



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:36 PM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

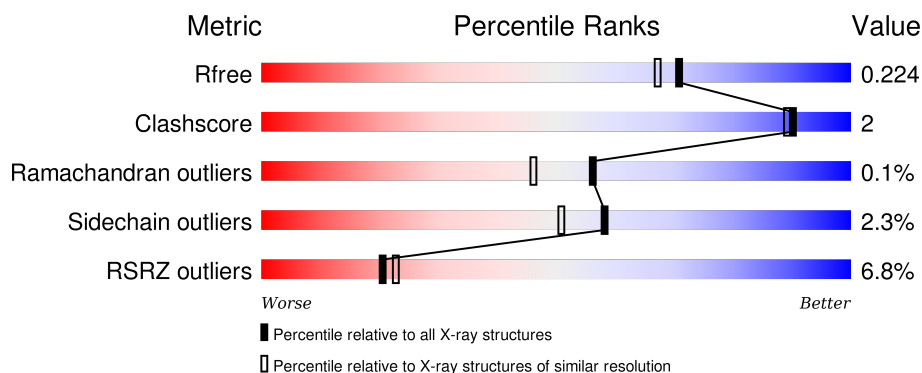
# 1 Overall quality at a glance ⓘ

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	406	<div> <div>7%</div> <div>84% 7% 9%</div> </div>
1	B	406	<div> <div>7%</div> <div>85% 6% • 8%</div> </div>
1	C	406	<div> <div>4%</div> <div>81% 7% 13%</div> </div>
1	D	406	<div> <div>7%</div> <div>84% 6% • 9%</div> </div>

## 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	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

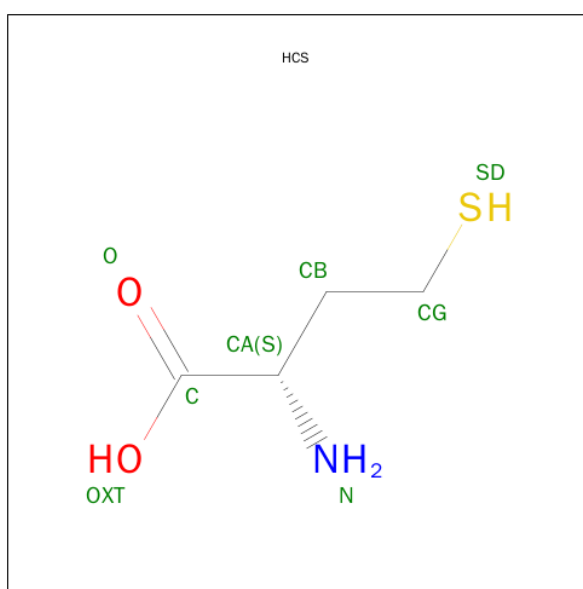
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).

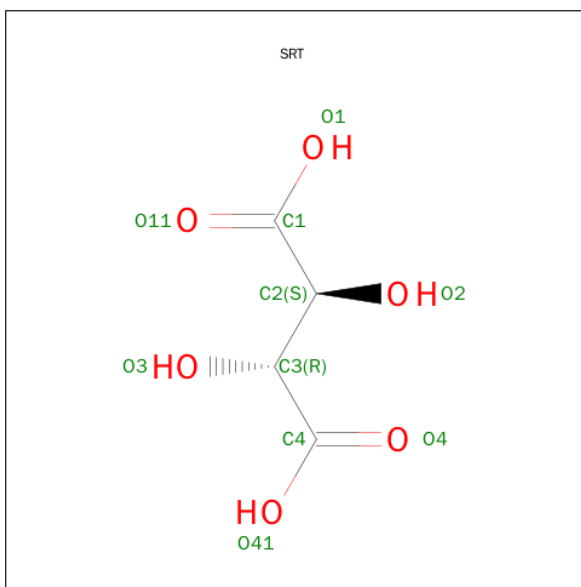
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total K 1 1	0	0
3	A	1	Total K 1 1	0	0
3	D	1	Total K 1 1	0	0
3	C	1	Total K 1 1	0	0

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



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:  $C_4H_6O_6$ ).

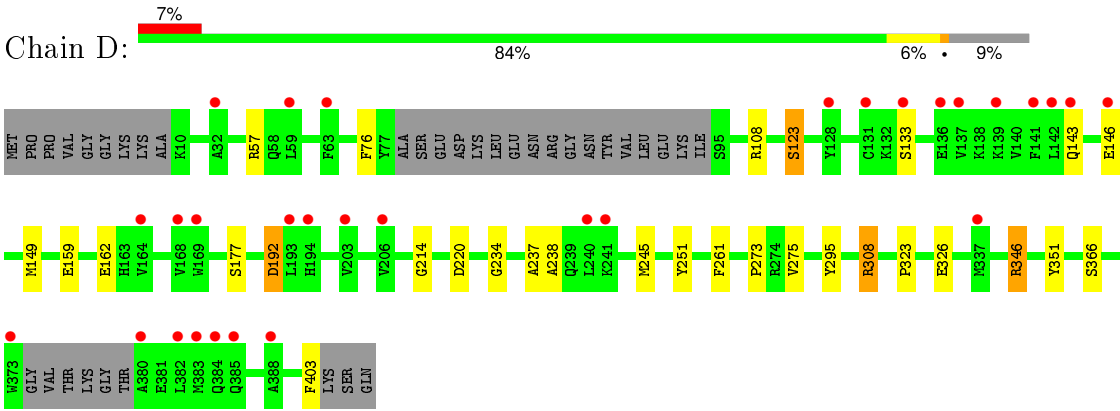


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			14	4	4	6		
5	D	1	Total	C	H	O	0	0
			13	4	3	6		

- 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		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.10 Å 102.62 Å 96.23 Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 1.89 Å)	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 <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 44.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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 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:B:22:ILE:HB	1:B:318:ARG:CD	2.40	0.52
1:A:273:PRO:HA	1:B:273:PRO:HA	1.92	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:B:314:LEU:O	1:B:318:ARG:HG3	2.14	0.46
1:A:340:LYS:NZ	6:A:965:HOH:O	2.49	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:C:162:GLU:HB3	1:C:193:LEU:HG	1.99	0.45
1:A:95:SER:N	1:A:98:GLU:OE1	2.50	0.45
1:D:234:GLY:O	1:D:237:ALA:O	2.36	0.44
1:A:250:ALA:HB2	1:A:302:PHE:CD1	2.52	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:B:65:ARG:HG2	1:B:324:ALA:HB2	2.01	0.43
1:A:183:ALA:O	1:A:213:ILE:HA	2.19	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:D:162:GLU:O	1:D:192:ASP:HB2	2.20	0.42
1:A:171:VAL:O	1:A:175:ILE:HG12	2.19	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:D:346:ARG:HD2	1:D:351:TYR:CZ	2.55	0.41
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: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 [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	366/406 (90%)	353 (96%)	12 (3%)	1 (0%)	46	35
1	B	367/406 (90%)	358 (98%)	8 (2%)	1 (0%)	46	35
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%)	56	46

All (2) Ramachandran outliers are listed below:

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

### 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	300/329 (91%)	295 (98%)	5 (2%)	68	64
1	B	299/329 (91%)	292 (98%)	7 (2%)	58	51
1	C	288/329 (88%)	280 (97%)	8 (3%)	51	41
1	D	300/329 (91%)	293 (98%)	7 (2%)	58	51
All	All	1187/1316 (90%)	1160 (98%)	27 (2%)	58	51

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 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 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	3,7,7	1.36	0	2,8,8	1.13	0
5	SRT	B	501	-	3,9,9	1.32	1 (33%)	6,12,12	2.32	2 (33%)
4	HCS	B	504	2	3,7,7	0.85	0	2,8,8	1.23	0
4	HCS	C	503	2	3,7,7	1.64	1 (33%)	2,8,8	1.19	0
5	SRT	D	501	-	3,9,9	2.41	2 (66%)	6,12,12	1.92	3 (50%)
4	HCS	D	504	2	3,7,7	1.02	0	2,8,8	1.20	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	-	0/3/7/7	0/0/0/0
5	SRT	B	501	-	-	0/4/12/12	0/0/0/0
4	HCS	B	504	2	-	0/3/7/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HCS	C	503	2	-	0/3/7/7	0/0/0/0
5	SRT	D	501	-	-	0/4/12/12	0/0/0/0
4	HCS	D	504	2	-	0/3/7/7	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	SRT	O2-C2	-3.48	1.35	1.42
5	D	501	SRT	O3-C3	-2.21	1.38	1.42
5	B	501	SRT	O3-C3	-2.12	1.38	1.42
4	C	503	HCS	CG-SD	2.36	1.89	1.80

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	SRT	C4-C3-C2	-4.19	104.75	113.35
5	D	501	SRT	C1-C2-C3	-2.88	107.45	113.35
5	D	501	SRT	O2-C2-C3	2.06	114.41	108.61
5	D	501	SRT	O2-C2-C1	2.31	117.03	111.21
5	B	501	SRT	O3-C3-C4	3.24	119.39	111.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	370/406 (91%)	0.31	27 (7%)	18	20	18, 30, 57, 76	0
1	B	373/406 (91%)	0.39	27 (7%)	18	20	19, 35, 59, 71	0
1	C	355/406 (87%)	0.28	16 (4%)	37	40	16, 26, 52, 82	0
1	D	371/406 (91%)	0.46	30 (8%)	15	16	18, 33, 59, 74	0
All	All	1469/1624 (90%)	0.36	100 (6%)	20	23	16, 30, 57, 82	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	77	TYR	6.7
1	C	396	GLU	5.7
1	C	129	LEU	5.6
1	A	126	PRO	5.5
1	B	403	PHE	5.3
1	D	384	GLN	4.3
1	C	373	TRP	4.2
1	D	131	CYS	4.1
1	D	142	LEU	3.9
1	D	193	LEU	3.8
1	D	388	ALA	3.8
1	A	77	TYR	3.7
1	B	133	SER	3.7
1	C	339	THR	3.7
1	C	397	LEU	3.6
1	D	373	TRP	3.6
1	B	140	VAL	3.5
1	C	93	LYS	3.5
1	A	133	SER	3.5
1	C	399	GLU	3.5
1	B	240	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	240	LEU	3.3
1	A	241	LYS	3.2
1	D	383	MET	3.2
1	D	194	HIS	3.2
1	B	126	PRO	3.1
1	D	137	VAL	3.1
1	A	383	MET	3.1
1	D	337	MET	3.1
1	D	164	VAL	3.0
1	D	168	VAL	3.0
1	B	169	TRP	3.0
1	B	139	LYS	3.0
1	C	337	MET	2.9
1	B	142	LEU	2.9
1	B	135	THR	2.9
1	B	337	MET	2.8
1	B	176	ALA	2.8
1	A	142	LEU	2.8
1	D	385	GLN	2.8
1	D	136	GLU	2.7
1	A	394	LEU	2.7
1	D	240	LEU	2.7
1	B	239	GLN	2.7
1	D	382	LEU	2.7
1	A	239	GLN	2.6
1	A	385	GLN	2.6
1	C	131	CYS	2.6
1	A	387	GLU	2.6
1	C	128	TYR	2.6
1	A	400	LYS	2.5
1	A	136	GLU	2.5
1	C	398	PHE	2.4
1	D	143	GLN	2.4
1	D	63	PHE	2.4
1	A	391	GLU	2.4
1	A	140	VAL	2.4
1	A	139	LYS	2.4
1	A	384	GLN	2.4
1	D	141	PHE	2.4
1	D	32	ALA	2.3
1	B	237	ALA	2.3
1	A	135	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	20	GLY	2.3
1	A	132	LYS	2.3
1	D	133	SER	2.3
1	D	59	LEU	2.3
1	B	382	LEU	2.3
1	A	386	LYS	2.3
1	B	388	ALA	2.3
1	B	375	VAL	2.2
1	B	207	LYS	2.2
1	A	389	THR	2.2
1	D	241	LYS	2.2
1	D	206	VAL	2.2
1	B	125	THR	2.2
1	B	402	LYS	2.2
1	C	130	SER	2.2
1	C	77	TYR	2.2
1	A	382	LEU	2.2
1	B	136	GLU	2.2
1	B	137	VAL	2.2
1	D	169	TRP	2.2
1	D	380	ALA	2.2
1	B	194	HIS	2.2
1	A	339	THR	2.2
1	B	241	LYS	2.2
1	D	139	LYS	2.2
1	A	375	VAL	2.1
1	C	137	VAL	2.1
1	D	128	TYR	2.1
1	D	203	VAL	2.1
1	B	339	THR	2.1
1	A	207	LYS	2.1
1	C	139	LYS	2.1
1	C	31	PHE	2.0
1	B	95	SER	2.0
1	A	137	VAL	2.0
1	A	194	HIS	2.0
1	D	146	GLU	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 [i](#)

There are no carbohydrates 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. 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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	SRT	B	501	10/10	0.86	0.13	0.87	31,40,45,45	0
3	K	D	503	1/1	0.99	0.16	0.43	26,26,26,26	0
5	SRT	D	501	10/10	0.92	0.14	0.38	28,35,37,40	0
4	HCS	A	703	8/8	0.95	0.11	-0.45	32,33,36,36	0
2	ZN	C	501	1/1	1.00	0.10	-0.49	25,25,25,25	0
2	ZN	B	502	1/1	1.00	0.09	-0.56	32,32,32,32	0
2	ZN	A	701	1/1	1.00	0.09	-1.06	31,31,31,31	0
3	K	B	503	1/1	1.00	0.08	-1.07	27,27,27,27	0
3	K	A	702	1/1	0.99	0.09	-1.18	23,23,23,23	0
4	HCS	D	504	8/8	0.95	0.11	-1.23	34,38,40,41	0
4	HCS	B	504	8/8	0.96	0.08	-1.28	31,36,36,38	0
4	HCS	C	503	8/8	0.98	0.08	-1.44	23,26,27,27	0
2	ZN	D	502	1/1	0.99	0.08	-1.63	32,32,32,32	0
3	K	C	502	1/1	1.00	0.10	-1.92	20,20,20,20	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.