WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Mar 26, 2024 – 10:07 AM EDT

PDB ID	:	4M3P
Title	:	Betaine-Homocysteine S-Methyltransferase from Homo sapiens complexed with Homocysteine
Authors	:	Koutmos, M.; Yamada, K.; Mladkova, J.; Paterova, J.; Diamond, C.E.; Tryon, K.; Jungwirth, P.; Garrow, T.A.; Jiracek, J.
Deposited on	:	2013-08-06
Resolution	:	1.90 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 (i) 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 (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1
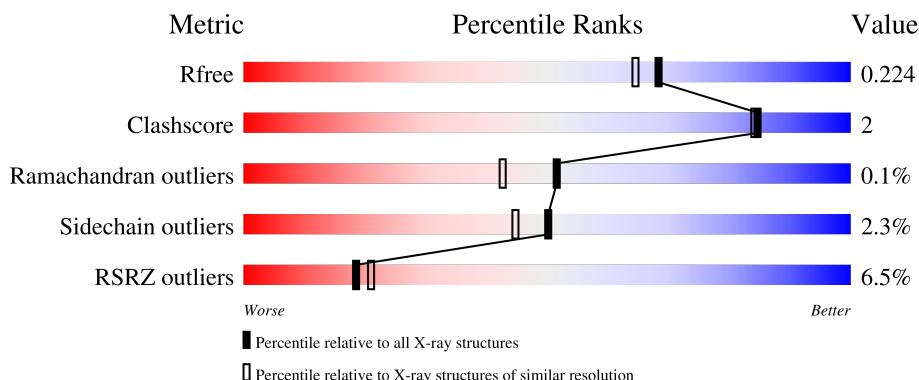
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
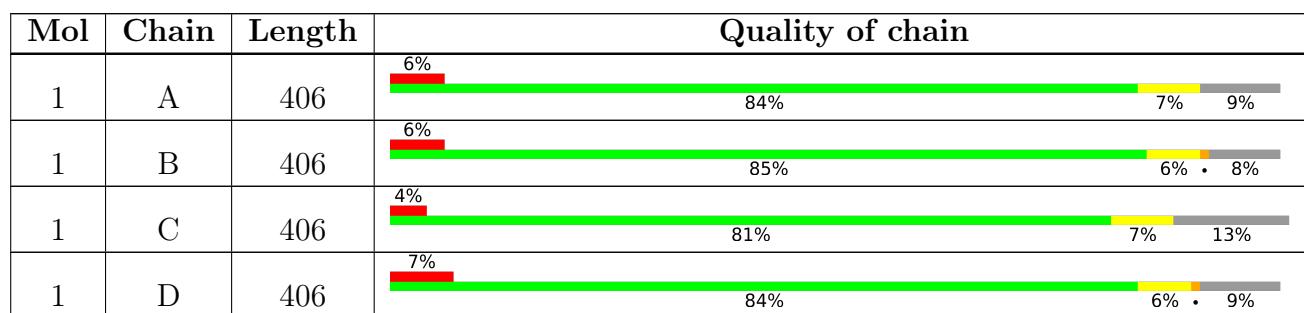
The reported resolution of this entry is 1.90 Å.

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	Percentile Ranks	Value
Rfree		0.224
Clashscore		2
Ramachandran outliers		0.1%
Sidechain outliers		2.3%
RSRZ outliers		6.5%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	406	6% / 84% / 7% / 9%
1	B	406	6% / 85% / 6% · 8%
1	C	406	4% / 81% / 7% / 13%
1	D	406	7% / 84% / 6% · 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SRT	D	501	-	X	-	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 23533 atoms, of which 11342 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 Betaine--homocysteine S-methyltransferase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	370	Total 5750	C 1844	H 2853	N 501	O 537	S 15	0	2	0
1	B	373	Total 5772	C 1853	H 2864	N 505	O 535	S 15	0	0	0
1	C	355	Total 5517	C 1776	H 2738	N 480	O 508	S 15	0	1	0
1	D	371	Total 5755	C 1851	H 2852	N 502	O 534	S 16	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	GLN	ARG	SEE REMARK 999	UNP Q93088
B	239	GLN	ARG	SEE REMARK 999	UNP Q93088
C	239	GLN	ARG	SEE REMARK 999	UNP Q93088
D	239	GLN	ARG	SEE REMARK 999	UNP Q93088
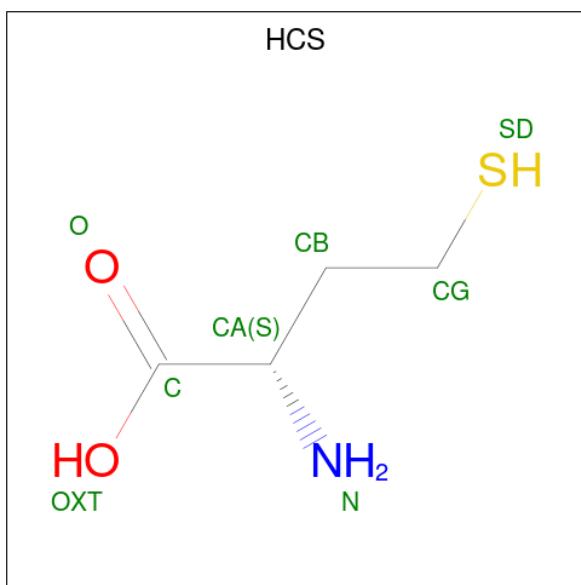
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).
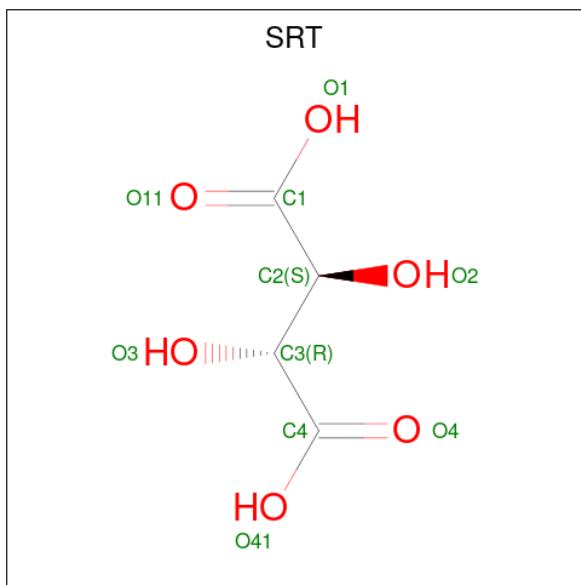
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	K 1	0	0
3	B	1	Total 1	K 1	0	0
3	C	1	Total 1	K 1	0	0
3	D	1	Total 1	K 1	0	0

- Molecule 4 is 2-AMINO-4-MERCAPTO-BUTYRIC ACID (three-letter code: HCS) (formula: $C_4H_9NO_2S$).

HCS

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 15	C 4	H 7	N 1	O 2	S 1	0	0
4	B	1	Total 15	C 4	H 7	N 1	O 2	S 1	0	0
4	C	1	Total 15	C 4	H 7	N 1	O 2	S 1	0	0
4	D	1	Total 15	C 4	H 7	N 1	O 2	S 1	0	0

- Molecule 5 is S,R MESO-TARTARIC ACID (three-letter code: SRT) (formula: $C_4H_6O_6$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total 14	C 4	H 4	O 6	0	0
5	D	1	Total 13	C 4	H 3	O 6	0	0
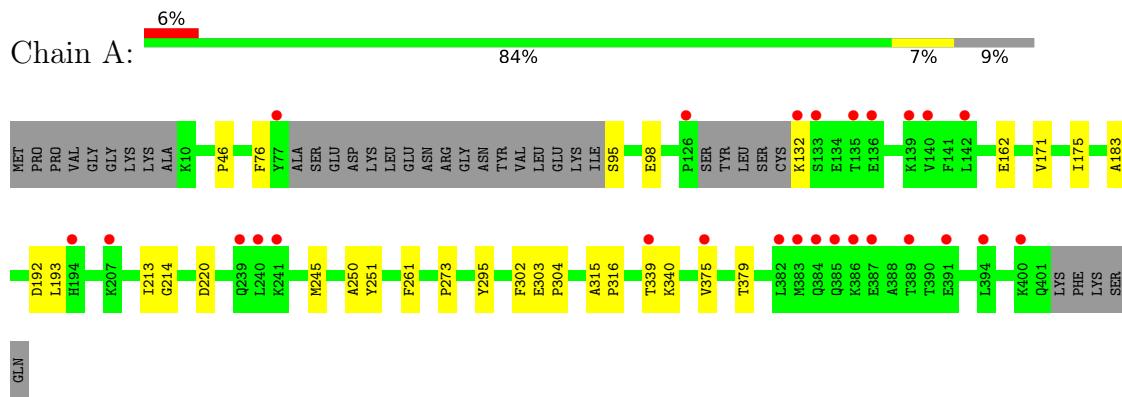
• Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	174	Total 174	O 174	0	0
6	B	141	Total 141	O 141	0	0
6	C	182	Total 182	O 182	0	0
6	D	147	Total 147	O 147	0	0
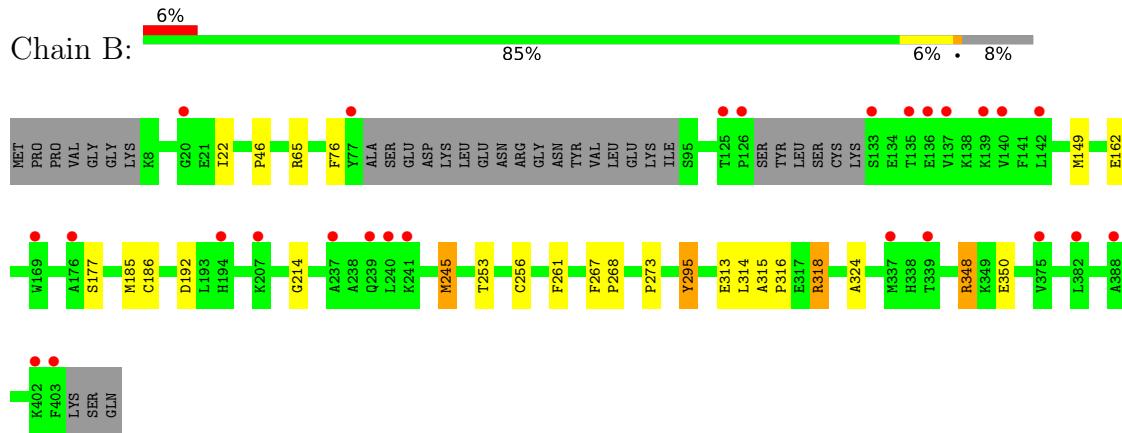
3 Residue-property plots ⓘ

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.
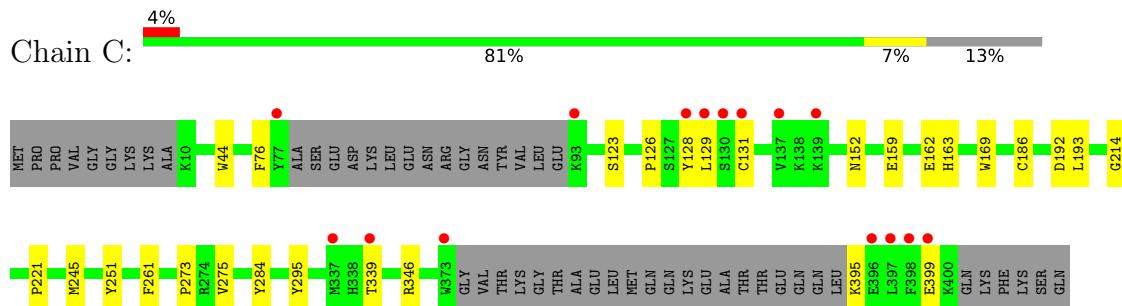
• Molecule 1: Betaine--homocysteine S-methyltransferase 1
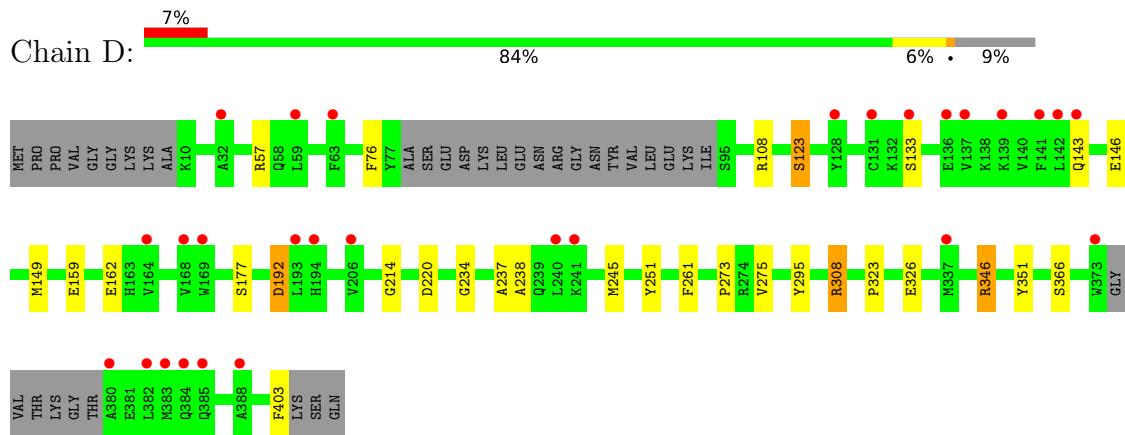
Chain A:

• Molecule 1: Betaine--homocysteine S-methyltransferase 1

Chain B:

• Molecule 1: Betaine--homocysteine S-methyltransferase 1

Chain C:

• Molecule 1: Betaine--homocysteine S-methyltransferase 1

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.10Å 102.62Å 96.23Å 90.00° 101.76° 90.00°	Depositor
Resolution (Å)	45.22 – 1.90 45.06 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.22-1.90) 99.0 (45.06-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.180 , 0.219 0.188 , 0.224	Depositor DCC
R_{free} test set	6476 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 44.0	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.48, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	23533	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 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: HCS, SRT, K, ZN

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	0.61	0/2972	0.67	0/4018
1	B	0.62	0/2978	0.69	1/4025 (0.0%)
1	C	0.67	2/2852 (0.1%)	0.72	1/3857 (0.0%)
1	D	0.63	0/2974	0.75	8/4020 (0.2%)
All	All	0.63	2/11776 (0.0%)	0.71	10/15920 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	169	TRP	CD2-CE2	5.12	1.47	1.41
1	C	44	TRP	CD2-CE2	5.05	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	308	ARG	NE-CZ-NH2	-11.36	114.62	120.30
1	D	308	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	D	346	ARG	NE-CZ-NH1	8.85	124.73	120.30
1	D	346	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	D	108	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	D	108	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	D	57	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	318	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	D	57	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	346	ARG	NE-CZ-NH1	5.06	122.83	120.30

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	2897	2853	2853	13	0
1	B	2908	2864	2863	14	0
1	C	2779	2738	2738	12	0
1	D	2903	2852	2851	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	8	7	7	0	0
4	B	8	7	7	0	0
4	C	8	7	7	0	0
4	D	8	7	7	0	0
5	B	10	4	4	0	0
5	D	10	3	3	0	0
6	A	174	0	0	1	0
6	B	141	0	0	1	0
6	C	182	0	0	1	0
6	D	147	0	0	2	0
All	All	12191	11342	11340	52	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 2.

All (52) 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:D:323:PRO:O	1:D:326:GLU:HG2	1.73	0.86
1:C:152:ASN:HB2	6:C:780:HOH:O	2.01	0.59
1:B:313:GLU:O	6:B:715:HOH:O	2.17	0.57
1:C:126:PRO:HG2	1:C:129:LEU:HD12	1.87	0.57
1:B:22:ILE:HB	1:B:318:ARG:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:ARG:HD2	6:D:745:HOH:O	2.04	0.56
1:D:149:MET:SD	1:D:177:SER:HB2	2.46	0.56
1:B:245:MET:HB2	1:B:295:TYR:HB3	1.87	0.55
1:C:123:SER:HA	1:C:159:GLU:O	2.08	0.54
1:C:126:PRO:CG	1:C:129:LEU:HD12	2.37	0.54
1:A:375:VAL:HG21	1:A:379:THR:HG21	1.89	0.54
1:D:403:PHE:O	6:D:716:HOH:O	2.19	0.53
1:A:339:THR:HG23	1:A:340:LYS:HG3	1.90	0.53
1:D:237:ALA:O	1:D:238:ALA:HB3	2.10	0.52
1:C:128:TYR:CD1	1:C:129:LEU:HG	2.45	0.52
1:A:273:PRO:HA	1:B:273:PRO:HA	1.92	0.52
1:B:22:ILE:HB	1:B:318:ARG:CD	2.40	0.52
1:B:348:ARG:NH2	1:B:350:GLU:HB2	2.26	0.50
1:B:149:MET:SD	1:B:177:SER:HB2	2.55	0.47
1:B:253:THR:HB	1:B:256:CYS:SG	2.54	0.47
1:C:214:GLY:HA3	1:C:245:MET:O	2.13	0.47
1:A:214:GLY:HA3	1:A:245:MET:O	2.14	0.47
1:A:340:LYS:NZ	6:A:965:HOH:O	2.49	0.46
1:B:314:LEU:O	1:B:318:ARG:HG3	2.14	0.46
1:B:162:GLU:HG3	1:B:186:CYS:SG	2.55	0.46
1:A:162:GLU:HB3	1:A:193:LEU:HG	1.98	0.46
1:C:163:HIS:NE2	1:C:193:LEU:HB2	2.31	0.45
1:A:95:SER:N	1:A:98:GLU:OE1	2.50	0.45
1:C:162:GLU:HB3	1:C:193:LEU:HG	1.99	0.45
1:A:250:ALA:HB2	1:A:302:PHE:CD1	2.52	0.44
1:D:234:GLY:O	1:D:237:ALA:O	2.36	0.44
1:D:346:ARG:HD2	1:D:351:TYR:CE2	2.53	0.44
1:C:251:TYR:CE1	1:C:275:VAL:HG22	2.52	0.43
1:A:183:ALA:O	1:A:213:ILE:HA	2.19	0.43
1:B:65:ARG:HG2	1:B:324:ALA:HB2	2.01	0.43
1:B:214:GLY:HA3	1:B:245:MET:O	2.18	0.43
1:A:315:ALA:N	1:A:316:PRO:CD	2.81	0.43
1:D:251:TYR:CE1	1:D:275:VAL:HG22	2.54	0.43
1:D:123:SER:HA	1:D:159:GLU:O	2.19	0.43
1:D:143:GLN:O	1:D:146:GLU:HB3	2.19	0.42
1:A:171:VAL:O	1:A:175:ILE:HG12	2.19	0.42
1:D:162:GLU:O	1:D:192:ASP:HB2	2.20	0.42
1:A:220:ASP:HB3	1:A:251:TYR:O	2.19	0.42
1:B:315:ALA:HB3	1:B:316:PRO:HD3	2.02	0.41
1:D:214:GLY:HA3	1:D:245:MET:O	2.20	0.41
1:C:162:GLU:HG3	1:C:186:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLU:HB3	1:A:304:PRO:CD	2.49	0.41
1:B:267:PHE:HA	1:B:268:PRO:HA	1.87	0.41
1:C:273:PRO:HA	1:D:273:PRO:HA	2.03	0.41
1:D:346:ARG:HD2	1:D:351:TYR:CZ	2.55	0.41
1:C:221:PRO:HB3	1:C:284:TYR:CD1	2.56	0.41
1:D:220:ASP:HB3	1:D:251:TYR:O	2.21	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	366/406 (90%)	353 (96%)	12 (3%)	1 (0%)	41	31
1	B	367/406 (90%)	358 (98%)	8 (2%)	1 (0%)	41	31
1	C	350/406 (86%)	338 (97%)	12 (3%)	0	100	100
1	D	365/406 (90%)	356 (98%)	9 (2%)	0	100	100
All	All	1448/1624 (89%)	1405 (97%)	41 (3%)	2 (0%)	51	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	46	PRO
1	A	46	PRO

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	300/329 (91%)	295 (98%)	5 (2%)	60	57
1	B	299/329 (91%)	292 (98%)	7 (2%)	50	45
1	C	288/329 (88%)	280 (97%)	8 (3%)	43	36
1	D	300/329 (91%)	293 (98%)	7 (2%)	50	45
All	All	1187/1316 (90%)	1160 (98%)	27 (2%)	50	45

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	PHE
1	A	132	LYS
1	A	192	ASP
1	A	261	PHE
1	A	295	TYR
1	B	76	PHE
1	B	185	MET
1	B	192	ASP
1	B	245	MET
1	B	261	PHE
1	B	295	TYR
1	B	348	ARG
1	C	76	PHE
1	C	131	CYS
1	C	192	ASP
1	C	261	PHE
1	C	295	TYR
1	C	339	THR
1	C	395	LYS
1	C	399	GLU
1	D	76	PHE
1	D	123	SER
1	D	133	SER
1	D	192	ASP
1	D	261	PHE
1	D	295	TYR
1	D	366	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	HCS	D	504	2	6,7,7	1.16	0	7,8,8	2.47	1 (14%)
4	HCS	B	504	2	6,7,7	1.20	0	7,8,8	2.95	1 (14%)
4	HCS	A	703	2	6,7,7	1.84	1 (16%)	7,8,8	2.03	1 (14%)
5	SRT	B	501	-	9,9,9	1.50	1 (11%)	12,12,12	2.31	5 (41%)
5	SRT	D	501	-	9,9,9	2.03	4 (44%)	12,12,12	1.73	4 (33%)
4	HCS	C	503	2	6,7,7	1.45	1 (16%)	7,8,8	1.75	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HCS	D	504	2	-	0/7/7/7	-
4	HCS	B	504	2	-	0/7/7/7	-
4	HCS	A	703	2	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SRT	B	501	-	-	7/12/12/12	-
5	SRT	D	501	-	-	7/12/12/12	-
4	HCS	C	503	2	-	0/7/7/7	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	HCS	CB-CA	3.27	1.60	1.53
5	D	501	SRT	O2-C2	-3.25	1.35	1.42
5	D	501	SRT	O4-C4	2.69	1.30	1.22
5	B	501	SRT	O4-C4	2.62	1.30	1.22
5	D	501	SRT	C3-C4	-2.43	1.49	1.52
4	C	503	HCS	CG-SD	2.33	1.89	1.80
5	D	501	SRT	O11-C1	2.17	1.28	1.22

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	504	HCS	CB-CG-SD	-7.13	106.31	113.74
4	D	504	HCS	CB-CG-SD	-6.19	107.30	113.74
4	A	703	HCS	CB-CG-SD	-4.30	109.27	113.74
5	B	501	SRT	O41-C4-C3	4.19	124.59	113.27
5	B	501	SRT	O3-C3-C4	4.16	119.39	110.66
4	C	503	HCS	CB-CG-SD	-3.75	109.84	113.74
5	D	501	SRT	O3-C3-C2	-3.24	103.79	110.23
5	B	501	SRT	O4-C4-C3	-3.21	113.18	121.63
5	D	501	SRT	O2-C2-C1	3.04	117.03	110.66
5	B	501	SRT	O2-C2-C3	-2.62	105.02	110.23
5	B	501	SRT	C2-C3-C4	-2.29	104.75	109.87
5	D	501	SRT	O2-C2-C3	2.10	114.41	110.23
5	D	501	SRT	O41-C4-C3	2.10	118.94	113.27

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	SRT	O11-C1-C2-O2
5	B	501	SRT	O2-C2-C3-O3
5	D	501	SRT	O1-C1-C2-O2
5	D	501	SRT	O11-C1-C2-O2
5	D	501	SRT	O2-C2-C3-O3

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	Atoms
5	B	501	SRT	O1-C1-C2-O2
5	B	501	SRT	C1-C2-C3-O3
5	D	501	SRT	O2-C2-C3-C4
5	B	501	SRT	O2-C2-C3-C4
5	D	501	SRT	O11-C1-C2-C3
5	D	501	SRT	O1-C1-C2-C3
5	B	501	SRT	C1-C2-C3-C4
5	D	501	SRT	C1-C2-C3-O3
5	B	501	SRT	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	370/406 (91%)	0.28	26 (7%)	16	18	18, 30, 57, 76	0
1	B	373/406 (91%)	0.35	26 (6%)	16	18	19, 34, 59, 71	0
1	C	355/406 (87%)	0.24	15 (4%)	36	39	16, 26, 52, 82	0
1	D	371/406 (91%)	0.42	28 (7%)	14	15	18, 33, 59, 74	0
All	All	1469/1624 (90%)	0.33	95 (6%)	18	21	16, 30, 57, 82	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	77	TYR	6.6
1	C	396	GLU	5.7
1	C	129	LEU	5.5
1	A	126	PRO	5.4
1	B	403	PHE	5.2
1	D	384	GLN	4.3
1	C	373	TRP	4.2
1	D	131	CYS	4.0
1	D	142	LEU	3.8
1	D	388	ALA	3.7
1	D	193	LEU	3.7
1	A	77	TYR	3.7
1	B	133	SER	3.6
1	C	339	THR	3.6
1	D	373	TRP	3.5
1	C	397	LEU	3.5
1	C	93	LYS	3.5
1	C	399	GLU	3.4
1	B	140	VAL	3.4
1	A	133	SER	3.4
1	B	240	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	240	LEU	3.3
1	A	241	LYS	3.1
1	D	383	MET	3.1
1	D	194	HIS	3.1
1	B	126	PRO	3.1
1	D	337	MET	3.0
1	A	383	MET	3.0
1	D	137	VAL	3.0
1	B	139	LYS	2.9
1	B	169	TRP	2.9
1	D	164	VAL	2.9
1	C	337	MET	2.9
1	D	168	VAL	2.9
1	B	135	THR	2.8
1	B	142	LEU	2.8
1	B	337	MET	2.8
1	D	385	GLN	2.7
1	B	176	ALA	2.7
1	D	136	GLU	2.7
1	A	142	LEU	2.7
1	B	239	GLN	2.6
1	A	394	LEU	2.6
1	D	240	LEU	2.6
1	A	239	GLN	2.6
1	A	385	GLN	2.6
1	D	382	LEU	2.6
1	A	387	GLU	2.5
1	C	131	CYS	2.5
1	C	128	TYR	2.5
1	A	400	LYS	2.4
1	A	136	GLU	2.4
1	A	391	GLU	2.4
1	D	143	GLN	2.4
1	C	398	PHE	2.4
1	D	63	PHE	2.3
1	A	139	LYS	2.3
1	A	384	GLN	2.3
1	A	140	VAL	2.3
1	D	141	PHE	2.3
1	B	20	GLY	2.3
1	A	135	THR	2.3
1	D	32	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	132	LYS	2.3
1	B	237	ALA	2.2
1	D	133	SER	2.2
1	A	386	LYS	2.2
1	B	207	LYS	2.2
1	D	241	LYS	2.2
1	B	382	LEU	2.2
1	D	59	LEU	2.2
1	A	389	THR	2.2
1	B	125	THR	2.2
1	B	388	ALA	2.2
1	B	402	LYS	2.2
1	B	375	VAL	2.2
1	D	206	VAL	2.2
1	C	77	TYR	2.1
1	C	130	SER	2.1
1	B	136	GLU	2.1
1	B	241	LYS	2.1
1	D	139	LYS	2.1
1	D	169	TRP	2.1
1	A	339	THR	2.1
1	A	382	LEU	2.1
1	D	380	ALA	2.1
1	B	194	HIS	2.1
1	D	128	TYR	2.1
1	B	137	VAL	2.1
1	A	375	VAL	2.0
1	C	137	VAL	2.0
1	A	207	LYS	2.0
1	C	139	LYS	2.0
1	B	339	THR	2.0
1	A	194	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

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, 95th 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	SRT	B	501	10/10	0.86	0.13	31,40,45,45	0
5	SRT	D	501	10/10	0.92	0.14	28,35,37,40	0
4	HCS	A	703	8/8	0.95	0.11	32,33,36,36	0
4	HCS	D	504	8/8	0.95	0.11	34,38,40,41	0
4	HCS	B	504	8/8	0.96	0.08	31,36,36,38	0
4	HCS	C	503	8/8	0.98	0.08	23,26,27,27	0
2	ZN	D	502	1/1	0.99	0.08	32,32,32,32	0
3	K	A	702	1/1	0.99	0.09	23,23,23,23	0
3	K	D	503	1/1	0.99	0.16	26,26,26,26	0
2	ZN	B	502	1/1	1.00	0.09	32,32,32,32	0
3	K	B	503	1/1	1.00	0.08	27,27,27,27	0
3	K	C	502	1/1	1.00	0.10	20,20,20,20	0
2	ZN	C	501	1/1	1.00	0.10	25,25,25,25	0
2	ZN	A	701	1/1	1.00	0.09	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.