



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 01:21 PM GMT

PDB ID : 3F5O
Title : Crystal Structure of hTHEM2(undecan-2-one-CoA)complex
Authors : Xu, H.; Gong, W.
Deposited on : 2008-11-04
Resolution : 1.70 Å(reported)

This is a wwPDB validation summary 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>

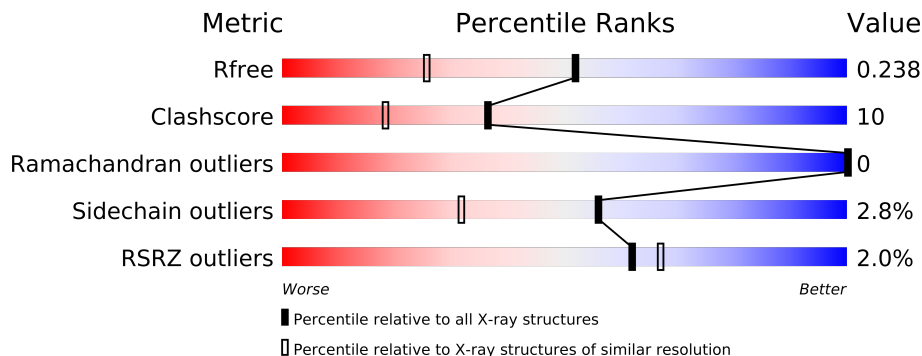
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
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)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.70 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	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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	148	
1	B	148	
1	C	148	
1	D	148	
1	E	148	
1	F	148	
1	G	148	
1	H	148	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	UOC	A	149	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	UOC	B	149	-	X
3	UOC	C	149	-	X
3	UOC	D	149	-	X
3	UOC	F	149	-	X
3	UOC	G	149	-	X
3	UOC	H	149	-	X
4	COA	B	150	-	X
5	P6G	B	1001	-	X
5	P6G	C	1001	-	X
5	P6G	E	1001	-	X
5	P6G	G	1001	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9600 atoms, of which 0 are hydrogen 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 Thioesterase superfamily member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	138	Total	C	N	O	S	0	3	0
			1039	651	180	198	10			
1	B	136	Total	C	N	O	S	0	4	0
			1025	643	182	192	8			
1	C	137	Total	C	N	O	S	0	4	0
			1036	650	182	195	9			
1	D	137	Total	C	N	O	S	0	5	0
			1025	643	177	195	10			
1	E	138	Total	C	N	O	S	0	1	0
			1021	639	178	196	8			
1	F	138	Total	C	N	O	S	0	1	0
			1024	639	181	196	8			
1	G	136	Total	C	N	O	S	0	3	0
			1017	642	177	189	9			
1	H	138	Total	C	N	O	S	0	5	0
			1036	651	181	194	10			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	LEU	-	EXPRESSION TAG	UNP Q9NPJ3
A	142	GLU	-	EXPRESSION TAG	UNP Q9NPJ3
A	143	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
A	144	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
A	145	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
A	146	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
A	147	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
A	148	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
B	141	LEU	-	EXPRESSION TAG	UNP Q9NPJ3
B	142	GLU	-	EXPRESSION TAG	UNP Q9NPJ3
B	143	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
B	144	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
B	145	HIS	-	EXPRESSION TAG	UNP Q9NPJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	146	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
B	147	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
B	148	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
C	141	LEU	-	EXPRESSION TAG	UNP Q9NPJ3
C	142	GLU	-	EXPRESSION TAG	UNP Q9NPJ3
C	143	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
C	144	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
C	145	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
C	146	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
C	147	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
C	148	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
D	141	LEU	-	EXPRESSION TAG	UNP Q9NPJ3
D	142	GLU	-	EXPRESSION TAG	UNP Q9NPJ3
D	143	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
D	144	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
D	145	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
D	146	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
D	147	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
D	148	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
E	141	LEU	-	EXPRESSION TAG	UNP Q9NPJ3
E	142	GLU	-	EXPRESSION TAG	UNP Q9NPJ3
E	143	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
E	144	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
E	145	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
E	146	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
E	147	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
E	148	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
F	141	LEU	-	EXPRESSION TAG	UNP Q9NPJ3
F	142	GLU	-	EXPRESSION TAG	UNP Q9NPJ3
F	143	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
F	144	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
F	145	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
F	146	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
F	147	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
F	148	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
G	141	LEU	-	EXPRESSION TAG	UNP Q9NPJ3
G	142	GLU	-	EXPRESSION TAG	UNP Q9NPJ3
G	143	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
G	144	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
G	145	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
G	146	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
G	147	HIS	-	EXPRESSION TAG	UNP Q9NPJ3

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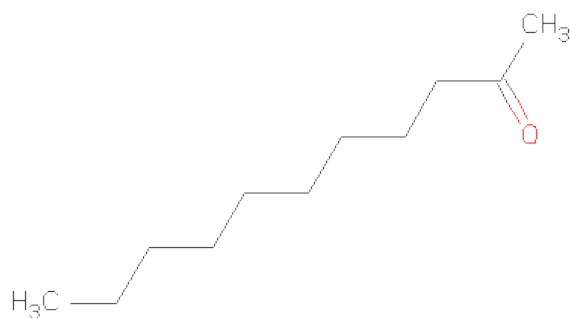
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Chain	Residue	Modelled	Actual	Comment	Reference
G	148	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
H	141	LEU	-	EXPRESSION TAG	UNP Q9NPJ3
H	142	GLU	-	EXPRESSION TAG	UNP Q9NPJ3
H	143	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
H	144	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
H	145	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
H	146	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
H	147	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
H	148	HIS	-	EXPRESSION TAG	UNP Q9NPJ3

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

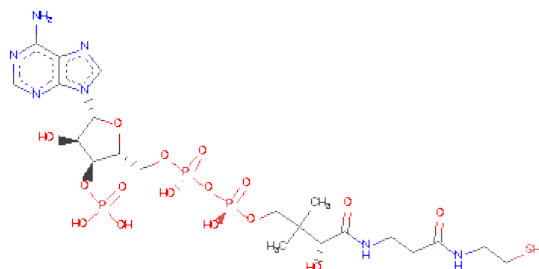
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0

- Molecule 3 is UNDECAN-2-ONE (three-letter code: UOC) (formula: C₁₁H₂₂O).



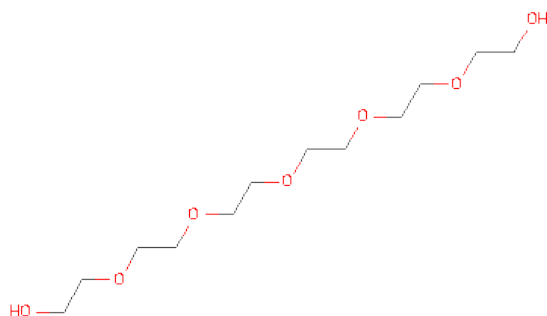
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	11	1		
3	B	1	Total	C	O	0	0
			12	11	1		
3	C	1	Total	C	O	0	0
			12	11	1		
3	D	1	Total	C	O	0	0
			12	11	1		
3	E	1	Total	C	O	0	0
			12	11	1		
3	F	1	Total	C	O	0	0
			12	11	1		
3	G	1	Total	C	O	0	0
			12	11	1		
3	H	1	Total	C	O	0	0
			12	11	1		

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			38	16	2	16	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	G	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	H	1	Total	C	N	O	P	S	0	0
			38	16	2	16	3	1		

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			15	10	5		
5	C	1	Total	C	O	0	0
			15	10	5		
5	E	1	Total	C	O	0	0
			15	10	5		
5	G	1	Total	C	O	0	0
			15	10	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	111	Total	O	0	0
			111	111		
6	B	95	Total	O	0	0
			95	95		
6	C	127	Total	O	0	0
			127	127		
6	D	92	Total	O	0	0
			92	92		
6	E	118	Total	O	0	0
			118	118		
6	F	107	Total	O	0	0
			107	107		
6	G	102	Total	O	0	0
			102	102		
6	H	98	Total	O	0	0
			98	98		

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: Thioesterase superfamily member 2

Chain A: 



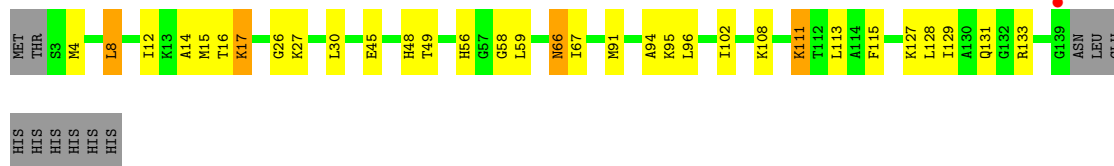
- Molecule 1: Thioesterase superfamily member 2

Chain B: 



- Molecule 1: Thioesterase superfamily member 2

Chain C: 



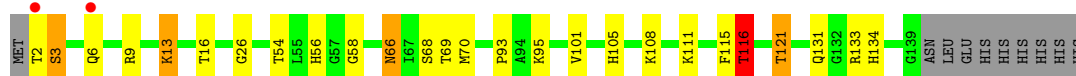
- Molecule 1: Thioesterase superfamily member 2

Chain D: 



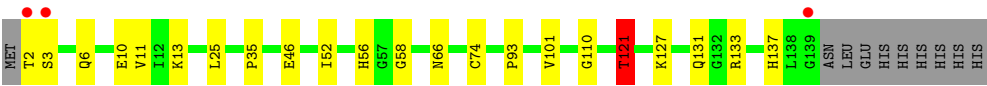
- Molecule 1: Thioesterase superfamily member 2

Chain E: 



- Molecule 1: Thioesterase superfamily member 2

Chain F: 



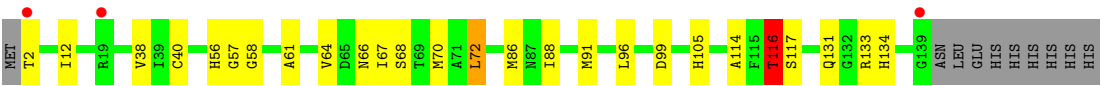
● Molecule 1: Thioesterase superfamily member 2

Chain G:



● Molecule 1: Thioesterase superfamily member 2

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.03Å 110.63Å 119.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.73 – 1.70 20.73 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.73-1.70) 98.9 (20.73-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.237 0.199 , 0.238	Depositor DCC
R_{free} test set	6645 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	3 of 132547 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9600	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.19 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3689e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: COA, UOC, P6G, CL

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	0/1055	0.68	0/1422
1	B	0.63	0/1048	0.75	0/1415
1	C	0.61	0/1059	0.71	0/1427
1	D	0.63	0/1050	0.71	0/1419
1	E	0.66	0/1034	0.75	2/1397 (0.1%)
1	F	0.64	0/1037	0.76	2/1401 (0.1%)
1	G	0.62	0/1037	0.69	0/1399
1	H	0.58	0/1062	0.74	1/1434 (0.1%)
All	All	0.62	0/8382	0.72	5/11314 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	116	THR	N-CA-CB	-5.93	99.04	110.30
1	H	116	THR	N-CA-CB	-5.81	99.26	110.30
1	E	116	THR	OG1-CB-CG2	5.72	123.17	110.00
1	F	121	THR	OG1-CB-CG2	5.54	122.75	110.00
1	F	121	THR	N-CA-CB	-5.23	100.37	110.30

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	1039	0	1090	19	0
1	B	1025	0	1074	19	0
1	C	1036	0	1092	32	0
1	D	1025	0	1068	23	0
1	E	1021	0	1062	32	0
1	F	1024	0	1073	18	0
1	G	1017	0	1058	15	0
1	H	1036	0	1087	37	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	12	0	20	5	0
3	B	12	0	21	0	0
3	C	12	0	21	1	0
3	D	12	0	21	1	0
3	E	12	0	21	2	0
3	F	12	0	21	0	0
3	G	12	0	21	1	0
3	H	12	0	21	2	0
4	A	38	0	26	6	0
4	B	48	0	31	1	0
4	C	48	0	31	0	0
4	D	48	0	31	0	0
4	E	48	0	31	1	0
4	F	48	0	31	3	0
4	G	48	0	31	5	0
4	H	38	0	26	3	0
5	B	15	0	16	0	0
5	C	15	0	16	0	0
5	E	15	0	16	1	0
5	G	15	0	16	1	0
6	A	111	0	0	1	0
6	B	95	0	0	3	0
6	C	127	0	0	0	0
6	D	92	0	0	1	0
6	E	118	0	0	5	0
6	F	107	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	102	0	0	1	0
6	H	98	0	0	1	0
All	All	9600	0	9073	184	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 10.

The worst 5 of 184 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:56:HIS:HD2	1:C:58:GLY:H	1.08	0.99
1:D:56:HIS:HD2	1:D:58:GLY:H	1.08	0.97
1:C:27:LYS:HE3	1:C:45:GLU:HG3	1.45	0.97
1:A:133:ARG:HE	1:D:131:GLN:HE21	1.10	0.96
1:F:133:ARG:HE	1:G:131:GLN:HE21	1.14	0.96

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	139/148 (94%)	136 (98%)	3 (2%)	0	100	100
1	B	138/148 (93%)	134 (97%)	4 (3%)	0	100	100
1	C	139/148 (94%)	137 (99%)	2 (1%)	0	100	100
1	D	140/148 (95%)	139 (99%)	1 (1%)	0	100	100
1	E	137/148 (93%)	133 (97%)	4 (3%)	0	100	100
1	F	137/148 (93%)	135 (98%)	2 (2%)	0	100	100
1	G	136/148 (92%)	134 (98%)	2 (2%)	0	100	100
1	H	141/148 (95%)	140 (99%)	1 (1%)	0	100	100
All	All	1107/1184 (94%)	1088 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	114/123 (93%)	113 (99%)	1 (1%)	87	79
1	B	111/123 (90%)	107 (96%)	4 (4%)	47	22
1	C	115/123 (94%)	108 (94%)	7 (6%)	26	8
1	D	112/123 (91%)	111 (99%)	1 (1%)	87	79
1	E	111/123 (90%)	105 (95%)	6 (5%)	31	11
1	F	113/123 (92%)	111 (98%)	2 (2%)	71	53
1	G	108/123 (88%)	108 (100%)	0	100	100
1	H	114/123 (93%)	110 (96%)	4 (4%)	48	23
All	All	898/984 (91%)	873 (97%)	25 (3%)	56	32

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	127	LYS
1	E	3	SER
1	H	99	ASP
1	D	96	LEU
1	E	13	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	66	ASN
1	E	66	ASN
1	H	66	ASN
1	D	131	GLN
1	E	56	HIS

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 27 ligands modelled in this entry, 7 are monoatomic - leaving 20 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$
3	UOC	A	149	4	11,11,11	1.06	1 (9%)	11,11,11	1.16	1 (9%)
4	COA	A	150	3	36,38,50	2.54	14 (38%)	52,56,75	2.30	14 (26%)
5	P6G	B	1001	-	12,14,18	0.72	0	11,13,17	0.37	0
3	UOC	B	149	4	11,11,11	0.47	0	11,11,11	0.85	0
4	COA	B	150	3	50,50,50	1.70	13 (26%)	75,75,75	2.19	12 (16%)
5	P6G	C	1001	-	12,14,18	0.67	0	11,13,17	0.64	0
3	UOC	C	149	4	11,11,11	0.62	0	11,11,11	0.60	0
4	COA	C	150	3	50,50,50	1.92	13 (26%)	75,75,75	1.80	15 (20%)
3	UOC	D	149	4	11,11,11	0.67	0	11,11,11	0.92	0
4	COA	D	150	3	50,50,50	2.14	13 (26%)	75,75,75	2.93	16 (21%)
5	P6G	E	1001	-	12,14,18	0.79	0	11,13,17	0.57	0
3	UOC	E	149	4	11,11,11	0.43	0	11,11,11	0.64	0
4	COA	E	150	3	50,50,50	2.13	14 (28%)	75,75,75	2.36	13 (17%)
3	UOC	F	149	4	11,11,11	0.46	0	11,11,11	1.33	1 (9%)
4	COA	F	150	3	50,50,50	1.86	12 (24%)	75,75,75	1.72	13 (17%)
5	P6G	G	1001	-	12,14,18	0.71	0	11,13,17	0.76	0
3	UOC	G	149	4	11,11,11	0.55	0	11,11,11	1.07	2 (18%)
4	COA	G	150	3	50,50,50	1.81	11 (22%)	75,75,75	1.84	15 (20%)
3	UOC	H	149	4	11,11,11	0.76	0	11,11,11	0.70	0
4	COA	H	150	3	36,38,50	1.73	9 (25%)	52,56,75	1.69	10 (19%)

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
3	UOC	A	149	4	-	0/9/9/9	0/0/0/0
4	COA	A	150	3	1/1/10/13	0/44/57/64	0/1/1/3
5	P6G	B	1001	-	-	0/12/12/16	0/0/0/0
3	UOC	B	149	4	-	0/9/9/9	0/0/0/0
4	COA	B	150	3	-	0/48/64/64	0/1/3/3
5	P6G	C	1001	-	-	0/12/12/16	0/0/0/0
3	UOC	C	149	4	-	0/9/9/9	0/0/0/0
4	COA	C	150	3	-	0/48/64/64	0/1/3/3
3	UOC	D	149	4	-	0/9/9/9	0/0/0/0
4	COA	D	150	3	-	0/48/64/64	0/1/3/3
5	P6G	E	1001	-	-	0/12/12/16	0/0/0/0
3	UOC	E	149	4	-	0/9/9/9	0/0/0/0
4	COA	E	150	3	-	0/48/64/64	0/1/3/3
3	UOC	F	149	4	-	0/9/9/9	0/0/0/0
4	COA	F	150	3	-	0/48/64/64	0/1/3/3
5	P6G	G	1001	-	-	0/12/12/16	0/0/0/0
3	UOC	G	149	4	-	0/9/9/9	0/0/0/0
4	COA	G	150	3	-	0/48/64/64	0/1/3/3
3	UOC	H	149	4	-	0/9/9/9	0/0/0/0
4	COA	H	150	3	-	1/44/57/64	0/1/1/3

The worst 5 of 100 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	150	COA	P2A-O3A	-8.01	1.45	1.59
4	A	150	COA	P1A-O3A	-7.77	1.45	1.59
4	E	150	COA	P2A-O3A	-6.24	1.48	1.59
4	C	150	COA	P2A-O3A	-6.08	1.48	1.59
4	F	150	COA	P2A-O3A	-5.92	1.49	1.59

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	150	COA	O4B-C1B-N9A	20.73	127.72	108.44
4	E	150	COA	O4B-C1B-N9A	-15.24	94.26	108.44
4	B	150	COA	O4B-C1B-N9A	11.26	118.91	108.44
4	A	150	COA	CBP-CAP-C9P	10.61	123.02	112.73
4	B	150	COA	N3A-C2A-N1A	-8.28	121.79	128.71

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	150	COA	CAP

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	150	COA	P3B-O3B-C3B-C4B

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	138/148 (93%)	-0.03	2 (1%) 72 78	18, 26, 36, 44	4 (2%)
1	B	136/148 (91%)	0.11	4 (2%) 49 54	18, 27, 37, 42	6 (4%)
1	C	137/148 (92%)	-0.14	1 (0%) 84 90	18, 24, 32, 43	6 (4%)
1	D	137/148 (92%)	0.02	4 (2%) 49 54	17, 25, 37, 45	3 (2%)
1	E	138/148 (93%)	-0.04	2 (1%) 72 78	18, 25, 34, 40	6 (4%)
1	F	138/148 (93%)	0.09	3 (2%) 59 64	17, 25, 37, 53	11 (7%)
1	G	136/148 (91%)	-0.02	2 (1%) 70 76	18, 26, 33, 38	9 (6%)
1	H	138/148 (93%)	0.04	3 (2%) 59 64	18, 27, 37, 45	1 (0%)
All	All	1098/1184 (92%)	0.00	21 (1%) 62 69	17, 25, 36, 53	46 (4%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2	THR	8.0
1	H	2	THR	7.2
1	H	139	GLY	5.6
1	F	139	GLY	5.5
1	E	2	THR	4.4

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
3	UOC	A	149	12/12	0.31	12.89	35,38,45,46	12
5	P6G	E	1001	15/19	0.27	6.33	63,67,70,70	0
3	UOC	G	149	12/12	0.25	5.98	37,45,50,51	0
5	P6G	G	1001	15/19	0.20	5.43	63,67,69,69	0
5	P6G	B	1001	15/19	0.28	4.79	72,77,79,79	0
3	UOC	D	149	12/12	0.17	4.25	29,38,49,51	0
3	UOC	B	149	12/12	0.20	3.99	36,46,52,52	0
4	COA	B	150	48/48	0.25	3.88	33,43,61,61	33
3	UOC	C	149	12/12	0.18	3.84	31,38,42,42	0
3	UOC	F	149	12/12	0.18	3.81	37,46,53,53	0
3	UOC	H	149	12/12	0.18	3.65	35,47,53,53	0
5	P6G	C	1001	15/19	0.23	2.77	48,52,53,53	0
4	COA	A	150	38/48	0.23	1.95	33,43,54,55	38
4	COA	G	150	48/48	0.18	1.80	28,45,56,57	30
4	COA	E	150	48/48	0.14	1.66	20,36,52,53	17
3	UOC	E	149	12/12	0.11	1.39	26,37,48,49	0
4	COA	F	150	48/48	0.19	1.21	32,43,56,56	27
4	COA	H	150	38/48	0.20	1.19	33,47,64,64	21
4	COA	C	150	48/48	0.14	0.70	22,34,48,48	17
4	COA	D	150	48/48	0.13	0.41	21,40,58,60	14
2	CL	A	151	1/1	0.08	-0.34	36,36,36,36	0
2	CL	D	151	1/1	0.04	-2.18	27,27,27,27	0
2	CL	F	151	1/1	0.03	-2.79	25,25,25,25	0
2	CL	G	151	1/1	0.03	-2.88	36,36,36,36	0
2	CL	C	151	1/1	0.03	-2.97	25,25,25,25	0
2	CL	E	151	1/1	0.04	-3.19	33,33,33,33	0
2	CL	H	151	1/1	0.03	-4.13	33,33,33,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.