



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:09 AM UTC

PDB ID : 3MJC / pdb_00003mjc
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

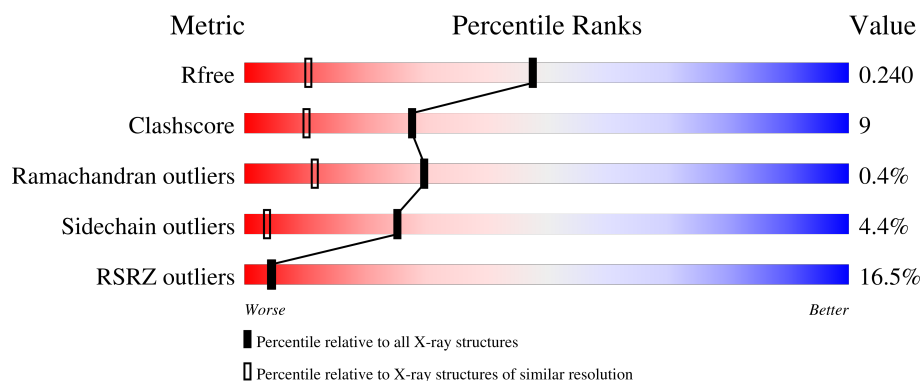
1 Overall quality at a glance

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}	180053	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (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 of 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	15% 70% 22% 5%
1	B	496	16% 73% 18% 5%

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:

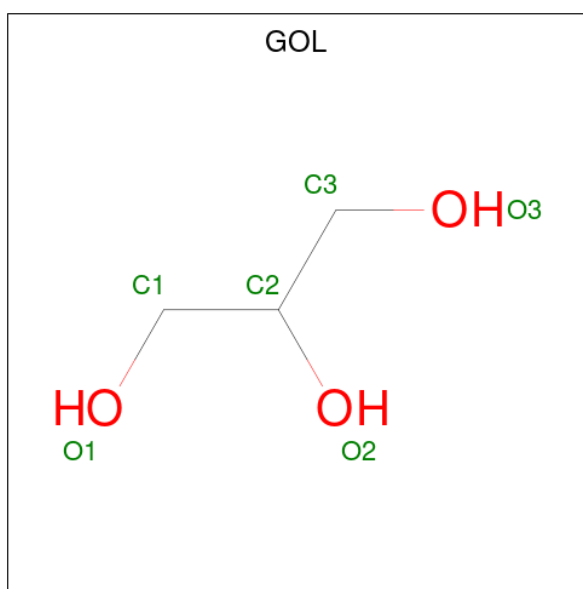
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q93NW7
A	-19	GLY	-	expression tag	UNP Q93NW7
A	-18	SER	-	expression tag	UNP Q93NW7
A	-17	SER	-	expression tag	UNP Q93NW7
A	-16	HIS	-	expression tag	UNP Q93NW7
A	-15	HIS	-	expression tag	UNP Q93NW7
A	-14	HIS	-	expression tag	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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

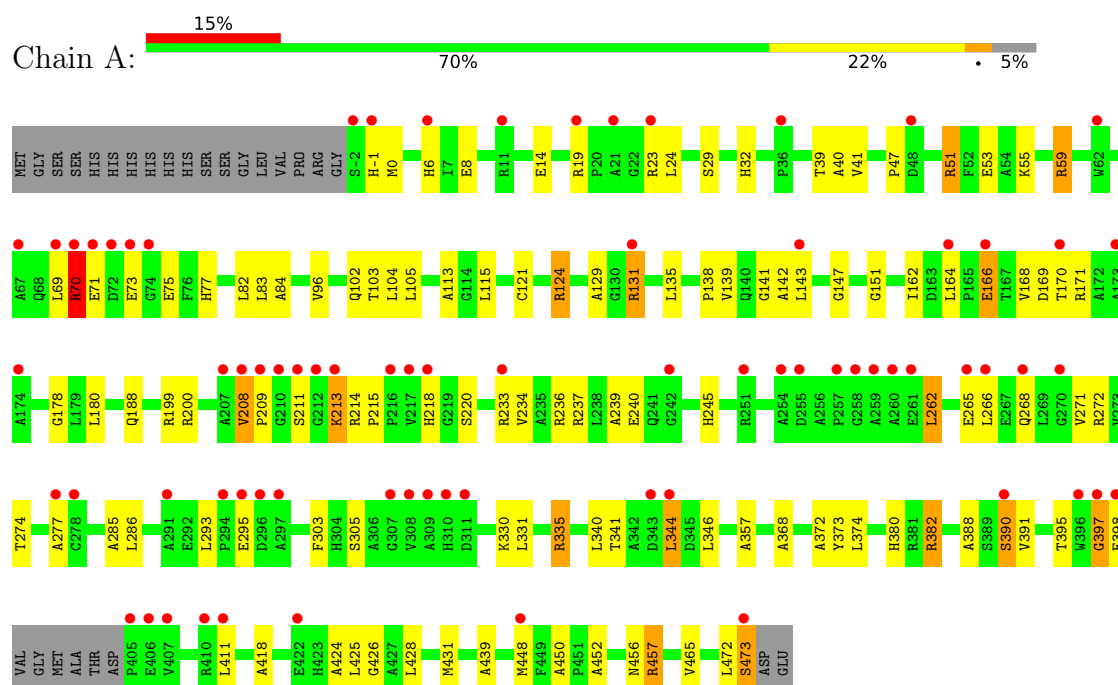
- Molecule 3 is water.

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

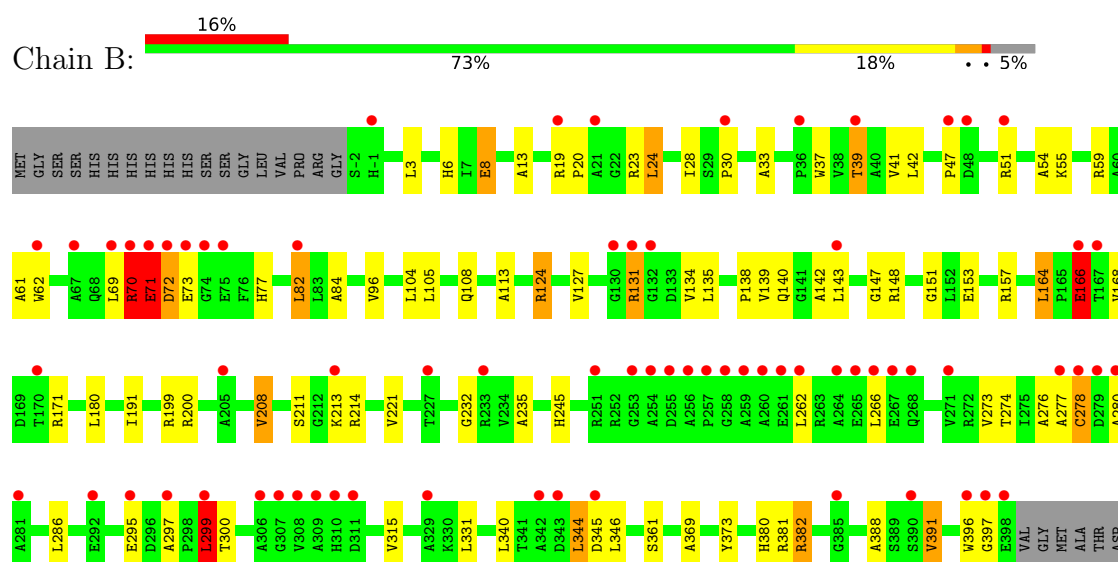
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: AmphB



• Molecule 1: AmphB





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 62.55 – 1.48	Depositor EDS
% Data completeness (in resolution range)	95.2 (62.55-1.48) 94.3 (62.55-1.48)	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 (4.74%)	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)	0.37 , 34.8	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 [i](#)

5.1 Standard geometry [i](#)

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	1.78	48/3495 (1.4%)	1.57	35/4772 (0.7%)
1	B	1.74	44/3495 (1.3%)	1.60	39/4772 (0.8%)
All	All	1.76	92/6990 (1.3%)	1.59	74/9544 (0.8%)

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	ARG	CZ-NH1	12.73	1.50	1.32
1	B	51	ARG	CZ-NH1	12.68	1.50	1.32
1	A	240	GLU	CB-CG	-9.19	1.24	1.52
1	B	51	ARG	CZ-NH2	9.01	1.45	1.33
1	A	96	VAL	N-CA	8.54	1.54	1.46
1	A	131	ARG	C-O	-8.42	1.13	1.24
1	A	103	THR	CA-CB	-8.33	1.40	1.53
1	A	208	VAL	CA-C	8.21	1.61	1.52
1	B	39	THR	CB-CG2	-7.79	1.26	1.52
1	A	450	ALA	CA-CB	7.63	1.62	1.53
1	B	39	THR	CB-OG1	-7.33	1.32	1.43
1	A	113	ALA	CA-CB	7.24	1.66	1.53
1	B	369	ALA	CA-CB	-7.10	1.42	1.53
1	A	51	ARG	CZ-NH2	7.05	1.42	1.33
1	B	142	ALA	CA-CB	7.04	1.64	1.53
1	B	452	ALA	CA-CB	-6.80	1.42	1.53
1	A	240	GLU	CA-CB	-6.65	1.42	1.53
1	A	6	HIS	CA-CB	-6.49	1.41	1.54
1	A	452	ALA	CA-CB	-6.45	1.43	1.53
1	B	70	ARG	C-O	-6.37	1.15	1.23
1	B	127	VAL	N-CA	6.33	1.53	1.46
1	B	131	ARG	C-O	-6.33	1.16	1.24
1	B	113	ALA	CA-C	-6.33	1.44	1.52
1	A	169	ASP	C-O	6.32	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	ARG	C-O	-6.31	1.15	1.24
1	A	178	GLY	N-CA	6.24	1.53	1.45
1	B	315	VAL	C-O	-6.23	1.16	1.24
1	B	54	ALA	CA-CB	6.17	1.60	1.52
1	B	104	LEU	C-O	-6.17	1.17	1.24
1	B	191	ILE	CA-C	6.08	1.60	1.52
1	A	439	ALA	CA-C	-6.03	1.45	1.52
1	A	465	VAL	N-CA	-6.00	1.41	1.46
1	B	8	GLU	CB-CG	-5.92	1.34	1.52
1	A	234	VAL	CA-CB	5.91	1.61	1.54
1	B	235	ALA	CA-CB	5.91	1.62	1.53
1	B	280	ALA	C-O	5.90	1.31	1.24
1	B	96	VAL	CA-CB	-5.88	1.48	1.53
1	A	424	ALA	N-CA	5.88	1.53	1.46
1	B	151	GLY	N-CA	5.87	1.53	1.45
1	A	305	SER	C-O	5.75	1.31	1.24
1	B	299	LEU	CG-CD2	-5.74	1.33	1.52
1	B	273	VAL	CA-C	-5.73	1.45	1.52
1	A	166	GLU	CB-CG	-5.73	1.35	1.52
1	B	457	ARG	CB-CG	-5.72	1.35	1.52
1	B	344	LEU	C-N	-5.72	1.26	1.33
1	A	102	GLN	C-O	-5.71	1.16	1.24
1	B	164	LEU	CA-C	-5.67	1.45	1.52
1	B	221	VAL	CA-C	-5.66	1.45	1.52
1	A	142	ALA	CA-CB	5.63	1.62	1.53
1	A	303	PHE	N-CA	5.63	1.53	1.46
1	A	104	LEU	N-CA	5.62	1.53	1.46
1	A	151	GLY	CA-C	5.58	1.58	1.52
1	A	418	ALA	CA-CB	5.57	1.62	1.53
1	B	151	GLY	CA-C	5.57	1.58	1.52
1	B	168	VAL	CA-C	5.56	1.57	1.52
1	A	372	ALA	CA-CB	5.55	1.62	1.53
1	A	293	LEU	C-N	5.52	1.41	1.33
1	A	121	CYS	C-O	5.50	1.30	1.24
1	B	199	ARG	CZ-NH2	5.48	1.40	1.33
1	A	29	SER	C-O	-5.47	1.17	1.24
1	B	418	ALA	CA-CB	5.41	1.61	1.53
1	A	331	LEU	CA-CB	5.39	1.61	1.53
1	B	457	ARG	CA-C	5.38	1.57	1.52
1	A	147	GLY	CA-C	5.37	1.58	1.52
1	A	456	ASN	CB-CG	-5.35	1.38	1.52
1	B	42	LEU	N-CA	5.29	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	315	VAL	CA-CB	5.29	1.60	1.54
1	A	357	ALA	C-O	-5.28	1.17	1.24
1	A	277	ALA	CA-C	5.27	1.59	1.52
1	B	62	TRP	CA-C	-5.26	1.46	1.52
1	A	285	ALA	CA-CB	5.25	1.61	1.53
1	B	153	GLU	N-CA	5.24	1.52	1.46
1	B	381	ARG	CA-C	-5.24	1.45	1.52
1	B	361	SER	C-O	5.22	1.29	1.23
1	A	124	ARG	CB-CG	5.21	1.68	1.52
1	A	129	ALA	CA-CB	5.18	1.61	1.53
1	A	215	PRO	C-O	-5.18	1.18	1.24
1	A	83	LEU	CA-C	-5.14	1.45	1.52
1	A	344	LEU	C-N	-5.13	1.26	1.33
1	B	131	ARG	C-N	-5.12	1.26	1.33
1	A	39	THR	CA-CB	5.12	1.61	1.53
1	A	395	THR	CA-CB	5.12	1.60	1.53
1	B	331	LEU	CA-CB	5.09	1.61	1.53
1	B	147	GLY	CA-C	5.08	1.57	1.52
1	B	134	VAL	CA-CB	-5.08	1.48	1.54
1	A	162	ILE	CA-CB	5.07	1.60	1.54
1	A	14	GLU	CA-C	-5.07	1.47	1.53
1	A	293	LEU	N-CA	5.05	1.52	1.45
1	B	6	HIS	CA-CB	-5.04	1.45	1.53
1	B	134	VAL	C-O	5.04	1.29	1.24
1	B	297	ALA	N-CA	5.04	1.53	1.46
1	A	368	ALA	C-O	5.03	1.29	1.24

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	LEU	CA-C-N	-16.28	96.67	123.37
1	B	344	LEU	C-N-CA	-16.28	96.67	123.37
1	A	344	LEU	CA-C-N	-15.20	102.23	123.20
1	A	344	LEU	C-N-CA	-15.20	102.23	123.20
1	B	124	ARG	CG-CD-NE	-11.16	87.45	112.00
1	A	382	ARG	NE-CZ-NH1	11.09	132.59	121.50
1	B	382	ARG	NE-CZ-NH2	-10.54	109.72	119.20
1	B	382	ARG	CD-NE-CZ	10.38	138.94	124.40
1	B	382	ARG	NE-CZ-NH1	10.37	131.87	121.50
1	A	382	ARG	NE-CZ-NH2	-10.14	110.07	119.20
1	B	382	ARG	CB-CG-CD	10.11	134.55	111.30
1	A	382	ARG	CB-CG-CD	9.50	133.16	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	ARG	NE-CZ-NH2	-9.38	110.76	119.20
1	A	382	ARG	CD-NE-CZ	9.04	137.05	124.40
1	A	272	ARG	NE-CZ-NH2	8.94	127.25	119.20
1	B	70	ARG	N-CA-C	-8.73	99.01	110.53
1	B	51	ARG	NE-CZ-NH2	-8.40	111.64	119.20
1	A	141	GLY	O-C-N	-7.93	114.03	122.19
1	B	131	ARG	O-C-N	-7.91	113.92	122.07
1	A	293	LEU	N-CA-C	7.76	119.49	109.64
1	A	214	ARG	CA-C-N	-7.63	112.52	120.38
1	A	214	ARG	C-N-CA	-7.63	112.52	120.38
1	B	131	ARG	CA-C-N	-7.40	106.91	121.41
1	B	131	ARG	C-N-CA	-7.40	106.91	121.41
1	A	239	ALA	CA-C-N	-7.38	109.09	120.31
1	A	239	ALA	C-N-CA	-7.38	109.09	120.31
1	B	61	ALA	N-CA-C	6.92	118.47	111.07
1	A	240	GLU	N-CA-C	6.87	119.79	111.82
1	A	51	ARG	NH1-CZ-NH2	6.56	127.83	119.30
1	B	131	ARG	N-CA-C	6.35	117.86	111.07
1	A	213	LYS	N-CA-C	-6.31	105.90	113.97
1	A	233	ARG	CG-CD-NE	-6.30	98.14	112.00
1	B	166	GLU	N-CA-CB	-6.29	100.87	110.12
1	B	208	VAL	CA-C-N	-6.29	113.80	120.03
1	B	208	VAL	C-N-CA	-6.29	113.80	120.03
1	B	391	VAL	CG1-CB-CG2	6.21	124.45	110.80
1	B	51	ARG	NH1-CZ-NH2	6.18	127.34	119.30
1	B	344	LEU	O-C-N	-6.17	114.66	122.43
1	A	344	LEU	N-CA-C	-6.11	100.89	110.36
1	B	344	LEU	N-CA-C	-6.05	101.03	110.17
1	B	142	ALA	CA-C-N	6.00	128.93	120.28
1	B	142	ALA	C-N-CA	6.00	128.93	120.28
1	A	271	VAL	N-CA-C	5.98	117.34	109.21
1	B	157	ARG	NE-CZ-NH1	-5.93	115.57	121.50
1	A	59	ARG	NE-CZ-NH2	5.92	124.53	119.20
1	A	372	ALA	CA-C-N	-5.90	112.37	120.28
1	A	372	ALA	C-N-CA	-5.90	112.37	120.28
1	B	278	CYS	N-CA-C	5.79	118.64	109.96
1	B	131	ARG	N-CA-CB	5.66	118.21	110.01
1	B	82	LEU	CD1-CG-CD2	-5.66	98.36	110.80
1	B	142	ALA	N-CA-C	5.59	118.14	111.71
1	A	390	SER	CA-CB-OG	-5.55	100.00	111.10
1	B	148	ARG	NE-CZ-NH2	-5.48	114.27	119.20
1	A	272	ARG	CB-CG-CD	5.40	123.73	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	GLY	N-CA-C	5.33	119.12	112.73
1	B	47	PRO	CB-CA-C	5.30	119.05	111.04
1	A	141	GLY	CA-C-O	5.27	125.83	120.45
1	A	39	THR	CA-CB-OG1	-5.25	101.72	109.60
1	B	51	ARG	CB-CG-CD	5.24	123.36	111.30
1	A	-1	HIS	CB-CA-C	5.24	119.49	110.79
1	A	47	PRO	CB-CA-C	5.21	118.91	111.04
1	B	62	TRP	N-CA-C	5.21	116.96	111.28
1	B	199	ARG	NE-CZ-NH1	5.18	126.68	121.50
1	A	218	HIS	N-CA-C	5.12	115.10	107.88
1	A	277	ALA	CA-C-N	5.12	128.12	120.95
1	A	277	ALA	C-N-CA	5.12	128.12	120.95
1	B	166	GLU	CA-C-N	-5.12	115.78	123.00
1	B	166	GLU	C-N-CA	-5.12	115.78	123.00
1	A	170	THR	CB-CA-C	5.07	120.41	110.67
1	A	457	ARG	CA-C-N	-5.07	115.35	120.31
1	A	457	ARG	C-N-CA	-5.07	115.35	120.31
1	B	396	TRP	N-CA-C	5.05	117.84	109.46
1	B	214	ARG	CA-C-N	-5.01	115.22	120.38
1	B	214	ARG	C-N-CA	-5.01	115.22	120.38

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	64	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	123	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 (123) 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: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: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:HD12	1:A:82:LEU:N	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
1:B:299:LEU:HD23	1:B:300:THR:N	2.17	0.60
1:B:24:LEU:HD22	1:B:24:LEU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:53:GLU:OE1	1:A:55:LYS:NZ	2.43	0.51
1:A:51:ARG:NH2	3:A:605:HOH:O	2.33	0.51
1:B:299:LEU:C	1:B:299:LEU:CD2	2.84	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: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:71:GLU:CG	1:B:72:ASP:H	2.26	0.48
1:B:286:LEU:HD23	1:B:340:LEU:HD12	1.95	0.48
1:A:220:SER:OG	1:A:245:HIS:HD2	1.97	0.47
1:A:236:ARG:NH2	3:A:684:HOH:O	2.21	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:299:LEU:HD23	1:B:299:LEU:C	2.41	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:A:208:VAL:HG23	1:A:211:SER:HG	1.73	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:H	1:A:398:GLU:HG3	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:O	1:A:70:ARG:HG3	2.18	0.43
1:A:209:PRO:HD2	1:B:13:ALA:HB2	1.99	0.43
1:A:262:LEU:HD22	1:A:266:LEU:HD13	2.00	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:HH11	1:A:457:ARG:HD2	1.70	0.43
1:A:24:LEU:N	1:A:24:LEU:CD2	2.82	0.43
1:A:237:ARG:HD2	1:A:425:LEU:CD1	2.41	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:397:GLY:O	1:A:398:GLU:C	2.63	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:276:ALA:C	1:B:278:CYS:H	2.29	0.40
1:B:41:VAL:CG2	1:B:164:LEU:CD1	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	43	22
1	B	466/496 (94%)	454 (97%)	9 (2%)	3 (1%)	21	6
All	All	932/992 (94%)	908 (97%)	20 (2%)	4 (0%)	30	11

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	330/351 (94%)	316 (96%)	14 (4%)	26	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	330/351 (94%)	315 (96%)	15 (4%)	24	3
All	All	660/702 (94%)	631 (96%)	29 (4%)	25	4

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	213	LYS
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	24	LEU
1	B	70	ARG
1	B	71	GLU
1	B	72	ASP
1	B	124	ARG
1	B	131	ARG
1	B	166	GLU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	65	GLN

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Mol	Chain	Res	Type
1	A	68	GLN
1	A	77	HIS
1	A	241	GLN
1	A	245	HIS
1	A	380	HIS
1	A	408	HIS
1	B	32	HIS
1	B	65	GLN
1	B	77	HIS
1	B	241	GLN
1	B	245	HIS
1	B	380	HIS
1	B	408	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 oligosaccharides 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	0.92	0	5,5,5	1.04	1 (20%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	476	GOL	O1-C1-C2	-2.08	101.03	110.38

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%)	0.97	74 (15%) 5 5	11, 20, 40, 56	0
1	B	470/496 (94%)	0.95	81 (17%) 4 4	11, 20, 40, 56	0
All	All	940/992 (94%)	0.96	155 (16%) 4 4	11, 20, 40, 56	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	PRO	5.7
1	A	407	VAL	5.2
1	B	397	GLY	5.0
1	B	396	TRP	4.9
1	B	278	CYS	4.8
1	B	74	GLY	4.8
1	A	294	PRO	4.7
1	B	131	ARG	4.7
1	A	295	GLU	4.5
1	A	397	GLY	4.5
1	A	277	ALA	4.4
1	A	308	VAL	4.3
1	B	407	VAL	4.2
1	A	72	ASP	4.1
1	A	307	GLY	4.1
1	B	277	ALA	4.1
1	A	473	SER	4.1
1	A	309	ALA	4.0
1	B	67	ALA	4.0
1	B	473	SER	3.9
1	A	131	ARG	3.9
1	B	342	ALA	3.9
1	A	278	CYS	3.9
1	A	211	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	212	GLY	3.8
1	B	307	GLY	3.8
1	B	257	PRO	3.8
1	A	74	GLY	3.7
1	B	308	VAL	3.7
1	B	71	GLU	3.7
1	A	210	GLY	3.7
1	A	208	VAL	3.6
1	B	72	ASP	3.6
1	B	166	GLU	3.6
1	A	213	LYS	3.6
1	B	422	GLU	3.6
1	A	70	ARG	3.6
1	B	406	GLU	3.5
1	A	448	MET	3.5
1	B	448	MET	3.5
1	A	265	GLU	3.5
1	A	406	GLU	3.5
1	A	398	GLU	3.5
1	B	343	ASP	3.4
1	A	-1	HIS	3.4
1	A	411	LEU	3.4
1	A	255	ASP	3.4
1	A	422	GLU	3.3
1	A	217	VAL	3.3
1	B	73	GLU	3.3
1	A	343	ASP	3.2
1	B	62	TRP	3.2
1	B	309	ALA	3.2
1	B	411	LEU	3.2
1	A	257	PRO	3.2
1	A	261	GLU	3.1
1	B	255	ASP	3.1
1	B	21	ALA	3.1
1	B	261	GLU	3.1
1	B	-1	HIS	3.0
1	A	143	LEU	3.0
1	A	296	ASP	3.0
1	B	251	ARG	3.0
1	B	143	LEU	3.0
1	A	390	SER	3.0
1	A	207	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	19	ARG	2.9
1	B	70	ARG	2.9
1	B	398	GLU	2.9
1	A	36	PRO	2.9
1	A	310	HIS	2.9
1	B	258	GLY	2.9
1	B	260	ALA	2.8
1	B	233	ARG	2.8
1	A	260	ALA	2.8
1	A	410	ARG	2.7
1	B	310	HIS	2.7
1	B	405	PRO	2.7
1	B	256	ALA	2.7
1	B	299	LEU	2.7
1	A	73	GLU	2.7
1	A	21	ALA	2.7
1	B	132	GLY	2.7
1	A	48	ASP	2.7
1	A	67	ALA	2.6
1	B	390	SER	2.6
1	A	297	ALA	2.6
1	B	205	ALA	2.6
1	B	329	ALA	2.6
1	B	259	ALA	2.6
1	A	251	ARG	2.6
1	A	-2	SER	2.6
1	B	82	LEU	2.6
1	A	170	THR	2.5
1	A	174	ALA	2.5
1	A	233	ARG	2.5
1	B	271	VAL	2.5
1	A	71	GLU	2.5
1	A	166	GLU	2.5
1	B	267	GLU	2.5
1	B	292	GLU	2.5
1	A	311	ASP	2.5
1	B	48	ASP	2.5
1	B	69	LEU	2.5
1	B	264	ALA	2.4
1	A	19	ARG	2.4
1	B	36	PRO	2.4
1	A	396	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	39	THR	2.4
1	B	306	ALA	2.4
1	B	213	LYS	2.4
1	B	385	GLY	2.4
1	B	262	LEU	2.4
1	B	295	GLU	2.4
1	B	170	THR	2.4
1	B	410	ARG	2.4
1	A	405	PRO	2.4
1	B	30	PRO	2.4
1	B	413	ARG	2.4
1	A	242	GLY	2.4
1	B	75	GLU	2.4
1	B	47	PRO	2.3
1	A	173	ALA	2.3
1	B	167	THR	2.3
1	A	270	GLY	2.3
1	B	311	ASP	2.3
1	A	259	ALA	2.3
1	A	6	HIS	2.3
1	A	23	ARG	2.2
1	B	227	THR	2.2
1	B	253	GLY	2.2
1	B	51	ARG	2.2
1	B	279	ASP	2.2
1	A	216	PRO	2.2
1	A	11	ARG	2.2
1	A	344	LEU	2.2
1	A	291	ALA	2.1
1	B	280	ALA	2.1
1	B	130	GLY	2.1
1	A	164	LEU	2.1
1	B	254	ALA	2.1
1	B	266	LEU	2.1
1	B	268	GLN	2.1
1	B	281	ALA	2.1
1	B	265	GLU	2.1
1	A	258	GLY	2.1
1	A	69	LEU	2.1
1	A	266	LEU	2.1
1	A	268	GLN	2.1
1	B	297	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	470	SER	2.0
1	B	345	ASP	2.0
1	A	62	TRP	2.0
1	A	218	HIS	2.0
1	A	254	ALA	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	GOL	B	476	6/6	0.96	0.06	21,23,26,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.