



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:36 PM UTC

PDB ID : 1S7M / pdb_00001s7m
Title : Crystal Structure of HiaBD1
Authors : Yeo, H.J.; Cotter, S.E.; Laarmann, S.; Juehne, T.; St Geme, J.W.; Waksman, G.
Deposited on : 2004-01-29
Resolution : 2.10 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 ⓘ 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:

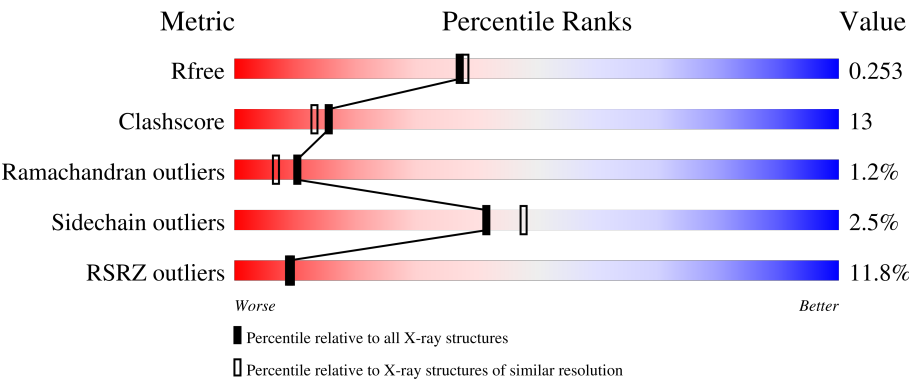
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 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	174	5% 69%21%•9%
1	B	174	18% 70%18%•10%
1	C	174	7% 72%17%•10%
1	D	174	8% 67%21%•9%
1	E	174	8% 63%23%•10%

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Mol	Chain	Length	Quality of chain
1	F	174	18% 66% 23% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7355 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 Hia.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	0	0	0
			1145	697	205	243			
1	B	157	Total	C	N	O	0	0	0
			1144	696	205	243			
1	C	157	Total	C	N	O	0	0	0
			1147	697	206	244			
1	D	158	Total	C	N	O	0	0	0
			1152	700	207	245			
1	E	157	Total	C	N	O	0	0	0
			1147	697	206	244			
1	F	157	Total	C	N	O	0	0	0
			1138	694	203	241			

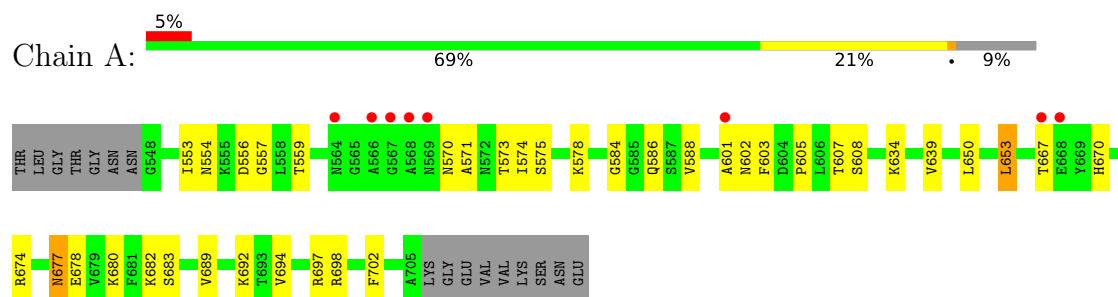
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	99	Total	O	0	0
			99	99		
2	B	84	Total	O	0	0
			84	84		
2	C	82	Total	O	0	0
			82	82		
2	D	73	Total	O	0	0
			73	73		
2	E	90	Total	O	0	0
			90	90		
2	F	54	Total	O	0	0
			54	54		

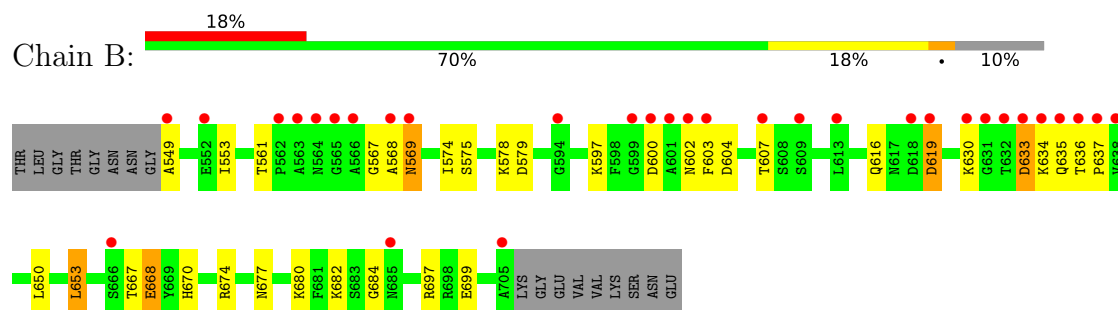
3 Residue-property plots [i](#)

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.

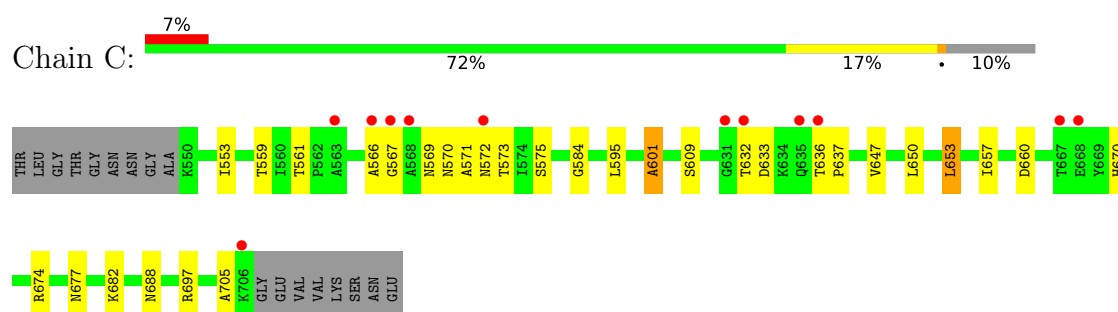
• Molecule 1: Hia



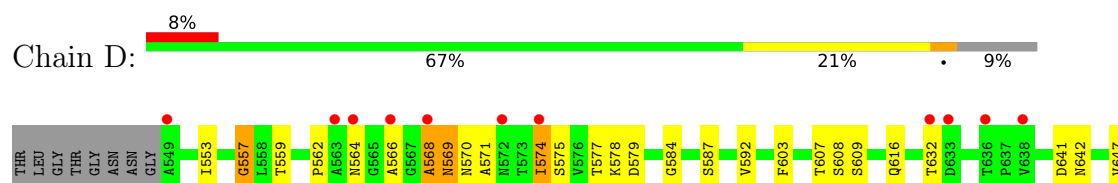
• Molecule 1: Hia

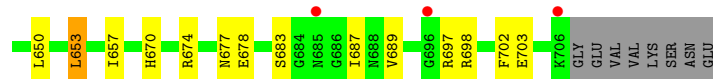


• Molecule 1: Hia

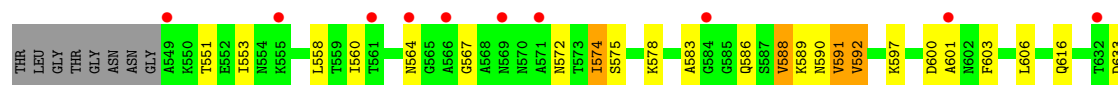


• Molecule 1: Hia

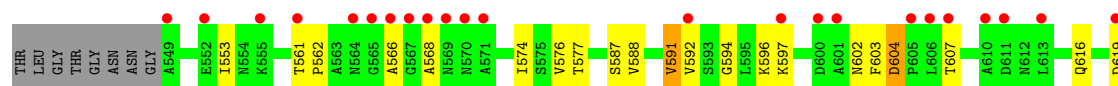




● Molecule 1: Hia



● Molecule 1: Hia



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.58Å 86.20Å 89.12Å 90.00° 99.08° 90.00°	Depositor
Resolution (Å)	44.00 – 2.10 44.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.1 (44.00-2.10) 96.2 (44.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.217 , 0.254 0.217 , 0.253	Depositor DCC
R_{free} test set	3587 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7355	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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 ⓘ

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	0.60	0/1156	1.04	7/1563 (0.4%)
1	B	0.57	0/1155	1.01	4/1562 (0.3%)
1	C	0.60	0/1158	1.05	6/1566 (0.4%)
1	D	0.51	0/1163	1.02	4/1573 (0.3%)
1	E	0.55	0/1158	1.06	7/1566 (0.4%)
1	F	0.52	0/1149	0.97	4/1554 (0.3%)
All	All	0.56	0/6939	1.03	32/9384 (0.3%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	601	ALA	N-CA-C	9.19	122.45	111.33
1	E	601	ALA	N-CA-C	8.59	121.59	111.71
1	C	609	SER	N-CA-C	-6.95	101.17	110.55
1	D	575	SER	N-CA-C	6.25	118.28	108.96
1	E	606	LEU	N-CA-C	5.96	119.66	112.38
1	A	608	SER	N-CA-C	5.94	119.77	110.32
1	F	604	ASP	CA-C-N	5.88	125.75	119.28
1	F	604	ASP	C-N-CA	5.88	125.75	119.28
1	B	604	ASP	CA-C-N	5.77	125.63	119.28
1	B	604	ASP	C-N-CA	5.77	125.63	119.28
1	C	575	SER	N-CA-C	5.74	117.79	109.07
1	D	609	SER	N-CA-C	-5.66	102.91	110.55
1	E	564	ASN	N-CA-C	5.61	119.82	113.15
1	A	557	GLY	N-CA-C	5.51	118.03	110.58
1	C	561	THR	CA-C-N	5.47	125.47	119.89
1	C	561	THR	C-N-CA	5.47	125.47	119.89
1	D	557	GLY	N-CA-C	5.46	117.80	110.43
1	A	698	ARG	N-CA-C	-5.45	100.22	108.67
1	A	588	VAL	N-CA-C	-5.43	99.33	107.37
1	E	574	ILE	N-CA-C	-5.41	100.59	108.17
1	F	594	GLY	N-CA-C	-5.31	107.89	115.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	SER	N-CA-C	5.29	117.30	108.99
1	E	575	SER	N-CA-C	5.29	116.88	108.79
1	D	608	SER	N-CA-C	5.21	118.56	110.17
1	F	620	ALA	N-CA-C	-5.18	105.81	111.82
1	B	575	SER	N-CA-C	5.17	116.93	109.07
1	C	682	LYS	N-CA-C	5.16	118.22	109.76
1	E	588	VAL	N-CA-C	-5.16	100.46	107.99
1	E	683	SER	N-CA-C	-5.08	102.96	110.48
1	A	677	ASN	N-CA-C	-5.05	102.59	110.42
1	A	697	ARG	N-CA-C	5.04	117.77	109.76
1	B	682	LYS	N-CA-C	5.03	118.00	109.76

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	1145	0	1121	26	0
1	B	1144	0	1122	34	0
1	C	1147	0	1123	22	0
1	D	1152	0	1128	45	0
1	E	1147	0	1126	54	0
1	F	1138	0	1114	42	0
2	A	99	0	0	3	0
2	B	84	0	0	5	0
2	C	82	0	0	4	0
2	D	73	0	0	8	0
2	E	90	0	0	5	0
2	F	54	0	0	2	0
All	All	7355	0	6734	182	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 13.

All (182) 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:B:607:THR:HA	1:B:634:LYS:HE2	1.40	1.02
1:B:674:ARG:H	1:B:677:ASN:HD22	1.06	1.01
1:A:674:ARG:H	1:A:677:ASN:HD22	1.01	0.98
1:C:567:GLY:HA3	1:C:572:ASN:HD22	1.31	0.95
1:C:674:ARG:H	1:C:677:ASN:HD22	1.09	0.95
1:D:674:ARG:H	1:D:677:ASN:HD22	0.98	0.94
1:F:674:ARG:H	1:F:677:ASN:ND2	1.67	0.91
1:E:674:ARG:H	1:E:677:ASN:HD22	1.08	0.90
1:D:574:ILE:HD11	1:F:576:VAL:HG13	1.54	0.89
1:B:600:ASP:HB3	2:B:418:HOH:O	1.73	0.88
1:F:674:ARG:N	1:F:677:ASN:HD22	1.70	0.88
1:D:674:ARG:H	1:D:677:ASN:ND2	1.75	0.85
1:F:674:ARG:H	1:F:677:ASN:HD22	0.90	0.85
1:D:574:ILE:HD11	1:F:576:VAL:CG1	2.10	0.82
1:D:674:ARG:N	1:D:677:ASN:HD22	1.80	0.78
1:E:600:ASP:HB3	2:E:117:HOH:O	1.84	0.76
1:A:674:ARG:H	1:A:677:ASN:ND2	1.83	0.76
1:B:674:ARG:H	1:B:677:ASN:ND2	1.85	0.75
1:E:588:VAL:HG12	1:E:591:VAL:CG2	2.17	0.75
1:A:650:LEU:HA	1:A:653:LEU:HD22	1.67	0.74
1:B:553:ILE:HG21	1:C:553:ILE:HD11	1.68	0.74
1:D:697:ARG:HD3	1:E:678:GLU:OE2	1.88	0.74
1:E:695:ASN:N	2:E:250:HOH:O	2.21	0.73
1:C:567:GLY:HA3	1:C:572:ASN:ND2	2.04	0.72
1:A:667:THR:HG22	2:A:336:HOH:O	1.89	0.72
1:D:641:ASP:HA	2:D:291:HOH:O	1.89	0.72
1:F:597:LYS:HE2	2:F:482:HOH:O	1.88	0.72
1:C:595:LEU:CD2	2:C:436:HOH:O	2.37	0.72
1:D:698:ARG:HH21	1:E:677:ASN:CG	1.99	0.71
1:A:674:ARG:N	1:A:677:ASN:HD22	1.82	0.71
1:E:704:LEU:HD22	1:F:686:GLY:HA3	1.72	0.70
1:F:604:ASP:OD2	1:F:607:THR:HG22	1.93	0.68
1:F:629:GLU:HG2	1:F:638:VAL:HG21	1.73	0.68
1:D:683:SER:HB3	1:D:689:VAL:H	1.58	0.68
1:B:668:GLU:H	1:B:668:GLU:CD	2.02	0.68
1:E:588:VAL:HG12	1:E:591:VAL:HG21	1.77	0.67
2:D:291:HOH:O	1:F:648:GLY:HA2	1.95	0.67
1:F:588:VAL:HG12	1:F:591:VAL:CG2	2.24	0.67
1:C:601:ALA:H	1:E:635:GLN:HE21	1.42	0.67
1:B:603:PHE:CD2	1:B:616:GLN:HG2	2.31	0.66
1:E:633:ASP:OD1	1:E:635:GLN:HB2	1.95	0.66
1:B:674:ARG:N	1:B:677:ASN:HD22	1.87	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:607:THR:HG23	2:F:129:HOH:O	1.96	0.66
1:D:683:SER:HB2	1:D:687:ILE:O	1.96	0.65
1:C:601:ALA:H	1:E:635:GLN:NE2	1.94	0.65
1:B:630:LYS:HB3	1:B:634:LYS:HA	1.79	0.64
1:D:571:ALA:O	1:D:584:GLY:HA2	1.98	0.64
1:C:674:ARG:N	1:C:677:ASN:HD22	1.90	0.64
1:E:674:ARG:N	1:E:677:ASN:HD22	1.88	0.64
1:B:607:THR:CA	1:B:634:LYS:HE2	2.21	0.64
1:C:650:LEU:HA	1:C:653:LEU:HD22	1.80	0.63
1:E:603:PHE:CD2	1:E:616:GLN:HG2	2.34	0.62
1:E:633:ASP:O	1:E:634:LYS:HB2	1.99	0.62
1:B:697:ARG:HH11	1:B:697:ARG:HB2	1.64	0.62
1:C:595:LEU:HD22	2:C:436:HOH:O	1.99	0.62
1:B:633:ASP:C	1:B:635:GLN:H	2.05	0.62
1:C:567:GLY:CA	1:C:572:ASN:HD22	2.09	0.62
1:D:698:ARG:HH11	1:E:671:ASP:CG	2.06	0.62
1:A:559:THR:HG23	1:A:573:THR:CG2	2.29	0.61
1:A:692:LYS:HG3	1:A:694:VAL:HG23	1.80	0.61
1:B:697:ARG:NH1	1:B:699:GLU:OE2	2.32	0.61
1:E:588:VAL:HG12	1:E:591:VAL:HG22	1.83	0.61
1:B:607:THR:O	1:B:634:LYS:HG2	2.01	0.61
1:A:574:ILE:HD13	1:A:584:GLY:HA3	1.83	0.61
1:D:698:ARG:HG2	1:E:678:GLU:O	2.01	0.61
1:A:570:ASN:O	1:A:573:THR:HB	2.01	0.60
1:E:674:ARG:H	1:E:677:ASN:ND2	1.91	0.59
1:B:650:LEU:HA	1:B:653:LEU:HD22	1.83	0.58
1:F:588:VAL:HG12	1:F:591:VAL:HG21	1.84	0.58
1:B:578:LYS:HG2	2:B:245:HOH:O	2.02	0.58
1:A:670:HIS:HE1	2:A:416:HOH:O	1.85	0.58
1:D:568:ALA:C	1:D:570:ASN:H	2.10	0.58
1:B:667:THR:HB	1:B:668:GLU:OE2	2.04	0.57
1:C:595:LEU:HD23	2:C:436:HOH:O	2.02	0.57
1:D:553:ILE:HD12	1:D:557:GLY:O	2.04	0.57
1:D:574:ILE:HG12	1:F:577:THR:O	2.04	0.57
1:B:578:LYS:HE3	1:B:579:ASP:OD1	2.05	0.56
1:F:596:LYS:HD2	1:F:629:GLU:OE2	2.06	0.56
1:D:559:THR:HG23	2:D:417:HOH:O	2.05	0.56
1:B:697:ARG:HB2	1:B:697:ARG:NH1	2.21	0.56
1:E:597:LYS:HE3	2:E:451:HOH:O	2.07	0.55
1:F:633:ASP:C	1:F:635:GLN:H	2.15	0.54
1:E:578:LYS:HA	1:F:574:ILE:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:ASP:C	1:B:635:GLN:N	2.65	0.54
1:D:698:ARG:NH1	1:E:671:ASP:CG	2.66	0.54
2:D:291:HOH:O	1:F:651:ARG:HD2	2.07	0.54
1:E:694:VAL:HG12	1:E:695:ASN:N	2.23	0.54
1:A:683:SER:HA	1:A:689:VAL:HG23	1.89	0.53
1:A:559:THR:HG23	1:A:573:THR:HG23	1.89	0.53
1:D:553:ILE:HD11	1:E:551:THR:HG21	1.91	0.53
1:A:678:GLU:CD	1:C:697:ARG:HD3	2.35	0.52
1:D:592:VAL:O	1:F:587:SER:HB3	2.08	0.52
1:D:698:ARG:NH1	1:E:671:ASP:OD1	2.41	0.52
1:B:602:ASN:HB2	2:B:418:HOH:O	2.09	0.52
1:E:704:LEU:HD13	1:F:687:ILE:HG13	1.92	0.52
1:D:702:PHE:O	1:E:684:GLY:HA3	2.11	0.51
1:F:588:VAL:HG12	1:F:591:VAL:HG22	1.92	0.51
1:B:578:LYS:HG3	1:B:579:ASP:OD1	2.11	0.50
1:E:567:GLY:HA3	1:E:572:ASN:ND2	2.26	0.50
1:D:650:LEU:HA	1:D:653:LEU:HD22	1.92	0.50
1:D:587:SER:HB3	1:E:592:VAL:O	2.11	0.50
1:C:566:ALA:O	1:C:570:ASN:HA	2.12	0.50
1:A:559:THR:HG23	1:A:573:THR:HG21	1.93	0.49
1:D:578:LYS:HA	1:E:574:ILE:HD13	1.94	0.49
1:A:702:PHE:O	1:B:684:GLY:HA3	2.12	0.49
1:A:682:LYS:HE2	2:C:188:HOH:O	2.13	0.48
1:E:678:GLU:HB2	1:F:621:TYR:OH	2.12	0.48
1:D:562:PRO:C	1:D:564:ASN:N	2.70	0.48
1:A:680:LYS:HG2	1:A:682:LYS:HG2	1.95	0.48
1:A:692:LYS:HG3	1:A:694:VAL:CG2	2.43	0.48
1:D:569:ASN:O	1:D:570:ASN:HB2	2.13	0.48
1:B:680:LYS:NZ	1:C:660:ASP:OD1	2.39	0.48
1:F:629:GLU:HG2	1:F:638:VAL:CG2	2.41	0.48
1:A:601:ALA:O	1:A:602:ASN:HB2	2.14	0.48
2:D:291:HOH:O	1:F:648:GLY:CA	2.58	0.48
1:E:558:LEU:HD12	1:F:553:ILE:HD11	1.96	0.47
1:D:607:THR:HG21	1:D:632:THR:HA	1.96	0.47
1:C:657:ILE:O	1:C:670:HIS:HA	2.15	0.46
1:E:574:ILE:HD12	1:E:574:ILE:N	2.31	0.46
1:F:607:THR:OG1	1:F:631:GLY:O	2.33	0.46
1:B:578:LYS:HG3	1:B:579:ASP:N	2.30	0.46
1:D:642:ASN:HB3	1:F:591:VAL:O	2.15	0.46
1:D:562:PRO:C	1:D:564:ASN:H	2.24	0.46
1:D:578:LYS:HD2	1:D:579:ASP:OD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:676:ALA:O	1:F:621:TYR:HE2	1.99	0.46
1:D:568:ALA:C	1:D:570:ASN:N	2.74	0.45
1:E:583:ALA:O	1:E:586:GLN:HG2	2.15	0.45
1:E:688:ASN:OD1	1:F:661:LYS:NZ	2.50	0.45
1:E:697:ARG:HB2	2:E:250:HOH:O	2.17	0.45
1:A:553:ILE:CD1	1:B:553:ILE:HD12	2.47	0.45
1:D:678:GLU:OE2	1:F:697:ARG:HD3	2.15	0.45
1:B:670:HIS:HE1	2:B:428:HOH:O	2.00	0.45
1:C:674:ARG:H	1:C:677:ASN:ND2	1.92	0.45
1:D:698:ARG:NH2	1:E:677:ASN:CG	2.73	0.44
1:C:571:ALA:O	1:C:584:GLY:HA2	2.17	0.44
2:D:456:HOH:O	1:E:586:GLN:CD	2.60	0.44
1:F:636:THR:HA	1:F:637:PRO:HD3	1.90	0.44
1:F:633:ASP:C	1:F:635:GLN:N	2.76	0.44
1:D:574:ILE:O	1:D:574:ILE:HG13	2.18	0.43
1:E:578:LYS:HA	1:F:574:ILE:HD13	2.00	0.43
1:E:589:LYS:O	1:E:590:ASN:C	2.61	0.43
1:A:554:ASN:OD1	1:A:556:ASP:N	2.44	0.43
1:A:603:PHE:O	1:A:605:PRO:HD3	2.18	0.43
2:D:291:HOH:O	1:F:647:VAL:HG12	2.18	0.43
1:F:561:THR:HA	1:F:562:PRO:HD3	1.86	0.43
1:B:635:GLN:OE1	1:B:635:GLN:HA	2.19	0.43
1:D:650:LEU:HD11	1:E:645:ALA:HB1	2.01	0.43
1:D:670:HIS:HE1	2:D:249:HOH:O	2.01	0.43
1:B:636:THR:HA	1:B:637:PRO:HD3	1.86	0.42
1:D:577:THR:HA	1:E:560:ILE:HD13	2.01	0.42
1:F:634:LYS:NZ	1:F:634:LYS:HB3	2.35	0.42
1:E:691:GLY:HA3	1:F:669:TYR:CD2	2.54	0.42
1:E:558:LEU:C	1:E:558:LEU:HD23	2.43	0.42
1:B:567:GLY:C	1:B:569:ASN:H	2.28	0.42
1:C:636:THR:HA	1:C:637:PRO:HD3	1.96	0.42
1:A:639:VAL:HG11	1:C:647:VAL:HG21	2.02	0.42
1:C:559:THR:HG23	1:C:573:THR:HG23	2.02	0.42
1:E:694:VAL:HG12	1:E:695:ASN:H	1.84	0.42
1:D:603:PHE:CD2	1:D:616:GLN:HG2	2.55	0.42
1:E:633:ASP:O	1:E:634:LYS:CB	2.67	0.42
1:E:694:VAL:HB	2:E:250:HOH:O	2.20	0.41
1:F:604:ASP:OD2	1:F:607:THR:CG2	2.67	0.41
1:D:647:VAL:HG21	1:E:639:VAL:HG11	2.00	0.41
1:F:604:ASP:CG	1:F:607:THR:HG22	2.45	0.41
1:E:688:ASN:ND2	1:E:705:ALA:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:603:PHE:CD2	1:F:616:GLN:HG2	2.56	0.41
1:A:578:LYS:HA	1:B:574:ILE:HD12	2.02	0.41
1:E:680:LYS:HD3	1:E:682:LYS:HD3	2.02	0.41
1:D:568:ALA:O	1:D:570:ASN:N	2.47	0.41
1:D:698:ARG:NH2	1:E:677:ASN:OD1	2.44	0.41
1:E:553:ILE:CD1	1:F:553:ILE:HD12	2.50	0.41
1:C:688:ASN:ND2	1:C:705:ALA:HB2	2.36	0.41
1:B:597:LYS:NZ	2:B:292:HOH:O	2.53	0.41
1:D:657:ILE:O	1:D:670:HIS:HA	2.21	0.41
1:E:657:ILE:O	1:E:670:HIS:HA	2.21	0.41
1:A:607:THR:HA	1:A:634:LYS:HG2	2.03	0.40
2:A:315:HOH:O	1:B:549:ALA:HB3	2.20	0.40
1:D:566:ALA:O	1:D:570:ASN:HA	2.21	0.40
1:D:703:GLU:CA	1:E:687:ILE:HD12	2.51	0.40
1:F:604:ASP:HB3	1:F:607:THR:HG22	2.03	0.40
1:A:571:ALA:O	1:A:584:GLY:HA2	2.21	0.40
1:B:549:ALA:HA	1:B:561:THR:O	2.22	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	156/174 (90%)	150 (96%)	6 (4%)	0	100	100
1	B	155/174 (89%)	145 (94%)	7 (4%)	3 (2%)	6	3
1	C	155/174 (89%)	148 (96%)	5 (3%)	2 (1%)	9	6
1	D	156/174 (90%)	148 (95%)	6 (4%)	2 (1%)	9	6
1	E	155/174 (89%)	147 (95%)	7 (4%)	1 (1%)	21	18
1	F	155/174 (89%)	146 (94%)	6 (4%)	3 (2%)	6	3
All	All	932/1044 (89%)	884 (95%)	37 (4%)	11 (1%)	10	7

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	569	ASN
1	C	632	THR
1	D	568	ALA
1	F	568	ALA
1	E	694	VAL
1	B	619	ASP
1	C	633	ASP
1	D	569	ASN
1	F	566	ALA
1	F	602	ASN
1	B	568	ALA

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	121/136 (89%)	119 (98%)	2 (2%)	53	62
1	B	122/136 (90%)	118 (97%)	4 (3%)	33	37
1	C	123/136 (90%)	121 (98%)	2 (2%)	55	64
1	D	123/136 (90%)	121 (98%)	2 (2%)	55	64
1	E	123/136 (90%)	119 (97%)	4 (3%)	33	37
1	F	120/136 (88%)	116 (97%)	4 (3%)	33	37
All	All	732/816 (90%)	714 (98%)	18 (2%)	42	48

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	586	GLN
1	A	653	LEU
1	B	619	ASP
1	B	633	ASP
1	B	653	LEU
1	B	668	GLU

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Mol	Chain	Res	Type
1	C	569	ASN
1	C	653	LEU
1	D	574	ILE
1	D	653	LEU
1	E	591	VAL
1	E	592	VAL
1	E	634	LYS
1	E	704	LEU
1	F	591	VAL
1	F	592	VAL
1	F	619	ASP
1	F	653	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	586	GLN
1	A	670	HIS
1	A	677	ASN
1	B	670	HIS
1	B	677	ASN
1	C	572	ASN
1	C	586	GLN
1	C	670	HIS
1	C	677	ASN
1	C	688	ASN
1	D	572	ASN
1	D	586	GLN
1	D	677	ASN
1	D	688	ASN
1	D	695	ASN
1	E	572	ASN
1	E	635	GLN
1	E	670	HIS
1	E	677	ASN
1	E	695	ASN
1	F	677	ASN

5.3.3 RNA ⓘ

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	158/174 (90%)	0.33	8 (5%) 33 35	15, 31, 48, 59	0
1	B	157/174 (90%)	0.90	32 (20%) 3 3	17, 35, 70, 80	0
1	C	157/174 (90%)	0.39	12 (7%) 20 21	14, 31, 62, 70	0
1	D	158/174 (90%)	0.71	14 (8%) 15 16	22, 37, 64, 69	0
1	E	157/174 (90%)	0.66	14 (8%) 15 16	24, 36, 52, 63	0
1	F	157/174 (90%)	1.11	31 (19%) 3 3	25, 39, 73, 81	0
All	All	944/1044 (90%)	0.68	111 (11%) 9 9	14, 35, 63, 81	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	631	GLY	5.4
1	F	569	ASN	4.9
1	C	563	ALA	4.8
1	B	602	ASN	4.7
1	B	636	THR	4.5
1	C	568	ALA	4.3
1	D	563	ALA	4.3
1	F	566	ALA	4.3
1	F	610	ALA	4.3
1	B	631	GLY	4.2
1	F	570	ASN	4.1
1	D	549	ALA	4.1
1	C	632	THR	4.0
1	F	636	THR	3.9
1	B	565	GLY	3.7
1	B	637	PRO	3.6
1	E	705	ALA	3.6
1	F	568	ALA	3.5
1	B	601	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	633	ASP	3.4
1	F	561	THR	3.3
1	A	568	ALA	3.3
1	F	631	GLY	3.2
1	B	630	LYS	3.2
1	B	566	ALA	3.2
1	F	549	ALA	3.2
1	D	696	GLY	3.2
1	F	632	THR	3.1
1	F	606	LEU	3.1
1	B	632	THR	3.1
1	B	564	ASN	3.1
1	C	636	THR	3.0
1	F	607	THR	3.0
1	D	633	ASP	3.0
1	B	568	ALA	2.9
1	D	568	ALA	2.9
1	B	563	ALA	2.9
1	F	638	VAL	2.8
1	F	567	GLY	2.8
1	B	609	SER	2.8
1	B	599	GLY	2.7
1	F	565	GLY	2.7
1	C	706	LYS	2.7
1	C	567	GLY	2.7
1	A	566	ALA	2.7
1	C	566	ALA	2.7
1	F	600	ASP	2.7
1	E	571	ALA	2.7
1	C	635	GLN	2.7
1	B	562	PRO	2.7
1	F	552	GLU	2.6
1	D	632	THR	2.6
1	F	705	ALA	2.6
1	F	564	ASN	2.6
1	F	605	PRO	2.5
1	B	603	PHE	2.5
1	A	569	ASN	2.4
1	B	552	GLU	2.4
1	B	638	VAL	2.4
1	E	549	ALA	2.4
1	C	572	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	633	ASP	2.4
1	E	694	VAL	2.4
1	F	592	VAL	2.4
1	D	706	LYS	2.4
1	B	685	ASN	2.4
1	E	564	ASN	2.4
1	F	555	LYS	2.4
1	F	630	LYS	2.4
1	F	637	PRO	2.4
1	F	601	ALA	2.3
1	B	619	ASP	2.3
1	A	667	THR	2.3
1	D	566	ALA	2.3
1	E	704	LEU	2.3
1	B	569	ASN	2.3
1	F	619	ASP	2.3
1	F	571	ALA	2.2
1	B	635	GLN	2.2
1	A	564	ASN	2.2
1	E	569	ASN	2.2
1	B	600	ASP	2.2
1	A	567	GLY	2.2
1	E	584	GLY	2.2
1	E	601	ALA	2.2
1	D	564	ASN	2.2
1	D	636	THR	2.2
1	B	705	ALA	2.2
1	B	613	LEU	2.2
1	C	667	THR	2.2
1	E	561	THR	2.2
1	F	611	ASP	2.2
1	C	668	GLU	2.1
1	D	638	VAL	2.1
1	E	676	ALA	2.1
1	A	668	GLU	2.1
1	D	572	ASN	2.1
1	E	632	THR	2.1
1	E	555	LYS	2.1
1	F	597	LYS	2.1
1	A	601	ALA	2.1
1	E	566	ALA	2.1
1	B	607	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	634	LYS	2.0
1	D	574	ILE	2.0
1	B	666	SER	2.0
1	B	549	ALA	2.0
1	D	685	ASN	2.0
1	F	613	LEU	2.0
1	B	618	ASP	2.0
1	B	594	GLY	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 [i](#)

There are no such residues in this entry.