



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:47 PM UTC

PDB ID : 3DIT / pdb_00003dit
Title : Crystal structure of MAD MH2 domain
Authors : Hao, R.; Wu, J.W.; Wang, Z.X.
Deposited on : 2008-06-20
Resolution : 3.20 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

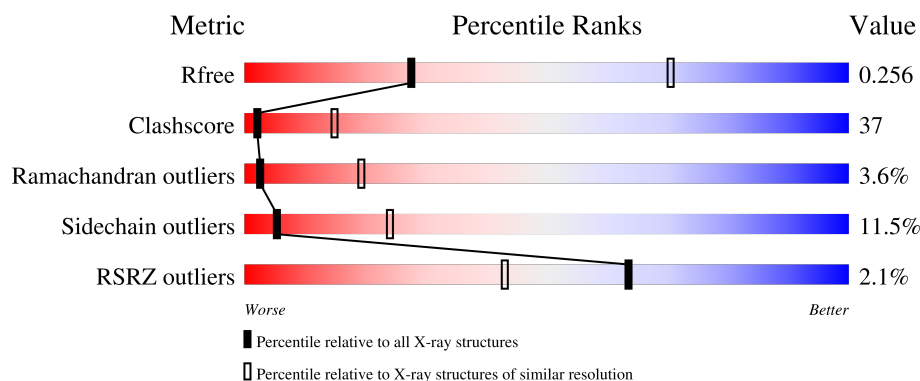
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	188	5% 43% 44% 11% ..
1	B	188	40% 44% 14% ..
1	C	188	5% 32% 59% 9% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4548 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 mothers against dpp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1482	931	263	275	13			
1	B	186	Total	C	N	O	S	0	0	0
			1481	932	262	274	13			
1	C	188	Total	C	N	O	S	0	0	0
			1495	939	265	278	13			

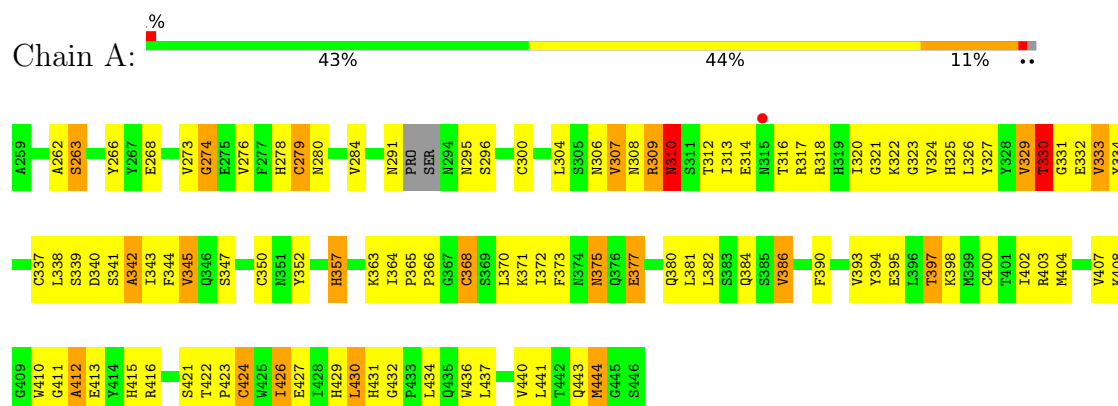
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	33	Total	O	0	0
			33	33		
2	B	35	Total	O	0	0
			35	35		
2	C	22	Total	O	0	0
			22	22		

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: Protein mothers against dpp





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	95.86Å 95.86Å 66.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20 50.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	85.0 (50.00-3.20) 89.9 (50.00-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.310 0.249 , 0.256	Depositor DCC
R_{free} test set	490 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 72.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l 0.037 for h,-h-k,-l 0.025 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	4548	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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	0.63	1/1519 (0.1%)	1.07	10/2059 (0.5%)
1	B	0.63	1/1519 (0.1%)	1.13	13/2060 (0.6%)
1	C	0.55	0/1534	1.13	16/2082 (0.8%)
All	All	0.60	2/4572 (0.0%)	1.11	39/6201 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	268	GLU	C-O	-8.84	1.14	1.24
1	A	444	MET	SD-CE	-5.24	1.66	1.79

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	269	LEU	N-CA-C	-10.83	91.97	108.00
1	C	269	LEU	CB-CA-C	-10.02	102.31	116.34
1	B	375	ASN	N-CA-C	8.88	120.96	111.28
1	C	396	LEU	N-CA-C	-8.06	103.34	113.01
1	B	396	LEU	N-CA-C	-7.66	103.91	113.18
1	B	270	ASN	CA-C-N	-7.27	112.54	122.86
1	B	270	ASN	C-N-CA	-7.27	112.54	122.86
1	A	415	HIS	N-CA-C	-6.98	103.28	111.03
1	C	375	ASN	N-CA-C	6.74	118.71	111.36
1	C	270	ASN	N-CA-C	-6.53	105.19	112.57
1	A	364	ILE	CA-C-N	6.44	127.02	120.38
1	A	364	ILE	C-N-CA	6.44	127.02	120.38
1	C	364	ILE	CA-C-N	6.39	126.97	120.38
1	C	364	ILE	C-N-CA	6.39	126.97	120.38
1	C	320	ILE	N-CA-C	-6.33	104.35	110.42
1	A	307	VAL	N-CA-C	-6.31	106.39	111.81
1	A	368	CYS	N-CA-C	6.29	117.99	110.19
1	A	357	HIS	N-CA-C	-6.27	100.45	109.48
1	C	390	PHE	N-CA-C	-6.14	104.51	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	320	ILE	N-CA-C	-6.13	104.53	110.72
1	B	345	VAL	N-CA-C	6.11	117.39	108.53
1	B	280	ASN	N-CA-C	-6.10	104.91	112.90
1	C	280	ASN	N-CA-C	-5.92	105.83	113.16
1	B	269	LEU	CB-CA-C	-5.88	109.81	116.63
1	A	345	VAL	N-CA-C	5.50	116.50	108.53
1	B	397	THR	N-CA-C	-5.47	105.47	111.82
1	C	368	CYS	N-CA-C	5.43	118.50	110.46
1	B	304	LEU	N-CA-C	5.35	116.99	110.41
1	C	432	GLY	CA-C-N	5.33	124.78	119.24
1	C	432	GLY	C-N-CA	5.33	124.78	119.24
1	C	417	GLN	N-CA-C	5.30	119.89	113.38
1	B	329	VAL	N-CA-C	5.27	115.57	107.77
1	B	269	LEU	N-CA-C	-5.25	99.21	108.08
1	A	422	THR	CA-C-N	5.24	125.05	119.28
1	A	422	THR	C-N-CA	5.24	125.05	119.28
1	C	357	HIS	N-CA-C	-5.16	103.17	110.29
1	A	340	ASP	N-CA-C	-5.14	106.84	113.01
1	C	410	TRP	N-CA-C	5.14	115.03	108.24
1	B	290	THR	N-CA-C	5.01	117.29	110.88

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	1482	0	1406	96	0
1	B	1481	0	1407	104	0
1	C	1495	0	1419	128	0
2	A	33	0	0	0	0
2	B	35	0	0	0	0
2	C	22	0	0	0	0
All	All	4548	0	4232	325	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 37.

All (325) 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:C:322:LYS:HB3	1:C:338:LEU:HB3	1.36	1.05
1:B:333:VAL:HG23	1:B:372:ILE:HG13	1.50	0.94
1:C:333:VAL:HG23	1:C:372:ILE:HG13	1.50	0.93
1:A:382:LEU:HD21	1:A:440:VAL:HG21	1.50	0.93
1:C:333:VAL:HG22	1:C:373:PHE:HB3	1.53	0.91
1:B:306:ASN:ND2	1:B:307:VAL:H	1.72	0.87
1:C:386:VAL:HG23	1:C:444:MET:HE3	1.57	0.87
1:C:348:ARG:HD2	1:C:399:MET:HG2	1.55	0.87
1:B:352:TYR:CZ	1:B:381:LEU:HD21	2.12	0.84
1:A:268:GLU:HG3	1:A:273:VAL:HG21	1.57	0.83
1:B:310:ASN:ND2	1:B:310:ASN:H	1.74	0.83
1:B:308:ASN:N	1:B:308:ASN:HD22	1.78	0.81
1:A:310:ASN:OD1	1:A:312:THR:HG22	1.80	0.81
1:C:374:ASN:HD22	1:C:377:GLU:HB2	1.46	0.81
1:B:333:VAL:HG22	1:B:373:PHE:HB3	1.62	0.80
1:A:268:GLU:OE1	1:A:313:ILE:HD13	1.83	0.79
1:B:302:GLY:HA2	1:B:317:ARG:NH2	1.98	0.79
1:C:337:CYS:SG	1:C:366:PRO:HA	2.24	0.77
1:A:394:TYR:O	1:A:397:THR:HB	1.83	0.77
1:B:310:ASN:H	1:B:310:ASN:HD22	1.28	0.77
1:C:394:TYR:O	1:C:397:THR:HB	1.86	0.76
1:B:374:ASN:OD1	1:B:377:GLU:HB2	1.86	0.75
1:C:309:ARG:HG2	1:C:310:ASN:H	1.52	0.74
1:C:380:GLN:HB3	1:C:384:GLN:HE21	1.51	0.74
1:C:268:GLU:HA	1:C:423:PRO:O	1.88	0.73
1:B:311:SER:O	1:B:315:ASN:HB2	1.89	0.73
1:B:333:VAL:HG22	1:B:373:PHE:CB	2.19	0.73
1:B:333:VAL:CG2	1:B:372:ILE:HG13	2.19	0.73
1:C:333:VAL:CG2	1:C:372:ILE:HG13	2.19	0.73
1:C:268:GLU:HG3	1:C:273:VAL:HG21	1.69	0.72
1:A:363:LYS:O	1:A:365:PRO:HD3	1.88	0.72
1:A:333:VAL:CG2	1:A:372:ILE:HG13	2.19	0.72
1:B:310:ASN:HD22	1:B:310:ASN:N	1.87	0.72
1:C:374:ASN:HD22	1:C:377:GLU:CB	2.03	0.72
1:C:352:TYR:CZ	1:C:381:LEU:HD21	2.24	0.72
1:C:382:LEU:HD21	1:C:440:VAL:HG21	1.70	0.72
1:C:390:PHE:CZ	1:C:441:LEU:HD22	2.25	0.72
1:B:307:VAL:HG23	1:B:308:ASN:ND2	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:ARG:HB3	1:B:421:SER:CB	2.20	0.71
1:A:320:ILE:O	1:A:339:SER:HB2	1.91	0.71
1:C:352:TYR:CE1	1:C:381:LEU:HD21	2.25	0.71
1:A:390:PHE:CZ	1:A:441:LEU:HD22	2.27	0.70
1:A:370:LEU:HD12	1:A:371:LYS:H	1.55	0.70
1:C:287:ASP:O	1:C:301:LEU:HD13	1.92	0.70
1:C:263:SER:OG	1:C:429:HIS:HB2	1.92	0.69
1:A:331:GLY:O	1:A:375:ASN:HB2	1.93	0.69
1:C:333:VAL:HG22	1:C:373:PHE:CB	2.21	0.69
1:B:345:VAL:HG22	1:B:404:MET:HB3	1.74	0.69
1:B:307:VAL:HG23	1:B:308:ASN:HD22	1.57	0.69
1:A:333:VAL:HG23	1:A:372:ILE:HG13	1.75	0.68
1:B:394:TYR:O	1:B:397:THR:HB	1.92	0.68
1:C:279:CYS:HB3	1:C:284:VAL:HG11	1.76	0.68
1:A:310:ASN:O	1:A:314:GLU:HB2	1.94	0.68
1:B:310:ASN:ND2	1:B:310:ASN:N	2.42	0.68
1:A:352:TYR:CE1	1:A:381:LEU:HD21	2.30	0.67
1:A:370:LEU:HD12	1:A:371:LYS:N	2.10	0.67
1:C:287:ASP:OD1	1:C:300:CYS:HA	1.93	0.67
1:B:347:SER:HB3	1:B:350:CYS:HB3	1.76	0.66
1:B:333:VAL:HG23	1:B:372:ILE:CG1	2.25	0.66
1:B:416:ARG:HB3	1:B:421:SER:HB3	1.76	0.66
1:C:374:ASN:HD22	1:C:377:GLU:CG	2.09	0.66
1:B:370:LEU:HD12	1:B:371:LYS:N	2.11	0.66
1:B:345:VAL:CG2	1:B:404:MET:HE2	2.26	0.65
1:A:408:LYS:HD2	1:A:416:ARG:NH2	2.12	0.65
1:C:363:LYS:O	1:C:365:PRO:HD3	1.97	0.65
1:A:408:LYS:HB3	1:A:416:ARG:CZ	2.26	0.65
1:C:264:ILE:HG23	1:C:428:ILE:HG12	1.78	0.65
1:A:310:ASN:ND2	1:A:313:ILE:HB	2.12	0.64
1:B:313:ILE:HG22	1:B:314:GLU:N	2.11	0.64
1:B:290:THR:HG22	1:B:290:THR:O	1.98	0.64
1:A:322:LYS:HB3	1:A:338:LEU:HB3	1.78	0.64
1:A:326:LEU:HD21	1:A:404:MET:CE	2.28	0.63
1:B:331:GLY:O	1:B:375:ASN:HB2	1.98	0.63
1:A:345:VAL:HG22	1:A:404:MET:HB3	1.79	0.63
1:C:266:TYR:CD2	1:C:273:VAL:HB	2.32	0.63
1:C:329:VAL:O	1:C:330:THR:HG22	1.99	0.63
1:A:395:GLU:C	1:A:397:THR:H	2.04	0.63
1:B:260:PHE:HD1	1:B:278:HIS:HB3	1.63	0.63
1:B:404:MET:HG3	1:B:426:ILE:HG13	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:CYS:HB3	1:B:284:VAL:HG11	1.80	0.62
1:C:386:VAL:CG2	1:C:444:MET:HE3	2.28	0.62
1:A:337:CYS:SG	1:A:343:ILE:HG13	2.40	0.62
1:A:333:VAL:HG22	1:A:373:PHE:HB3	1.82	0.61
1:A:337:CYS:HA	1:A:343:ILE:HD12	1.81	0.61
1:B:352:TYR:CE1	1:B:381:LEU:HD21	2.35	0.61
1:A:263:SER:HB3	1:A:278:HIS:HD2	1.66	0.61
1:A:400:CYS:CB	1:A:434:LEU:HG	2.30	0.61
1:C:431:HIS:O	1:C:432:GLY:C	2.43	0.61
1:A:427:GLU:HG2	1:A:429:HIS:CE1	2.37	0.60
1:C:380:GLN:HB3	1:C:384:GLN:NE2	2.15	0.60
1:C:345:VAL:HG11	1:C:372:ILE:CG2	2.32	0.60
1:B:268:GLU:HG3	1:B:273:VAL:HG21	1.82	0.60
1:A:307:VAL:C	1:A:309:ARG:H	2.10	0.59
1:C:353:HIS:C	1:C:353:HIS:CD2	2.80	0.59
1:B:370:LEU:HD12	1:B:371:LYS:H	1.66	0.59
1:B:437:LEU:O	1:B:441:LEU:HD12	2.01	0.59
1:B:306:ASN:CG	1:B:307:VAL:H	2.09	0.59
1:C:300:CYS:SG	1:C:303:GLN:HG2	2.43	0.59
1:C:334:TYR:OH	1:C:371:LYS:HD3	2.03	0.59
1:C:430:LEU:HB3	1:C:433:PRO:HD2	1.85	0.59
1:A:333:VAL:HG23	1:A:372:ILE:CG1	2.33	0.58
1:A:390:PHE:CE1	1:A:441:LEU:HD22	2.39	0.58
1:C:291:ASN:HB2	1:C:298:ARG:NH2	2.18	0.58
1:C:310:ASN:HD21	1:C:313:ILE:H	1.50	0.57
1:A:310:ASN:ND2	1:A:313:ILE:H	2.01	0.57
1:C:390:PHE:CE1	1:C:441:LEU:HD22	2.40	0.57
1:A:395:GLU:C	1:A:397:THR:N	2.58	0.57
1:C:374:ASN:ND2	1:C:377:GLU:OE2	2.38	0.57
1:C:309:ARG:NH1	1:C:317:ARG:NH1	2.53	0.57
1:A:279:CYS:HB3	1:A:284:VAL:HG11	1.87	0.57
1:B:290:THR:HG23	1:B:303:GLN:HA	1.86	0.57
1:C:290:THR:HG23	1:C:303:GLN:HB3	1.86	0.57
1:A:403:ARG:HB3	1:A:403:ARG:NH1	2.20	0.56
1:B:267:TYR:CE1	1:B:272:ARG:HB2	2.40	0.56
1:C:337:CYS:SG	1:C:343:ILE:HG13	2.44	0.56
1:C:404:MET:O	1:C:404:MET:HG3	2.06	0.56
1:A:306:ASN:HD22	1:A:307:VAL:H	1.54	0.56
1:C:344:PHE:O	1:C:404:MET:HB2	2.06	0.56
1:C:374:ASN:ND2	1:C:377:GLU:CG	2.69	0.56
1:B:291:ASN:HB3	1:B:300:CYS:SG	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:ASN:ND2	1:C:313:ILE:H	2.04	0.55
1:A:284:VAL:HG23	1:A:284:VAL:O	2.06	0.55
1:B:268:GLU:HA	1:B:423:PRO:O	2.07	0.55
1:C:393:VAL:HG13	1:C:441:LEU:HD21	1.87	0.55
1:C:353:HIS:HB2	1:C:377:GLU:OE1	2.07	0.55
1:A:341:SER:O	1:A:342:ALA:O	2.25	0.55
1:A:404:MET:CG	1:A:426:ILE:HD11	2.36	0.55
1:B:273:VAL:HG12	1:B:304:LEU:HD13	1.89	0.55
1:A:333:VAL:HG22	1:A:373:PHE:CB	2.36	0.55
1:A:344:PHE:CE2	1:A:363:LYS:HB2	2.42	0.55
1:C:268:GLU:O	1:C:269:LEU:HB2	2.06	0.55
1:C:334:TYR:CZ	1:C:371:LYS:HD3	2.42	0.55
1:A:309:ARG:O	1:A:310:ASN:HB3	2.05	0.54
1:A:352:TYR:CZ	1:A:381:LEU:HD21	2.43	0.54
1:B:310:ASN:O	1:B:314:GLU:HB2	2.08	0.54
1:B:308:ASN:N	1:B:308:ASN:ND2	2.46	0.54
1:B:436:TRP:O	1:B:440:VAL:HG23	2.07	0.54
1:B:320:ILE:O	1:B:339:SER:HB2	2.08	0.54
1:B:400:CYS:CB	1:B:434:LEU:HG	2.38	0.53
1:C:345:VAL:HG11	1:C:372:ILE:HG22	1.90	0.53
1:A:306:ASN:HD22	1:A:307:VAL:N	2.06	0.53
1:B:416:ARG:HB3	1:B:421:SER:HB2	1.89	0.53
1:C:262:ALA:HA	1:C:429:HIS:O	2.08	0.53
1:C:333:VAL:HG23	1:C:372:ILE:CG1	2.33	0.53
1:C:436:TRP:O	1:C:440:VAL:HG23	2.08	0.53
1:A:274:GLY:HA3	1:A:304:LEU:HD13	1.90	0.53
1:C:260:PHE:CD1	1:C:278:HIS:HB3	2.43	0.53
1:C:374:ASN:ND2	1:C:377:GLU:HB2	2.21	0.53
1:A:263:SER:HG	1:A:431:HIS:HE2	1.57	0.53
1:A:324:VAL:HG22	1:A:325:HIS:N	2.24	0.52
1:B:268:GLU:O	1:B:269:LEU:C	2.51	0.52
1:C:440:VAL:O	1:C:444:MET:HG3	2.09	0.52
1:B:322:LYS:HB3	1:B:338:LEU:HB3	1.90	0.52
1:C:359:SER:O	1:C:360:THR:C	2.50	0.52
1:C:374:ASN:ND2	1:C:377:GLU:H	2.08	0.52
1:C:353:HIS:C	1:C:355:GLY:H	2.18	0.52
1:B:380:GLN:O	1:B:381:LEU:C	2.53	0.52
1:C:324:VAL:HB	1:C:343:ILE:HD13	1.90	0.52
1:A:330:THR:CG2	1:A:330:THR:O	2.58	0.52
1:B:306:ASN:ND2	1:B:307:VAL:N	2.50	0.52
1:A:310:ASN:HD22	1:A:313:ILE:HB	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:HIS:C	1:B:353:HIS:CD2	2.87	0.52
1:A:382:LEU:HD21	1:A:440:VAL:CG2	2.32	0.51
1:C:337:CYS:HA	1:C:343:ILE:HD12	1.91	0.51
1:A:310:ASN:CG	1:A:312:THR:HG22	2.34	0.51
1:A:377:GLU:O	1:A:380:GLN:HB2	2.10	0.51
1:C:400:CYS:SG	1:C:433:PRO:HB2	2.51	0.51
1:A:416:ARG:HB3	1:A:421:SER:HB2	1.92	0.51
1:A:395:GLU:HG2	1:A:398:LYS:HE3	1.93	0.51
1:A:404:MET:O	1:A:426:ILE:HG12	2.10	0.50
1:C:281:ASN:OD1	1:C:282:ASN:N	2.44	0.50
1:A:326:LEU:HD21	1:A:404:MET:HE1	1.93	0.50
1:A:386:VAL:HG13	1:A:444:MET:HE3	1.93	0.50
1:B:365:PRO:O	1:B:368:CYS:HB2	2.12	0.50
1:B:394:TYR:CD1	1:B:394:TYR:C	2.88	0.50
1:A:410:TRP:CD1	1:A:411:GLY:N	2.80	0.50
1:C:445:GLY:O	1:C:446:SER:O	2.29	0.50
1:A:431:HIS:O	1:A:432:GLY:C	2.52	0.50
1:A:347:SER:HB3	1:A:350:CYS:HB3	1.93	0.50
1:A:412:ALA:O	1:A:413:GLU:HG2	2.12	0.49
1:C:341:SER:CB	1:C:407:VAL:HG22	2.42	0.49
1:B:404:MET:SD	1:B:426:ILE:HD11	2.52	0.49
1:B:306:ASN:CG	1:B:307:VAL:N	2.70	0.49
1:A:306:ASN:HD21	1:A:308:ASN:HB2	1.78	0.48
1:A:307:VAL:C	1:A:309:ARG:N	2.70	0.48
1:A:400:CYS:HB3	1:A:434:LEU:HG	1.95	0.48
1:B:260:PHE:HD2	1:B:260:PHE:N	2.11	0.48
1:C:341:SER:HB2	1:C:407:VAL:HG22	1.95	0.48
1:A:339:SER:OG	1:A:341:SER:N	2.42	0.48
1:B:441:LEU:O	1:B:444:MET:HB3	2.14	0.48
1:C:397:THR:HA	1:C:437:LEU:CD2	2.43	0.48
1:B:339:SER:O	1:B:366:PRO:HB3	2.13	0.48
1:B:281:ASN:OD1	1:B:282:ASN:N	2.47	0.48
1:A:331:GLY:C	1:A:332:GLU:HG2	2.38	0.48
1:B:378:PHE:O	1:B:379:ALA:C	2.57	0.48
1:C:348:ARG:NH2	1:C:398:LYS:HD2	2.29	0.48
1:C:374:ASN:ND2	1:C:377:GLU:CB	2.75	0.48
1:B:260:PHE:N	1:B:260:PHE:CD2	2.81	0.48
1:B:291:ASN:ND2	1:B:300:CYS:SG	2.83	0.48
1:A:397:THR:HA	1:A:437:LEU:CD2	2.44	0.48
1:C:283:SER:OG	1:C:325:HIS:NE2	2.39	0.47
1:B:363:LYS:O	1:B:365:PRO:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:PHE:HA	1:C:362:CYS:O	2.14	0.47
1:B:376:GLN:NE2	1:B:380:GLN:HE21	2.12	0.47
1:A:310:ASN:HD22	1:A:310:ASN:N	2.11	0.47
1:B:397:THR:HA	1:B:437:LEU:CD2	2.45	0.47
1:C:300:CYS:C	1:C:301:LEU:HD12	2.40	0.47
1:C:416:ARG:HB3	1:C:421:SER:HB3	1.97	0.47
1:C:335:ALA:HB2	1:C:372:ILE:HD13	1.97	0.47
1:C:310:ASN:C	1:C:310:ASN:HD22	2.23	0.46
1:B:269:LEU:HD23	1:B:269:LEU:HA	1.77	0.46
1:B:337:CYS:HA	1:B:343:ILE:HD12	1.97	0.46
1:B:395:GLU:HG2	1:B:398:LYS:HE3	1.97	0.46
1:C:374:ASN:ND2	1:C:377:GLU:HG3	2.31	0.46
1:C:321:GLY:C	1:C:323:GLY:H	2.24	0.46
1:A:334:TYR:CZ	1:A:371:LYS:HD3	2.50	0.46
1:C:274:GLY:HA3	1:C:304:LEU:HD22	1.98	0.46
1:A:327:TYR:HB2	1:A:334:TYR:HB2	1.98	0.46
1:C:291:ASN:HB2	1:C:298:ARG:CZ	2.46	0.46
1:B:334:TYR:CE1	1:B:371:LYS:HB2	2.51	0.46
1:C:285:ILE:N	1:C:285:ILE:HD12	2.31	0.46
1:C:301:LEU:O	1:C:317:ARG:NH2	2.49	0.46
1:C:345:VAL:HG11	1:C:372:ILE:HG21	1.97	0.45
1:A:339:SER:OG	1:A:341:SER:O	2.30	0.45
1:B:324:VAL:HG21	1:B:404:MET:HE1	1.98	0.45
1:B:376:GLN:HE22	1:B:380:GLN:NE2	2.13	0.45
1:B:442:THR:C	1:B:444:MET:N	2.73	0.45
1:A:416:ARG:HG3	1:A:416:ARG:NH1	2.30	0.45
1:C:395:GLU:C	1:C:397:THR:N	2.71	0.45
1:A:357:HIS:CE1	1:B:322:LYS:NZ	2.84	0.45
1:B:354:HIS:C	1:C:311:SER:HB2	2.42	0.45
1:A:329:VAL:C	1:A:331:GLY:H	2.25	0.45
1:B:381:LEU:O	1:B:385:SER:HB2	2.16	0.45
1:C:266:TYR:HD2	1:C:273:VAL:HB	1.79	0.45
1:B:404:MET:HG3	1:B:426:ILE:CG1	2.46	0.45
1:A:310:ASN:ND2	1:A:310:ASN:C	2.74	0.45
1:A:365:PRO:O	1:A:368:CYS:HB2	2.17	0.45
1:B:400:CYS:HB3	1:B:434:LEU:HG	1.99	0.44
1:C:353:HIS:C	1:C:355:GLY:N	2.75	0.44
1:B:300:CYS:HB2	1:B:303:GLN:HG2	1.99	0.44
1:B:356:PHE:CE2	1:C:310:ASN:OD1	2.70	0.44
1:C:281:ASN:OD1	1:C:283:SER:N	2.49	0.44
1:C:414:TYR:O	1:C:417:GLN:NE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:THR:C	1:A:318:ARG:H	2.25	0.44
1:B:320:ILE:O	1:B:339:SER:CB	2.65	0.44
1:C:285:ILE:HD12	1:C:285:ILE:H	1.83	0.44
1:C:418:ASP:OD2	1:C:419:VAL:N	2.51	0.44
1:B:266:TYR:CD2	1:B:301:LEU:HD22	2.53	0.44
1:C:380:GLN:O	1:C:381:LEU:C	2.60	0.44
1:B:309:ARG:HB3	1:B:314:GLU:OE1	2.18	0.44
1:B:352:TYR:OH	1:B:381:LEU:HD21	2.16	0.44
1:B:382:LEU:HD13	1:B:437:LEU:HD12	2.00	0.44
1:C:410:TRP:O	1:C:414:TYR:HD2	2.01	0.44
1:A:266:TYR:OH	1:A:424:CYS:HB3	2.18	0.43
1:C:337:CYS:HA	1:C:343:ILE:CD1	2.48	0.43
1:A:386:VAL:CG2	1:A:440:VAL:HG11	2.48	0.43
1:C:309:ARG:CG	1:C:310:ASN:H	2.24	0.43
1:C:315:ASN:HD22	1:C:315:ASN:HA	1.57	0.43
1:B:350:CYS:O	1:B:350:CYS:SG	2.77	0.43
1:B:315:ASN:HD22	1:B:315:ASN:HA	1.50	0.43
1:C:311:SER:O	1:C:315:ASN:HB2	2.18	0.43
1:C:400:CYS:CB	1:C:434:LEU:HG	2.48	0.43
1:C:434:LEU:O	1:C:435:GLN:C	2.60	0.43
1:C:441:LEU:O	1:C:444:MET:HB2	2.18	0.43
1:B:268:GLU:HG3	1:B:273:VAL:CG2	2.47	0.43
1:B:268:GLU:O	1:B:269:LEU:HB2	2.19	0.43
1:B:277:PHE:CD1	1:B:299:CYS:HB2	2.53	0.43
1:B:403:ARG:HG2	1:B:403:ARG:HH11	1.84	0.43
1:C:320:ILE:O	1:C:339:SER:HB2	2.17	0.43
1:A:436:TRP:O	1:A:440:VAL:HG23	2.18	0.43
1:C:310:ASN:HD21	1:C:313:ILE:CB	2.32	0.43
1:A:316:THR:HG21	1:A:423:PRO:HG2	2.01	0.43
1:C:321:GLY:C	1:C:323:GLY:N	2.75	0.43
1:B:261:TRP:CE3	1:B:262:ALA:HB2	2.54	0.43
1:A:402:ILE:HD12	1:A:430:LEU:CD2	2.49	0.42
1:B:353:HIS:C	1:B:355:GLY:H	2.28	0.42
1:C:353:HIS:C	1:C:353:HIS:HD2	2.27	0.42
1:C:374:ASN:HD22	1:C:377:GLU:CD	2.27	0.42
1:C:385:SER:O	1:C:386:VAL:C	2.59	0.42
1:A:306:ASN:ND2	1:A:307:VAL:N	2.68	0.42
1:C:348:ARG:CD	1:C:399:MET:HG2	2.39	0.42
1:C:395:GLU:C	1:C:397:THR:H	2.26	0.42
1:A:365:PRO:O	1:A:366:PRO:C	2.62	0.42
1:B:344:PHE:CE2	1:B:363:LYS:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:LEU:HD12	1:C:371:LYS:N	2.34	0.42
1:B:316:THR:C	1:B:318:ARG:H	2.28	0.42
1:C:310:ASN:HD21	1:C:313:ILE:HG13	1.84	0.42
1:C:345:VAL:HG22	1:C:404:MET:HB3	2.01	0.42
1:C:310:ASN:ND2	1:C:310:ASN:N	2.67	0.42
1:C:437:LEU:HD12	1:C:437:LEU:HA	1.88	0.42
1:A:380:GLN:O	1:A:384:GLN:HB2	2.20	0.42
1:B:316:THR:C	1:B:318:ARG:N	2.77	0.42
1:B:376:GLN:NE2	1:B:380:GLN:NE2	2.68	0.41
1:B:309:ARG:HG2	1:B:313:ILE:HG21	2.03	0.41
1:C:314:GLU:OE1	1:C:314:GLU:HA	2.21	0.41
1:B:302:GLY:HA2	1:B:317:ARG:HH22	1.81	0.41
1:B:319:HIS:O	1:B:341:SER:HB2	2.21	0.41
1:C:263:SER:HA	1:C:277:PHE:O	2.21	0.41
1:C:281:ASN:ND2	1:C:297:ASP:OD2	2.53	0.41
1:C:386:VAL:HG13	1:C:387:ASN:N	2.36	0.41
1:A:262:ALA:HB2	1:A:430:LEU:HD12	2.02	0.41
1:A:309:ARG:HG3	1:A:313:ILE:HG21	2.03	0.41
1:B:263:SER:HB2	1:B:278:HIS:HD2	1.86	0.41
1:A:268:GLU:OE2	1:A:309:ARG:NH2	2.53	0.41
1:C:349:ASN:HD22	1:C:399:MET:CE	2.33	0.41
1:A:397:THR:HA	1:A:437:LEU:HD21	2.01	0.41
1:A:321:GLY:C	1:A:323:GLY:N	2.79	0.41
1:C:274:GLY:CA	1:C:304:LEU:HD22	2.50	0.41
1:C:316:THR:HG21	1:C:423:PRO:HG2	2.02	0.41
1:B:273:VAL:O	1:B:274:GLY:O	2.38	0.41
1:B:378:PHE:C	1:B:380:GLN:N	2.76	0.41
1:C:261:TRP:CE3	1:C:262:ALA:HB2	2.55	0.41
1:C:306:ASN:ND2	1:C:307:VAL:H	2.19	0.41
1:C:353:HIS:CB	1:C:377:GLU:OE1	2.68	0.41
1:A:276:VAL:O	1:A:276:VAL:HG13	2.20	0.41
1:A:268:GLU:OE2	1:A:317:ARG:HD2	2.21	0.40
1:A:337:CYS:HA	1:A:343:ILE:CD1	2.48	0.40
1:A:393:VAL:HG11	1:A:444:MET:SD	2.61	0.40
1:C:321:GLY:O	1:C:323:GLY:N	2.54	0.40
1:B:419:VAL:HG22	1:B:425:TRP:CD2	2.56	0.40
1:C:264:ILE:HA	1:C:427:GLU:O	2.21	0.40
1:A:310:ASN:HD21	1:A:313:ILE:H	1.70	0.40
1:A:386:VAL:O	1:A:444:MET:CE	2.69	0.40
1:B:277:PHE:CG	1:B:299:CYS:HB2	2.56	0.40
1:C:310:ASN:ND2	1:C:313:ILE:HB	2.36	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	182/188 (97%)	153 (84%)	20 (11%)	9 (5%)	1	13
1	B	182/188 (97%)	148 (81%)	30 (16%)	4 (2%)	5	29
1	C	186/188 (99%)	151 (81%)	28 (15%)	7 (4%)	2	18
All	All	550/564 (98%)	452 (82%)	78 (14%)	20 (4%)	2	19

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	SER
1	A	342	ALA
1	B	342	ALA
1	C	263	SER
1	C	296	SER
1	C	310	ASN
1	C	342	ALA
1	A	330	THR
1	A	412	ALA
1	B	274	GLY
1	A	295	ASN
1	C	388	ASN
1	C	412	ALA
1	A	274	GLY
1	A	309	ARG
1	A	310	ASN
1	B	412	ALA
1	C	322	LYS
1	B	407	VAL
1	A	407	VAL

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	165/167 (99%)	148 (90%)	17 (10%)	7	28
1	B	165/167 (99%)	139 (84%)	26 (16%)	2	13
1	C	167/167 (100%)	153 (92%)	14 (8%)	10	38
All	All	497/501 (99%)	440 (88%)	57 (12%)	5	24

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	SER
1	A	279	CYS
1	A	280	ASN
1	A	291	ASN
1	A	300	CYS
1	A	310	ASN
1	A	329	VAL
1	A	330	THR
1	A	333	VAL
1	A	375	ASN
1	A	377	GLU
1	A	386	VAL
1	A	397	THR
1	A	424	CYS
1	A	426	ILE
1	A	430	LEU
1	A	443	GLN
1	B	279	CYS
1	B	280	ASN
1	B	291	ASN
1	B	295	ASN
1	B	299	CYS
1	B	303	GLN
1	B	308	ASN
1	B	310	ASN
1	B	312	THR

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Mol	Chain	Res	Type
1	B	313	ILE
1	B	315	ASN
1	B	329	VAL
1	B	330	THR
1	B	333	VAL
1	B	371	LYS
1	B	376	GLN
1	B	377	GLU
1	B	385	SER
1	B	387	ASN
1	B	397	THR
1	B	404	MET
1	B	407	VAL
1	B	424	CYS
1	B	430	LEU
1	B	434	LEU
1	B	435	GLN
1	C	264	ILE
1	C	279	CYS
1	C	310	ASN
1	C	315	ASN
1	C	329	VAL
1	C	375	ASN
1	C	397	THR
1	C	413	GLU
1	C	424	CYS
1	C	426	ILE
1	C	430	LEU
1	C	436	TRP
1	C	443	GLN
1	C	446	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	HIS
1	A	294	ASN
1	A	306	ASN
1	A	310	ASN
1	A	315	ASN
1	A	351	ASN
1	A	357	HIS

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Mol	Chain	Res	Type
1	A	429	HIS
1	B	278	HIS
1	B	291	ASN
1	B	306	ASN
1	B	308	ASN
1	B	310	ASN
1	B	315	ASN
1	B	351	ASN
1	B	376	GLN
1	B	380	GLN
1	B	387	ASN
1	B	417	GLN
1	B	429	HIS
1	C	294	ASN
1	C	303	GLN
1	C	306	ASN
1	C	308	ASN
1	C	310	ASN
1	C	315	ASN
1	C	349	ASN
1	C	351	ASN
1	C	374	ASN
1	C	384	GLN
1	C	387	ASN
1	C	443	GLN

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 oligosaccharides 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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	186/188 (98%)	0.14	1 (0%) 87 76	11, 42, 100, 166	0
1	B	186/188 (98%)	0.30	2 (1%) 78 61	9, 53, 109, 148	0
1	C	188/188 (100%)	0.65	9 (4%) 35 22	22, 66, 181, 198	0
All	All	560/564 (99%)	0.36	12 (2%) 63 43	9, 54, 148, 198	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	415	HIS	3.7
1	C	294	ASN	3.2
1	C	297	ASP	3.2
1	C	308	ASN	3.1
1	C	304	LEU	3.1
1	C	306	ASN	2.7
1	C	301	LEU	2.6
1	B	296	SER	2.4
1	B	403	ARG	2.2
1	C	296	SER	2.2
1	A	315	ASN	2.1
1	C	312	THR	2.1

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.