



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:19 PM UTC

PDB ID : 1RD5 / pdb_00001rd5
Title : Crystal structure of Tryptophan synthase alpha chain homolog BX1: a member of the chemical plant defense system
Authors : Kulik, V.; Hartmann, E.; Weyand, M.; Frey, M.; Gierl, A.; Niks, D.; Dunn, M.F.; Schlichting, I.
Deposited on : 2003-11-05
Resolution : 2.02 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

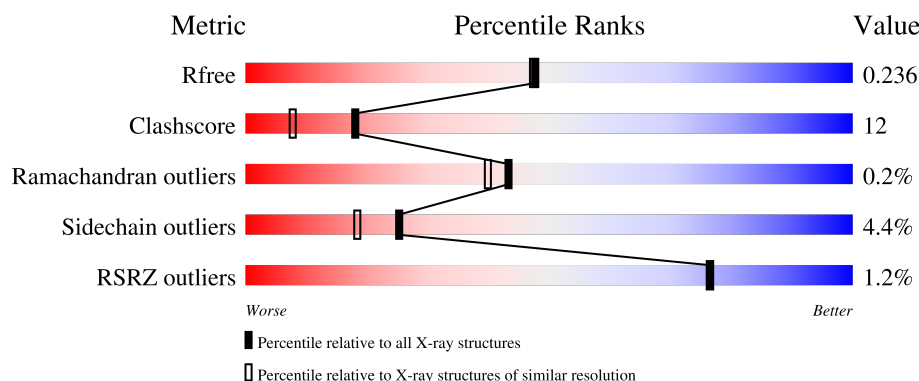
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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 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	262	
1	B	262	

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
2	MLA	A	302	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4092 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.

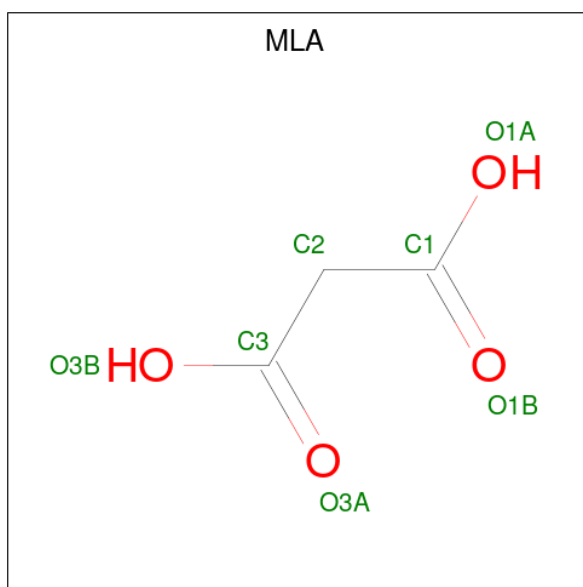
- Molecule 1 is a protein called Tryptophan synthase alpha chain, chloroplast.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	4	0
			1955	1237	338	368	12			
1	B	248	Total	C	N	O	S	0	4	0
			1875	1187	327	349	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P42390
A	108	PHE	SER	SEE REMARK 999	UNP P42390
A	113	LYS	GLU	SEE REMARK 999	UNP P42390
A	262	GLY	PRO	SEE REMARK 999	UNP P42390
B	1	MET	-	initiating methionine	UNP P42390
B	108	PHE	SER	SEE REMARK 999	UNP P42390
B	113	LYS	GLU	SEE REMARK 999	UNP P42390
B	262	GLY	PRO	SEE REMARK 999	UNP P42390

- Molecule 2 is MALONIC ACID (CCD ID: MLA) (formula: C₃H₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	3	4		
2	B	1	Total	C	O	0	0
			7	3	4		

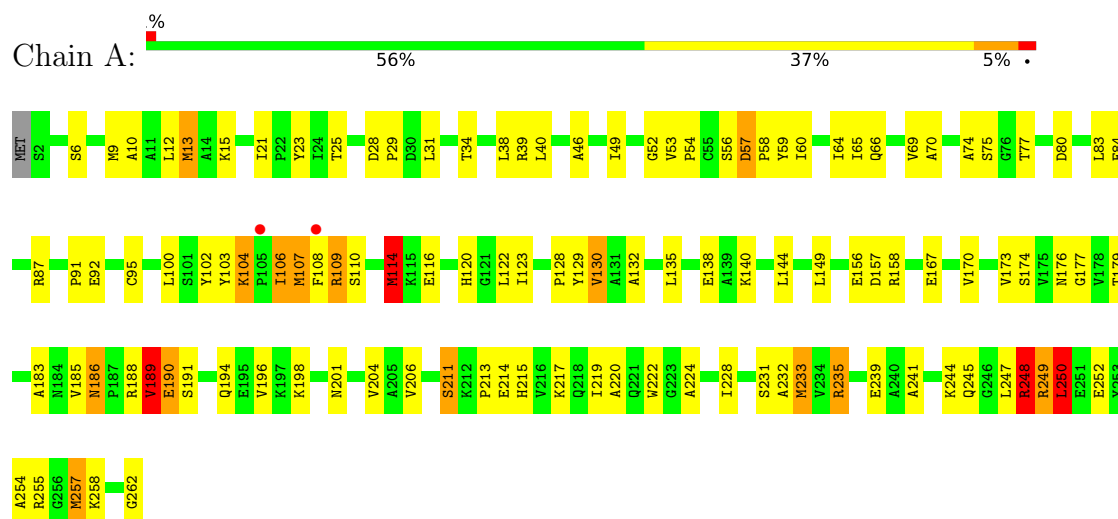
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	130	Total	O	0	0
			130	130		
3	B	118	Total	O	0	0
			118	118		

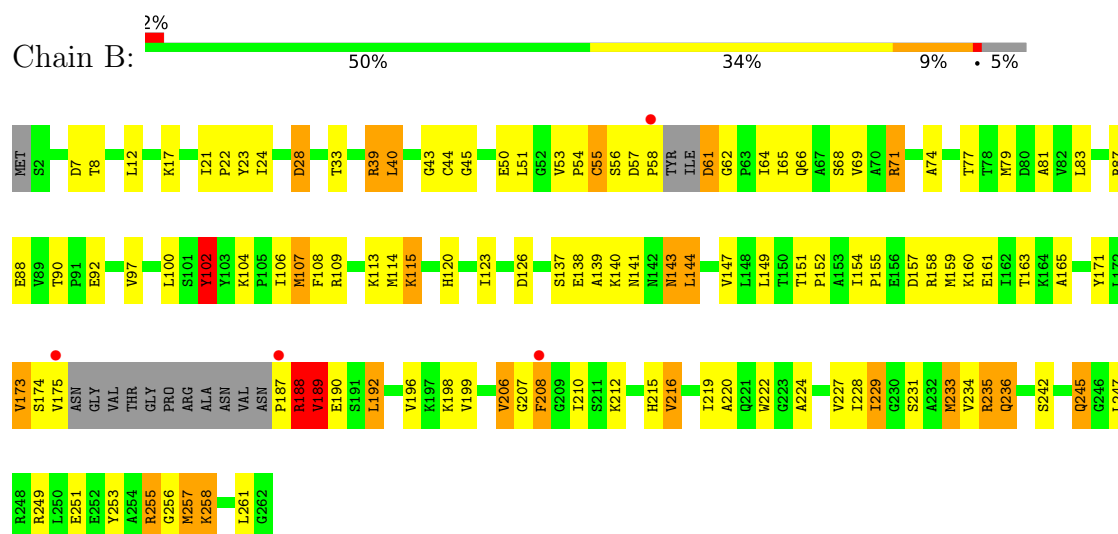
3 Residue-property plots [i](#)

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: Tryptophan synthase alpha chain, chloroplast



- Molecule 1: Tryptophan synthase alpha chain, chloroplast



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	91.09Å 159.81Å 162.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.02 25.00 – 2.02	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.02) 94.7 (25.00-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.245 , 0.299 0.180 , 0.236	Depositor DCC
R_{free} test set	1851 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4092	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 4.36% 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: MLA

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	2.46	91/2013 (4.5%)	1.75	32/2735 (1.2%)
1	B	2.41	97/1931 (5.0%)	1.84	41/2614 (1.6%)
All	All	2.44	188/3944 (4.8%)	1.79	73/5349 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	MET	SD-CE	-19.92	1.29	1.79
1	A	109	ARG	CA-CB	12.94	1.72	1.53
1	B	114	MET	SD-CE	-12.67	1.47	1.79
1	B	257	MET	SD-CE	-10.86	1.52	1.79
1	A	108	PHE	CA-CB	9.99	1.69	1.53
1	A	107	MET	SD-CE	9.97	2.04	1.79
1	B	107	MET	CG-SD	9.43	2.04	1.80
1	A	109	ARG	C-O	9.28	1.35	1.24
1	A	49	ILE	CA-CB	-8.82	1.43	1.54
1	A	177	GLY	CA-C	8.62	1.60	1.52
1	B	55	CYS	CA-C	8.49	1.63	1.52
1	A	132	ALA	CA-C	8.43	1.63	1.52
1	A	255	ARG	NE-CZ	8.15	1.42	1.33
1	A	220	ALA	CA-CB	8.14	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	LYS	N-CA	8.10	1.54	1.46
1	B	229	ILE	CA-CB	-8.08	1.43	1.53
1	A	106	ILE	CG1-CD1	-8.00	1.20	1.51
1	B	196	VAL	CA-CB	-7.99	1.44	1.54
1	B	155	PRO	C-O	7.88	1.33	1.23
1	A	104	LYS	CA-C	7.86	1.61	1.52
1	B	90	THR	CA-C	7.80	1.62	1.52
1	A	104	LYS	CA-CB	7.71	1.62	1.53
1	B	234	VAL	C-O	-7.61	1.15	1.24
1	A	196	VAL	CA-C	7.56	1.62	1.52
1	B	24	ILE	N-CA	7.53	1.54	1.46
1	B	206	VAL	N-CA	-7.48	1.37	1.46
1	A	77	THR	CA-C	7.41	1.62	1.52
1	B	90	THR	C-O	-7.22	1.17	1.24
1	B	198	LYS	CA-CB	7.19	1.64	1.53
1	A	170	VAL	CA-CB	7.17	1.63	1.54
1	B	74	ALA	C-O	-7.17	1.15	1.24
1	B	207	GLY	CA-C	-7.10	1.44	1.52
1	A	257	MET	SD-CE	-7.06	1.61	1.79
1	A	254	ALA	N-CA	-7.05	1.38	1.46
1	A	91	PRO	C-O	-7.02	1.15	1.24
1	A	60	ILE	CA-CB	7.02	1.63	1.54
1	B	161	GLU	C-O	7.01	1.32	1.24
1	B	7	ASP	C-O	-7.00	1.16	1.24
1	B	210	ILE	CA-C	6.97	1.60	1.52
1	B	102	TYR	CG-CD2	6.97	1.53	1.39
1	B	173	VAL	CB-CG1	-6.95	1.29	1.52
1	A	149	LEU	CG-CD2	-6.89	1.29	1.52
1	B	39	ARG	C-O	-6.88	1.16	1.24
1	B	106	ILE	CA-CB	6.88	1.63	1.54
1	B	33	THR	CA-CB	6.84	1.64	1.53
1	A	83	LEU	C-O	6.84	1.32	1.24
1	A	186	ASN	CA-C	6.83	1.60	1.52
1	A	249	ARG	NE-CZ	6.79	1.40	1.33
1	A	158	ARG	CD-NE	6.77	1.55	1.46
1	B	212	LYS	CA-C	6.77	1.60	1.52
1	A	206	VAL	CA-CB	-6.76	1.45	1.54
1	B	215	HIS	C-O	-6.74	1.15	1.24
1	B	104	LYS	C-O	-6.73	1.18	1.24
1	B	108	PHE	CA-C	6.72	1.61	1.52
1	B	28	ASP	C-O	6.70	1.32	1.24
1	A	258	LYS	CD-CE	6.68	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	VAL	CA-CB	-6.62	1.46	1.54
1	A	224	ALA	CA-CB	-6.62	1.42	1.53
1	A	70	ALA	CA-CB	6.62	1.63	1.53
1	B	21	ILE	CA-C	6.60	1.59	1.52
1	A	25	THR	CA-C	-6.56	1.44	1.52
1	A	224	ALA	CA-C	6.56	1.61	1.52
1	A	196	VAL	C-O	-6.55	1.16	1.24
1	B	58	PRO	CA-C	6.55	1.66	1.52
1	A	108	PHE	CA-C	6.49	1.61	1.52
1	A	247	LEU	CA-C	6.47	1.61	1.52
1	A	231	SER	CB-OG	6.45	1.55	1.42
1	A	140	LYS	CA-C	6.45	1.61	1.52
1	B	231	SER	N-CA	-6.44	1.38	1.46
1	A	65	ILE	C-O	-6.44	1.16	1.24
1	B	228	ILE	C-O	6.44	1.31	1.24
1	B	104	LYS	CG-CD	6.43	1.71	1.52
1	A	87	ARG	NE-CZ	6.43	1.40	1.33
1	B	107	MET	CB-CG	-6.43	1.33	1.52
1	B	229	ILE	CG1-CD1	-6.42	1.26	1.51
1	B	257	MET	CG-SD	6.35	1.96	1.80
1	A	46	ALA	CA-CB	-6.33	1.43	1.53
1	A	25	THR	CA-CB	6.28	1.62	1.53
1	A	194	GLN	CG-CD	6.26	1.67	1.52
1	B	51	LEU	C-O	6.26	1.30	1.24
1	A	233	MET	CG-SD	6.25	1.96	1.80
1	A	60	ILE	CA-C	6.21	1.60	1.52
1	B	12	LEU	C-O	-6.20	1.17	1.24
1	A	95	CYS	CA-C	6.18	1.61	1.52
1	B	53	VAL	C-N	-6.17	1.27	1.33
1	B	137	SER	CA-CB	6.16	1.63	1.53
1	A	109	ARG	CA-C	6.12	1.60	1.52
1	B	50	GLU	CA-CB	-6.07	1.44	1.53
1	B	174	SER	N-CA	6.07	1.53	1.46
1	B	64	ILE	CA-C	-6.06	1.45	1.52
1	B	165	ALA	CA-CB	6.00	1.63	1.53
1	B	154	ILE	C-O	-6.00	1.16	1.24
1	B	242	SER	N-CA	6.00	1.51	1.46
1	A	53	VAL	CA-C	-6.00	1.48	1.53
1	A	235[A]	ARG	CA-C	5.96	1.60	1.52
1	A	235[B]	ARG	CA-C	5.96	1.60	1.52
1	B	212	LYS	CE-NZ	5.95	1.67	1.49
1	B	62	GLY	C-O	-5.94	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	LYS	CD-CE	5.94	1.70	1.52
1	B	234	VAL	CA-C	-5.93	1.45	1.52
1	A	13	MET	CB-CG	-5.92	1.34	1.52
1	B	235[A]	ARG	N-CA	-5.92	1.39	1.46
1	B	235[B]	ARG	N-CA	-5.92	1.39	1.46
1	A	100	LEU	CA-CB	-5.91	1.45	1.53
1	B	207	GLY	C-O	-5.89	1.18	1.23
1	A	57	ASP	C-O	-5.88	1.17	1.24
1	A	123	ILE	C-O	5.87	1.30	1.24
1	B	196	VAL	CA-C	5.86	1.60	1.52
1	A	194	GLN	CA-C	5.85	1.60	1.52
1	B	109	ARG	CA-C	-5.85	1.45	1.53
1	B	160	LYS	CG-CD	5.85	1.70	1.52
1	A	130	VAL	CB-CG2	-5.81	1.33	1.52
1	A	248	ARG	NE-CZ	5.79	1.39	1.33
1	B	141	ASN	C-O	-5.75	1.16	1.24
1	B	219	ILE	CA-CB	-5.73	1.47	1.54
1	A	189	VAL	CA-CB	-5.73	1.46	1.54
1	A	241	ALA	CA-C	5.73	1.60	1.52
1	B	154	ILE	CA-C	-5.72	1.48	1.53
1	A	66	GLN	CA-C	5.70	1.60	1.52
1	B	227	VAL	CA-C	-5.69	1.45	1.52
1	A	138	GLU	CA-C	5.67	1.60	1.52
1	B	81	ALA	C-O	5.67	1.30	1.24
1	B	144	LEU	CA-CB	-5.67	1.45	1.53
1	A	176	ASN	C-O	5.64	1.30	1.23
1	A	252	GLU	N-CA	5.61	1.53	1.46
1	B	123	ILE	CA-CB	5.61	1.61	1.54
1	B	224	ALA	N-CA	-5.60	1.39	1.46
1	B	234	VAL	CA-CB	5.59	1.61	1.54
1	B	140	LYS	CA-C	5.59	1.59	1.52
1	A	92	GLU	C-O	-5.59	1.16	1.24
1	A	12	LEU	C-O	-5.58	1.17	1.24
1	A	190	GLU	CA-CB	5.56	1.61	1.53
1	B	109	ARG	CZ-NH1	5.55	1.40	1.32
1	A	10	ALA	CA-CB	-5.53	1.44	1.53
1	A	186	ASN	CG-OD1	5.52	1.34	1.23
1	B	44	CYS	C-O	-5.52	1.16	1.24
1	B	97	VAL	CA-CB	5.52	1.60	1.54
1	A	110	SER	C-O	5.52	1.30	1.23
1	B	144	LEU	CG-CD1	-5.52	1.34	1.52
1	B	188	ARG	CG-CD	5.50	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	TYR	CA-C	5.50	1.59	1.52
1	A	34	THR	C-O	-5.50	1.17	1.24
1	A	188	ARG	CD-NE	5.48	1.53	1.46
1	B	189	VAL	CA-CB	5.47	1.61	1.54
1	A	38	LEU	CA-C	5.46	1.60	1.52
1	B	40	LEU	CB-CG	-5.43	1.42	1.53
1	A	21	ILE	CA-CB	5.42	1.61	1.54
1	B	114	MET	N-CA	-5.41	1.40	1.46
1	A	249	ARG	CZ-NH1	5.38	1.40	1.32
1	B	66	GLN	CA-C	5.38	1.59	1.52
1	B	102	TYR	CD1-CE1	5.38	1.54	1.38
1	B	143	ASN	C-O	5.36	1.30	1.23
1	A	103	TYR	CB-CG	-5.35	1.39	1.51
1	B	233	MET	C-O	-5.35	1.18	1.24
1	B	216	VAL	CA-C	5.35	1.59	1.52
1	A	75	SER	CA-C	5.33	1.60	1.52
1	B	107	MET	C-O	-5.31	1.18	1.24
1	B	190	GLU	CA-C	5.31	1.59	1.52
1	A	6	SER	CA-CB	5.29	1.61	1.53
1	A	201	ASN	CA-C	-5.27	1.45	1.52
1	B	126	ASP	N-CA	-5.26	1.38	1.46
1	A	39	ARG	NE-CZ	5.24	1.38	1.33
1	B	187	PRO	CA-C	5.23	1.64	1.52
1	B	198	LYS	CD-CE	5.23	1.68	1.52
1	B	147	VAL	C-O	-5.21	1.18	1.24
1	B	245	GLN	CA-C	5.21	1.59	1.52
1	B	220	ALA	CA-CB	-5.21	1.45	1.53
1	B	189	VAL	C-O	5.19	1.31	1.24
1	B	102	TYR	CG-CD1	5.19	1.50	1.39
1	B	219	ILE	C-O	-5.18	1.18	1.24
1	B	43	GLY	N-CA	5.17	1.52	1.45
1	A	84	GLU	CD-OE2	5.16	1.35	1.25
1	A	214	GLU	CA-C	5.14	1.59	1.52
1	A	190	GLU	C-O	-5.14	1.18	1.24
1	B	236	GLN	CA-C	5.14	1.59	1.52
1	A	255	ARG	CG-CD	5.13	1.67	1.52
1	B	79	MET	N-CA	-5.12	1.40	1.46
1	A	239	GLU	N-CA	5.11	1.52	1.46
1	A	84	GLU	CG-CD	5.10	1.64	1.52
1	A	156	GLU	C-O	-5.08	1.18	1.24
1	B	39	ARG	CZ-NH1	5.06	1.39	1.32
1	A	173	VAL	N-CA	-5.06	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	149	LEU	CG-CD2	-5.05	1.35	1.52
1	A	198	LYS	CG-CD	5.05	1.67	1.52
1	A	248	ARG	CD-NE	5.04	1.53	1.46
1	B	247	LEU	C-O	-5.04	1.18	1.24
1	B	61	ASP	CA-C	5.02	1.63	1.52
1	A	114	MET	C-O	-5.01	1.18	1.24

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ASP	CB-CA-C	13.25	135.27	110.10
1	B	233	MET	N-CA-C	-9.68	100.68	111.14
1	B	207	GLY	CA-C-O	-9.24	113.11	122.26
1	B	54	PRO	CA-C-O	-9.04	110.34	120.92
1	A	250	LEU	CD1-CG-CD2	-7.75	93.74	110.80
1	B	257	MET	CG-SD-CE	-7.52	84.36	100.90
1	A	108	PHE	N-CA-C	7.48	120.49	111.82
1	B	77	THR	N-CA-C	7.41	121.01	109.96
1	B	157	ASP	N-CA-CB	7.40	120.99	110.12
1	A	196	VAL	N-CA-C	-7.37	103.67	110.82
1	B	54	PRO	O-C-N	7.17	130.63	123.03
1	A	104	LYS	CD-CE-NZ	-6.95	89.66	111.90
1	A	213	PRO	CA-C-O	-6.91	109.13	120.05
1	B	66	GLN	CA-CB-CG	6.89	127.87	114.10
1	A	59	TYR	N-CA-C	6.74	120.95	112.87
1	B	71	ARG	CB-CA-C	-6.66	99.53	110.85
1	B	192	LEU	CA-C-O	6.65	127.47	120.42
1	B	56	SER	CA-CB-OG	-6.62	97.86	111.10
1	B	140	LYS	N-CA-C	-6.56	104.05	111.07
1	B	256	GLY	N-CA-C	-6.42	104.55	112.77
1	A	53	VAL	CA-C-O	6.34	122.89	119.15
1	B	17	LYS	CD-CE-NZ	-6.31	91.72	111.90
1	A	84	GLU	CB-CG-CD	6.17	123.09	112.60
1	B	115	LYS	CD-CE-NZ	-6.09	92.40	111.90
1	B	231	SER	CB-CA-C	6.01	120.77	110.79
1	B	62	GLY	CA-C-N	5.95	125.15	118.97
1	B	62	GLY	C-N-CA	5.95	125.15	118.97
1	B	143	ASN	N-CA-C	5.84	119.49	111.54
1	A	185	VAL	N-CA-C	-5.84	102.05	109.58
1	B	137	SER	N-CA-C	-5.81	104.54	111.69
1	B	247	LEU	N-CA-C	5.78	118.04	111.11
1	B	199	VAL	N-CA-C	5.76	118.54	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	VAL	CA-C-O	5.75	122.92	119.19
1	B	258	LYS	N-CA-CB	5.74	118.33	110.01
1	A	109	ARG	CA-C-O	5.70	127.19	120.69
1	A	191	SER	CA-CB-OG	-5.66	99.78	111.10
1	A	109	ARG	N-CA-C	5.62	118.70	109.76
1	B	81	ALA	N-CA-C	5.57	117.35	111.28
1	B	100	LEU	CB-CA-C	5.56	119.30	110.19
1	A	179	THR	CA-C-N	5.49	130.49	121.87
1	A	179	THR	C-N-CA	5.49	130.49	121.87
1	B	206	VAL	CA-C-N	-5.46	113.81	122.65
1	B	206	VAL	C-N-CA	-5.46	113.81	122.65
1	A	149	LEU	CB-CA-C	-5.45	100.32	109.65
1	A	189	VAL	CA-CB-CG1	5.39	119.56	110.40
1	A	80	ASP	N-CA-C	5.38	117.14	111.28
1	B	53	VAL	CB-CA-C	-5.34	104.86	110.53
1	B	107	MET	N-CA-C	5.32	117.50	111.11
1	A	54	PRO	CA-C-O	5.31	127.39	121.34
1	B	255[A]	ARG	CB-CG-CD	5.30	123.49	111.30
1	B	255[B]	ARG	CB-CG-CD	5.30	123.49	111.30
1	B	231	SER	CA-CB-OG	-5.30	100.51	111.10
1	B	66	GLN	N-CA-C	-5.28	105.42	111.07
1	A	248	ARG	N-CA-C	-5.24	105.57	111.28
1	A	128	PRO	CA-C-O	-5.21	115.39	121.34
1	A	239	GLU	N-CA-C	5.19	119.30	112.92
1	B	173	VAL	CA-C-N	-5.17	114.91	122.19
1	B	173	VAL	C-N-CA	-5.17	114.91	122.19
1	A	56	SER	CA-C-N	-5.14	117.19	122.85
1	A	56	SER	C-N-CA	-5.14	117.19	122.85
1	A	31	LEU	N-CA-C	5.14	117.78	111.82
1	A	74	ALA	N-CA-C	5.13	118.80	112.54
1	A	106	ILE	O-C-N	5.12	127.80	122.17
1	A	156	GLU	N-CA-C	5.12	117.25	111.11
1	B	83	LEU	N-CA-C	-5.08	105.93	111.82
1	B	61	ASP	O-C-N	-5.07	114.89	123.00
1	A	179	THR	OG1-CB-CG2	-5.03	99.23	109.30
1	A	217	LYS	N-CA-CB	5.03	117.52	110.12
1	A	52	GLY	CA-C-N	5.02	126.21	122.59
1	A	52	GLY	C-N-CA	5.02	126.21	122.59
1	B	8	THR	N-CA-C	-5.01	105.71	111.07
1	B	113	LYS	N-CA-C	5.01	116.74	111.28
1	A	233	MET	CB-CA-C	-5.01	102.34	110.85

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Peptide
1	B	206	VAL	Peptide
1	B	61	ASP	Peptide

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	1955	0	2007	38	0
1	B	1875	0	1931	57	0
2	A	7	0	3	2	0
2	B	7	0	2	0	0
3	A	130	0	0	13	0
3	B	118	0	0	8	0
All	All	4092	0	3943	95	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 12.

All (95) 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:15[B]:LYS:CE	1:A:15[B]:LYS:NZ	1.72	1.50
1:B:107:MET:CG	1:B:107:MET:SD	2.04	1.45
1:A:107:MET:CE	1:A:107:MET:SD	2.04	1.44
1:A:57:ASP:HB3	3:A:383:HOH:O	1.60	0.99
1:A:157:ASP:HB2	3:A:376:HOH:O	1.70	0.92
1:B:68:SER:HA	1:B:71:ARG:NH1	1.87	0.88
1:B:216:VAL:HG21	1:B:257:MET:HE1	1.62	0.81
1:B:251:GLU:OE2	1:B:255[A]:ARG:CZ	2.33	0.76
1:B:107:MET:HB2	1:B:107:MET:CE	2.17	0.75
1:A:57:ASP:CB	3:A:383:HOH:O	2.26	0.73
1:B:55:CYS:O	1:B:69:VAL:HG11	1.88	0.72
1:B:107:MET:SD	1:B:107:MET:CB	2.75	0.71
1:A:262:GLY:C	3:A:397:HOH:O	2.33	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:CYS:HB3	1:B:102:TYR:CE2	2.32	0.65
1:A:58:PRO:HG3	1:A:69:VAL:HG11	1.77	0.65
1:B:39:ARG:NE	1:B:92:GLU:OE1	2.30	0.65
1:B:107:MET:CE	1:B:107:MET:CB	2.75	0.64
1:B:236:GLN:HE21	1:B:249:ARG:HB3	1.62	0.63
1:A:233:MET:CE	1:A:250:LEU:HG	2.29	0.63
1:A:248:ARG:HD3	3:A:404:HOH:O	1.99	0.62
1:B:251:GLU:OE2	1:B:255[A]:ARG:NH1	2.32	0.62
1:B:65:ILE:HG13	1:B:208:PHE:CE2	2.35	0.62
1:A:250:LEU:C	1:A:250:LEU:HD23	2.26	0.60
1:B:107:MET:CG	1:B:107:MET:CE	2.79	0.60
1:A:248:ARG:CZ	3:A:373:HOH:O	2.50	0.59
1:B:245:GLN:OE1	3:B:364:HOH:O	2.16	0.58
1:B:102:TYR:H	1:B:102:TYR:HD2	1.51	0.58
1:A:104:LYS:HE3	1:B:57:ASP:O	2.04	0.57
1:A:23:TYR:CD2	1:A:23:TYR:C	2.83	0.57
1:A:257:MET:HA	1:A:257:MET:HE2	1.87	0.56
1:B:151:THR:HB	1:B:152:PRO:HD2	1.88	0.56
1:B:235[B]:ARG:NH1	3:B:367:HOH:O	2.39	0.56
1:B:107:MET:HB2	1:B:107:MET:HE3	1.86	0.55
1:A:233:MET:HE1	1:A:250:LEU:HG	1.90	0.54
1:A:186:ASN:O	1:A:189:VAL:HG13	2.08	0.53
1:A:235[B]:ARG:NH2	3:A:430:HOH:O	2.42	0.53
1:A:167:GLU:HG3	3:A:385:HOH:O	2.08	0.53
1:B:45:GLY:HA3	1:B:258:LYS:HD2	1.91	0.52
1:B:40:LEU:HD11	1:B:251:GLU:HB2	1.91	0.52
1:B:28:ASP:OD1	1:B:71:ARG:HD2	2.09	0.52
1:A:183:ALA:O	1:A:215:HIS:CE1	2.63	0.52
1:B:216:VAL:HG21	1:B:257:MET:CE	2.38	0.51
1:B:28:ASP:OD2	1:B:71:ARG:NH1	2.44	0.51
1:B:216:VAL:HG12	1:B:261:LEU:HD21	1.92	0.51
1:A:57:ASP:CG	3:A:383:HOH:O	2.52	0.51
1:A:174:SER:O	3:A:405:HOH:O	2.19	0.50
1:B:151:THR:HB	1:B:152:PRO:CD	2.42	0.50
1:A:120[A]:HIS:CD2	3:A:319:HOH:O	2.65	0.49
1:A:233:MET:HE3	1:A:233:MET:HA	1.94	0.49
1:B:138:GLU:OE2	3:B:338:HOH:O	2.20	0.48
1:A:116:GLU:HG3	3:A:407:HOH:O	2.13	0.48
1:B:87[A]:ARG:NH2	3:B:396:HOH:O	2.36	0.48
1:B:65:ILE:HG13	1:B:208:PHE:HE2	1.77	0.48
1:B:236:GLN:NE2	1:B:249:ARG:HB3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LEU:HD11	1:B:251:GLU:HG3	1.95	0.48
1:B:255[B]:ARG:NH1	3:B:360:HOH:O	2.48	0.47
2:A:302:MLA:C3	1:B:158[B]:ARG:HH21	2.27	0.46
1:A:114:MET:HE1	1:A:122:LEU:HD13	1.97	0.46
1:A:245:GLN:HG2	1:A:249:ARG:HD3	1.98	0.46
1:A:190:GLU:HG3	1:A:222:TRP:CD1	2.51	0.45
1:B:189:VAL:HG22	1:B:222:TRP:CE3	2.52	0.45
1:B:40:LEU:HD11	1:B:251:GLU:CB	2.47	0.45
1:A:58:PRO:HA	1:A:102:TYR:CZ	2.52	0.45
1:B:107:MET:CB	1:B:107:MET:HE3	2.42	0.45
1:B:115:LYS:HE2	1:B:143:ASN:O	2.17	0.45
1:B:188:ARG:O	1:B:188:ARG:HG3	2.17	0.44
1:B:158[A]:ARG:HG2	3:B:412:HOH:O	2.18	0.44
1:A:211:SER:HB3	1:A:232:ALA:CB	2.48	0.44
1:A:211:SER:HB3	1:A:232:ALA:HB2	1.99	0.44
1:B:39:ARG:CD	1:B:92:GLU:OE1	2.66	0.44
1:B:55:CYS:HB3	1:B:102:TYR:CD2	2.53	0.44
1:B:188:ARG:CD	1:B:192:LEU:HD21	2.48	0.44
1:B:139:ALA:HB1	1:B:144:LEU:O	2.18	0.43
1:B:171:TYR:CE1	1:B:173:VAL:HG12	2.54	0.43
3:A:395:HOH:O	1:B:158[A]:ARG:HD3	2.18	0.43
1:B:235[A]:ARG:NH2	3:B:411:HOH:O	2.51	0.43
1:A:245:GLN:HG3	1:A:248:ARG:NH1	2.34	0.43
2:A:302:MLA:O1B	2:A:302:MLA:O3A	2.36	0.43
1:A:129:TYR:CD1	1:A:129:TYR:C	2.97	0.43
1:B:23:TYR:CD2	1:B:23:TYR:C	2.97	0.43
1:A:28:ASP:HA	1:A:29:PRO:HA	1.90	0.42
1:A:9:MET:O	1:A:13:MET:HG3	2.20	0.42
1:B:68:SER:HA	1:B:71:ARG:HH11	1.73	0.42
1:B:159:MET:O	1:B:163:THR:HG23	2.20	0.41
1:B:188:ARG:HG3	1:B:192:LEU:HG	2.02	0.41
1:B:151:THR:CB	1:B:152:PRO:CD	2.99	0.41
1:B:158[B]:ARG:NH1	3:B:336:HOH:O	2.53	0.41
1:A:106:ILE:HG21	1:A:106:ILE:HD13	1.82	0.41
1:A:190:GLU:HG3	1:A:222:TRP:CG	2.56	0.41
1:B:22:PRO:HB3	1:B:233:MET:HE3	2.03	0.41
1:B:39:ARG:HE	1:B:92:GLU:CD	2.29	0.41
1:A:228:ILE:HD12	1:A:228:ILE:N	2.36	0.41
1:B:107:MET:HB2	1:B:107:MET:HE2	1.98	0.40
1:B:65:ILE:CG1	1:B:208:PHE:HE2	2.34	0.40

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	263/262 (100%)	260 (99%)	3 (1%)	0	100	100
1	B	246/262 (94%)	242 (98%)	3 (1%)	1 (0%)	30	22
All	All	509/524 (97%)	502 (99%)	6 (1%)	1 (0%)	43	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	208	PHE

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	212/211 (100%)	201 (95%)	11 (5%)	21	13
1	B	204/211 (97%)	197 (97%)	7 (3%)	32	28
All	All	416/422 (99%)	398 (96%)	18 (4%)	25	19

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	64	ILE
1	A	114	MET
1	A	130	VAL
1	A	135	LEU

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Mol	Chain	Res	Type
1	A	144	LEU
1	A	189	VAL
1	A	211	SER
1	A	219	ILE
1	A	248	ARG
1	A	250	LEU
1	B	88	GLU
1	B	102	TYR
1	B	120	HIS
1	B	175	VAL
1	B	188	ARG
1	B	189	VAL
1	B	229	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	215	HIS
1	B	66	GLN
1	B	141	ASN
1	B	236	GLN

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](#)

2 ligands are 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	MLA	B	301	-	6,6,6	1.75	1 (16%)	7,7,7	1.37	1 (14%)
2	MLA	A	302	-	6,6,6	2.26	4 (66%)	7,7,7	3.20	3 (42%)

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	MLA	B	301	-	-	2/4/4/4	-
2	MLA	A	302	-	-	4/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	302	MLA	O1B-C1	3.76	1.34	1.22
2	B	301	MLA	O3A-C3	3.26	1.32	1.22
2	A	302	MLA	C2-C3	2.45	1.54	1.51
2	A	302	MLA	O3B-C3	2.13	1.37	1.30
2	A	302	MLA	O3A-C3	2.11	1.29	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	302	MLA	O3A-C3-C2	-6.03	104.94	122.11
2	A	302	MLA	O3B-C3-C2	5.30	130.92	114.51
2	B	301	MLA	O3B-C3-O3A	2.55	129.88	123.33
2	A	302	MLA	O1A-C1-O1B	2.24	129.10	123.33

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	MLA	O1A-C1-C2-C3
2	A	302	MLA	C1-C2-C3-O3B
2	B	301	MLA	C1-C2-C3-O3B
2	B	301	MLA	C1-C2-C3-O3A
2	A	302	MLA	O1B-C1-C2-C3
2	A	302	MLA	C1-C2-C3-O3A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	MLA	2	0

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 [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	261/262 (99%)	-0.35	2 (0%) 82 83	11, 20, 31, 46	4 (1%)
1	B	248/262 (94%)	-0.10	4 (1%) 70 70	10, 21, 33, 46	4 (1%)
All	All	509/524 (97%)	-0.22	6 (1%) 76 76	10, 20, 32, 46	8 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	PHE	3.5
1	B	58	PRO	3.4
1	B	187	PRO	3.1
1	B	175	VAL	2.9
1	B	208	PHE	2.2
1	A	105	PRO	2.1

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	MLA	A	302	7/7	0.81	0.14	50,51,55,66	0
2	MLA	B	301	7/7	0.87	0.10	44,49,56,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.