



Full wwPDB X-ray Structure Validation Report

Sep 29, 2014 – 04:51 PM 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

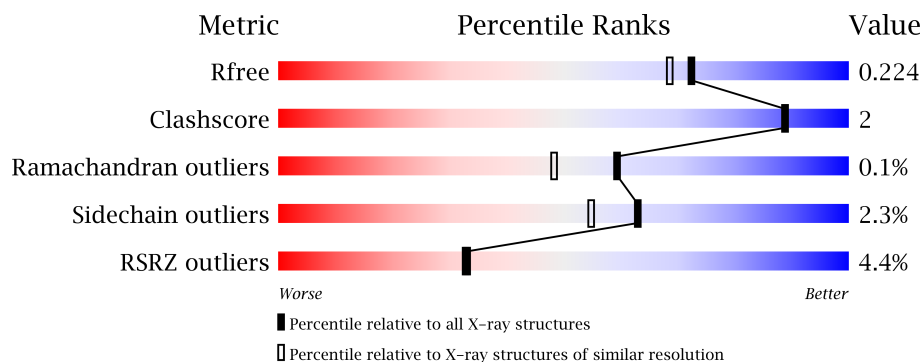
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23828
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23828

1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	406	
1	B	406	
1	C	406	
1	D	406	

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 deuterium.

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--homocysteineS-methyltransferase 1.

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

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

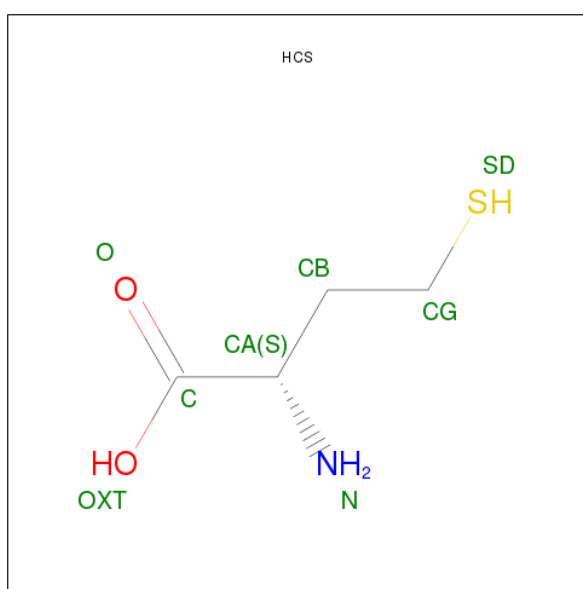
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

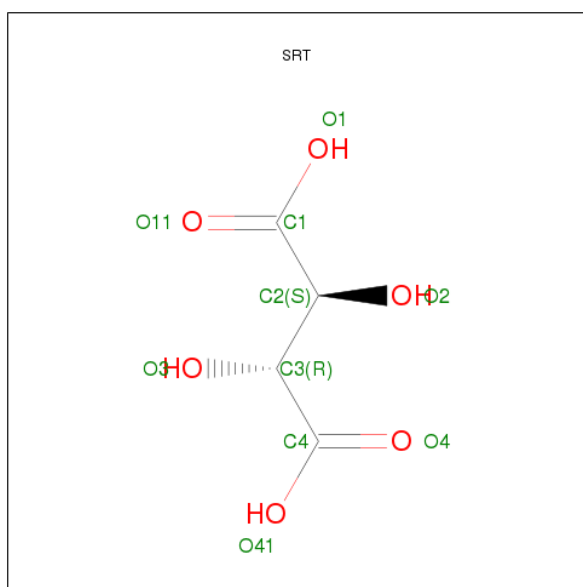
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total K 1 1	0	0
3	A	1	Total K 1 1	0	0
3	D	1	Total K 1 1	0	0
3	C	1	Total K 1 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H N O S 15 4 7 1 2 1	0	0
4	B	1	Total C H N O S 15 4 7 1 2 1	0	0
4	C	1	Total C H N O S 15 4 7 1 2 1	0	0
4	D	1	Total C H N O S 15 4 7 1 2 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	C	H	O	0	0
			14	4	4	6		
5	D	1	Total	C	H	O	0	0
			13	4	3	6		

- Molecule 6 is water.

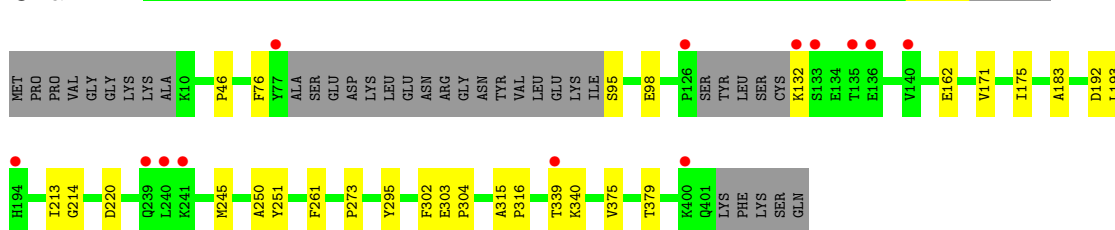
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	174	Total	O	0	0
			174	174		
6	B	141	Total	O	0	0
			141	141		
6	C	182	Total	O	0	0
			182	182		
6	D	147	Total	O	0	0
			147	147		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

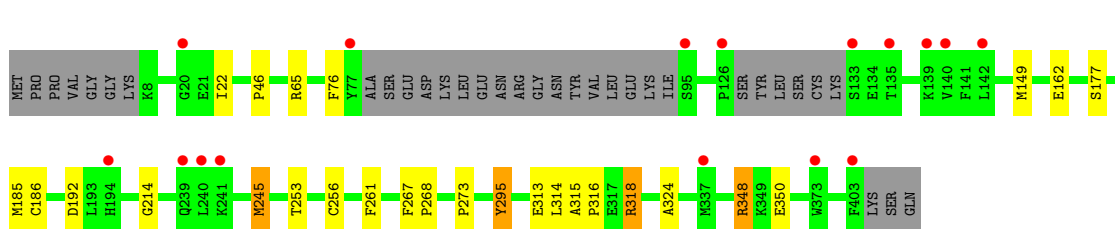
- Molecule 1: Betaine--homocysteineS-methyltransferase 1

Chain A:



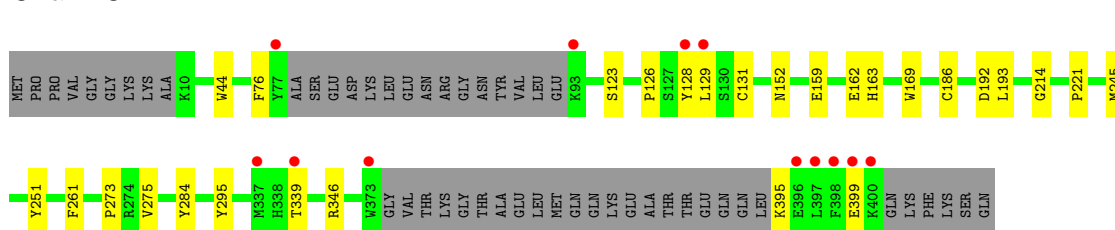
- Molecule 1: Betaine--homocysteineS-methyltransferase 1

Chain B:



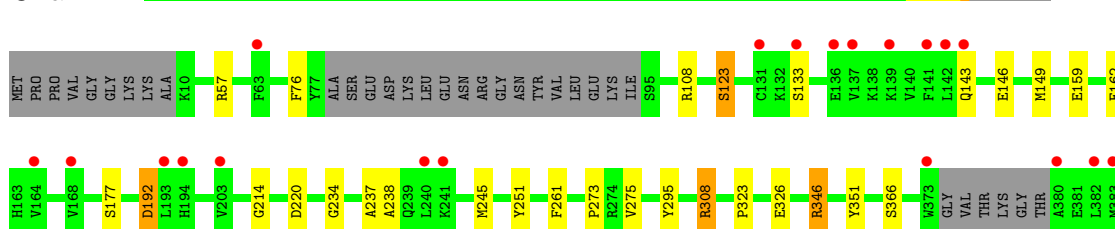
- Molecule 1: Betaine--homocysteineS-methyltransferase 1

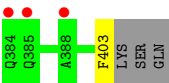
Chain C:



- Molecule 1: Betaine--homocysteineS-methyltransferase 1

Chain D:





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (5.30%)	DCC
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 38.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 128582 reflections	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.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HCS, ZN, K, SRT

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2897	2853	0	13	0
1	B	2908	2864	0	14	0
1	C	2779	2738	0	12	0
1	D	2903	2852	0	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	0	0	0
4	B	8	7	0	0	0
4	C	8	7	0	0	0
4	D	8	7	0	0	0
5	B	10	4	0	0	0
5	D	10	3	0	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	0	52	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (52) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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	1.91	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: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:B:149:MET:SD	1:B:177:SER:HB2	2.55	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:A:162:GLU:HB3	1:A:193:LEU:HG	1.98	0.46
1:B:162:GLU:HG3	1:B:186:CYS:SG	2.55	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
1:A:303:GLU:HB3	1:A:304:PRO:CD	2.49	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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%)	50	37
1	B	367/406 (90%)	358 (98%)	8 (2%)	1 (0%)	50	37
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%)	59	48

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%)	73	68
1	B	299/329 (91%)	292 (98%)	7 (2%)	63	55
1	C	288/329 (88%)	280 (97%)	8 (3%)	56	45
1	D	300/329 (91%)	293 (98%)	7 (2%)	63	55
All	All	1187/1316 (90%)	1160 (98%)	27 (2%)	63	55

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

Some 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 chains 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 carbohydrates 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	A	703	2	7,7,7	1.60	2 (28%)	8,8,8	0.97	0
5	SRT	B	501	-	9,9,9	1.47	1 (11%)	12,12,12	2.13	4 (33%)
4	HCS	B	504	2	7,7,7	1.33	1 (14%)	8,8,8	1.27	0
4	HCS	C	503	2	7,7,7	1.47	2 (28%)	8,8,8	0.87	0
5	SRT	D	501	-	9,9,9	2.05	4 (44%)	12,12,12	1.65	3 (25%)
4	HCS	D	504	2	7,7,7	1.32	1 (14%)	8,8,8	1.08	0

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	A	703	2	-	0/7/7/7	0/0/0/0
5	SRT	B	501	-	-	0/12/12/12	0/0/0/0
4	HCS	B	504	2	-	0/7/7/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HCS	C	503	2	-	0/7/7/7	0/0/0/0
5	SRT	D	501	-	-	0/12/12/12	0/0/0/0
4	HCS	D	504	2	-	0/7/7/7	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	SRT	O2-C2	-3.33	1.35	1.42
4	D	504	HCS	CA-C	2.65	1.62	1.53
5	D	501	SRT	C3-C4	-2.63	1.49	1.52
4	C	503	HCS	CA-C	2.50	1.62	1.53
5	D	501	SRT	O4-C4	2.43	1.30	1.22
5	B	501	SRT	O4-C4	2.36	1.30	1.22
4	A	703	HCS	CA-C	2.36	1.61	1.53
4	B	504	HCS	CA-C	2.30	1.61	1.53
4	C	503	HCS	CG-SD	2.23	1.89	1.80
4	A	703	HCS	CB-CA	2.07	1.60	1.54
5	D	501	SRT	O3-C3	-2.03	1.38	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	SRT	O3-C3-C4	4.02	119.39	110.78
5	B	501	SRT	O41-C4-C3	3.81	124.59	113.81
5	D	501	SRT	O3-C3-C2	-3.12	103.79	110.19
5	D	501	SRT	O2-C2-C1	2.92	117.03	110.78
5	B	501	SRT	O4-C4-C3	-2.83	113.18	121.26
5	B	501	SRT	O2-C2-C3	-2.52	105.02	110.19
5	D	501	SRT	O2-C2-C3	2.06	114.41	110.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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%)	0.27	13 (3%) 42 43	18, 30, 57, 76	0
1	B	373/406 (91%)	0.31	16 (4%) 34 34	19, 35, 59, 71	0
1	C	355/406 (87%)	0.15	12 (3%) 43 44	16, 26, 52, 82	0
1	D	371/406 (91%)	0.33	23 (6%) 20 20	18, 33, 59, 74	0
All	All	1469/1624 (90%)	0.27	64 (4%) 33 33	16, 30, 57, 82	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	77	TYR	6.2
1	C	396	GLU	5.5
1	A	126	PRO	5.2
1	B	403	PHE	4.3
1	C	129	LEU	3.9
1	C	373	TRP	3.9
1	C	397	LEU	3.9
1	A	77	TYR	3.8
1	D	373	TRP	3.7
1	D	142	LEU	3.5
1	B	133	SER	3.5
1	A	241	LYS	3.5
1	C	93	LYS	3.4
1	D	131	CYS	3.3
1	A	133	SER	3.2
1	B	126	PRO	3.2
1	C	399	GLU	3.1
1	D	193	LEU	3.1
1	A	240	LEU	3.0
1	D	384	GLN	3.0
1	B	240	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	194	HIS	2.8
1	D	164	VAL	2.8
1	D	383	MET	2.8
1	D	240	LEU	2.7
1	B	241	LYS	2.7
1	D	203	VAL	2.6
1	B	20	GLY	2.6
1	C	398	PHE	2.5
1	A	136	GLU	2.5
1	C	339	THR	2.5
1	A	239	GLN	2.5
1	D	136	GLU	2.5
1	C	128	TYR	2.5
1	B	135	THR	2.4
1	B	95	SER	2.4
1	D	63	PHE	2.4
1	B	140	VAL	2.4
1	C	77	TYR	2.3
1	C	337	MET	2.3
1	A	140	VAL	2.3
1	B	139	LYS	2.3
1	D	241	LYS	2.3
1	D	382	LEU	2.2
1	B	337	MET	2.2
1	D	137	VAL	2.2
1	D	168	VAL	2.2
1	D	133	SER	2.2
1	A	400	LYS	2.2
1	D	143	GLN	2.2
1	D	388	ALA	2.1
1	A	339	THR	2.1
1	C	400	LYS	2.1
1	B	142	LEU	2.1
1	A	132	LYS	2.1
1	D	139	LYS	2.1
1	D	380	ALA	2.1
1	D	385	GLN	2.1
1	B	194	HIS	2.1
1	A	135	THR	2.0
1	B	239	GLN	2.0
1	D	141	PHE	2.0
1	A	194	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	373	TRP	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 carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	SRT	B	501	10/10	0.14	0.38	31,40,45,45	0
5	SRT	D	501	10/10	0.14	-0.16	28,35,37,40	0
2	ZN	C	501	1/1	0.09	-0.19	25,25,25,25	0
3	K	D	503	1/1	0.14	-0.42	26,26,26,26	0
2	ZN	B	502	1/1	0.09	-0.90	32,32,32,32	0
4	HCS	D	504	8/8	0.11	-0.98	34,38,40,41	0
4	HCS	A	703	8/8	0.10	-1.04	32,33,36,36	0
4	HCS	C	503	8/8	0.08	-1.15	23,26,27,27	0
2	ZN	A	701	1/1	0.09	-1.40	31,31,31,31	0
4	HCS	B	504	8/8	0.08	-1.42	31,36,36,38	0
3	K	A	702	1/1	0.09	-1.49	23,23,23,23	0
2	ZN	D	502	1/1	0.07	-1.57	32,32,32,32	0
3	K	B	503	1/1	0.08	-1.72	27,27,27,27	0
3	K	C	502	1/1	0.08	-1.85	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.