



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:33 am BST

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 X-ray Structure Validation 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

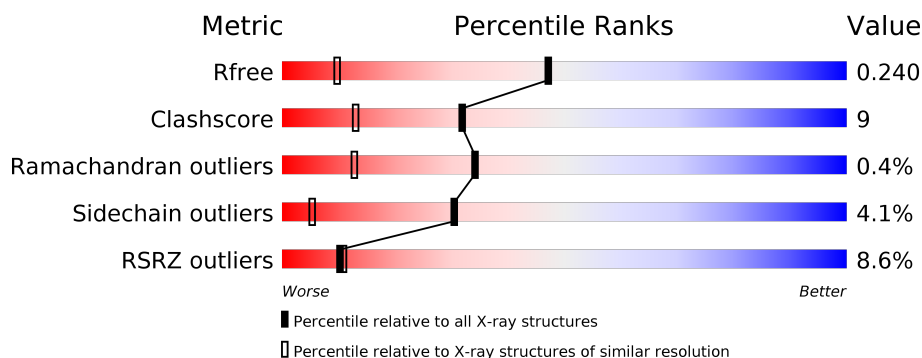
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (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 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	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 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 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:

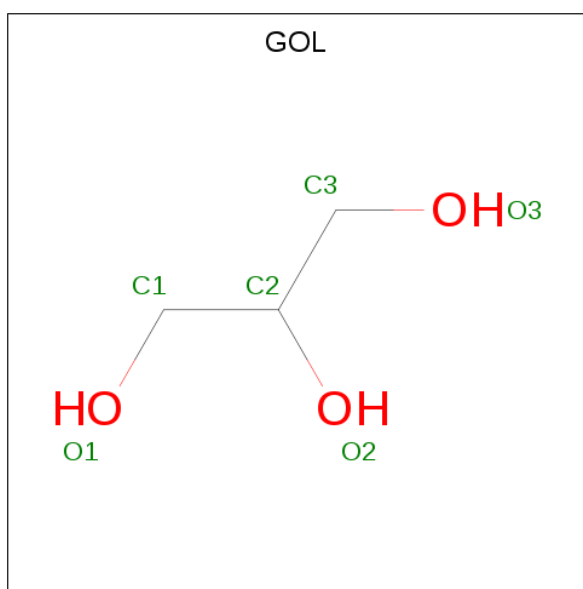
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q93NW7
A	-19	GLY	-	EXPRESSION TAG	UNP Q93NW7
A	-18	SER	-	EXPRESSION TAG	UNP Q93NW7
A	-17	SER	-	EXPRESSION TAG	UNP Q93NW7
A	-16	HIS	-	EXPRESSION TAG	UNP Q93NW7
A	-15	HIS	-	EXPRESSION TAG	UNP Q93NW7
A	-14	HIS	-	EXPRESSION TAG	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: $C_3H_8O_3$).



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

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 0.211 , 0.240	Depositor DCC
R_{free} test set	7468 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.063 for h,-k,h-l	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.

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

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 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	3426	0	3389	63	0
1	B	3426	0	3389	60	0
2	B	6	0	8	0	0
3	A	248	0	0	11	0
3	B	264	0	0	10	0
All	All	7370	0	6786	122	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 9.

All (122) 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:A:208:VAL:HG23	1:A:211:SER:OG	1.44	1.18
1:A:448:MET:HG3	3:A:642:HOH:O	1.55	1.05
1:B:208:VAL:HG23	1:B:211:SER:OG	1.57	1.04
1:B:39:THR:HB	3:B:569:HOH:O	1.67	0.93
1:B:448:MET:HG3	3:B:669:HOH:O	1.68	0.93
1:A:23:ARG:NH1	1:A:73:GLU:HB3	1.91	0.86
1:A:237:ARG:HD2	1:A:425:LEU:HD13	1.59	0.85
1:A:139:VAL:HG22	3:A:577:HOH:O	1.76	0.84
1:A:265:GLU:HG2	3:A:684:HOH:O	1.79	0.82
1:A:208:VAL:HG23	1:A:211:SER:HG	1.42	0.81
1:B:23:ARG:NH1	1:B:73:GLU:HB3	1.99	0.78
1:B:70:ARG:O	1:B:71:GLU:CB	2.29	0.76
1:B:208:VAL:HG23	1:B:211:SER:HG	1.48	0.75
1:B:41:VAL:CG2	1:B:164:LEU:HD11	2.16	0.75
1:B:139:VAL:HG22	3:B:574:HOH:O	1.87	0.75
1:B:391:VAL:HG21	1:B:428:LEU:HD13	1.69	0.74
1:B:70:ARG:O	1:B:71:GLU:HB3	1.88	0.71
1:A:245:HIS:HE1	1:A:274:THR:OG1	1.74	0.71
1:A:70:ARG:HH11	1:A:75:GLU:HA	1.57	0.70
1:A:24:LEU:HD23	3:A:654:HOH:O	1.93	0.69
1:A:472:LEU:O	1:A:473:SER:HB2	1.93	0.69
1:B:346:LEU:HD13	3:B:642:HOH:O	1.93	0.68
1:B:245:HIS:HE1	1:B:274:THR:OG1	1.76	0.67
1:B:59:ARG:HB2	1:B:105:LEU:HD22	1.77	0.67
1:B:420:GLU:HG3	3:B:656:HOH:O	1.96	0.66
1:A:59:ARG:HB2	1:A:105:LEU:HD22	1.77	0.65
1:A:23:ARG:HH12	1:A:73:GLU:HB3	1.61	0.65
1:B:41:VAL:HG21	1:B:164:LEU:HD11	1.76	0.65
1:B:84:ALA:HB2	1:B:143:LEU:CD1	2.27	0.64
1:A:41:VAL:CG2	1:A:164:LEU:HD11	2.27	0.63
1:B:208:VAL:CG2	1:B:211:SER:OG	2.40	0.63
1:A:82:LEU:N	1:A:82:LEU:HD12	2.13	0.62
1:B:344:LEU:HB2	1:B:346:LEU:HD11	1.81	0.62
1:A:208:VAL:CG2	1:A:211:SER:OG	2.37	0.62
1:B:344:LEU:HB2	1:B:346:LEU:CD1	2.30	0.62
1:B:166:GLU:HB3	3:B:639:HOH:O	1.98	0.61
1:A:344:LEU:HB2	1:A:346:LEU:CD1	2.31	0.61
1:B:391:VAL:HG21	1:B:428:LEU:CD1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:LEU:HD23	1:B:300:THR:N	2.17	0.60
1:B:24:LEU:N	1:B:24:LEU:HD22	2.17	0.60
1:A:24:LEU:HD22	1:A:24:LEU:N	2.19	0.58
1:B:24:LEU:HD23	3:B:562:HOH:O	2.04	0.58
1:A:208:VAL:HG23	1:A:211:SER:CB	2.34	0.57
1:A:84:ALA:HB2	1:A:143:LEU:CD1	2.35	0.56
1:B:69:LEU:O	1:B:73:GLU:HG2	2.05	0.56
1:A:59:ARG:HB2	1:A:105:LEU:CD2	2.35	0.56
1:B:71:GLU:CG	1:B:72:ASP:N	2.68	0.56
1:B:77:HIS:HE1	1:B:180:LEU:O	1.89	0.55
1:B:84:ALA:HB2	1:B:143:LEU:HD13	1.88	0.55
1:A:69:LEU:O	1:A:73:GLU:HG2	2.06	0.55
1:A:391:VAL:HG22	1:A:431:MET:SD	2.47	0.54
1:A:237:ARG:CD	1:A:425:LEU:HD13	2.36	0.53
1:A:237:ARG:CD	1:A:425:LEU:HB3	2.38	0.53
1:B:71:GLU:HG3	1:B:72:ASP:N	2.22	0.53
1:A:344:LEU:HB2	1:A:346:LEU:HD12	1.90	0.52
1:B:140:GLN:O	1:B:143:LEU:HB2	2.09	0.52
1:A:70:ARG:HD2	1:A:115:LEU:HG	1.91	0.52
1:B:407:VAL:O	1:B:411:LEU:HD23	2.10	0.52
1:B:37:TRP:CE3	1:B:164:LEU:HD12	2.45	0.52
1:B:382:ARG:HD3	1:B:388:ALA:O	2.09	0.51
1:A:51:ARG:NH2	3:A:605:HOH:O	2.33	0.51
1:A:265:GLU:CG	3:A:684:HOH:O	2.45	0.51
1:B:472:LEU:O	1:B:473:SER:HB2	2.11	0.50
1:A:391:VAL:HG21	1:A:428:LEU:HD13	1.92	0.50
1:B:422:GLU:CG	3:B:656:HOH:O	2.59	0.50
1:B:84:ALA:CB	1:B:143:LEU:CD1	2.90	0.49
1:B:135:LEU:O	1:B:380:HIS:HD2	1.95	0.49
1:A:41:VAL:HG21	1:A:164:LEU:HD11	1.94	0.49
1:A:448:MET:CG	3:A:642:HOH:O	2.31	0.49
1:A:135:LEU:O	1:A:380:HIS:HD2	1.95	0.49
1:A:53:GLU:OE1	1:A:55:LYS:NZ	2.43	0.49
1:B:138:PRO:HB2	1:B:373:TYR:CE1	2.48	0.49
1:B:23:ARG:HH12	1:B:73:GLU:HB3	1.73	0.49
1:B:82:LEU:HD12	1:B:82:LEU:N	2.28	0.49
1:A:77:HIS:HE1	1:A:180:LEU:O	1.96	0.48
1:B:286:LEU:HD23	1:B:340:LEU:HD12	1.95	0.48
1:B:71:GLU:CG	1:B:72:ASP:H	2.26	0.48
1:A:236:ARG:NH2	3:A:684:HOH:O	2.21	0.47
1:A:220:SER:OG	1:A:245:HIS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:GLU:HG3	3:B:656:HOH:O	2.15	0.47
1:B:39:THR:CB	3:B:569:HOH:O	2.42	0.47
1:A:391:VAL:HG21	1:A:428:LEU:CD1	2.45	0.47
1:B:8:GLU:HG3	1:B:200:ARG:HB2	1.96	0.47
1:B:19:ARG:HG3	1:B:20:PRO:HD2	1.97	0.47
1:B:346:LEU:HD12	1:B:346:LEU:N	2.29	0.47
1:B:70:ARG:O	1:B:71:GLU:CG	2.63	0.47
1:A:32:HIS:HD2	3:A:676:HOH:O	1.97	0.46
1:A:341:THR:HB	1:A:346:LEU:HD11	1.98	0.46
1:B:70:ARG:O	1:B:71:GLU:HG2	2.14	0.46
1:A:0:MET:SD	1:A:426:GLY:HA3	2.56	0.46
1:A:346:LEU:HD13	3:A:655:HOH:O	2.15	0.46
1:B:299:LEU:CD2	1:B:299:LEU:C	2.84	0.45
1:A:382:ARG:HD3	1:A:388:ALA:O	2.15	0.45
1:B:208:VAL:HG23	1:B:208:VAL:O	2.16	0.45
1:A:138:PRO:HB2	1:A:373:TYR:CE1	2.52	0.45
1:B:24:LEU:N	1:B:24:LEU:CD2	2.80	0.45
1:A:344:LEU:HB2	1:A:346:LEU:HD11	1.99	0.44
1:A:398:GLU:HG3	1:A:398:GLU:H	1.46	0.44
1:A:188:GLN:OE1	1:A:199:ARG:HD3	2.17	0.44
1:A:19:ARG:HD3	3:A:718:HOH:O	2.17	0.44
1:A:70:ARG:HG3	1:A:70:ARG:O	2.18	0.43
1:A:262:LEU:HD22	1:A:266:LEU:HD13	2.00	0.43
1:A:209:PRO:HD2	1:B:13:ALA:HB2	1.99	0.43
1:B:391:VAL:HG22	1:B:431:MET:SD	2.58	0.43
1:A:84:ALA:HB2	1:A:143:LEU:HD13	1.99	0.43
1:A:8:GLU:HG3	1:A:200:ARG:HB2	2.01	0.43
1:A:457:ARG:HD2	1:A:457:ARG:HH11	1.70	0.43
1:A:237:ARG:HD2	1:A:425:LEU:CD1	2.41	0.43
1:A:24:LEU:N	1:A:24:LEU:CD2	2.82	0.43
1:B:28:ILE:CG2	1:B:33:ALA:HB2	2.49	0.42
1:A:237:ARG:HD2	1:A:425:LEU:HB3	2.01	0.42
1:B:105:LEU:HD23	1:B:108:GLN:OE1	2.20	0.42
1:A:70:ARG:HH11	1:A:75:GLU:CA	2.29	0.42
1:A:84:ALA:CB	1:A:143:LEU:CD1	2.97	0.42
1:A:330:LYS:HD2	1:A:374:LEU:HD11	2.02	0.42
1:A:335:ARG:HH21	1:A:335:ARG:HD3	1.55	0.41
1:A:286:LEU:HD23	1:A:340:LEU:HD12	2.02	0.41
1:A:40:ALA:HB1	1:A:168:VAL:HB	2.03	0.41
1:B:3:LEU:O	1:B:441:ILE:HA	2.22	0.40
1:B:299:LEU:C	1:B:299:LEU:HD23	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:VAL:CG2	1:B:164:LEU:CD1	2.94	0.40
1:B:30:PRO:HG3	1:B:55:LYS:HG2	2.03	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	466/496 (94%)	454 (97%)	11 (2%)	1 (0%)	47	23
1	B	466/496 (94%)	454 (97%)	9 (2%)	3 (1%)	25	7
All	All	932/992 (94%)	908 (97%)	20 (2%)	4 (0%)	34	13

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 [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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	330/351 (94%)	316 (96%)	14 (4%)	30	5
1	B	330/351 (94%)	317 (96%)	13 (4%)	32	6
All	All	660/702 (94%)	633 (96%)	27 (4%)	30	5

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
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. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	77	HIS
1	A	102	GLN
1	A	241	GLN
1	A	245	HIS
1	A	380	HIS
1	A	434	ASN
1	B	32	HIS
1	B	77	HIS
1	B	102	GLN
1	B	241	GLN
1	B	245	HIS
1	B	380	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	0.88	0	5,5,5	0.96	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	-

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.

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, 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%)	0.62	41 (8%)	10 10	11, 20, 40, 56	0
1	B	470/496 (94%)	0.61	40 (8%)	10 11	11, 20, 40, 56	0
All	All	940/992 (94%)	0.61	81 (8%)	10 11	11, 20, 40, 56	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	407	VAL	6.3
1	B	397	GLY	5.4
1	A	131	ARG	5.3
1	A	209	PRO	4.8
1	A	212	GLY	4.8
1	B	131	ARG	4.8
1	B	398	GLU	4.6
1	A	295	GLU	4.6
1	A	398	GLU	4.5
1	B	407	VAL	4.1
1	A	406	GLU	4.0
1	A	473	SER	4.0
1	B	473	SER	4.0
1	B	405	PRO	4.0
1	A	-1	HIS	3.9
1	B	406	GLU	3.9
1	A	397	GLY	3.8
1	B	396	TRP	3.8
1	B	258	GLY	3.7
1	A	213	LYS	3.5
1	B	342	ALA	3.5
1	A	294	PRO	3.5
1	A	405	PRO	3.4
1	B	310	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	310	HIS	3.3
1	A	261	GLU	3.2
1	B	448	MET	3.2
1	A	211	SER	3.1
1	A	217	VAL	3.1
1	B	21	ALA	3.1
1	B	71	GLU	3.0
1	A	296	ASP	3.0
1	B	413	ARG	3.0
1	B	227	THR	3.0
1	A	343	ASP	3.0
1	B	261	GLU	3.0
1	B	166	GLU	2.9
1	B	251	ARG	2.9
1	B	62	TRP	2.9
1	A	342	ALA	2.8
1	A	472	LEU	2.7
1	A	265	GLU	2.7
1	B	410	ARG	2.7
1	A	308	VAL	2.7
1	B	72	ASP	2.7
1	B	422	GLU	2.7
1	A	307	GLY	2.7
1	A	422	GLU	2.7
1	B	-1	HIS	2.7
1	A	251	ARG	2.6
1	A	309	ALA	2.6
1	B	295	GLU	2.6
1	B	256	ALA	2.6
1	A	208	VAL	2.6
1	A	72	ASP	2.6
1	A	411	LEU	2.5
1	A	413	ARG	2.5
1	B	309	ALA	2.5
1	B	58	ASP	2.4
1	A	210	GLY	2.4
1	A	410	ARG	2.4
1	B	411	LEU	2.4
1	A	448	MET	2.4
1	A	408	HIS	2.4
1	B	257	PRO	2.3
1	A	21	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	255	ASP	2.3
1	B	265	GLU	2.3
1	B	213	LYS	2.2
1	B	161	LEU	2.2
1	A	67	ALA	2.1
1	B	307	GLY	2.1
1	A	216	PRO	2.1
1	B	180	LEU	2.1
1	A	215	PRO	2.1
1	A	11	ARG	2.0
1	B	308	VAL	2.0
1	B	409	ASP	2.0
1	A	166	GLU	2.0
1	B	19	ARG	2.0
1	B	262	LEU	2.0

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 [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. 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(\AA^2)	Q<0.9
2	GOL	B	476	6/6	0.95	0.08	21,23,26,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.