



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 09:03 am BST

PDB ID : 6HSM
Title : Structure of partially reduced RsrR in space group P2(1)2(1)2(1)
Authors : Volbeda, A.; Fontecilla-Camps, J.C.
Deposited on : 2018-10-01
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

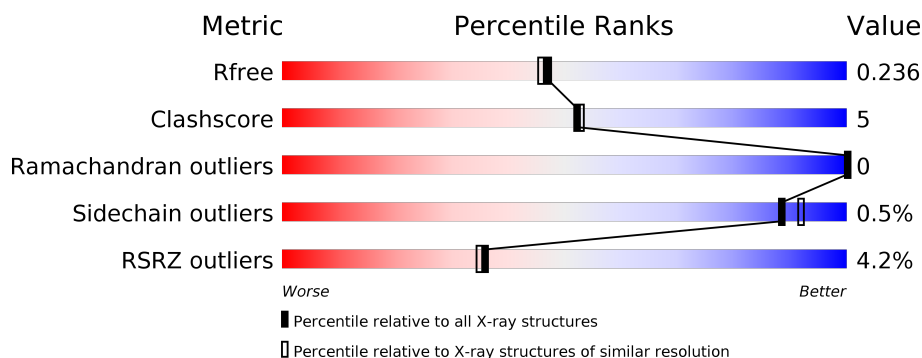
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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 $\leq 5\%$. 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	166	<div> <div style="width: 5%; background-color: red;"></div> <div style="width: 93%; background-color: green;"></div> <div style="width: 2%; background-color: yellow;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>5% •</div>
1	B	166	<div> <div style="width: 2%; background-color: red;"></div> <div style="width: 93%; background-color: green;"></div> <div style="width: 5%; background-color: yellow;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>5% •</div>
1	C	166	<div> <div style="width: 2%; background-color: red;"></div> <div style="width: 86%; background-color: green;"></div> <div style="width: 8%; background-color: yellow;"></div> <div style="width: 4%; background-color: grey;"></div> </div> <div>8% • 5%</div>
1	D	166	<div> <div style="width: 5%; background-color: red;"></div> <div style="width: 91%; background-color: green;"></div> <div style="width: 4%; background-color: yellow;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>5% •</div>
1	E	166	<div> <div style="width: 5%; background-color: red;"></div> <div style="width: 91%; background-color: green;"></div> <div style="width: 4%; background-color: yellow;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>5% •</div>
1	F	166	<div> <div style="width: 5%; background-color: red;"></div> <div style="width: 89%; background-color: green;"></div> <div style="width: 7%; background-color: yellow;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>7% 5%</div>

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Mol	Chain	Length	Quality of chain
1	G	166	
1	H	166	

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
3	MPD	B	206	-	-	X	-
3	MPD	C	201	-	-	X	-
4	GOL	A	208[A]	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10355 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Rrf2 family transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	8	0
			1242	789	218	227	8			
1	D	160	Total	C	N	O	S	0	4	0
			1167	733	204	222	8			
1	B	163	Total	C	N	O	S	0	2	0
			1191	749	212	222	8			
1	C	158	Total	C	N	O	S	0	7	0
			1173	741	207	217	8			
1	E	159	Total	C	N	O	S	0	5	0
			1173	739	207	219	8			
1	G	156	Total	C	N	O	S	0	6	0
			1169	743	205	213	8			
1	F	158	Total	C	N	O	S	0	7	0
			1184	749	208	219	8			
1	H	158	Total	C	N	O	S	0	4	0
			1162	733	201	220	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	161	HIS	-	expression tag	UNP F2RGC9
A	162	HIS	-	expression tag	UNP F2RGC9
A	163	HIS	-	expression tag	UNP F2RGC9
A	164	HIS	-	expression tag	UNP F2RGC9
A	165	HIS	-	expression tag	UNP F2RGC9
A	166	HIS	-	expression tag	UNP F2RGC9
D	161	HIS	-	expression tag	UNP F2RGC9
D	162	HIS	-	expression tag	UNP F2RGC9
D	163	HIS	-	expression tag	UNP F2RGC9
D	164	HIS	-	expression tag	UNP F2RGC9
D	165	HIS	-	expression tag	UNP F2RGC9
D	166	HIS	-	expression tag	UNP F2RGC9
B	161	HIS	-	expression tag	UNP F2RGC9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	162	HIS	-	expression tag	UNP F2RGC9
B	163	HIS	-	expression tag	UNP F2RGC9
B	164	HIS	-	expression tag	UNP F2RGC9
B	165	HIS	-	expression tag	UNP F2RGC9
B	166	HIS	-	expression tag	UNP F2RGC9
C	161	HIS	-	expression tag	UNP F2RGC9
C	162	HIS	-	expression tag	UNP F2RGC9
C	163	HIS	-	expression tag	UNP F2RGC9
C	164	HIS	-	expression tag	UNP F2RGC9
C	165	HIS	-	expression tag	UNP F2RGC9
C	166	HIS	-	expression tag	UNP F2RGC9
E	161	HIS	-	expression tag	UNP F2RGC9
E	162	HIS	-	expression tag	UNP F2RGC9
E	163	HIS	-	expression tag	UNP F2RGC9
E	164	HIS	-	expression tag	UNP F2RGC9
E	165	HIS	-	expression tag	UNP F2RGC9
E	166	HIS	-	expression tag	UNP F2RGC9
G	161	HIS	-	expression tag	UNP F2RGC9
G	162	HIS	-	expression tag	UNP F2RGC9
G	163	HIS	-	expression tag	UNP F2RGC9
G	164	HIS	-	expression tag	UNP F2RGC9
G	165	HIS	-	expression tag	UNP F2RGC9
G	166	HIS	-	expression tag	UNP F2RGC9
F	161	HIS	-	expression tag	UNP F2RGC9
F	162	HIS	-	expression tag	UNP F2RGC9
F	163	HIS	-	expression tag	UNP F2RGC9
F	164	HIS	-	expression tag	UNP F2RGC9
F	165	HIS	-	expression tag	UNP F2RGC9
F	166	HIS	-	expression tag	UNP F2RGC9
H	161	HIS	-	expression tag	UNP F2RGC9
H	162	HIS	-	expression tag	UNP F2RGC9
H	163	HIS	-	expression tag	UNP F2RGC9
H	164	HIS	-	expression tag	UNP F2RGC9
H	165	HIS	-	expression tag	UNP F2RGC9
H	166	HIS	-	expression tag	UNP F2RGC9

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	E	1	Total	Fe	S	0	0
			4	2	2		
2	E	1	Total	Fe	S	0	0
			4	2	2		
2	F	1	Total	Fe	S	0	0
			4	2	2		
2	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	1
			8	6	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			6	3	3		
4	D	1	Total	C	O	0	1
			12	6	6		
4	C	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

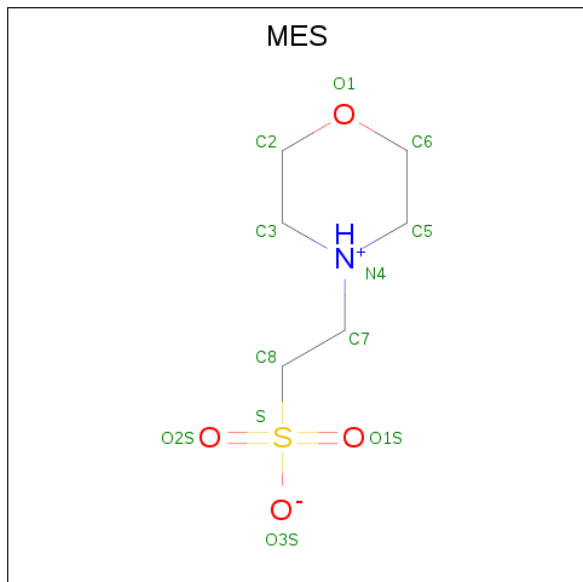
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		
5	F	1	Total	Cl	0	0
			1	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	90	Total	O	0	4
			91	91		
8	D	98	Total	O	0	4
			100	100		
8	B	81	Total	O	0	2
			82	82		
8	C	72	Total	O	0	1
			72	72		
8	E	83	Total	O	0	2
			83	83		
8	G	65	Total	O	0	1
			66	66		
8	F	60	Total	O	0	3
			60	60		
8	H	32	Total	O	0	1
			32	32		

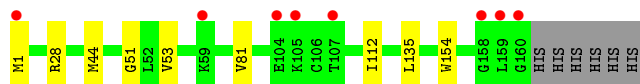
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

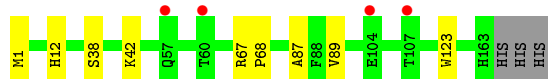
- Molecule 1: Rrf2 family transcriptional regulator



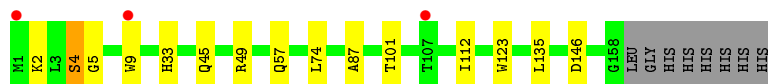
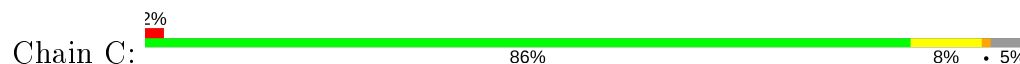
- Molecule 1: Rrf2 family transcriptional regulator



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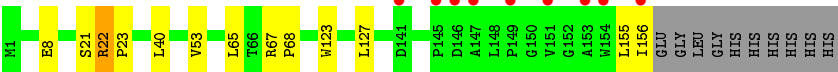
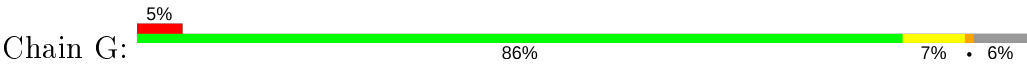
- Molecule 1: Rrf2 family transcriptional regulator



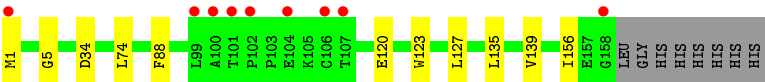
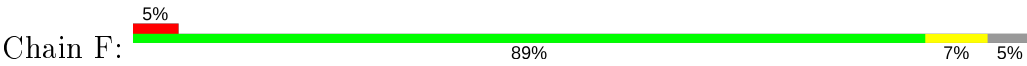
- Molecule 1: Rrf2 family transcriptional regulator



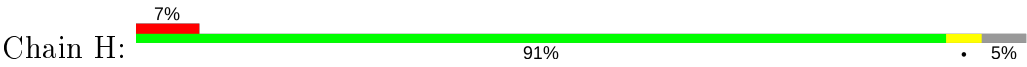
- Molecule 1: Rrf2 family transcriptional regulator



• Molecule 1: Rrf2 family transcriptional regulator



• Molecule 1: Rrf2 family transcriptional regulator



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.65Å 129.84Å 170.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.66 – 2.00 48.66 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.66-2.00) 99.7 (48.66-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.195 , 0.230 0.203 , 0.236	Depositor DCC
R_{free} test set	5015 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10355	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, MG, CL, MPD, FES, MES

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	0.54	0/1294	0.71	0/1770
1	B	0.54	0/1222	0.67	0/1671
1	C	0.54	0/1212	0.70	0/1658
1	D	0.55	0/1195	0.71	0/1635
1	E	0.53	0/1207	0.68	0/1649
1	F	0.47	0/1224	0.64	0/1675
1	G	0.52	0/1212	0.71	0/1659
1	H	0.48	0/1196	0.64	0/1636
All	All	0.52	0/9762	0.68	0/13353

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1242	0	1274	9	0
1	B	1191	0	1206	15	0
1	C	1173	0	1198	21	0
1	D	1167	0	1180	9	0
1	E	1173	0	1206	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1184	0	1204	9	0
1	G	1169	0	1213	9	0
1	H	1162	0	1187	6	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
2	E	8	0	0	0	0
2	F	8	0	0	0	0
3	A	48	0	84	9	0
3	B	48	0	84	22	0
3	C	16	0	28	8	0
3	D	48	0	84	11	0
3	E	8	0	14	0	0
3	F	16	0	28	3	0
3	G	24	0	42	3	0
3	H	16	0	26	8	0
4	A	6	0	8	0	0
4	C	6	0	8	1	0
4	D	12	0	16	0	0
4	E	6	0	8	2	0
4	F	6	0	8	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	B	1	0	0	0	0
7	E	12	0	13	0	0
8	A	91	0	0	1	0
8	B	82	0	0	0	0
8	C	72	0	0	2	0
8	D	100	0	0	0	0
8	E	83	0	0	0	0
8	F	60	0	0	2	0
8	G	66	0	0	0	0
8	H	32	0	0	0	0
All	All	10355	0	10119	109	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 5.

The worst 5 of 109 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)
3:H:202[B]:MPD:H53	3:H:202[B]:MPD:HM1	1.39	1.01
3:A:205:MPD:H12	3:A:205:MPD:H53	1.45	0.99
3:H:201:MPD:HM1	3:H:201:MPD:H53	1.48	0.94
3:C:201:MPD:HM3	1:F:5:GLY:H	1.36	0.89
3:D:206:MPD:H13	3:D:206:MPD:H52	1.55	0.89

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	170/166 (102%)	169 (99%)	1 (1%)	0	100	100
1	B	163/166 (98%)	160 (98%)	3 (2%)	0	100	100
1	C	161/166 (97%)	159 (99%)	2 (1%)	0	100	100
1	D	161/166 (97%)	158 (98%)	3 (2%)	0	100	100
1	E	161/166 (97%)	157 (98%)	4 (2%)	0	100	100
1	F	162/166 (98%)	157 (97%)	5 (3%)	0	100	100
1	G	160/166 (96%)	157 (98%)	3 (2%)	0	100	100
1	H	160/166 (96%)	158 (99%)	2 (1%)	0	100	100
All	All	1298/1328 (98%)	1275 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	131/125 (105%)	131 (100%)	0	100	100
1	B	123/125 (98%)	123 (100%)	0	100	100
1	C	122/125 (98%)	121 (99%)	1 (1%)	81	86
1	D	121/125 (97%)	121 (100%)	0	100	100
1	E	123/125 (98%)	122 (99%)	1 (1%)	81	86
1	F	123/125 (98%)	122 (99%)	1 (1%)	81	86
1	G	123/125 (98%)	120 (98%)	3 (2%)	49	51
1	H	121/125 (97%)	121 (100%)	0	100	100
All	All	987/1000 (99%)	981 (99%)	6 (1%)	88	90

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	21	SER
1	F	34	ASP
1	G	22[A]	ARG
1	E	34	ASP
1	G	22[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	57	GLN
1	G	95	GLN
1	H	79	GLN

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 47 ligands modelled in this entry, 4 are monoatomic - leaving 43 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	$\# Z > 2$
2	FES	A	209	1	0,4,4	0.00	-	-		
4	GOL	A	208[A]	-	5,5,5	0.19	0	5,5,5	0.10	0
3	MPD	E	203	-	7,7,7	0.13	0	9,10,10	0.32	0
3	MPD	D	201	-	7,7,7	0.34	0	9,10,10	0.55	0
3	MPD	D	204	-	7,7,7	0.17	0	9,10,10	0.43	0
2	FES	A	201	1	0,4,4	0.00	-	-		
3	MPD	D	202	-	7,7,7	0.23	0	9,10,10	0.60	0
3	MPD	A	206	-	7,7,7	0.19	0	9,10,10	0.43	0
3	MPD	G	201	-	7,7,7	0.20	0	9,10,10	0.38	0
3	MPD	D	203	-	7,7,7	0.20	0	9,10,10	0.44	0
2	FES	B	201	1	0,4,4	0.00	-	-		
3	MPD	A	204	-	7,7,7	0.27	0	9,10,10	0.35	0
2	FES	F	201	1	0,4,4	0.00	-	-		
4	GOL	D	207[A]	-	5,5,5	0.19	0	5,5,5	0.43	0
3	MPD	A	203	-	7,7,7	0.28	0	9,10,10	0.30	0
3	MPD	D	205	-	7,7,7	0.14	0	9,10,10	0.40	0
3	MPD	G	203	-	7,7,7	0.20	0	9,10,10	0.54	0
3	MPD	D	206	-	7,7,7	0.27	0	9,10,10	0.41	0
3	MPD	A	202	-	7,7,7	0.30	0	9,10,10	0.43	0
3	MPD	B	207	-	7,7,7	0.19	0	9,10,10	0.65	0
3	MPD	F	202	-	7,7,7	0.30	0	9,10,10	0.37	0
3	MPD	A	205	-	7,7,7	0.31	0	9,10,10	0.47	0
4	GOL	F	204	-	5,5,5	0.18	0	5,5,5	0.16	0
3	MPD	B	204	-	7,7,7	0.31	0	9,10,10	0.45	0
4	GOL	C	203	-	5,5,5	0.12	0	5,5,5	0.31	0
3	MPD	B	205	-	7,7,7	0.19	0	9,10,10	0.44	0
4	GOL	E	204	-	5,5,5	0.10	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MPD	G	202	-	7,7,7	0.20	0	9,10,10	0.40	0
3	MPD	H	201	-	7,7,7	0.21	0	9,10,10	0.35	0
3	MPD	B	206	-	7,7,7	0.31	0	9,10,10	0.42	0
3	MPD	H	202[B]	-	7,7,7	0.15	0	9,10,10	0.36	0
3	MPD	F	203	-	7,7,7	0.20	0	9,10,10	0.31	0
3	MPD	B	203	-	7,7,7	0.36	0	9,10,10	0.54	0
4	GOL	D	207[B]	-	5,5,5	0.20	0	5,5,5	0.22	0
2	FES	E	201	1	0,4,4	0.00	-	-		
2	FES	F	206	1	0,4,4	0.00	-	-		
3	MPD	A	207	-	7,7,7	0.18	0	9,10,10	0.73	0
2	FES	E	202	1	0,4,4	0.00	-	-		
3	MPD	C	202	-	7,7,7	0.19	0	9,10,10	0.33	0
2	FES	B	210	1	0,4,4	0.00	-	-		
3	MPD	B	202	-	7,7,7	0.38	0	9,10,10	0.54	0
7	MES	E	205	-	12,12,12	0.72	0	14,16,16	0.75	0
3	MPD	C	201	-	7,7,7	0.17	0	9,10,10	0.55	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
2	FES	A	209	1	-	-	0/1/1/1
4	GOL	A	208[A]	-	-	2/4/4/4	-
3	MPD	E	203	-	-	1/5/5/5	-
3	MPD	D	201	-	-	5/5/5/5	-
3	MPD	D	204	-	-	4/5/5/5	-
2	FES	A	201	1	-	-	0/1/1/1
3	MPD	D	202	-	-	1/5/5/5	-
3	MPD	A	206	-	-	1/5/5/5	-
3	MPD	G	201	-	-	4/5/5/5	-
3	MPD	D	203	-	-	0/5/5/5	-
4	GOL	D	207[B]	-	-	4/4/4/4	-
3	MPD	A	204	-	-	1/5/5/5	-
2	FES	F	201	1	-	-	0/1/1/1
2	FES	B	201	1	-	-	0/1/1/1
4	GOL	D	207[A]	-	-	2/4/4/4	-
3	MPD	A	203	-	-	3/5/5/5	-
3	MPD	D	205	-	-	4/5/5/5	-
3	MPD	G	203	-	-	5/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	D	206	-	-	4/5/5/5	-
3	MPD	A	202	-	-	0/5/5/5	-
3	MPD	B	207	-	-	5/5/5/5	-
2	FES	B	210	1	-	-	0/1/1/1
3	MPD	A	205	-	-	1/5/5/5	-
4	GOL	F	204	-	-	0/4/4/4	-
3	MPD	B	204	-	-	2/5/5/5	-
4	GOL	C	203	-	-	3/4/4/4	-
3	MPD	B	205	-	-	0/5/5/5	-
4	GOL	E	204	-	-	3/4/4/4	-
3	MPD	G	202	-	-	2/5/5/5	-
2	FES	F	206	1	-	-	0/1/1/1
3	MPD	B	206	-	-	3/5/5/5	-
3	MPD	H	202[B]	-	-	1/5/5/5	-
3	MPD	F	203	-	-	2/5/5/5	-
3	MPD	B	203	-	-	2/5/5/5	-
2	FES	E	201	1	-	-	0/1/1/1
3	MPD	H	201	-	-	1/5/5/5	-
3	MPD	A	207	-	-	2/5/5/5	-
2	FES	E	202	1	-	-	0/1/1/1
3	MPD	C	202	-	-	2/5/5/5	-
3	MPD	F	202	-	-	1/5/5/5	-
3	MPD	B	202	-	-	2/5/5/5	-
7	MES	E	205	-	-	3/6/14/14	0/1/1/1
3	MPD	C	201	-	-	2/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 78 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	201	MPD	C1-C2-C3-C4
3	D	201	MPD	O2-C2-C3-C4
3	D	204	MPD	CM-C2-C3-C4
3	D	202	MPD	C2-C3-C4-C5
3	G	201	MPD	O2-C2-C3-C4

There are no ring outliers.

23 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	201	MPD	2	0
3	D	204	MPD	2	0
3	G	201	MPD	1	0
3	D	203	MPD	2	0
3	A	204	MPD	1	0
3	A	203	MPD	3	0
3	D	205	MPD	2	0
3	D	206	MPD	3	0
3	F	202	MPD	1	0
3	A	205	MPD	2	0
4	C	203	GOL	1	0
3	B	205	MPD	1	0
4	E	204	GOL	2	0
3	G	202	MPD	2	0
3	H	201	MPD	3	0
3	B	206	MPD	17	0
3	H	202[B]	MPD	5	0
3	F	203	MPD	2	0
3	B	203	MPD	1	0
3	A	207	MPD	3	0
3	C	202	MPD	1	0
3	B	202	MPD	3	0
3	C	201	MPD	7	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	164/166 (98%)	0.08	1 (0%) 89 88	27, 36, 54, 82	0
1	B	163/166 (98%)	-0.03	4 (2%) 57 56	31, 44, 76, 99	0
1	C	158/166 (95%)	0.13	3 (1%) 66 65	35, 47, 70, 82	2 (1%)
1	D	160/166 (96%)	0.31	8 (5%) 28 28	30, 38, 74, 99	1 (0%)
1	E	159/166 (95%)	0.09	8 (5%) 28 28	30, 42, 72, 93	1 (0%)
1	F	158/166 (95%)	0.29	9 (5%) 23 23	35, 49, 76, 89	1 (0%)
1	G	156/166 (93%)	0.08	9 (5%) 23 22	31, 46, 80, 90	0
1	H	158/166 (95%)	0.52	12 (7%) 13 13	42, 57, 88, 111	0
All	All	1276/1328 (96%)	0.18	54 (4%) 36 35	27, 45, 75, 111	5 (0%)

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	158	GLY	5.9
1	F	99[A]	LEU	5.3
1	C	1	MET	5.1
1	E	59	LYS	4.8
1	H	58	GLY	4.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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. 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
3	MPD	D	204	8/8	0.61	0.26	62,68,73,75	0
3	MPD	H	202[B]	8/8	0.61	0.37	53,55,57,60	8
4	GOL	C	203	6/6	0.69	0.32	79,81,82,83	0
4	GOL	F	204	6/6	0.71	0.21	78,80,81,82	0
7	MES	E	205	12/12	0.73	0.26	68,86,89,90	0
4	GOL	A	208[A]	6/6	0.74	0.51	43,44,44,45	6
3	MPD	B	207	8/8	0.75	0.17	67,70,72,72	0
4	GOL	E	204	6/6	0.75	0.21	77,79,80,80	0
3	MPD	A	207	8/8	0.76	0.24	73,74,79,79	0
3	MPD	G	201	8/8	0.78	0.26	72,74,74,75	0
3	MPD	A	204	8/8	0.79	0.27	59,60,62,63	0
3	MPD	D	202	8/8	0.79	0.27	71,74,77,78	0
3	MPD	D	205	8/8	0.80	0.24	65,71,73,73	0
3	MPD	D	203	8/8	0.80	0.27	84,90,93,96	0
3	MPD	G	203	8/8	0.81	0.17	57,62,63,64	0
3	MPD	B	205	8/8	0.81	0.21	79,80,81,82	0
3	MPD	C	201	8/8	0.81	0.26	47,50,54,57	0
3	MPD	G	202	8/8	0.83	0.18	81,83,84,84	0
3	MPD	F	203	8/8	0.84	0.23	75,77,79,79	0
5	CL	B	208	1/1	0.84	0.13	66,66,66,66	0
3	MPD	H	201	8/8	0.85	0.32	80,83,83,84	0
3	MPD	C	202	8/8	0.85	0.34	94,95,96,97	0
3	MPD	B	202	8/8	0.85	0.24	74,75,77,78	0
5	CL	D	208	1/1	0.85	0.13	54,54,54,54	1
3	MPD	B	204	8/8	0.85	0.22	70,77,77,80	0
3	MPD	A	202	8/8	0.86	0.17	61,65,66,66	0
3	MPD	A	206	8/8	0.86	0.20	66,67,69,70	0
3	MPD	B	203	8/8	0.87	0.22	71,73,75,76	0
5	CL	F	205	1/1	0.87	0.10	67,67,67,67	0
4	GOL	D	207[B]	6/6	0.88	0.30	50,52,55,57	6
4	GOL	D	207[A]	6/6	0.88	0.30	54,55,57,58	6
3	MPD	D	206	8/8	0.90	0.18	70,72,77,78	0
6	MG	B	209	1/1	0.90	0.18	56,56,56,56	1
3	MPD	A	205	8/8	0.91	0.17	79,81,82,82	0
3	MPD	A	203	8/8	0.91	0.20	67,70,78,79	0
3	MPD	F	202	8/8	0.92	0.22	81,83,86,86	0
3	MPD	E	203	8/8	0.92	0.16	71,71,73,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MPD	B	206	8/8	0.92	0.39	73,74,81,82	0
3	MPD	D	201	8/8	0.93	0.16	57,57,60,61	0
2	FES	A	201	4/4	0.99	0.10	32,33,34,35	0
2	FES	B	201	4/4	0.99	0.07	38,39,39,41	0
2	FES	B	210	4/4	0.99	0.11	38,40,41,44	0
2	FES	F	201	4/4	0.99	0.10	45,45,48,49	0
2	FES	E	201	4/4	0.99	0.10	33,34,35,36	0
2	FES	F	206	4/4	0.99	0.05	44,45,45,47	0
2	FES	E	202	4/4	1.00	0.09	33,34,34,35	0
2	FES	A	209	4/4	1.00	0.12	30,30,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.