



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:10 AM UTC

PDB ID : 4LO8 / pdb_00004lo8
Title : HA70(D3)-HA17
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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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

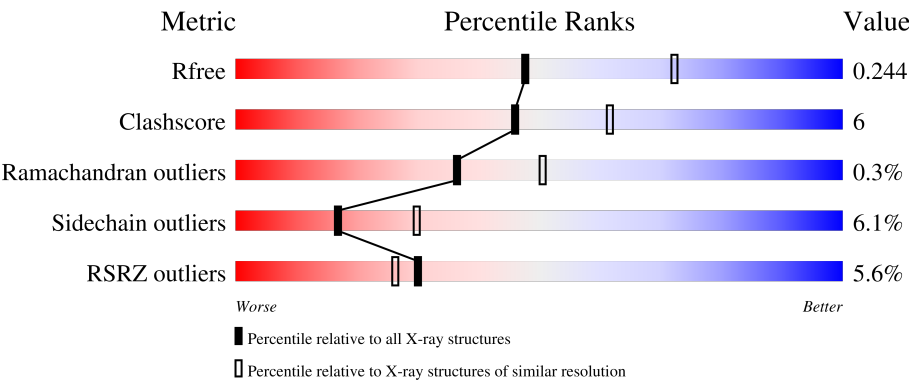
1 Overall quality at a glance i

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	254	5% 76% 13% • 8%
1	C	254	6% 73% 16% • 8%
1	E	254	12% 73% 17% • 8%
1	G	254	5% 74% 16% • 8%
2	B	147	% 88% 7% • •

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Mol	Chain	Length	Quality of chain
2	D	147	2% 84% 13%
2	F	147	5% 82% 12%
2	H	147	% 78% 18%

2 Entry composition

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

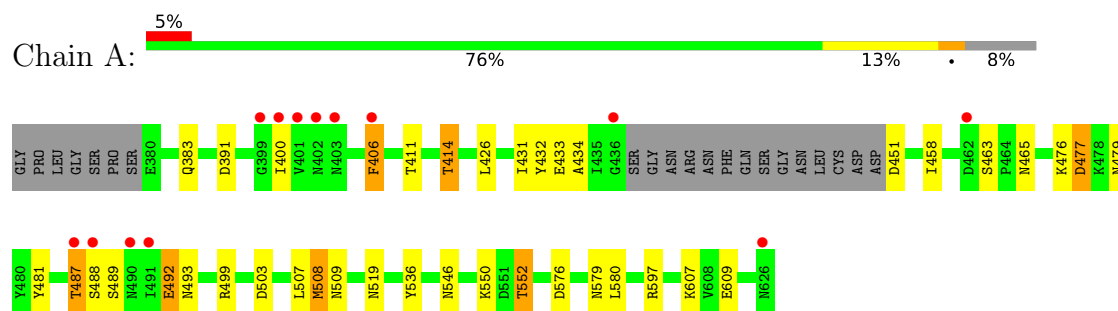
- Molecule 3 is water.

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		

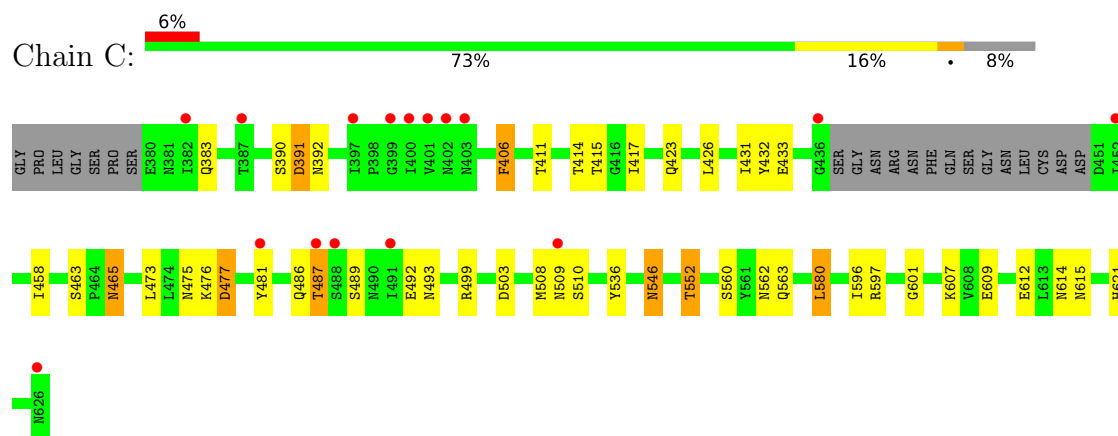
3 Residue-property plots

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.

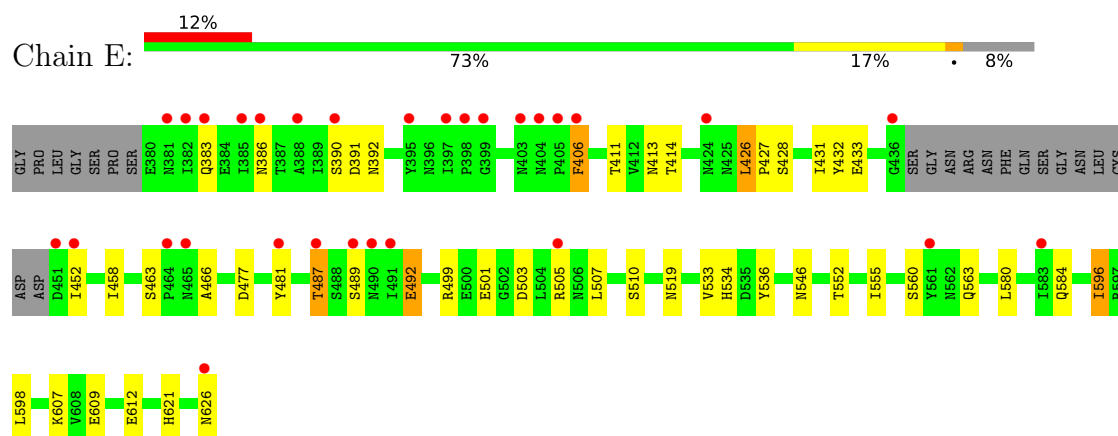
• Molecule 1: HA-70



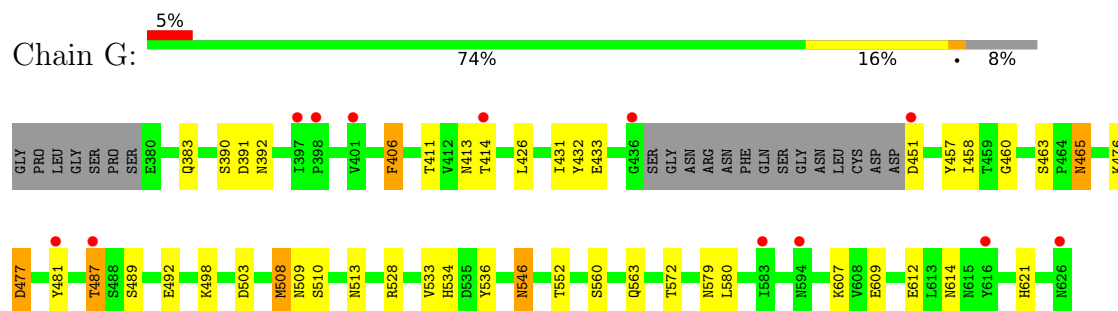
• Molecule 1: HA-70



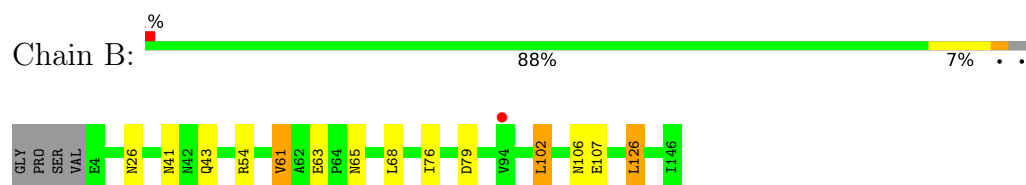
• Molecule 1: HA-70



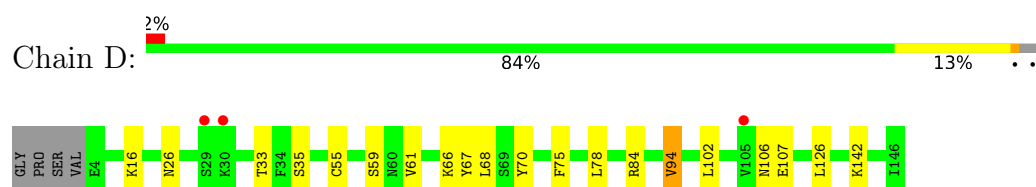
- Molecule 1: HA-70



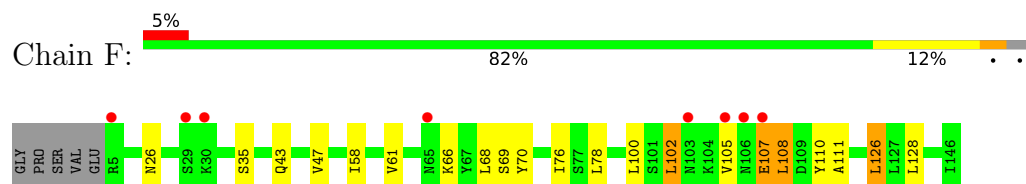
- Molecule 2: HA-17



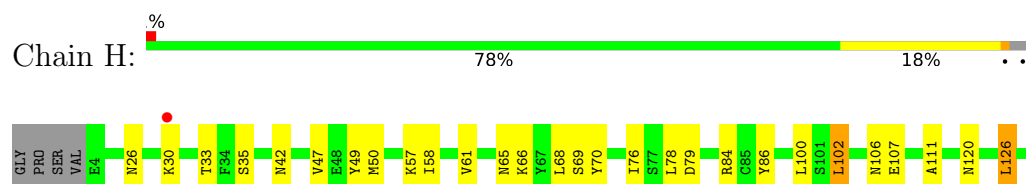
- Molecule 2: HA-17



- Molecule 2: HA-17



- Molecule 2: HA-17



4 Data and refinement statistics

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 45.78 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.78-2.40) 99.4 (45.78-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.197 , 0.249 0.196 , 0.244	Depositor DCC
R_{free} test set	3181 reflections (5.05%)	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 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/1923	0.72	0/2619
1	C	0.26	0/1923	0.72	0/2619
1	E	0.27	0/1923	0.72	0/2619
1	G	0.27	0/1923	0.70	0/2619
2	B	0.28	0/1210	0.70	2/1643 (0.1%)
2	D	0.28	0/1210	0.68	0/1643
2	F	0.28	0/1201	0.69	0/1631
2	H	0.28	0/1210	0.68	0/1643
All	All	0.27	0/12523	0.71	2/17036 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	63	GLU	CA-C-N	5.15	124.94	119.28
2	B	63	GLU	C-N-CA	5.15	124.94	119.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1889	0	1849	23	0
1	C	1889	0	1849	26	0
1	E	1889	0	1849	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1889	0	1849	24	0
2	B	1180	0	1141	9	0
2	D	1180	0	1141	11	0
2	F	1171	0	1135	12	0
2	H	1180	0	1141	18	0
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	140	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 (140) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:THR:C	1:A:489:SER:H	2.15	0.54
1:E:560:SER:HG	1:E:621:HIS:HE2	1.56	0.54
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
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:E:487:THR:C	1:E:489:SER:H	2.17	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: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
1:C:560:SER:HG	1:C:621:HIS:HE2	1.59	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:E:428:SER:OG	1:E:466:ALA:O	2.27	0.48
1:G:536:TYR:CD1	1:G:607:LYS:HE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:415:THR:HG23	1:C:475:ASN:HA	1.97	0.47
1:C:487:THR:C	1:C:489:SER:H	2.22	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:G:487:THR:C	1:G:489:SER:H	2.24	0.46
1:G:457:TYR:OH	1:G:460:GLY:O	2.32	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:50:MET:HE1	2:H:86:TYR:CD2	2.55	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
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

5.3.1 Protein backbone

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%)	30	43
1	C	229/254 (90%)	215 (94%)	13 (6%)	1 (0%)	30	43
1	E	229/254 (90%)	216 (94%)	12 (5%)	1 (0%)	30	43
1	G	229/254 (90%)	217 (95%)	11 (5%)	1 (0%)	30	43
2	B	141/147 (96%)	133 (94%)	8 (6%)	0	100	100
2	D	141/147 (96%)	135 (96%)	5 (4%)	1 (1%)	18	28
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%)	36	50

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

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%)	199 (93%)	16 (7%)	13	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	215/232 (93%)	198 (92%)	17 (8%)	11	19
1	E	215/232 (93%)	200 (93%)	15 (7%)	14	24
1	G	215/232 (93%)	201 (94%)	14 (6%)	15	27
2	B	135/138 (98%)	130 (96%)	5 (4%)	30	51
2	D	135/138 (98%)	130 (96%)	5 (4%)	30	51
2	F	134/138 (97%)	128 (96%)	6 (4%)	24	42
2	H	135/138 (98%)	127 (94%)	8 (6%)	18	31
All	All	1399/1480 (94%)	1313 (94%)	86 (6%)	17	30

All (86) 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	492	GLU
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	61	VAL
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	414	THR
1	C	417	ILE
1	C	423	GLN
1	C	426	LEU
1	C	463	SER

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Mol	Chain	Res	Type
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	580	LEU
1	C	596	ILE
2	D	16	LYS
2	D	33	THR
2	D	61	VAL
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	477	ASP
1	E	487	THR
1	E	492	GLU
1	E	507	LEU
1	E	519	ASN
1	E	546	ASN
1	E	552	THR
1	E	596	ILE
2	F	61	VAL
2	F	68	LEU
2	F	102	LEU
2	F	107	GLU
2	F	108	LEU
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

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Mol	Chain	Res	Type
1	G	463	SER
1	G	465	ASN
1	G	477	ASP
1	G	487	THR
1	G	492	GLU
1	G	508	MET
1	G	546	ASN
1	G	552	THR
2	H	33	THR
2	H	61	VAL
2	H	65	ASN
2	H	68	LEU
2	H	79	ASP
2	H	84	ARG
2	H	102	LEU
2	H	126	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	392	ASN
1	A	413	ASN
1	A	519	ASN
1	A	534	HIS
1	A	588	HIS
2	B	26	ASN
2	B	53	ASN
2	B	131	ASN
1	C	392	ASN
1	C	423	GLN
1	C	496	GLN
1	C	534	HIS
2	D	26	ASN
2	D	118	ASN
2	D	120	ASN
2	D	131	ASN
1	E	392	ASN
1	E	423	GLN
1	E	425	ASN
1	E	519	ASN
1	E	534	HIS
2	F	26	ASN

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Mol	Chain	Res	Type
2	F	42	ASN
2	F	53	ASN
2	F	124	GLN
2	F	131	ASN
1	G	392	ASN
1	G	423	GLN
1	G	534	HIS
2	H	26	ASN
2	H	53	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	233/254 (91%)	0.03	13 (5%)	30 26	17, 39, 102, 140	4 (1%)
1	C	233/254 (91%)	0.43	16 (6%)	23 19	28, 66, 136, 173	6 (2%)
1	E	233/254 (91%)	0.38	30 (12%)	7 5	17, 53, 115, 149	6 (2%)
1	G	233/254 (91%)	0.45	12 (5%)	33 29	26, 68, 131, 175	5 (2%)
2	B	143/147 (97%)	-0.06	1 (0%)	84 81	26, 42, 78, 109	0
2	D	143/147 (97%)	-0.20	3 (2%)	63 59	28, 41, 68, 92	0
2	F	142/147 (96%)	-0.05	8 (5%)	30 26	26, 43, 78, 108	0
2	H	143/147 (97%)	-0.13	1 (0%)	84 81	29, 44, 70, 112	0
All	All	1503/1604 (93%)	0.16	84 (5%)	30 26	17, 49, 113, 175	21 (1%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	400	ILE	5.0
2	F	105	VAL	4.5
1	C	401	VAL	4.1
1	G	481	TYR	4.1
1	C	402	ASN	4.0
2	F	107	GLU	4.0
1	C	481	TYR	4.0
1	C	399	GLY	3.7
1	A	491	ILE	3.6
1	C	491	ILE	3.6
1	C	400	ILE	3.5
1	E	491	ILE	3.5
1	C	397	ILE	3.3
1	A	626	ASN	3.2
1	E	505	ARG	3.2
1	E	397	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	385	ILE	3.2
1	E	398	PRO	3.2
1	C	436	GLY	3.2
2	D	29	SER	3.0
1	C	452	ILE	3.0
1	E	481	TYR	2.9
1	E	403	ASN	2.9
1	C	382	ILE	2.9
1	E	626	ASN	2.8
2	D	105	VAL	2.8
1	G	398	PRO	2.7
1	G	401	VAL	2.7
1	C	403	ASN	2.7
1	G	626	ASN	2.7
2	B	94	VAL	2.7
1	E	399	GLY	2.7
1	E	405	PRO	2.7
1	E	452	ILE	2.7
2	F	106	ASN	2.7
1	G	436	GLY	2.6
1	G	397	ILE	2.6
2	H	30	LYS	2.6
1	E	404	ASN	2.6
1	E	561	TYR	2.6
1	E	487	THR	2.6
2	D	30	LYS	2.6
1	A	488	SER	2.6
1	A	399	GLY	2.6
1	E	406	PHE	2.6
1	A	490	ASN	2.6
1	E	382	ILE	2.5
1	A	401	VAL	2.5
1	C	387	THR	2.5
1	G	616	TYR	2.4
1	A	436	GLY	2.4
2	F	30	LYS	2.4
1	G	594	ASN	2.4
2	F	65	ASN	2.4
1	C	488	SER	2.3
1	C	509	ASN	2.3
1	E	465	ASN	2.3
1	A	487	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	487	THR	2.3
2	F	5	ARG	2.3
1	E	583	ILE	2.3
1	A	403	ASN	2.3
1	E	390	SER	2.3
1	C	626	ASN	2.2
1	A	402	ASN	2.2
2	F	103	ASN	2.2
1	G	487	THR	2.2
1	E	451	ASP	2.2
1	A	406	PHE	2.2
1	E	383	GLN	2.2
1	G	414	THR	2.2
1	G	451	ASP	2.2
1	E	381	ASN	2.1
1	E	490	ASN	2.1
1	E	464	PRO	2.1
1	E	436	GLY	2.1
1	E	489	SER	2.1
1	E	386	ASN	2.0
1	G	583	ILE	2.0
1	E	388	ALA	2.0
1	E	424	ASN	2.0
1	A	462	ASP	2.0
1	E	395	TYR	2.0
2	F	29	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.