F	0	GLY	-	expression tag	UNP Q45878
F	1	PRO	-	expression tag	UNP Q45878
H	0	GLY	-	expression tag	UNP Q45878
H	1	PRO	-	expression tag	UNP Q45878

- Molecule 3 is water.

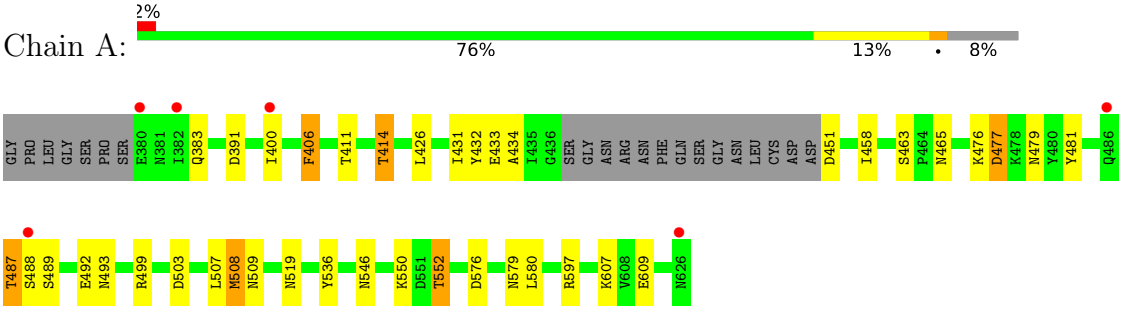
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	75	Total	O	0	0
			75	75		
3	B	43	Total	O	0	0
			43	43		
3	C	45	Total	O	0	0
			45	45		
3	D	51	Total	O	0	0
			51	51		
3	E	66	Total	O	0	0
			66	66		
3	F	47	Total	O	0	0
			47	47		
3	G	40	Total	O	0	0
			40	40		
3	H	46	Total	O	0	0
			46	46		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

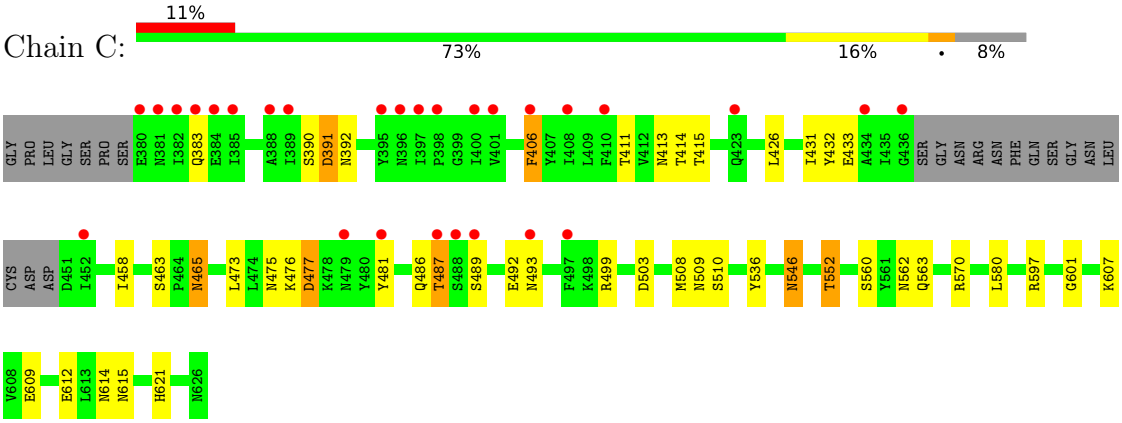
• Molecule 1: HA-70

Chain A:



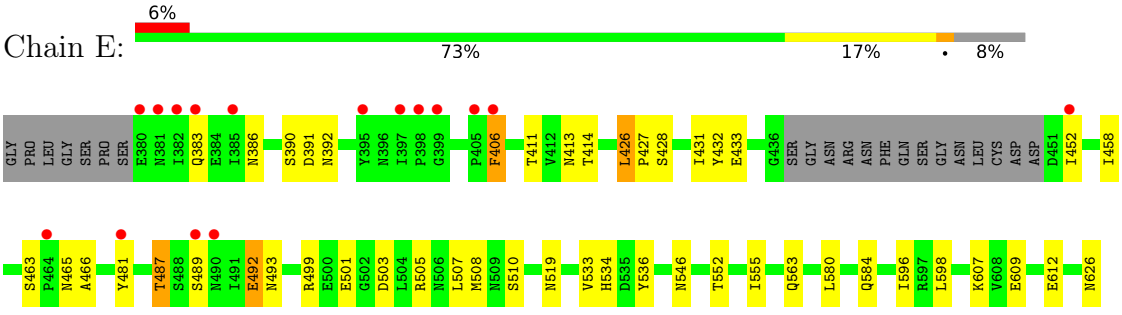
• Molecule 1: HA-70

Chain C:



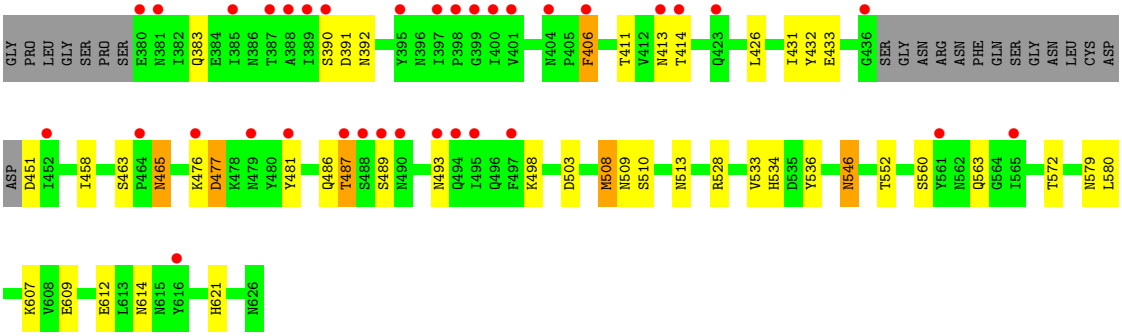
• Molecule 1: HA-70

Chain E:

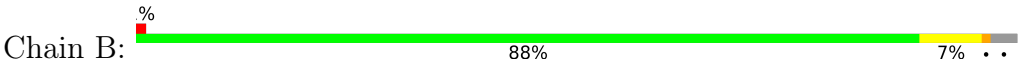


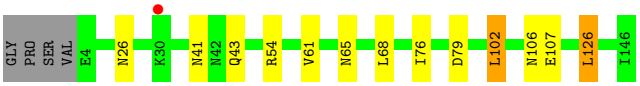
• Molecule 1: HA-70

Chain G:

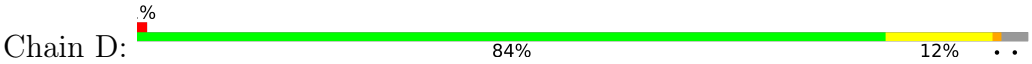


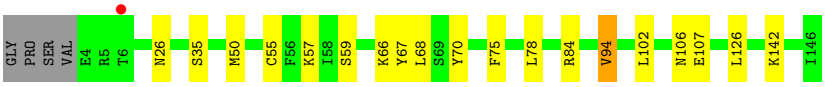
• Molecule 2: HA-17



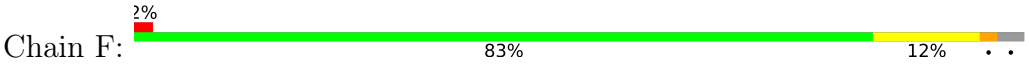


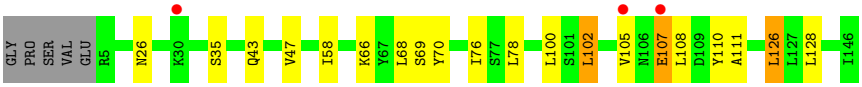
• Molecule 2: HA-17



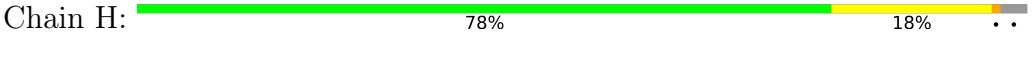


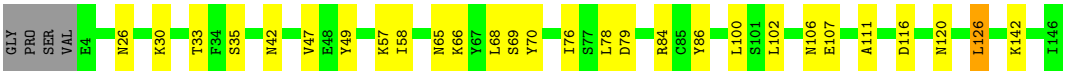
• Molecule 2: HA-17





• Molecule 2: HA-17





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	45.81Å 228.86Å 78.72Å 90.00° 92.05° 90.00°	Depositor
Resolution (Å)	45.78 – 2.40 46.27 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.78-2.40) 99.4 (46.27-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.197 , 0.249 0.194 , 0.243	Depositor DCC
R_{free} test set	3181 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	1.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12680	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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

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	0.24	0/1923	0.45	0/2619
1	C	0.23	0/1923	0.45	0/2619
1	E	0.23	0/1923	0.45	0/2619
1	G	0.23	0/1923	0.44	0/2619
2	B	0.24	0/1210	0.42	0/1643
2	D	0.24	0/1210	0.41	0/1643
2	F	0.24	0/1201	0.42	0/1631
2	H	0.24	0/1210	0.41	0/1643
All	All	0.24	0/12523	0.43	0/17036

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

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	1889	0	1849	23	0
1	C	1889	0	1849	26	0
1	E	1889	0	1849	27	0
1	G	1889	0	1849	23	0
2	B	1180	0	1141	9	0
2	D	1180	0	1141	12	0
2	F	1171	0	1135	12	0
2	H	1180	0	1141	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	75	0	0	2	0
3	B	43	0	0	1	0
3	C	45	0	0	0	0
3	D	51	0	0	1	0
3	E	66	0	0	3	0
3	F	47	0	0	0	0
3	G	40	0	0	0	0
3	H	46	0	0	3	0
All	All	12680	0	11954	138	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 6.

All (138) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:505:ARG:NH2	2:H:57:LYS:HE2	1.38	1.36
1:E:505:ARG:HH22	2:H:57:LYS:CE	1.65	1.07
1:E:505:ARG:NH2	2:H:57:LYS:CE	2.32	0.80
1:A:550:LYS:NZ	3:A:755:HOH:O	2.20	0.75
1:G:546:ASN:OD1	2:H:142:LYS:NZ	2.19	0.74
1:G:560:SER:HG	1:G:621:HIS:HE2	1.36	0.73
1:E:505:ARG:HH22	2:H:57:LYS:HE2	0.73	0.72
1:C:383:GLN:HG3	1:C:406:PHE:HE2	1.56	0.69
1:E:386:ASN:ND2	3:E:748:HOH:O	2.21	0.69
1:C:546:ASN:OD1	2:D:142:LYS:NZ	2.26	0.68
1:A:400:ILE:O	1:A:400:ILE:HG22	1.93	0.67
1:G:383:GLN:HG3	1:G:406:PHE:HE2	1.63	0.63
1:G:503:ASP:HB3	1:G:580:LEU:HB2	1.83	0.60
2:D:50:MET:HE1	2:D:57:LYS:HB3	1.84	0.58
1:C:552:THR:HG22	1:C:597:ARG:HH11	1.69	0.57
1:E:503:ASP:HB3	1:E:580:LEU:HB2	1.87	0.56
1:C:477:ASP:N	1:C:477:ASP:OD1	2.38	0.56
2:F:76:ILE:HG13	2:F:126:LEU:HD13	1.87	0.56
1:C:433:GLU:HB2	1:C:458:ILE:HD11	1.88	0.55
1:E:383:GLN:HG3	1:E:406:PHE:HE2	1.70	0.55
1:G:433:GLU:HB2	1:G:458:ILE:HD11	1.89	0.55
2:D:66:LYS:HB3	2:D:78:LEU:HD22	1.88	0.54
2:H:120:ASN:HA	3:H:208:HOH:O	2.08	0.54
2:H:26:ASN:HD21	2:H:35:SER:HB2	1.73	0.54
2:H:47:VAL:HG22	2:H:58:ILE:HG12	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:477:ASP:N	1:G:477:ASP:OD1	2.41	0.54
1:A:503:ASP:HB3	1:A:580:LEU:HB2	1.91	0.53
2:F:107:GLU:HB2	2:H:30:LYS:HD2	1.89	0.53
1:A:391:ASP:HA	1:A:499:ARG:HB2	1.90	0.53
1:G:390:SER:O	1:G:392:ASN:N	2.40	0.53
1:E:432:TYR:HB2	1:E:481:TYR:HB2	1.91	0.53
1:E:563:GLN:HB3	1:E:612:GLU:HB3	1.91	0.52
1:C:383:GLN:HG3	1:C:406:PHE:CE2	2.43	0.52
2:F:66:LYS:HB3	2:F:78:LEU:HD22	1.90	0.52
1:A:400:ILE:O	1:A:400:ILE:CG2	2.57	0.52
1:G:510:SER:HB3	1:G:536:TYR:HB2	1.92	0.51
1:G:383:GLN:HG3	1:G:406:PHE:CE2	2.45	0.51
1:E:499:ARG:NH2	1:E:501:GLU:OE2	2.43	0.51
1:A:552:THR:HG22	1:A:597:ARG:HH11	1.74	0.51
1:A:576:ASP:OD1	2:B:54:ARG:NH2	2.38	0.51
2:H:66:LYS:HB3	2:H:78:LEU:HD22	1.92	0.51
1:C:510:SER:HB3	1:C:536:TYR:HB2	1.93	0.51
1:C:503:ASP:HB3	1:C:580:LEU:HB2	1.94	0.50
1:A:487:THR:C	1:A:489:SER:H	2.15	0.50
1:C:476:LYS:HG3	1:C:477:ASP:OD1	2.13	0.49
1:E:433:GLU:OE1	3:E:753:HOH:O	2.20	0.49
1:G:431:ILE:HG23	1:G:458:ILE:HB	1.94	0.49
2:H:76:ILE:HG13	2:H:126:LEU:HD13	1.94	0.49
1:A:414:THR:HA	1:A:476:LYS:HE2	1.94	0.49
1:C:431:ILE:HG23	1:C:458:ILE:HB	1.95	0.49
2:H:49:TYR:O	3:H:245:HOH:O	2.20	0.49
1:A:383:GLN:HG3	1:A:406:PHE:HE2	1.77	0.48
2:B:107:GLU:OE2	2:F:105:VAL:HB	2.13	0.48
2:B:76:ILE:HG13	2:B:126:LEU:HD13	1.94	0.48
2:F:100:LEU:HD23	2:F:111:ALA:HB2	1.96	0.48
1:G:533:VAL:HG12	1:G:534:HIS:CD2	2.49	0.48
2:H:100:LEU:HD23	2:H:111:ALA:HB2	1.95	0.48
1:G:536:TYR:CD1	1:G:607:LYS:HE2	2.49	0.48
1:E:428:SER:OG	1:E:466:ALA:O	2.27	0.48
2:D:106:ASN:HB3	2:D:107:GLU:H	1.51	0.47
1:E:426:LEU:HD22	1:E:427:PRO:HA	1.95	0.47
1:A:536:TYR:CE1	1:A:609:GLU:HB2	2.49	0.47
1:G:476:LYS:HG3	1:G:477:ASP:OD1	2.14	0.47
1:G:563:GLN:HB3	1:G:612:GLU:HB3	1.96	0.47
1:A:476:LYS:HG3	1:A:477:ASP:OD1	2.14	0.47
1:C:390:SER:O	1:C:392:ASN:N	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:THR:HG23	1:C:475:ASN:HA	1.97	0.47
1:C:560:SER:HG	1:C:621:HIS:HE2	1.63	0.47
1:E:487:THR:C	1:E:489:SER:H	2.17	0.47
2:D:75:PHE:HE1	2:F:108:LEU:HD21	1.79	0.47
1:C:465:ASN:OD1	1:C:465:ASN:N	2.47	0.47
1:E:383:GLN:HG3	1:E:406:PHE:CE2	2.50	0.46
1:G:508:MET:HA	1:G:509:ASN:HA	1.66	0.46
1:C:536:TYR:CD1	1:C:607:LYS:HE2	2.50	0.46
1:E:555:ILE:HG13	1:E:598:LEU:HD12	1.98	0.46
2:F:110:TYR:HB3	2:F:128:LEU:HG	1.97	0.46
2:B:79:ASP:OD2	3:B:232:HOH:O	2.20	0.46
1:C:563:GLN:HB3	1:C:612:GLU:HB3	1.98	0.46
2:F:102:LEU:HD23	2:F:102:LEU:HA	1.82	0.46
1:A:508:MET:HA	1:A:509:ASN:HA	1.70	0.46
2:D:55:CYS:HA	3:D:232:HOH:O	2.16	0.46
1:A:536:TYR:CD1	1:A:607:LYS:HE2	2.51	0.45
1:A:434:ALA:HB3	1:A:479:ASN:HB2	1.99	0.45
1:C:391:ASP:HA	1:C:499:ARG:HB2	1.97	0.45
1:E:431:ILE:HG23	1:E:458:ILE:HB	1.98	0.45
1:C:432:TYR:HB2	1:C:481:TYR:HB2	1.98	0.45
1:G:536:TYR:CE1	1:G:609:GLU:HB2	2.51	0.45
1:E:536:TYR:CD1	1:E:607:LYS:HE2	2.52	0.44
2:H:42:ASN:ND2	3:H:233:HOH:O	2.29	0.44
1:G:465:ASN:OD1	1:G:465:ASN:N	2.50	0.44
2:D:70:TYR:CZ	2:D:84:ARG:HD2	2.52	0.44
2:F:69:SER:OG	2:F:70:TYR:N	2.50	0.44
2:H:106:ASN:HB3	2:H:107:GLU:H	1.50	0.44
1:E:390:SER:O	1:E:392:ASN:N	2.50	0.44
1:E:492:GLU:H	1:E:492:GLU:HG2	1.48	0.44
2:D:26:ASN:HD21	2:D:35:SER:HB2	1.83	0.43
2:D:78:LEU:HD23	2:D:78:LEU:HA	1.89	0.43
1:A:552:THR:HG21	1:A:597:ARG:HD3	2.00	0.43
1:C:473:LEU:HB2	1:C:508:MET:SD	2.58	0.43
1:G:432:TYR:HB2	1:G:481:TYR:HB2	2.01	0.43
2:B:41:ASN:O	2:B:61:VAL:HG22	2.19	0.43
1:C:508:MET:HA	1:C:509:ASN:HA	1.68	0.43
1:C:536:TYR:CE1	1:C:609:GLU:HB2	2.53	0.43
1:C:612:GLU:HG2	1:C:614:ASN:OD1	2.19	0.43
2:D:102:LEU:HD23	2:D:102:LEU:HA	1.84	0.42
2:F:47:VAL:HG22	2:F:58:ILE:HG12	2.01	0.42
1:C:487:THR:C	1:C:489:SER:H	2.22	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:612:GLU:HG2	1:G:614:ASN:OD1	2.19	0.42
2:H:86:TYR:HB3	2:H:102:LEU:HD22	2.00	0.42
2:D:59:SER:HB3	2:D:67:TYR:CE1	2.54	0.42
1:G:392:ASN:HD21	1:G:498:LYS:NZ	2.18	0.42
1:A:477:ASP:OD1	1:A:477:ASP:N	2.52	0.42
1:A:579:ASN:ND2	3:A:735:HOH:O	2.52	0.42
1:C:601:GLY:O	2:D:94:VAL:HG23	2.20	0.41
1:E:584:GLN:OE1	1:E:596:ILE:HD12	2.20	0.41
2:F:26:ASN:HB3	2:F:43:GLN:HG2	2.01	0.41
2:H:69:SER:OG	2:H:70:TYR:N	2.53	0.41
1:C:552:THR:HG21	1:C:597:ARG:HB3	2.02	0.41
1:E:533:VAL:HG12	1:E:534:HIS:CD2	2.56	0.41
1:A:383:GLN:HG3	1:A:406:PHE:CE2	2.55	0.41
1:A:433:GLU:HB2	1:A:458:ILE:HD11	2.02	0.41
2:F:26:ASN:HD21	2:F:35:SER:HB2	1.85	0.41
1:A:431:ILE:HG23	1:A:458:ILE:HB	2.02	0.41
1:E:433:GLU:HB2	1:E:458:ILE:HD11	2.02	0.41
1:E:510:SER:HB3	1:E:536:TYR:HB2	2.02	0.41
1:E:626:ASN:ND2	3:E:730:HOH:O	2.53	0.41
2:B:106:ASN:HB3	2:B:107:GLU:H	1.69	0.41
1:G:487:THR:C	1:G:489:SER:H	2.24	0.41
2:B:126:LEU:HD23	2:B:126:LEU:HA	1.92	0.41
1:C:562:ASN:OD1	1:C:615:ASN:N	2.54	0.41
1:E:426:LEU:HD22	1:E:426:LEU:HA	1.92	0.41
1:E:536:TYR:CE1	1:E:609:GLU:HB2	2.56	0.41
1:G:572:THR:OG1	1:G:579:ASN:HB2	2.20	0.41
1:G:513:ASN:OD1	1:G:528:ARG:NE	2.54	0.41
2:B:102:LEU:HA	2:B:102:LEU:HD23	1.82	0.40
1:A:492:GLU:H	1:A:492:GLU:HG2	1.68	0.40
1:A:432:TYR:HB2	1:A:481:TYR:HB2	2.04	0.40
2:B:26:ASN:ND2	2:B:43:GLN:HE21	2.19	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	229/254 (90%)	217 (95%)	11 (5%)	1 (0%)	34	48
1	C	229/254 (90%)	215 (94%)	13 (6%)	1 (0%)	34	48
1	E	229/254 (90%)	216 (94%)	12 (5%)	1 (0%)	34	48
1	G	229/254 (90%)	217 (95%)	11 (5%)	1 (0%)	34	48
2	B	141/147 (96%)	133 (94%)	8 (6%)	0	100	100
2	D	141/147 (96%)	135 (96%)	5 (4%)	1 (1%)	22	32
2	F	140/147 (95%)	133 (95%)	7 (5%)	0	100	100
2	H	141/147 (96%)	135 (96%)	6 (4%)	0	100	100
All	All	1479/1604 (92%)	1401 (95%)	73 (5%)	5 (0%)	41	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	94	VAL
1	E	391	ASP
1	G	391	ASP
1	C	391	ASP
1	A	488	SER

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	215/232 (93%)	200 (93%)	15 (7%)	15	24
1	C	215/232 (93%)	200 (93%)	15 (7%)	15	24
1	E	215/232 (93%)	199 (93%)	16 (7%)	13	22
1	G	215/232 (93%)	200 (93%)	15 (7%)	15	24
2	B	135/138 (98%)	131 (97%)	4 (3%)	41	61
2	D	135/138 (98%)	133 (98%)	2 (2%)	65	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	134/138 (97%)	130 (97%)	4 (3%)	41 61
2	H	135/138 (98%)	128 (95%)	7 (5%)	23 38
All	All	1399/1480 (94%)	1321 (94%)	78 (6%)	21 34

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	406	PHE
1	A	411	THR
1	A	414	THR
1	A	426	LEU
1	A	451	ASP
1	A	463	SER
1	A	465	ASN
1	A	477	ASP
1	A	487	THR
1	A	493	ASN
1	A	507	LEU
1	A	508	MET
1	A	519	ASN
1	A	546	ASN
1	A	552	THR
2	B	65	ASN
2	B	68	LEU
2	B	102	LEU
2	B	126	LEU
1	C	406	PHE
1	C	411	THR
1	C	413	ASN
1	C	414	THR
1	C	426	LEU
1	C	463	SER
1	C	465	ASN
1	C	477	ASP
1	C	486	GLN
1	C	487	THR
1	C	492	GLU
1	C	493	ASN
1	C	546	ASN
1	C	552	THR
1	C	570	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	68	LEU
2	D	126	LEU
1	E	406	PHE
1	E	411	THR
1	E	413	ASN
1	E	414	THR
1	E	426	LEU
1	E	452	ILE
1	E	463	SER
1	E	465	ASN
1	E	487	THR
1	E	492	GLU
1	E	493	ASN
1	E	507	LEU
1	E	508	MET
1	E	519	ASN
1	E	546	ASN
1	E	552	THR
2	F	68	LEU
2	F	102	LEU
2	F	107	GLU
2	F	126	LEU
1	G	406	PHE
1	G	411	THR
1	G	413	ASN
1	G	414	THR
1	G	426	LEU
1	G	451	ASP
1	G	463	SER
1	G	465	ASN
1	G	477	ASP
1	G	486	GLN
1	G	487	THR
1	G	493	ASN
1	G	508	MET
1	G	546	ASN
1	G	552	THR
2	H	33	THR
2	H	65	ASN
2	H	68	LEU
2	H	79	ASP
2	H	84	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	116	ASP
2	H	126	LEU

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

Mol	Chain	Res	Type
1	A	392	ASN
1	A	534	HIS
2	B	26	ASN
1	C	392	ASN
2	D	26	ASN
2	D	118	ASN
1	E	392	ASN
1	E	534	HIS
2	F	26	ASN
1	G	392	ASN
1	G	534	HIS
2	H	26	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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	233/254 (91%)	-0.23	6 (2%) 56 54	17, 39, 106, 140	4 (1%)
1	C	233/254 (91%)	0.60	28 (12%) 4 3	28, 66, 144, 173	6 (2%)
1	E	233/254 (91%)	0.08	16 (6%) 16 15	17, 53, 116, 149	6 (2%)
1	G	233/254 (91%)	0.62	35 (15%) 2 1	26, 68, 151, 175	5 (2%)
2	B	143/147 (97%)	-0.25	1 (0%) 87 86	26, 42, 78, 109	0
2	D	143/147 (97%)	-0.34	1 (0%) 87 86	28, 41, 68, 92	0
2	F	142/147 (96%)	-0.29	3 (2%) 63 61	26, 43, 78, 108	0
2	H	143/147 (97%)	-0.33	0 100 100	29, 44, 70, 112	0
All	All	1503/1604 (93%)	0.05	90 (5%) 21 20	17, 49, 118, 175	21 (1%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	380	GLU	11.8
1	C	400	ILE	9.9
1	C	397	ILE	7.9
1	C	481	TYR	7.8
1	G	397	ILE	7.6
1	G	400	ILE	7.5
1	C	383	GLN	7.0
1	C	398	PRO	6.5
1	G	490	ASN	6.4
1	E	398	PRO	6.2
1	G	380	GLU	5.7
1	C	406	PHE	5.5
1	G	481	TYR	5.3
1	C	381	ASN	5.2
1	G	487	THR	5.2
1	G	404	ASN	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	401	VAL	5.0
1	G	399	GLY	4.9
1	C	488	SER	4.7
1	C	385	ILE	4.7
1	C	382	ILE	4.6
1	A	488	SER	4.5
1	E	382	ILE	4.4
1	C	395	TYR	4.3
2	F	105	VAL	4.2
1	C	436	GLY	4.2
1	G	388	ALA	4.2
1	G	413	ASN	4.0
1	G	464	PRO	4.0
1	G	489	SER	4.0
1	E	383	GLN	3.9
1	G	406	PHE	3.8
1	C	396	ASN	3.8
1	C	401	VAL	3.7
1	G	398	PRO	3.5
1	G	414	THR	3.5
1	C	487	THR	3.3
1	E	397	ILE	3.3
1	G	488	SER	3.2
1	A	380	GLU	3.2
1	E	481	TYR	3.1
1	C	497	PHE	3.0
1	G	497	PHE	3.0
1	E	381	ASN	2.9
1	C	434	ALA	2.9
1	G	476	LYS	2.9
1	A	626	ASN	2.8
1	E	399	GLY	2.8
1	G	389	ILE	2.8
2	F	107	GLU	2.8
1	G	423	GLN	2.8
1	C	423	GLN	2.8
1	G	616	TYR	2.7
2	F	30	LYS	2.7
1	E	385	ILE	2.7
1	E	405	PRO	2.7
1	G	390	SER	2.6
1	C	389	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	395	TYR	2.6
1	C	489	SER	2.6
1	E	490	ASN	2.6
1	C	493	ASN	2.6
1	G	385	ILE	2.5
1	E	489	SER	2.5
1	C	410	PHE	2.4
1	C	384	GLU	2.4
1	A	400	ILE	2.3
1	E	464	PRO	2.3
1	E	406	PHE	2.3
1	G	479	ASN	2.2
1	A	382	ILE	2.2
1	C	408	ILE	2.2
1	G	561	TYR	2.2
1	G	493	ASN	2.2
1	E	452	ILE	2.2
1	G	565	ILE	2.2
1	G	381	ASN	2.2
1	G	495	ILE	2.2
1	G	387	THR	2.1
1	E	380	GLU	2.1
1	C	452	ILE	2.1
1	C	388	ALA	2.1
1	C	479	ASN	2.1
1	G	494	GLN	2.1
2	B	30	LYS	2.1
1	G	452	ILE	2.1
1	G	395	TYR	2.0
2	D	6	THR	2.0
1	G	436	GLY	2.0
1	A	486	GLN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.