Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2022 – 04:57 pm BST

PDB ID	:	7ZVU
Title	:	HUMAN PRMT5:MEP50 Crystal Structure With MTA and Fragment Bound
Authors	:	Ahmad, M.U.; Koelmel, W.; Arkhipova, V.; Lawson, J.D.; Smith, C.R.; Gunn, R.J.
Deposited on	:	2022-05-17
Resolution	:	1.95 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:

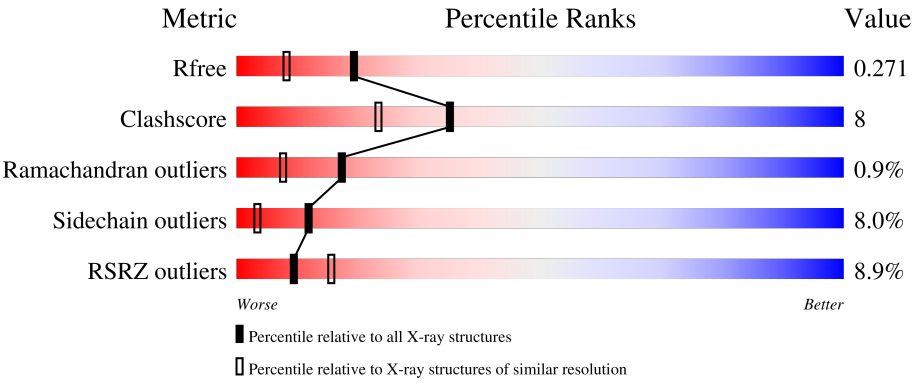
MolProbity	:	4.02b-467
Mogul	:	FAILED
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	645	5% 75% 19%
2	B	350	15% 64% 22% 11%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7793 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 arginine N-methyltransferase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	625	Total	C	N	O	S	0	3	0
			5083	3252	872	934	25			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP O14744
A	-6	ASP	-	expression tag	UNP O14744
A	-5	TYR	-	expression tag	UNP O14744
A	-4	LYS	-	expression tag	UNP O14744
A	-3	ASP	-	expression tag	UNP O14744
A	-2	ASP	-	expression tag	UNP O14744
A	-1	ASP	-	expression tag	UNP O14744
A	0	ASP	-	expression tag	UNP O14744
A	1	LYS	-	expression tag	UNP O14744

- Molecule 2 is a protein called Methylosome protein 50.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	310	Total	C	N	O	S	0	1	0
			2345	1471	401	458	15			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP Q9BQA1
B	-6	HIS	-	expression tag	UNP Q9BQA1
B	-5	HIS	-	expression tag	UNP Q9BQA1
B	-4	HIS	-	expression tag	UNP Q9BQA1
B	-3	HIS	-	expression tag	UNP Q9BQA1
B	-2	HIS	-	expression tag	UNP Q9BQA1
B	-1	HIS	-	expression tag	UNP Q9BQA1

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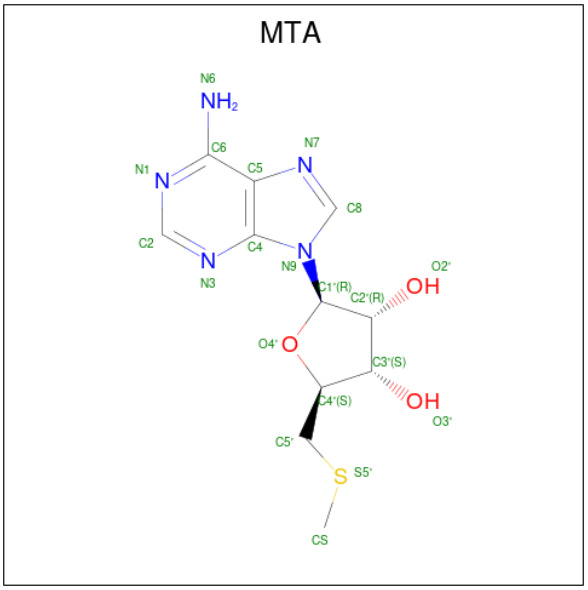
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP Q9BQA1
B	1	HIS	-	expression tag	UNP Q9BQA1

- Molecule 3 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (three-letter code: MTA) (formula: $C_{11}H_{15}N_5O_3S$) (labeled as "Ligand of Interest" by depositor).

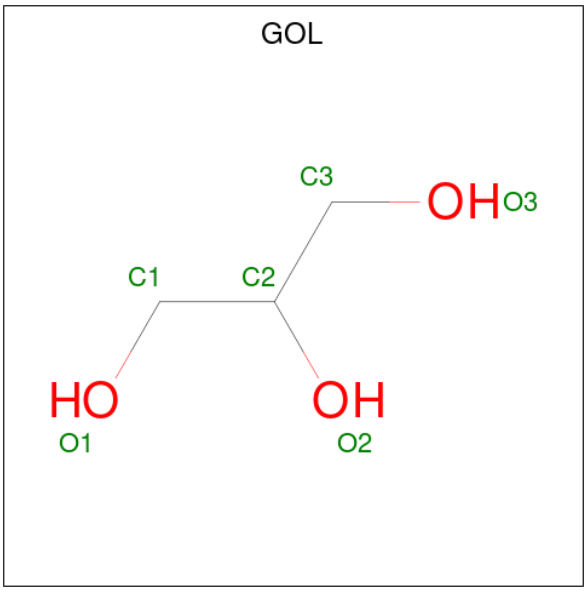


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

- Molecule 4 is UNKNOWN LIGAND (three-letter code: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			20	14	6		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

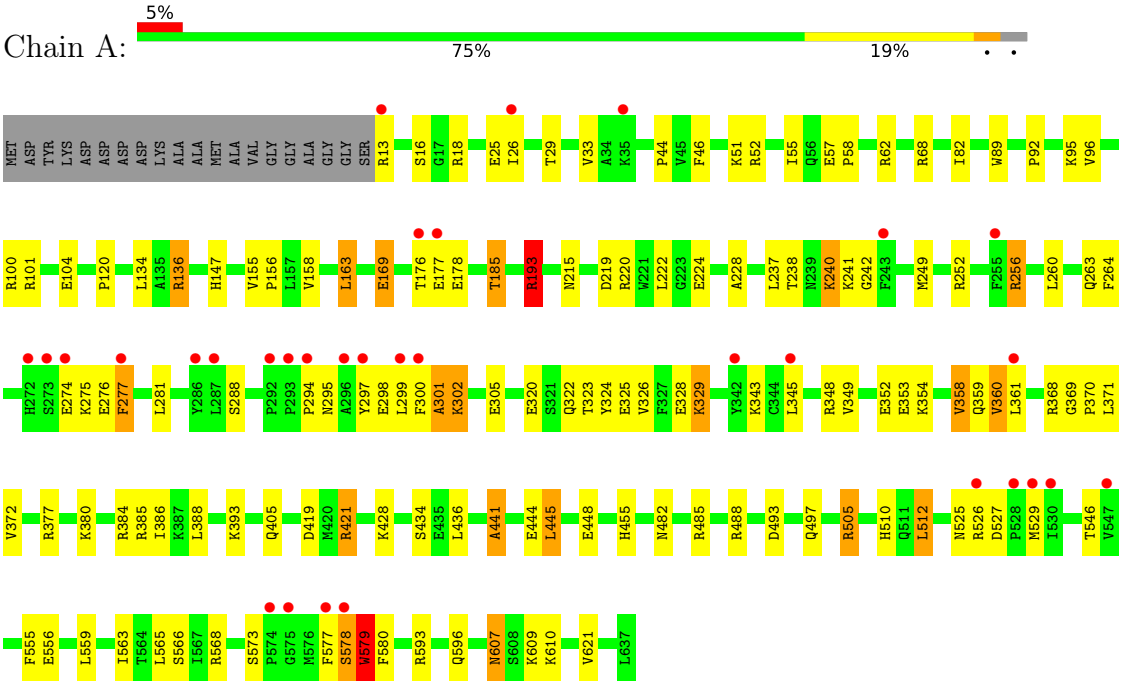
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	256	Total O 256 256	0	0
6	B	57	Total O 57 57	0	0

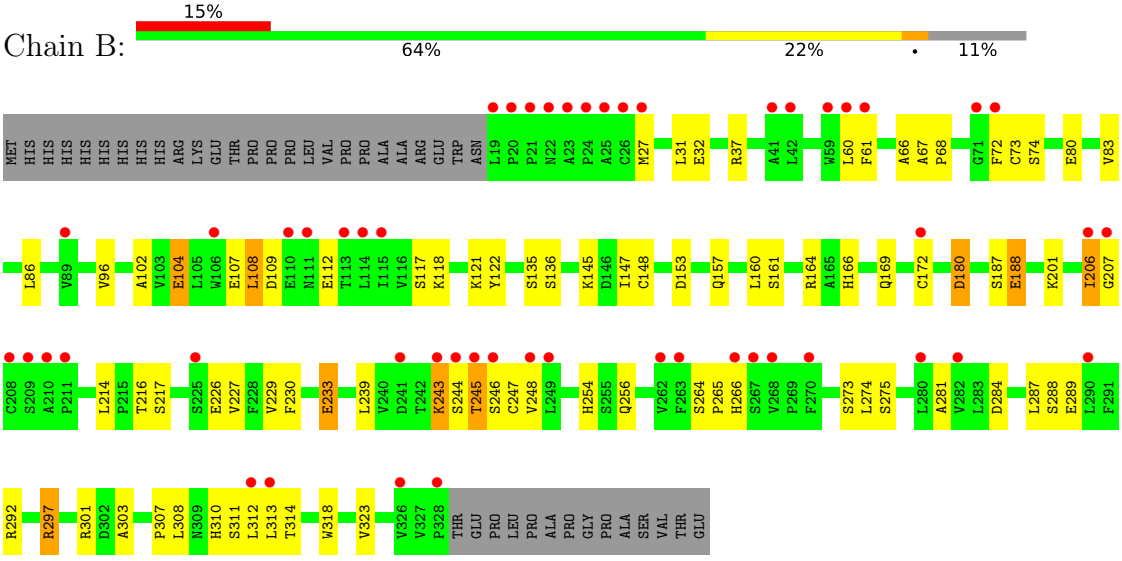
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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 arginine N-methyltransferase 5



• Molecule 2: Methylosome protein 50



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	105.15Å 139.16Å 178.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.75 – 1.95 109.75 – 1.95	Depositor EDS
% Data completeness (in resolution range)	62.2 (109.75-1.95) 62.2 (109.75-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.64 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.237 , 0.266 0.242 , 0.271	Depositor DCC
R_{free} test set	3096 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	35.5	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7793	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, UNL, MTA

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	0.86	4/5228 (0.1%)	0.99	14/7111 (0.2%)
2	B	0.88	3/2402 (0.1%)	0.89	1/3283 (0.0%)
All	All	0.87	7/7630 (0.1%)	0.96	15/10394 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	GLU	CD-OE2	-6.61	1.18	1.25
1	A	224	GLU	CD-OE1	-6.52	1.18	1.25
2	B	80	GLU	CD-OE2	6.06	1.32	1.25
1	A	320	GLU	CD-OE1	-5.78	1.19	1.25
2	B	233	GLU	CD-OE2	5.37	1.31	1.25
1	A	325	GLU	CD-OE2	-5.15	1.20	1.25
2	B	188	GLU	CD-OE2	-5.04	1.20	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	607	ASN	CB-CA-C	-9.01	92.38	110.40
1	A	193	ARG	NE-CZ-NH1	-8.22	116.19	120.30
1	A	62	ARG	NE-CZ-NH1	-7.73	116.43	120.30
1	A	256	ARG	NE-CZ-NH1	6.97	123.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	136	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	A	485	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	488	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	568	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	421	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	A	100	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	B	227	VAL	CA-CB-CG2	5.36	118.94	110.90
1	A	215	ASN	CB-CA-C	-5.33	99.75	110.40
1	A	493	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	A	68	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	193	ARG	NH1-CZ-NH2	5.02	124.92	119.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169[A]	GLU	Sidechain

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	5083	0	4978	77	0
2	B	2345	0	2260	46	0
3	A	20	0	15	0	0
4	A	20	0	0	1	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	256	0	0	9	0
6	B	57	0	0	6	0
All	All	7793	0	7269	121	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 8.

All (121) 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:A:578:SER:O	1:A:579:TRP:HB2	1.26	1.08
1:A:578:SER:O	1:A:579:TRP:CB	2.02	1.03
1:A:185:THR:HG22	6:A:922:HOH:O	1.72	0.89
2:B:201:LYS:O	6:B:501:HOH:O	1.97	0.81
1:A:156:PRO:O	1:A:185:THR:HG21	1.81	0.80
1:A:324:TYR:CB	1:A:368:ARG:HD2	2.16	0.76
2:B:60:LEU:HD22	2:B:108:LEU:HD21	1.69	0.75
1:A:348:ARG:HE	1:A:359:GLN:HE22	1.36	0.72
1:A:297:TYR:CD2	1:A:577:PHE:HA	2.25	0.72
2:B:27:MET:HE3	2:B:31:LEU:HD21	1.73	0.71
2:B:32:GLU:OE1	6:B:502:HOH:O	2.07	0.71
1:A:302:LYS:O	1:A:305:GLU:OE1	2.12	0.68
1:A:419:ASP:OD1	1:A:421:ARG:HD3	1.94	0.68
1:A:358:VAL:HA	1:A:385:ARG:O	1.96	0.66
2:B:157:GLN:OE1	6:B:503:HOH:O	2.12	0.66
1:A:238:THR:HG22	1:A:242:GLY:HA2	1.78	0.64
1:A:324:TYR:HB2	1:A:368:ARG:HD2	1.80	0.64
1:A:348:ARG:HE	1:A:359:GLN:NE2	1.96	0.64
1:A:294:PRO:HB2	1:A:298:GLU:HB2	1.81	0.61
1:A:156:PRO:O	1:A:185:THR:CG2	2.50	0.60
1:A:343:LYS:HE3	1:A:563:ILE:HD11	1.83	0.60
2:B:109:ASP:HB3	2:B:112:GLU:H	1.67	0.60
2:B:27:MET:HE2	2:B:68:PRO:HB2	1.84	0.59
2:B:169:GLN:NE2	6:B:507:HOH:O	2.29	0.59
2:B:102:ALA:HB2	2:B:122:TYR:CD1	2.38	0.58
1:A:377:ARG:O	1:A:380:LYS:HG3	2.02	0.58
2:B:172[B]:CYS:SG	2:B:216:THR:O	2.62	0.57
1:A:158:VAL:HG11	1:A:163:LEU:HD13	1.85	0.57
1:A:324:TYR:HB3	1:A:368:ARG:HD2	1.86	0.57
2:B:109:ASP:HB3	2:B:112:GLU:N	2.21	0.56
1:A:444:GLU:OE2	4:A:702:UNL:N3	2.39	0.56
1:A:322:GLN:O	1:A:326:VAL:HG13	2.05	0.55
2:B:60:LEU:CD2	2:B:108:LEU:HD21	2.35	0.54
1:A:18:ARG:NH2	1:A:277:PHE:CZ	2.75	0.54
2:B:32:GLU:HG2	2:B:83:VAL:O	2.08	0.54
1:A:565:LEU:HA	1:A:573:SER:OG	2.07	0.54
1:A:607:ASN:HB3	1:A:609:LYS:H	1.71	0.54
1:A:29:THR:O	1:A:33:VAL:HG13	2.07	0.54
1:A:222:LEU:HD12	1:A:510:HIS:CG	2.44	0.53
1:A:295:ASN:OD1	1:A:297:TYR:HB3	2.08	0.53
1:A:434:SER:HB2	1:A:436:LEU:HG	1.91	0.53
1:A:444:GLU:O	1:A:445:LEU:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ILE:HD13	6:A:919:HOH:O	2.08	0.52
1:A:301:ALA:HB1	1:A:505:ARG:HG3	1.91	0.52
1:A:360:VAL:HG11	1:A:428:LYS:O	2.10	0.52
1:A:448:GLU:O	6:A:803:HOH:O	2.19	0.52
1:A:300:PHE:HE1	1:A:329:LYS:HE2	1.76	0.51
1:A:577:PHE:CD1	1:A:578:SER:N	2.79	0.51
2:B:135:SER:OG	2:B:180:ASP:OD2	2.25	0.51
1:A:147:HIS:HB3	6:A:928:HOH:O	2.11	0.50
1:A:44:PRO:HB2	1:A:46:PHE:O	2.11	0.50
1:A:607:ASN:HB2	1:A:610:LYS:H	1.75	0.50
1:A:240:LYS:H	1:A:240:LYS:CE	2.25	0.50
1:A:386:ILE:HG13	1:A:386:ILE:O	2.12	0.49
1:A:349:VAL:HG23	1:A:384:ARG:HE	1.77	0.49
2:B:109:ASP:O	2:B:112:GLU:HG2	2.12	0.49
1:A:228:ALA:HA	1:A:263:GLN:O	2.12	0.49
1:A:596:GLN:OE1	6:A:804:HOH:O	2.20	0.49
1:A:297:TYR:CE2	1:A:577:PHE:HA	2.47	0.49
1:A:607:ASN:CB	1:A:609:LYS:H	2.25	0.49
2:B:102:ALA:HA	2:B:121:LYS:O	2.13	0.48
2:B:148:CYS:SG	2:B:164:ARG:HG2	2.53	0.48
1:A:527:ASP:HB3	1:A:529:MET:O	2.14	0.48
2:B:96:VAL:HB	2:B:104:GLU:HG3	1.95	0.48
1:A:294:PRO:HB2	1:A:298:GLU:CB	2.43	0.48
2:B:281:ALA:HB2	2:B:292:ARG:NH1	2.29	0.48
1:A:219:ASP:O	1:A:222:LEU:HG	2.14	0.48
1:A:512:LEU:HG	1:A:546:THR:HG21	1.95	0.48
1:A:82:ILE:O	1:A:120:PRO:HD2	2.15	0.47
2:B:303:ALA:HB1	2:B:313:LEU:HD11	1.95	0.47
1:A:101:ARG:NH1	6:A:821:HOH:O	2.48	0.46
1:A:240:LYS:H	1:A:240:LYS:HE2	1.80	0.46
2:B:229:VAL:HG12	2:B:239:LEU:HA	1.98	0.46
2:B:217:SER:O	2:B:230:PHE:HA	2.15	0.46
1:A:455:HIS:HD2	6:A:1008:HOH:O	1.99	0.46
2:B:264:SER:HB2	2:B:266:HIS:HD2	1.81	0.46
1:A:249:MET:SD	1:A:252:ARG:HD3	2.56	0.45
1:A:441:ALA:HB2	1:A:555:PHE:HB2	1.98	0.45
1:A:276:GLU:HG3	1:A:277:PHE:N	2.32	0.45
1:A:163:LEU:HD12	1:A:163:LEU:HA	1.79	0.45
2:B:66:ALA:HB1	2:B:72:PHE:HB2	1.98	0.45
2:B:244:SER:HB3	2:B:246:SER:HB3	1.98	0.45
1:A:328:GLU:OE2	1:A:368:ARG:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LYS:HG2	1:A:89:TRP:CD2	2.52	0.45
1:A:556:GLU:HG2	1:A:566:SER:HB2	1.99	0.45
2:B:145:LYS:HA	2:B:169:GLN:HB3	1.99	0.45
1:A:372:VAL:HG13	1:A:388:LEU:HD13	1.98	0.44
2:B:254:HIS:CG	2:B:275:SER:HB2	2.51	0.44
2:B:265:PRO:HB2	2:B:310:HIS:CE1	2.53	0.44
1:A:345:LEU:O	1:A:349:VAL:HG22	2.18	0.44
1:A:371:LEU:HB2	6:A:872:HOH:O	2.18	0.44
2:B:32:GLU:OE2	2:B:301:ARG:HD3	2.18	0.44
1:A:16:SER:HA	1:A:264:PHE:O	2.18	0.44
1:A:369:GLY:N	1:A:370:PRO:CD	2.81	0.43
1:A:323:THR:O	1:A:326:VAL:HG22	2.18	0.43
2:B:166:HIS:ND1	2:B:187:SER:HB3	2.34	0.43
2:B:243:LYS:HA	2:B:243:LYS:NZ	2.33	0.43
2:B:153:ASP:HB2	2:B:160:LEU:HD21	2.01	0.43
2:B:307:PRO:O	2:B:310:HIS:CD2	2.72	0.42
1:A:26:ILE:HG22	6:B:512:HOH:O	2.18	0.42
1:A:352:GLU:HG2	1:A:353:GLU:N	2.34	0.42
2:B:61:PHE:CG	2:B:67:ALA:HB2	2.54	0.42
2:B:264:SER:HB2	2:B:266:HIS:CD2	2.54	0.42
1:A:349:VAL:HG23	1:A:384:ARG:NE	2.35	0.42
2:B:244:SER:C	2:B:246:SER:N	2.73	0.41
2:B:289:GLU:OE2	2:B:292:ARG:HB2	2.20	0.41
1:A:240:LYS:H	1:A:240:LYS:HZ3	1.68	0.41
2:B:301:ARG:HD2	2:B:318:TRP:NE1	2.35	0.41
2:B:314:THR:HA	2:B:323:VAL:O	2.20	0.41
1:A:92:PRO:HG2	1:A:134:LEU:HD12	2.02	0.41
2:B:188:GLU:HG2	2:B:214:LEU:HD13	2.01	0.41
1:A:58:PRO:HG3	2:B:297:ARG:HA	2.02	0.41
1:A:260:LEU:HD12	1:A:260:LEU:HA	1.84	0.41
2:B:86:LEU:HD11	2:B:96:VAL:HG22	2.03	0.41
2:B:206:ILE:HG13	2:B:207:GLY:N	2.35	0.41
1:A:193:ARG:HH11	1:A:193:ARG:HD3	1.62	0.41
1:A:505:ARG:HG2	1:A:580:PHE:CD1	2.56	0.40
2:B:256:GLN:NE2	6:B:511:HOH:O	2.54	0.40
2:B:284:ASP:OD2	2:B:288:SER:HB2	2.21	0.40
1:A:96:VAL:HG21	2:B:233:GLU:HG3	2.03	0.40
1:A:104:GLU:HB3	6:A:1033:HOH:O	2.22	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	626/645 (97%)	590 (94%)	31 (5%)	5 (1%)	19 9
2	B	309/350 (88%)	299 (97%)	7 (2%)	3 (1%)	15 6
All	All	935/995 (94%)	889 (95%)	38 (4%)	8 (1%)	17 8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	579	TRP
2	B	147	ILE
1	A	578	SER
2	B	248	VAL
1	A	358	VAL
1	A	441	ALA
1	A	301	ALA
2	B	245	THR

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	561/570 (98%)	517 (92%)	44 (8%)	12 3
2	B	264/298 (89%)	241 (91%)	23 (9%)	10 2
All	All	825/868 (95%)	758 (92%)	67 (8%)	12 3

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	25	GLU
1	A	52	ARG
1	A	57	GLU
1	A	95	LYS
1	A	136	ARG
1	A	155	VAL
1	A	163	LEU
1	A	169[A]	GLU
1	A	169[B]	GLU
1	A	176	THR
1	A	177	GLU
1	A	178	GLU
1	A	185	THR
1	A	193	ARG
1	A	220	ARG
1	A	237	LEU
1	A	240	LYS
1	A	241	LYS
1	A	256	ARG
1	A	274	GLU
1	A	275	LYS
1	A	277	PHE
1	A	281	LEU
1	A	288	SER
1	A	299	LEU
1	A	302	LYS
1	A	329	LYS
1	A	354	LYS
1	A	360	VAL
1	A	361	LEU
1	A	393	LYS
1	A	405	GLN
1	A	445	LEU
1	A	482	ASN
1	A	497	GLN
1	A	505	ARG
1	A	512	LEU
1	A	525	ASN
1	A	526	ARG
1	A	559	LEU
1	A	579	TRP
1	A	593	ARG

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Mol	Chain	Res	Type
1	A	621	VAL
2	B	37	ARG
2	B	73	CYS
2	B	74	SER
2	B	104	GLU
2	B	107	GLU
2	B	108	LEU
2	B	117	SER
2	B	118	LYS
2	B	136	SER
2	B	161	SER
2	B	180	ASP
2	B	206	ILE
2	B	226	GLU
2	B	243	LYS
2	B	245	THR
2	B	247	CYS
2	B	273	SER
2	B	274	LEU
2	B	287	LEU
2	B	297	ARG
2	B	308	LEU
2	B	311	SER
2	B	312	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	56	GLN
1	A	251	GLN
1	A	289	GLN
1	A	336	GLN
1	A	359	GLN
1	A	525	ASN
2	B	139	GLN
2	B	157	GLN
2	B	224	GLN
2	B	266	HIS
2	B	294	GLN
2	B	310	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

Mogul failed to run properly - this section is therefore empty.

5.5 Carbohydrates

Mogul failed to run properly - this section is therefore empty.

5.6 Ligand geometry

Mogul failed to run properly - this section is therefore empty.

5.7 Other polymers

Mogul failed to run properly - this section is therefore empty.

5.8 Polymer linkage issues

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	625/645 (96%)	0.72	32 (5%) 28 37	17, 26, 60, 112	0
2	B	310/350 (88%)	1.10	51 (16%) 1 2	19, 34, 69, 100	0
All	All	935/995 (93%)	0.84	83 (8%) 9 15	17, 29, 67, 112	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	21	PRO	8.3
2	B	19	LEU	6.7
1	A	293	PRO	6.3
2	B	268	VAL	6.3
2	B	26	CYS	6.2
1	A	294	PRO	6.2
2	B	209	SER	5.7
2	B	23	ALA	5.4
1	A	13	ARG	5.3
2	B	114	LEU	5.2
1	A	277	PHE	5.1
2	B	207	GLY	5.1
2	B	248	VAL	5.0
1	A	177	GLU	5.0
1	A	577	PHE	4.8
2	B	110	GLU	4.7
2	B	210	ALA	4.7
1	A	296	ALA	4.6
1	A	299	LEU	4.4
1	A	529	MET	4.3
2	B	208	CYS	4.2
2	B	312	LEU	4.1
1	A	300	PHE	4.1
2	B	24	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	244	SER	3.9
2	B	60	LEU	3.8
2	B	290	LEU	3.8
2	B	270	PHE	3.7
1	A	297	TYR	3.6
1	A	575	GLY	3.5
2	B	22	ASN	3.5
2	B	59	TRP	3.4
2	B	206	ILE	3.4
2	B	106	TRP	3.4
1	A	273	SER	3.3
2	B	243	LYS	3.3
1	A	243	PHE	3.3
1	A	526	ARG	3.2
2	B	246	SER	3.2
2	B	326	VAL	3.0
2	B	61	PHE	3.0
2	B	113	THR	3.0
1	A	578	SER	3.0
1	A	176	THR	2.9
1	A	342	TYR	2.9
2	B	282	VAL	2.9
2	B	20	PRO	2.9
2	B	71	GLY	2.8
2	B	328	PRO	2.8
2	B	115	ILE	2.8
2	B	111	ASN	2.8
1	A	361	LEU	2.7
2	B	280	LEU	2.7
2	B	262	VAL	2.7
1	A	286	TYR	2.6
2	B	211	PRO	2.6
2	B	313	LEU	2.5
2	B	25	ALA	2.4
1	A	345	LEU	2.4
2	B	72	PHE	2.4
1	A	292	PRO	2.4
2	B	266	HIS	2.4
2	B	27	MET	2.4
2	B	241	ASP	2.4
2	B	41	ALA	2.3
1	A	530	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	255	PHE	2.2
1	A	574	PRO	2.2
2	B	225	SER	2.2
2	B	267	SER	2.2
1	A	274	GLU	2.2
1	A	547	VAL	2.2
2	B	245	THR	2.1
1	A	272	HIS	2.1
2	B	172[A]	CYS	2.1
1	A	287	LEU	2.1
2	B	42	LEU	2.1
2	B	249	LEU	2.1
2	B	89	VAL	2.0
1	A	35	LYS	2.0
1	A	528	PRO	2.0
2	B	263	PHE	2.0
1	A	26	ILE	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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	A	703	6/6	0.85	0.21	46,50,58,67	0
5	GOL	B	401	6/6	0.90	0.23	65,69,72,73	0
4	UNL	A	702	20/-	0.97	0.14	16,22,29,32	0
3	MTA	A	701	20/20	0.98	0.14	16,18,20,21	0

6.5 Other polymers (i)

There are no such residues in this entry.