Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:56 PM GMT

PDB ID	:	1RD5
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

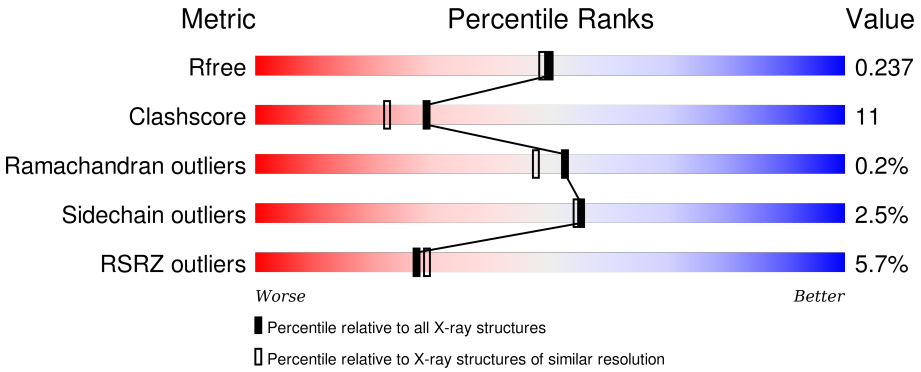
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	5% 69% 24% 6% •
1	B	262	6% 65% 23% 6% • 5%

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.

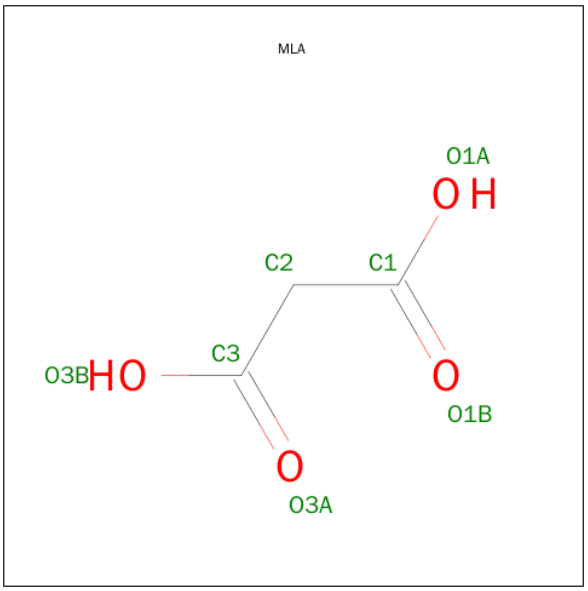
- Molecule 1 is a protein called Tryptophan synthase alpha chain, chloroplast.

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 MET	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 MET	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 (three-letter code: MLA) (formula: $C_3H_4O_4$).



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

- Molecule 3 is water.

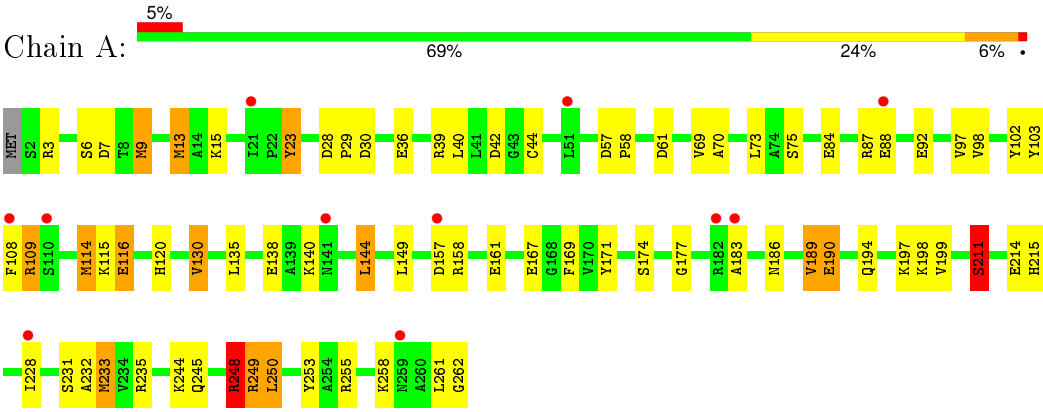
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	130	Total O 130 130	0	0
3	B	118	Total O 118 118	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

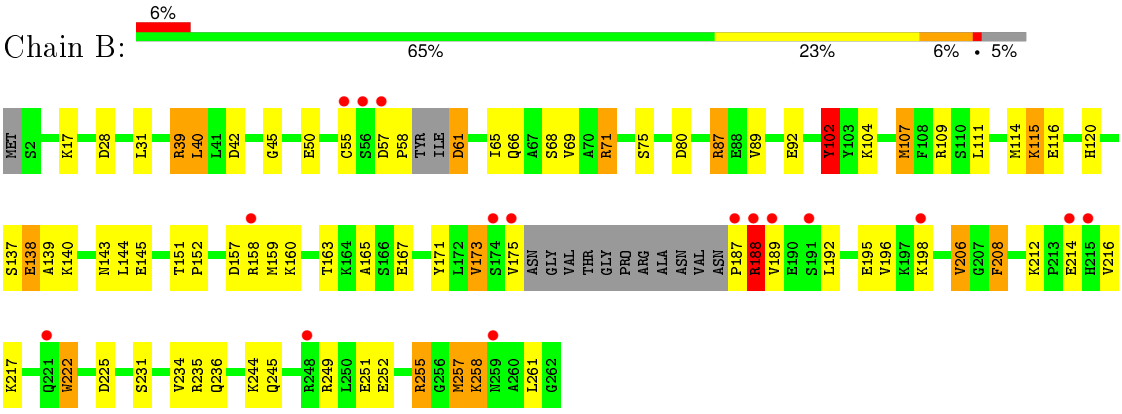
- Molecule 1: Tryptophan synthase alpha chain, chloroplast

Chain A:



- Molecule 1: Tryptophan synthase alpha chain, chloroplast

Chain B:



4 Data and refinement statistics (i)

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 24.17 – 2.02	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.02) 94.3 (24.17-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.245 , 0.299 0.180 , 0.237	Depositor DCC
R_{free} test set	1850 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 48.5	EDS
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 37002 reflections	Xtriage
F_o,F_c correlation	0.96	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.94	57/2013 (2.8%)	1.47	23/2735 (0.8%)
1	B	1.98	50/1931 (2.6%)	1.59	25/2614 (1.0%)
All	All	1.96	107/3944 (2.7%)	1.53	48/5349 (0.9%)

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 (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	102	TYR	CG-CD2	11.41	1.53	1.39
1	B	173	VAL	CB-CG1	-11.06	1.29	1.52
1	B	102	TYR	CD1-CE1	10.29	1.54	1.39
1	A	231	SER	CB-OG	9.85	1.55	1.42
1	A	130	VAL	CB-CG2	-9.28	1.33	1.52
1	B	107	MET	CG-SD	8.92	2.04	1.81
1	A	84	GLU	CD-OE2	8.64	1.35	1.25
1	A	114	MET	SD-CE	-8.59	1.29	1.77
1	A	84	GLU	CG-CD	8.56	1.64	1.51
1	B	102	TYR	CG-CD1	8.53	1.50	1.39
1	A	258	LYS	CD-CE	8.50	1.72	1.51
1	A	109	ARG	CA-CB	8.46	1.72	1.53
1	B	116	GLU	CD-OE2	8.34	1.34	1.25
1	A	103	TYR	CB-CG	-7.85	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	GLU	CD-OE2	7.67	1.34	1.25
1	B	116	GLU	CD-OE1	7.63	1.34	1.25
1	A	244	LYS	CD-CE	7.61	1.70	1.51
1	B	252	GLU	CD-OE2	7.54	1.33	1.25
1	B	206	VAL	CB-CG1	-7.34	1.37	1.52
1	A	36	GLU	CD-OE2	7.28	1.33	1.25
1	B	212	LYS	CE-NZ	7.26	1.67	1.49
1	A	194	GLN	CG-CD	7.24	1.67	1.51
1	A	108	PHE	CA-CB	7.24	1.69	1.53
1	A	222	TRP	CB-CG	-7.18	1.37	1.50
1	B	234	VAL	CB-CG2	-7.14	1.37	1.52
1	B	167	GLU	CD-OE2	7.09	1.33	1.25
1	B	89	VAL	CB-CG2	7.00	1.67	1.52
1	B	58	PRO	CA-C	6.93	1.66	1.52
1	B	137	SER	CA-CB	6.91	1.63	1.52
1	A	255	ARG	NE-CZ	6.89	1.42	1.33
1	B	188	ARG	CG-CD	6.80	1.69	1.51
1	B	198	LYS	CD-CE	6.75	1.68	1.51
1	A	44	CYS	CB-SG	6.73	1.93	1.82
1	B	75	SER	CB-OG	6.73	1.51	1.42
1	B	50	GLU	CD-OE1	6.72	1.33	1.25
1	A	97	VAL	CB-CG1	6.58	1.66	1.52
1	A	220	ALA	CA-CB	6.51	1.66	1.52
1	B	231	SER	CB-OG	-6.45	1.33	1.42
1	B	102	TYR	CB-CG	6.44	1.61	1.51
1	A	88	GLU	CG-CD	6.43	1.61	1.51
1	A	255	ARG	CG-CD	6.36	1.67	1.51
1	A	109	ARG	C-O	6.23	1.35	1.23
1	B	195	GLU	CD-OE2	6.19	1.32	1.25
1	B	115	LYS	CD-CE	6.11	1.66	1.51
1	B	138	GLU	CD-OE1	6.08	1.32	1.25
1	A	84	GLU	CD-OE1	6.06	1.32	1.25
1	A	92	GLU	CD-OE1	6.05	1.32	1.25
1	A	197	LYS	CE-NZ	6.01	1.64	1.49
1	A	87	ARG	CG-CD	6.01	1.67	1.51
1	A	149	LEU	CG-CD2	-5.95	1.29	1.51
1	B	257	MET	CG-SD	5.95	1.96	1.81
1	A	138	GLU	CD-OE2	5.92	1.32	1.25
1	A	233	MET	CG-SD	5.86	1.96	1.81
1	B	140	LYS	CD-CE	5.83	1.65	1.51
1	B	39	ARG	CG-CD	5.80	1.66	1.51
1	A	249	ARG	NE-CZ	5.75	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	109	ARG	CZ-NH1	5.75	1.40	1.33
1	A	116	GLU	CG-CD	5.74	1.60	1.51
1	A	6	SER	CA-CB	5.73	1.61	1.52
1	B	107	MET	CB-CG	-5.68	1.33	1.51
1	B	104	LYS	CG-CD	5.67	1.71	1.52
1	B	17	LYS	CD-CE	5.67	1.65	1.51
1	B	244	LYS	CE-NZ	5.65	1.63	1.49
1	A	75	SER	CB-OG	5.62	1.49	1.42
1	A	211	SER	CB-OG	-5.59	1.34	1.42
1	A	249	ARG	CZ-NH1	5.57	1.40	1.33
1	B	187	PRO	CA-C	5.54	1.64	1.52
1	A	199	VAL	CB-CG2	-5.53	1.41	1.52
1	B	214	GLU	CD-OE1	5.50	1.31	1.25
1	B	196	VAL	CB-CG1	5.49	1.64	1.52
1	A	248	ARG	CG-CD	5.46	1.65	1.51
1	B	214	GLU	CG-CD	5.46	1.60	1.51
1	A	158	ARG	CD-NE	5.46	1.55	1.46
1	A	87	ARG	NE-CZ	5.44	1.40	1.33
1	B	102	TYR	CE1-CZ	5.41	1.45	1.38
1	A	169	PHE	CD1-CE1	-5.38	1.28	1.39
1	A	84	GLU	CB-CG	5.36	1.62	1.52
1	B	114	MET	SD-CE	-5.35	1.47	1.77
1	A	177	GLY	CA-C	5.35	1.60	1.51
1	A	70	ALA	CA-CB	5.32	1.63	1.52
1	A	214	GLU	CG-CD	5.28	1.59	1.51
1	B	145	GLU	CD-OE1	-5.28	1.19	1.25
1	A	98	VAL	CB-CG2	-5.24	1.41	1.52
1	A	258	LYS	CE-NZ	5.24	1.62	1.49
1	B	61	ASP	CB-CG	5.23	1.62	1.51
1	B	39	ARG	CZ-NH1	5.22	1.39	1.33
1	A	3	ARG	CG-CD	5.22	1.65	1.51
1	A	13	MET	CB-CG	-5.21	1.34	1.51
1	A	190	GLU	CD-OE1	5.21	1.31	1.25
1	B	50	GLU	CD-OE2	5.20	1.31	1.25
1	A	140	LYS	CD-CE	5.19	1.64	1.51
1	B	140	LYS	CE-NZ	5.18	1.62	1.49
1	B	175	VAL	CB-CG2	5.18	1.63	1.52
1	B	160	LYS	CG-CD	5.16	1.70	1.52
1	B	258	LYS	CB-CG	5.16	1.66	1.52
1	A	140	LYS	CE-NZ	5.13	1.61	1.49
1	B	222	TRP	CB-CG	5.12	1.59	1.50
1	A	161	GLU	CD-OE1	5.11	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	165	ALA	CA-CB	5.10	1.63	1.52
1	A	23	TYR	CB-CG	5.08	1.59	1.51
1	A	253	TYR	CD1-CE1	5.07	1.47	1.39
1	B	102	TYR	CD2-CE2	5.04	1.47	1.39
1	A	115	LYS	CD-CE	5.04	1.63	1.51
1	B	217	LYS	CD-CE	5.03	1.63	1.51
1	A	88	GLU	CD-OE1	5.01	1.31	1.25
1	A	92	GLU	CG-CD	5.01	1.59	1.51
1	A	104	LYS	CB-CG	5.01	1.66	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	61	ASP	CB-CA-C	12.43	135.27	110.40
1	B	257	MET	CG-SD-CE	-9.90	84.36	100.20
1	A	104	LYS	CD-CE-NZ	-9.58	89.66	111.70
1	B	39	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	B	17	LYS	CD-CE-NZ	-8.69	91.72	111.70
1	A	3	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	B	115	LYS	CD-CE-NZ	-8.39	92.40	111.70
1	B	42	ASP	CB-CG-OD2	7.76	125.29	118.30
1	A	73	LEU	CB-CG-CD1	-7.52	98.21	111.00
1	B	87[A]	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	B	87[B]	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	A	171	TYR	CB-CG-CD1	7.43	125.46	121.00
1	A	149	LEU	CB-CG-CD1	7.38	123.55	111.00
1	A	39	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	61	ASP	CB-CG-OD2	6.78	124.40	118.30
1	A	255	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	30	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	158	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	B	40	LEU	CA-CB-CG	6.70	130.71	115.30
1	A	248	ARG	NE-CZ-NH2	6.63	123.61	120.30
1	B	66	GLN	CA-CB-CG	6.58	127.87	113.40
1	B	31	LEU	CB-CG-CD1	-6.54	99.88	111.00
1	B	244	LYS	CD-CE-NZ	-6.42	96.92	111.70
1	B	50	GLU	OE1-CD-OE2	6.24	130.79	123.30
1	A	171	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	B	111	LEU	CB-CG-CD2	6.02	121.23	111.00
1	B	40	LEU	CB-CG-CD1	-5.97	100.84	111.00
1	A	7	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	42	ASP	CB-CG-OD2	5.88	123.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	255[A]	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	255[B]	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	225	ASP	CB-CG-OD1	5.82	123.54	118.30
1	A	9	MET	CG-SD-CE	5.78	109.44	100.20
1	A	189	VAL	CA-CB-CG1	5.78	119.56	110.90
1	B	157	ASP	N-CA-CB	5.77	120.99	110.60
1	A	144	LEU	CA-CB-CG	5.70	128.41	115.30
1	B	61	ASP	CA-C-N	5.67	127.55	116.20
1	A	261	LEU	CB-CG-CD1	-5.64	101.41	111.00
1	B	231	SER	CB-CA-C	5.61	120.77	110.10
1	A	250	LEU	CD1-CG-CD2	-5.59	93.74	110.50
1	B	31	LEU	CB-CG-CD2	5.51	120.36	111.00
1	A	198	LYS	CD-CE-NZ	5.46	124.25	111.70
1	B	71	ARG	CB-CA-C	-5.44	99.53	110.40
1	A	73	LEU	CB-CG-CD2	5.39	120.16	111.00
1	A	149	LEU	CB-CA-C	-5.20	100.32	110.20
1	A	87	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	140	LYS	CD-CE-NZ	5.07	123.36	111.70
1	B	80	ASP	CB-CG-OD1	5.02	122.82	118.30

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	35	0
1	B	1875	0	1931	54	0
2	A	7	0	3	2	0
2	B	7	0	2	0	0
3	A	130	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	118	0	0	8	0
All	All	4092	0	3943	89	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 11.

All (89) 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:SD	1:A:107:MET:CE	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:251:GLU:OE2	1:B:255[A]:ARG:CZ	2.33	0.76
1:B:107:MET:CE	1:B:107:MET:HB2	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:CB	1:B:107:MET:SD	2.75	0.71
1:A:262:GLY:C	3:A:397:HOH:O	2.33	0.67
1:B:55:CYS:HB3	1:B:102:TYR:CE2	2.32	0.65
1:B:39:ARG:NE	1:B:92:GLU:OE1	2.30	0.65
1:A:58:PRO:HG3	1:A:69:VAL:HG11	1.77	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:B:251:GLU:OE2	1:B:255[A]:ARG:NH1	2.32	0.62
1:A:248:ARG:HD3	3:A:404:HOH:O	1.99	0.62
1:B:65:ILE:HG13	1:B:208:PHE:CE2	2.35	0.62
1:B:107:MET:CE	1:B:107:MET:CG	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: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:A:250:LEU:C	1:A:250:LEU:HD23	2.26	0.56
1:A:233:MET:HE1	1:A:250:LEU:HG	1.88	0.55
1:B:107:MET:HE3	1:B:107:MET:HB2	1.87	0.54
1:A:186:ASN:O	1:A:189:VAL:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235[B]:ARG:NH2	3:A:430:HOH:O	2.42	0.53
1:B:216:VAL:HG21	1:B:257:MET:CE	2.38	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:A:23:TYR:CD2	1:A:23:TYR:C	2.83	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: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: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: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
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
1:A:233:MET:HA	1:A:233:MET:HE3	1.96	0.47
1:B:216:VAL:HG21	1:B:257:MET:HE3	1.96	0.46
2:A:302:MLA:C3	1:B:158[B]:ARG:HH21	2.27	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:188:ARG:O	1:B:188:ARG:HG3	2.17	0.45
1:B:115:LYS:HE2	1:B:143:ASN:O	2.17	0.45
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:55:CYS:HB3	1:B:102:TYR:CD2	2.53	0.44
1:B:39:ARG:CD	1:B:92:GLU:OE1	2.66	0.44
1:B:188:ARG:CD	1:B:192:LEU:HD21	2.48	0.44
1:B:107:MET:HE3	1:B:107:MET:CB	2.43	0.43
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
1:B:235[A]:ARG:NH2	3:B:411:HOH:O	2.51	0.43
3:A:395:HOH:O	1:B:158[A]:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:28:ASP:HA	1:A:29:PRO:HA	1.90	0.42
1:A:57:ASP:CG	3:A:383:HOH:O	2.52	0.42
1:B:107:MET:HB2	1:B:107:MET:HE2	1.97	0.42
1:B:68:SER:HA	1:B:71:ARG:HH11	1.73	0.42
1:A:9:MET:O	1:A:13:MET:HG3	2.20	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:HD13	1:A:106:ILE:HG21	1.82	0.41
1:A:190:GLU:HG3	1:A:222:TRP:CG	2.56	0.41
1:A:228:ILE:N	1:A:228:ILE:HD12	2.36	0.41
1:B:65:ILE:CG1	1:B:208:PHE:HE2	2.34	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	263/262 (100%)	260 (99%)	3 (1%)	0	100	100
1	B	246/262 (94%)	242 (98%)	3 (1%)	1 (0%)	39	32
All	All	509/524 (97%)	502 (99%)	6 (1%)	1 (0%)	52	47

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	208	PHE

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	212/211 (100%)	205 (97%)	7 (3%)	45 42
1	B	204/211 (97%)	201 (98%)	3 (2%)	72 74
All	All	416/422 (99%)	406 (98%)	10 (2%)	55 56

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	114	MET
1	A	130	VAL
1	A	135	LEU
1	A	144	LEU
1	A	211	SER
1	A	248	ARG
1	B	102	TYR
1	B	120	HIS
1	B	188	ARG

Some 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	141	ASN
1	B	142	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 carbohydrates 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	A	302	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	B	301	-	0,6,6	0.00	-	0,7,7	0.00	-

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	A	302	-	-	0/0/4/4	0/0/0/0
2	MLA	B	301	-	-	0/0/4/4	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.

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

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, 95^{th} 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%)	0.25	13 (4%)	32	34	11, 21, 31, 46	0
1	B	248/262 (94%)	0.34	16 (6%)	22	23	10, 21, 33, 46	0
All	All	509/524 (97%)	0.30	29 (5%)	27	29	10, 21, 32, 46	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	PHE	5.9
1	B	175	VAL	5.3
1	A	182	ARG	5.0
1	B	188	ARG	3.5
1	B	174	SER	3.4
1	A	110	SER	3.1
1	B	55	CYS	3.1
1	A	107	MET	3.0
1	A	105	PRO	2.9
1	A	141[A]	ASN	2.9
1	B	187	PRO	2.9
1	A	51	LEU	2.8
1	B	158[A]	ARG	2.7
1	B	189	VAL	2.7
1	B	56	SER	2.7
1	B	57	ASP	2.7
1	A	157	ASP	2.5
1	B	215	HIS	2.4
1	B	221	GLN	2.3
1	A	88	GLU	2.3
1	B	198	LYS	2.3
1	A	183	ALA	2.3
1	B	191	SER	2.2
1	B	248	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	214	GLU	2.2
1	A	21	ILE	2.1
1	A	259	ASN	2.0
1	B	259	ASN	2.0
1	A	228	ILE	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. 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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	MLA	A	302	7/7	0.80	0.24	0.76	50,51,55,66	0
2	MLA	B	301	7/7	0.90	0.14	-0.25	44,49,56,60	0

6.5 Other polymers (i)

There are no such residues in this entry.