



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:58 AM GMT

PDB ID : 3MJC
Title : Structure of A-type Ketoreductases from Modular Polyketide Synthase
Authors : Zheng, J.; Taylor, C.A.; Piasecki, S.K.; Keatinge-Clay, A.T.
Deposited on : 2010-04-12
Resolution : 1.48 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>

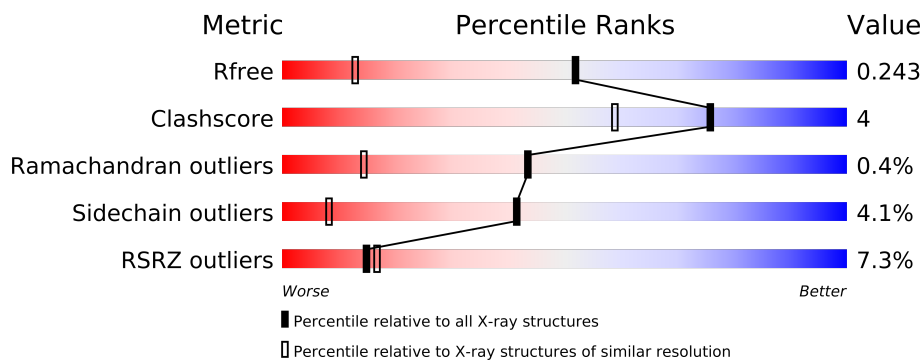
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 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 1.48 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	2222 (1.50-1.46)
Clashscore	79885	2555 (1.50-1.46)
Ramachandran outliers	78287	2496 (1.50-1.46)
Sidechain outliers	78261	2494 (1.50-1.46)
RSRZ outliers	66119	2223 (1.50-1.46)

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	496	
1	B	496	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7370 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 AmphB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3426	2140	629	649	8			
1	B	470	Total	C	N	O	S	0	0	0
			3426	2140	629	649	8			

There are 42 discrepancies between the modelled and reference sequences:

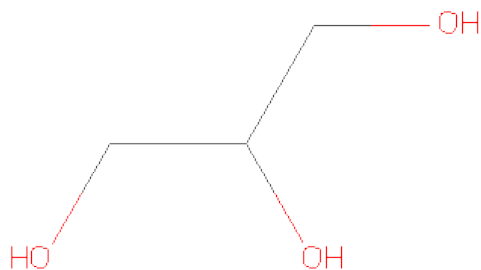
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q93NW7
A	-19	GLY	-	EXPRESSION TAG	UNP Q93NW7
A	-18	SER	-	EXPRESSION TAG	UNP Q93NW7
A	-17	SER	-	EXPRESSION TAG	UNP Q93NW7
A	-16	HIS	-	EXPRESSION TAG	UNP Q93NW7
A	-15	HIS	-	EXPRESSION TAG	UNP Q93NW7
A	-14	HIS	-	EXPRESSION TAG	UNP Q93NW7
A	-13	HIS	-	EXPRESSION TAG	UNP Q93NW7
A	-12	HIS	-	EXPRESSION TAG	UNP Q93NW7
A	-11	HIS	-	EXPRESSION TAG	UNP Q93NW7
A	-10	SER	-	EXPRESSION TAG	UNP Q93NW7
A	-9	SER	-	EXPRESSION TAG	UNP Q93NW7
A	-8	GLY	-	EXPRESSION TAG	UNP Q93NW7
A	-7	LEU	-	EXPRESSION TAG	UNP Q93NW7
A	-6	VAL	-	EXPRESSION TAG	UNP Q93NW7
A	-5	PRO	-	EXPRESSION TAG	UNP Q93NW7
A	-4	ARG	-	EXPRESSION TAG	UNP Q93NW7
A	-3	GLY	-	EXPRESSION TAG	UNP Q93NW7
A	-2	SER	-	EXPRESSION TAG	UNP Q93NW7
A	-1	HIS	-	EXPRESSION TAG	UNP Q93NW7
A	0	MET	-	EXPRESSION TAG	UNP Q93NW7
B	-20	MET	-	EXPRESSION TAG	UNP Q93NW7
B	-19	GLY	-	EXPRESSION TAG	UNP Q93NW7
B	-18	SER	-	EXPRESSION TAG	UNP Q93NW7
B	-17	SER	-	EXPRESSION TAG	UNP Q93NW7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	EXPRESSION TAG	UNP Q93NW7
B	-15	HIS	-	EXPRESSION TAG	UNP Q93NW7
B	-14	HIS	-	EXPRESSION TAG	UNP Q93NW7
B	-13	HIS	-	EXPRESSION TAG	UNP Q93NW7
B	-12	HIS	-	EXPRESSION TAG	UNP Q93NW7
B	-11	HIS	-	EXPRESSION TAG	UNP Q93NW7
B	-10	SER	-	EXPRESSION TAG	UNP Q93NW7
B	-9	SER	-	EXPRESSION TAG	UNP Q93NW7
B	-8	GLY	-	EXPRESSION TAG	UNP Q93NW7
B	-7	LEU	-	EXPRESSION TAG	UNP Q93NW7
B	-6	VAL	-	EXPRESSION TAG	UNP Q93NW7
B	-5	PRO	-	EXPRESSION TAG	UNP Q93NW7
B	-4	ARG	-	EXPRESSION TAG	UNP Q93NW7
B	-3	GLY	-	EXPRESSION TAG	UNP Q93NW7
B	-2	SER	-	EXPRESSION TAG	UNP Q93NW7
B	-1	HIS	-	EXPRESSION TAG	UNP Q93NW7
B	0	MET	-	EXPRESSION TAG	UNP Q93NW7

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is water.

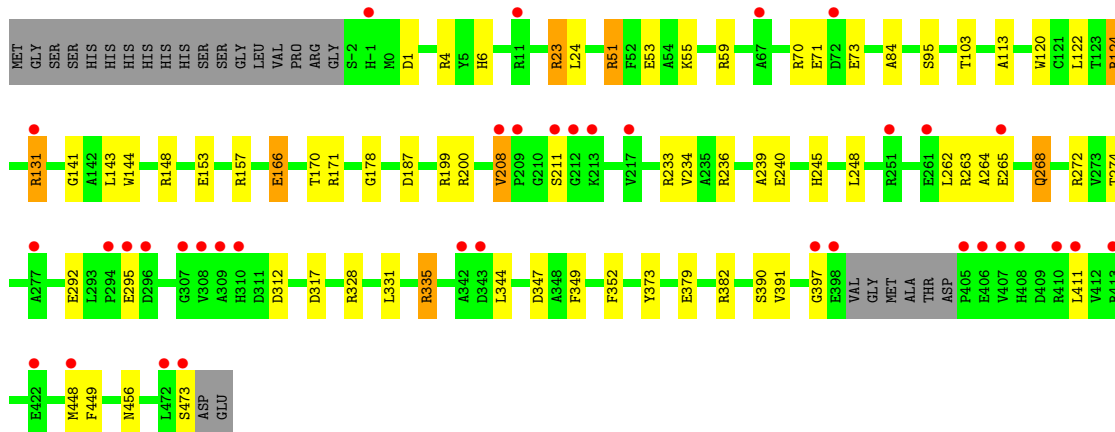
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	248	Total 248	O 248	0	0
3	B	264	Total 264	O 264	0	0

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.

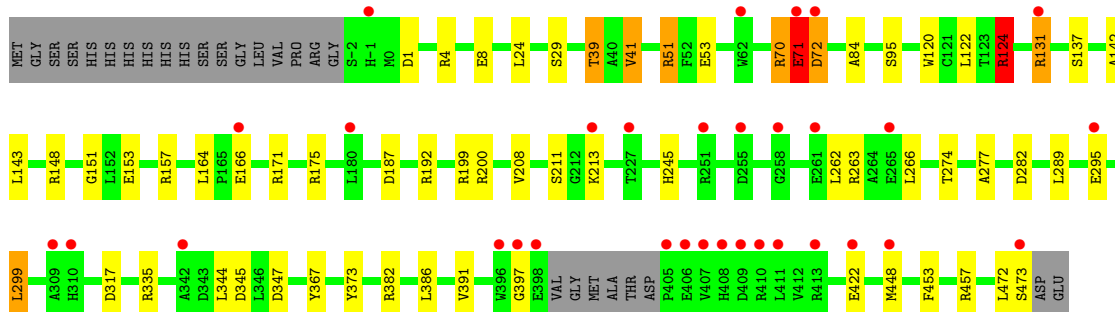
• Molecule 1: AmphB

Chain A: 



• Molecule 1: AmphB

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.47Å 63.75Å 71.55Å 72.79° 67.30° 89.82°	Depositor
Resolution (Å)	62.55 – 1.48 44.03 – 1.48	Depositor EDS
% Data completeness (in resolution range)	95.2 (62.55-1.48) 94.3 (44.03-1.48)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.213 , 0.243 0.213 , 0.243	Depositor DCC
R_{free} test set	7468 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 41.1	EDS
Estimated twinning fraction	0.063 for h,-k,h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 148637 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7370	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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: GOL

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	1.44	22/3495 (0.6%)	1.47	45/4772 (0.9%)
1	B	1.41	17/3495 (0.5%)	1.50	41/4772 (0.9%)
All	All	1.43	39/6990 (0.6%)	1.48	86/9544 (0.9%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	GLU	CB-CG	-14.35	1.24	1.52
1	A	51	ARG	CZ-NH1	13.48	1.50	1.33
1	B	51	ARG	CZ-NH1	13.43	1.50	1.33
1	B	51	ARG	CZ-NH2	9.31	1.45	1.33
1	B	8	GLU	CB-CG	-9.18	1.34	1.52
1	A	166	GLU	CB-CG	-8.89	1.35	1.52
1	B	39	THR	CB-CG2	-7.72	1.26	1.52
1	B	120	TRP	CG-CD1	7.64	1.47	1.36
1	A	51	ARG	CZ-NH2	7.35	1.42	1.33
1	B	166	GLU	CB-CG	-7.17	1.38	1.52
1	A	113	ALA	CA-CB	6.76	1.66	1.52
1	B	457	ARG	CB-CG	-6.39	1.35	1.52
1	A	144	TRP	CG-CD1	6.04	1.45	1.36
1	B	137	SER	CB-OG	5.95	1.50	1.42
1	B	142	ALA	CA-CB	5.91	1.64	1.52
1	A	95	SER	CB-OG	5.81	1.49	1.42
1	B	199	ARG	CZ-NH2	5.79	1.40	1.33
1	B	367	TYR	CG-CD1	5.78	1.46	1.39
1	A	124	ARG	CB-CG	5.75	1.68	1.52
1	B	39	THR	CB-OG1	-5.61	1.32	1.43
1	A	6	HIS	CA-CB	-5.60	1.41	1.53
1	A	456	ASN	CB-CG	-5.38	1.38	1.51
1	A	120	TRP	CG-CD1	5.36	1.44	1.36
1	A	240	GLU	CA-CB	-5.32	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	53	GLU	CG-CD	-5.32	1.44	1.51
1	A	349	PHE	CE1-CZ	5.28	1.47	1.37
1	A	391	VAL	CB-CG2	5.22	1.63	1.52
1	B	95	SER	CB-OG	5.22	1.49	1.42
1	B	29	SER	CB-OG	5.20	1.49	1.42
1	A	379	GLU	CD-OE1	-5.18	1.20	1.25
1	B	41	VAL	CB-CG1	-5.17	1.42	1.52
1	A	292	GLU	CB-CG	-5.16	1.42	1.52
1	A	379	GLU	CB-CG	5.14	1.61	1.52
1	A	103	THR	CA-CB	-5.12	1.40	1.53
1	A	234	VAL	CB-CG1	5.06	1.63	1.52
1	A	449	PHE	CD1-CE1	5.06	1.49	1.39
1	A	178	GLY	N-CA	5.04	1.53	1.46
1	A	131	ARG	C-O	-5.00	1.13	1.23
1	B	151	GLY	N-CA	5.00	1.53	1.46

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	ARG	NE-CZ-NH1	24.57	132.59	120.30
1	B	382	ARG	NE-CZ-NH1	23.15	131.87	120.30
1	B	382	ARG	NE-CZ-NH2	-21.17	109.72	120.30
1	A	382	ARG	NE-CZ-NH2	-20.46	110.07	120.30
1	A	51	ARG	NE-CZ-NH2	-19.07	110.76	120.30
1	B	51	ARG	NE-CZ-NH2	-17.32	111.64	120.30
1	A	272	ARG	NE-CZ-NH2	13.90	127.25	120.30
1	B	199	ARG	NE-CZ-NH1	12.77	126.68	120.30
1	B	148	ARG	NE-CZ-NH2	-12.06	114.27	120.30
1	B	200	ARG	NE-CZ-NH1	12.03	126.31	120.30
1	B	124	ARG	CG-CD-NE	-11.60	87.45	111.80
1	A	199	ARG	NE-CZ-NH1	11.10	125.85	120.30
1	B	382	ARG	CD-NE-CZ	10.96	138.94	123.60
1	B	200	ARG	NE-CZ-NH2	-10.73	114.94	120.30
1	B	4	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	B	344	LEU	C-N-CA	-10.01	96.67	121.70
1	A	382	ARG	CD-NE-CZ	9.61	137.05	123.60
1	B	157	ARG	NE-CZ-NH1	-9.46	115.57	120.30
1	B	382	ARG	CB-CG-CD	8.83	134.55	111.60
1	A	124	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	A	148	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	B	347	ASP	CB-CG-OD2	-8.54	110.62	118.30
1	B	391	VAL	CG1-CB-CG2	8.47	124.45	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ARG	NE-CZ-NH2	8.45	124.53	120.30
1	B	148	ARG	NE-CZ-NH1	8.43	124.52	120.30
1	A	382	ARG	CB-CG-CD	8.29	133.16	111.60
1	B	192	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	344	LEU	C-N-CA	-7.79	102.23	121.70
1	B	124	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	B	175	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	51	ARG	NH1-CZ-NH2	7.66	127.83	119.40
1	A	148	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	B	131	ARG	C-N-CA	-7.33	106.91	122.30
1	A	347	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	B	51	ARG	NH1-CZ-NH2	7.22	127.34	119.40
1	A	263	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	B	289	LEU	CB-CG-CD2	-7.14	98.86	111.00
1	A	122	LEU	CB-CG-CD2	7.08	123.03	111.00
1	B	199	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	B	457	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	A	153	GLU	OE1-CD-OE2	-6.93	114.98	123.30
1	A	312	ASP	CB-CG-OD2	-6.89	112.09	118.30
1	A	200	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	A	335	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	B	1	ASP	CB-CG-OD1	6.65	124.28	118.30
1	A	157	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	A	233	ARG	CG-CD-NE	-6.50	98.14	111.80
1	A	187	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	B	282	ASP	CB-CG-OD1	6.33	124.00	118.30
1	B	453	PHE	CB-CG-CD1	-6.25	116.43	120.80
1	A	373	TYR	CD1-CE1-CZ	-6.06	114.34	119.80
1	A	4	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	59	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	A	208	VAL	CG1-CB-CG2	-5.97	101.35	110.90
1	A	1	ASP	CB-CG-OD1	5.87	123.59	118.30
1	A	352	PHE	CB-CG-CD2	-5.87	116.69	120.80
1	B	317	ASP	CB-CG-OD1	-5.86	113.03	118.30
1	A	248	LEU	CB-CG-CD1	-5.76	101.21	111.00
1	A	331	LEU	CB-CG-CD1	-5.74	101.24	111.00
1	A	335	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	B	122	LEU	CB-CG-CD2	5.71	120.70	111.00
1	A	317	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	272	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	A	170	THR	CA-CB-CG2	-5.57	104.61	112.40
1	A	1	ASP	CB-CG-OD2	-5.53	113.33	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	GLU	OE1-CD-OE2	-5.50	116.70	123.30
1	B	335	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	131	ARG	O-C-N	-5.46	113.92	123.20
1	A	141	GLY	O-C-N	-5.42	114.03	122.70
1	A	157	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	B	166	GLU	N-CA-CB	-5.41	100.87	110.60
1	A	263	ARG	NE-CZ-NH2	5.39	123.00	120.30
1	A	187	ASP	CB-CG-OD2	5.32	123.08	118.30
1	B	386	LEU	CB-CG-CD2	-5.29	102.01	111.00
1	B	453	PHE	CZ-CE2-CD2	-5.27	113.78	120.10
1	B	263	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	B	472	LEU	CB-CG-CD1	-5.15	102.24	111.00
1	A	124	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	187	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	200	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	373	TYR	CD1-CE1-CZ	-5.10	115.21	119.80
1	A	391	VAL	CG1-CB-CG2	5.06	119.00	110.90
1	A	239	ALA	C-N-CA	-5.05	109.09	121.70
1	B	344	LEU	O-C-N	-5.03	114.66	122.70
1	A	328	ARG	NE-CZ-NH1	-5.01	117.79	120.30
1	B	457	ARG	NE-CZ-NH2	-5.00	117.80	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	3426	0	0	12	0
1	B	3426	0	0	15	0
2	B	6	0	0	0	0
3	A	248	0	0	5	0
3	B	264	0	0	6	0
All	All	7370	0	0	27	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 4.

All (27) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:448:MET:CG	3:A:642:HOH:O	2.31	0.77
1:B:70:ARG:O	1:B:71:GLU:CB	2.29	0.76
1:A:208:VAL:CG2	1:A:211:SER:OG	2.37	0.73
1:A:236:ARG:NH2	3:A:684:HOH:O	2.21	0.72
1:B:208:VAL:CG2	1:B:211:SER:OG	2.40	0.70
1:B:39:THR:CB	3:B:569:HOH:O	2.42	0.66
1:A:51:ARG:NE	3:A:605:HOH:O	2.30	0.65
1:A:265:GLU:CG	3:A:684:HOH:O	2.45	0.64
1:B:448:MET:CG	3:B:669:HOH:O	2.47	0.63
1:A:51:ARG:NH2	3:A:605:HOH:O	2.33	0.61
1:B:71:GLU:CG	1:B:72:ASP:N	2.68	0.56
1:B:51:ARG:NH2	3:B:549:HOH:O	2.42	0.53
1:A:53:GLU:OE1	1:A:55:LYS:NZ	2.43	0.51
1:A:245:HIS:CE1	1:A:274:THR:OG1	2.65	0.50
1:B:84:ALA:CB	1:B:143:LEU:CD1	2.90	0.50
1:B:422:GLU:CG	3:B:656:HOH:O	2.59	0.50
1:B:245:HIS:CE1	1:B:274:THR:OG1	2.66	0.48
1:B:124:ARG:NH1	3:B:601:HOH:O	2.46	0.47
1:B:70:ARG:O	1:B:71:GLU:CG	2.63	0.47
1:B:51:ARG:NE	3:B:549:HOH:O	2.48	0.46
1:B:41:VAL:CG2	1:B:164:LEU:CD1	2.94	0.46
1:B:299:LEU:CD2	1:B:299:LEU:C	2.84	0.45
1:B:24:LEU:CD2	1:B:24:LEU:N	2.80	0.45
1:A:264:ALA:O	1:A:268:GLN:NE2	2.51	0.44
1:A:84:ALA:CB	1:A:143:LEU:CD1	2.97	0.43
1:A:24:LEU:N	1:A:24:LEU:CD2	2.82	0.43
1:A:23:ARG:NH1	1:A:73:GLU:CB	2.84	0.41

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	466/496 (94%)	454 (97%)	11 (2%)	1 (0%)	56	25
1	B	466/496 (94%)	454 (97%)	9 (2%)	3 (1%)	33	9
All	All	932/992 (94%)	908 (97%)	20 (2%)	4 (0%)	43	14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	71	GLU
1	B	277	ALA
1	A	397	GLY
1	B	397	GLY

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	330/351 (94%)	316 (96%)	14 (4%)	40	8
1	B	330/351 (94%)	317 (96%)	13 (4%)	43	9
All	All	660/702 (94%)	633 (96%)	27 (4%)	41	8

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

Mol	Chain	Res	Type
1	A	23	ARG
1	A	70	ARG
1	A	71	GLU
1	A	124	ARG
1	A	131	ARG
1	A	166	GLU
1	A	171	ARG
1	A	262	LEU
1	A	268	GLN
1	A	295	GLU
1	A	335	ARG
1	A	390	SER
1	A	411	LEU

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Mol	Chain	Res	Type
1	A	473	SER
1	B	70	ARG
1	B	71	GLU
1	B	72	ASP
1	B	124	ARG
1	B	131	ARG
1	B	171	ARG
1	B	213	LYS
1	B	262	LEU
1	B	266	LEU
1	B	295	GLU
1	B	299	LEU
1	B	345	ASP
1	B	473	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 ⓘ

1 ligand is modelled in this entry.

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	GOL	B	476	-	5,5,5	0.80	0	5,5,5	0.87	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	GOL	B	476	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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	470/496 (94%)	0.49	37 (7%) 13 14	11, 20, 40, 56	0
1	B	470/496 (94%)	0.50	32 (6%) 17 19	11, 20, 40, 56	0
All	All	940/992 (94%)	0.49	69 (7%) 15 17	11, 20, 40, 56	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	407	VAL	6.6
1	B	407	VAL	5.7
1	A	131	ARG	5.5
1	B	397	GLY	5.4
1	B	131	ARG	5.4
1	B	398	GLU	5.0
1	A	295	GLU	4.8
1	B	405	PRO	4.6
1	A	398	GLU	4.4
1	A	-1	HIS	4.3
1	B	473	SER	4.2
1	B	342	ALA	4.1
1	A	406	GLU	4.0
1	A	209	PRO	4.0
1	B	406	GLU	3.9
1	A	212	GLY	3.9
1	A	473	SER	3.6
1	A	294	PRO	3.5
1	B	310	HIS	3.5
1	A	397	GLY	3.4
1	B	396	TRP	3.4
1	A	405	PRO	3.3
1	A	217	VAL	3.3
1	A	296	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	251	ARG	3.1
1	A	343	ASP	3.1
1	B	411	LEU	3.1
1	A	213	LYS	3.1
1	A	411	LEU	3.0
1	B	258	GLY	3.0
1	A	310	HIS	2.9
1	B	448	MET	2.9
1	A	265	GLU	2.8
1	B	62	TRP	2.8
1	B	295	GLU	2.8
1	B	261	GLU	2.8
1	B	-1	HIS	2.7
1	B	71	GLU	2.7
1	A	261	GLU	2.6
1	B	422	GLU	2.6
1	A	211	SER	2.6
1	B	166	GLU	2.6
1	A	208	VAL	2.5
1	A	308	VAL	2.5
1	B	410	ARG	2.5
1	A	309	ALA	2.5
1	A	342	ALA	2.4
1	A	307	GLY	2.4
1	A	448	MET	2.4
1	A	422	GLU	2.4
1	B	413	ARG	2.4
1	A	408	HIS	2.3
1	B	72	ASP	2.3
1	B	408	HIS	2.3
1	A	472	LEU	2.3
1	A	251	ARG	2.2
1	A	413	ARG	2.2
1	B	227	THR	2.2
1	B	213	LYS	2.2
1	B	309	ALA	2.2
1	A	11	ARG	2.1
1	B	409	ASP	2.1
1	B	255	ASP	2.1
1	B	180	LEU	2.1
1	A	72	ASP	2.1
1	A	410	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	265	GLU	2.1
1	A	67	ALA	2.0
1	A	277	ALA	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(\AA^2)	Q<0.9
2	GOL	B	476	6/6	0.07	-2.21	21,23,26,27	0

6.5 Other polymers ⓘ

There are no such residues in this entry.