



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2017 – 06:12 PM EDT

PDB ID : 5VYZ
Title : Crystal structure of Lactococcus lactis pyruvate carboxylase in complex with cyclic-di-AMP
Authors : Choi, P.H.; Tong, L.
Deposited on : unknown
Resolution : 2.30 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029824

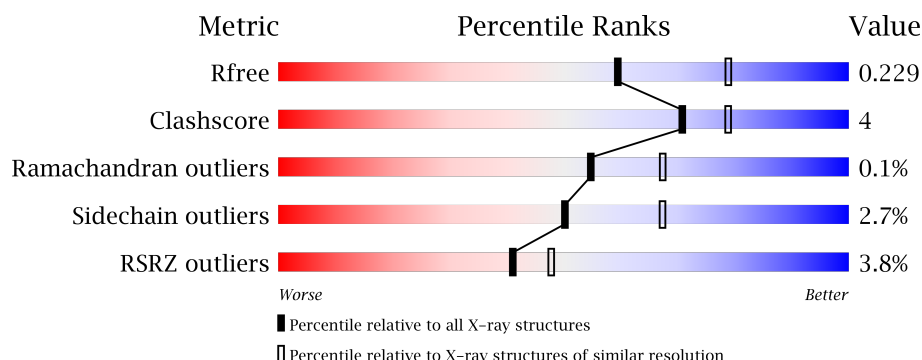
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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 $\leq 5\%$. 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	1145	<div> <div>3%</div> <div>87%</div> <div>12%</div> <div>•</div> </div>
1	B	1145	<div> <div>3%</div> <div>89%</div> <div>10%</div> <div>•</div> </div>
1	C	1145	<div> <div>3%</div> <div>84%</div> <div>10%</div> <div>• 5%</div> </div>
1	D	1145	<div> <div>5%</div> <div>90%</div> <div>9%</div> <div>•</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36479 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 Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1144	Total	C	N	O	S	0	0	0
			8956	5677	1547	1697	35			
1	B	1142	Total	C	N	O	S	0	0	0
			8934	5665	1539	1695	35			
1	C	1083	Total	C	N	O	S	0	0	0
			8520	5406	1470	1612	32			
1	D	1144	Total	C	N	O	S	0	0	0
			8946	5670	1544	1697	35			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP A0A089XIW4
A	-6	LEU	-	expression tag	UNP A0A089XIW4
A	-5	VAL	-	expression tag	UNP A0A089XIW4
A	-4	PRO	-	expression tag	UNP A0A089XIW4
A	-3	ARG	-	expression tag	UNP A0A089XIW4
A	-2	GLY	-	expression tag	UNP A0A089XIW4
A	-1	SER	-	expression tag	UNP A0A089XIW4
A	0	HIS	-	expression tag	UNP A0A089XIW4
A	1055	ALA	THR	conflict	UNP A0A089XIW4
B	-7	GLY	-	expression tag	UNP A0A089XIW4
B	-6	LEU	-	expression tag	UNP A0A089XIW4
B	-5	VAL	-	expression tag	UNP A0A089XIW4
B	-4	PRO	-	expression tag	UNP A0A089XIW4
B	-3	ARG	-	expression tag	UNP A0A089XIW4
B	-2	GLY	-	expression tag	UNP A0A089XIW4
B	-1	SER	-	expression tag	UNP A0A089XIW4
B	0	HIS	-	expression tag	UNP A0A089XIW4
B	1055	ALA	THR	conflict	UNP A0A089XIW4
C	-7	GLY	-	expression tag	UNP A0A089XIW4
C	-6	LEU	-	expression tag	UNP A0A089XIW4
C	-5	VAL	-	expression tag	UNP A0A089XIW4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP A0A089XIW4
C	-3	ARG	-	expression tag	UNP A0A089XIW4
C	-2	GLY	-	expression tag	UNP A0A089XIW4
C	-1	SER	-	expression tag	UNP A0A089XIW4
C	0	HIS	-	expression tag	UNP A0A089XIW4
C	1055	ALA	THR	conflict	UNP A0A089XIW4
D	-7	GLY	-	expression tag	UNP A0A089XIW4
D	-6	LEU	-	expression tag	UNP A0A089XIW4
D	-5	VAL	-	expression tag	UNP A0A089XIW4
D	-4	PRO	-	expression tag	UNP A0A089XIW4
D	-3	ARG	-	expression tag	UNP A0A089XIW4
D	-2	GLY	-	expression tag	UNP A0A089XIW4
D	-1	SER	-	expression tag	UNP A0A089XIW4
D	0	HIS	-	expression tag	UNP A0A089XIW4
D	1055	ALA	THR	conflict	UNP A0A089XIW4

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

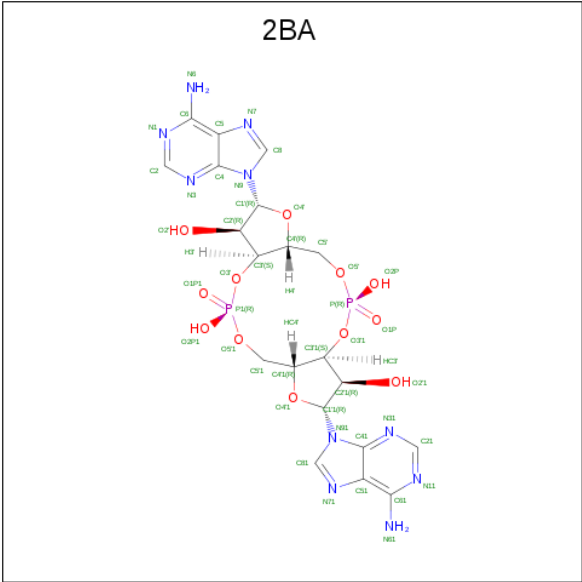


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is (2R,3R,3aS,5R,7aR,9R,10R,10aS,12R,14aR)-2,9-bis(6-amino-9H-purin-9-yl)octahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-3,5,10,12-tetraol 5,12-dioxide (three-letter code: 2BA) (formula: $C_{20}H_{24}N_{10}O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			44	20	10	12	2		
5	D	1	Total	C	N	O	P	0	0
			44	20	10	12	2		

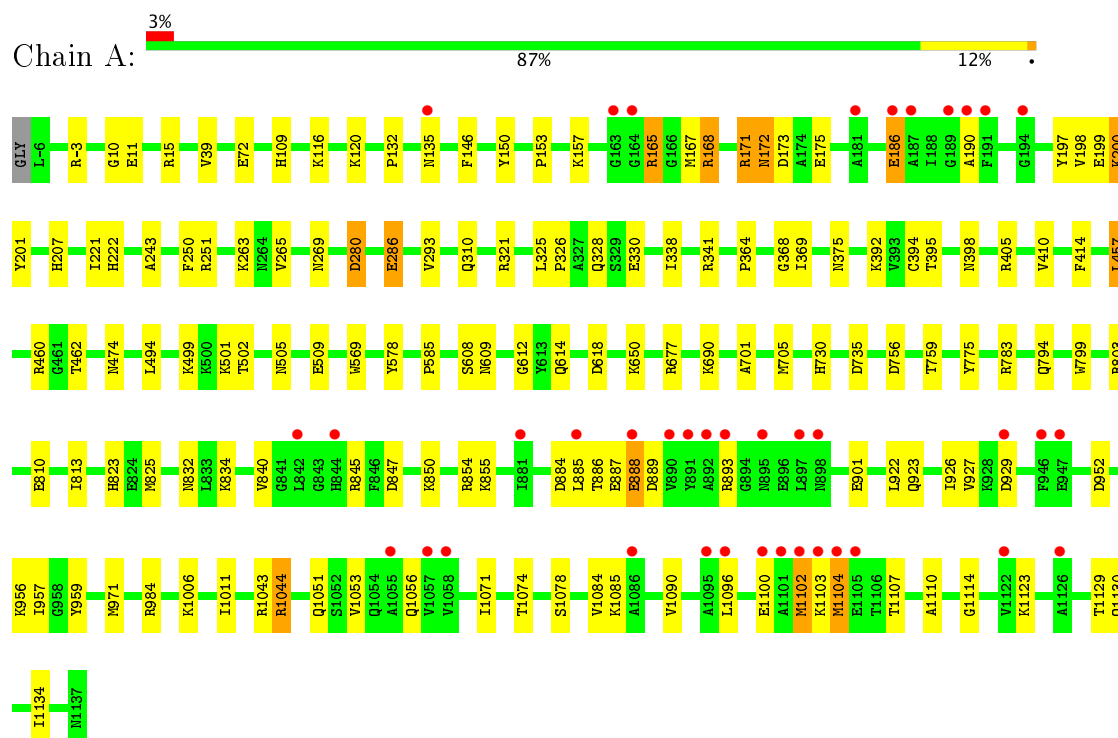
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	210	Total	O	0	0
			210	210		
6	B	243	Total	O	0	0
			243	243		
6	C	220	Total	O	0	0
			220	220		
6	D	246	Total	O	0	0
			246	246		

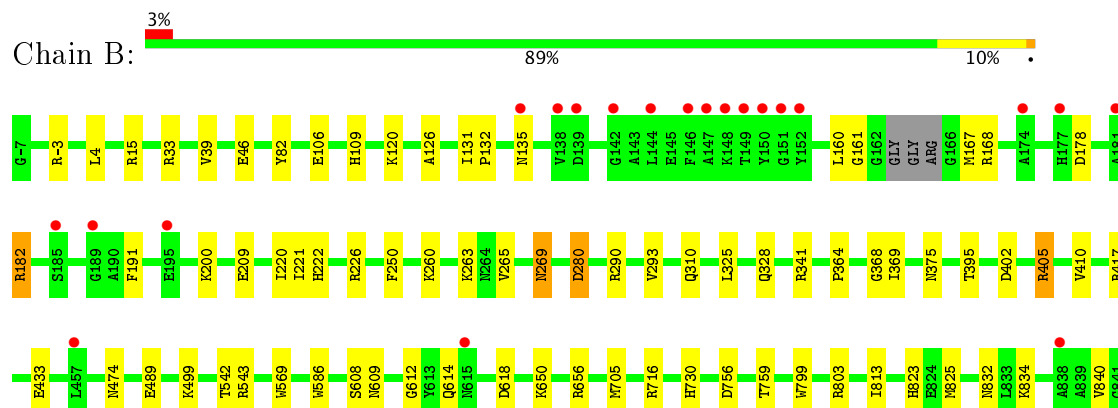
3 Residue-property plots [i](#)

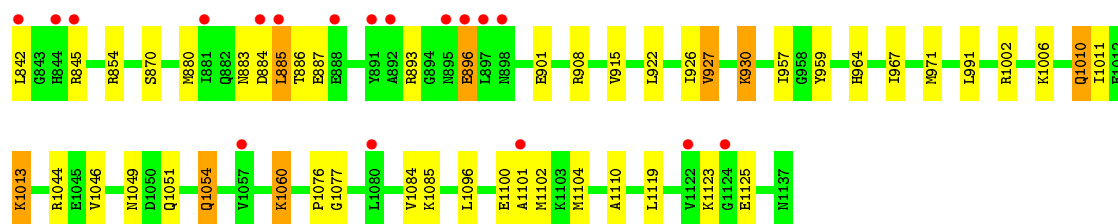
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Pyruvate carboxylase

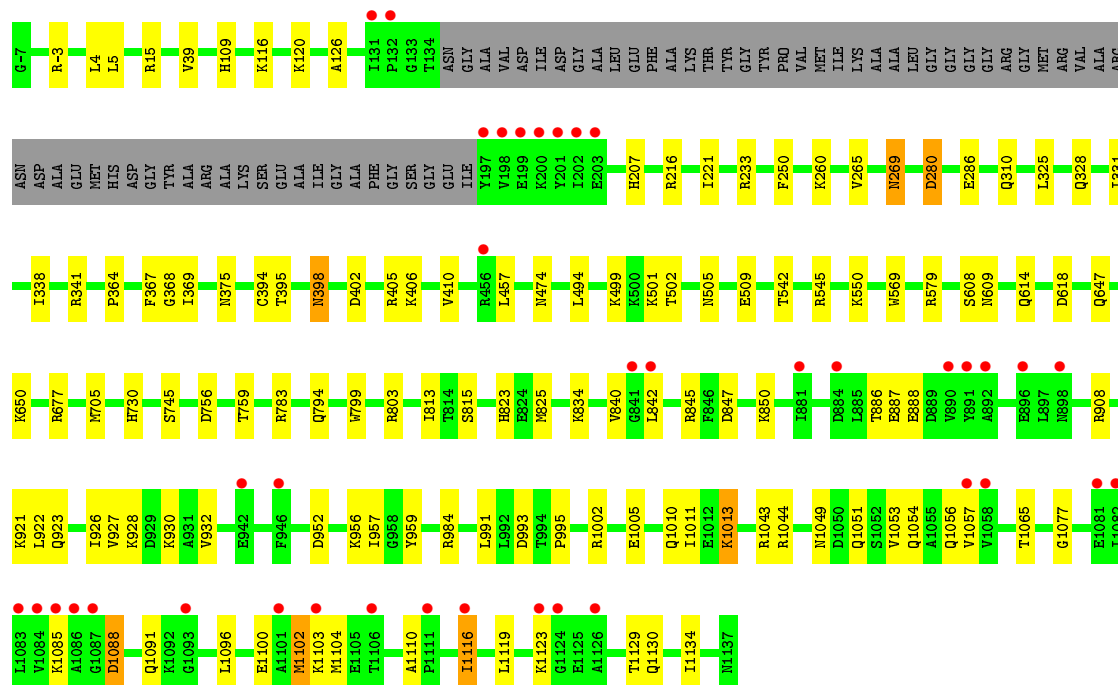
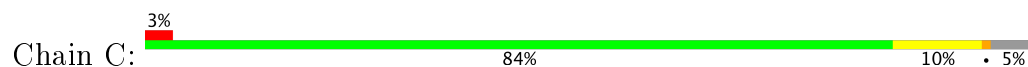


• Molecule 1: Pyruvate carboxylase

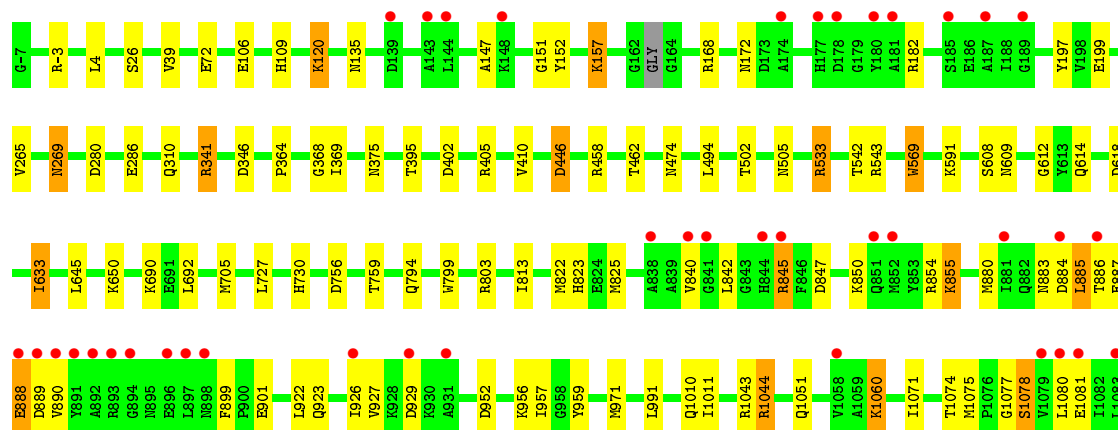
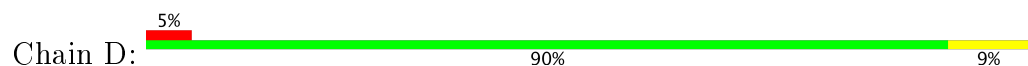


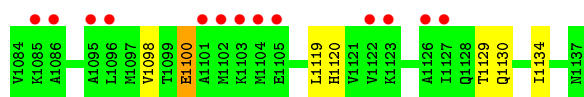


• Molecule 1: Pyruvate carboxylase



• Molecule 1: Pyruvate carboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	97.27Å 130.43Å 133.37Å 66.08° 89.05° 70.60°	Depositor
Resolution (Å)	48.60 – 2.30 48.55 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.5 (48.60-2.30) 75.9 (48.55-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.183 , 0.221 0.193 , 0.229	Depositor DCC
R_{free} test set	11253 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	36479	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: MG, MN, 2BA, ADP

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	0.82	1/9130 (0.0%)	0.86	19/12354 (0.2%)
1	B	0.80	2/9107 (0.0%)	0.85	21/12323 (0.2%)
1	C	0.80	1/8686 (0.0%)	0.87	18/11756 (0.2%)
1	D	0.81	1/9119 (0.0%)	0.87	15/12338 (0.1%)
All	All	0.81	5/36042 (0.0%)	0.86	73/48771 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	402	ASP	CB-CG	6.17	1.64	1.51
1	C	1005	GLU	CD-OE1	-5.51	1.19	1.25
1	B	209	GLU	CD-OE1	5.12	1.31	1.25
1	B	402	ASP	CB-CG	5.11	1.62	1.51
1	A	810	GLU	CD-OE1	5.08	1.31	1.25

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	341	ARG	NE-CZ-NH1	-13.67	113.47	120.30
1	D	341	ARG	NE-CZ-NH2	13.02	126.81	120.30
1	D	-3	ARG	NE-CZ-NH2	-9.55	115.52	120.30
1	C	-3	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	A	341	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	B	405	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	D	633	ILE	CA-CB-CG1	-7.96	95.88	111.00
1	A	-3	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	-3	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	C	1043	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	A	1043	ARG	NE-CZ-NH1	7.77	124.18	120.30
1	C	-3	ARG	NE-CZ-NH1	7.69	124.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	-3	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	D	1044	ARG	NE-CZ-NH1	-7.59	116.50	120.30
1	B	716	ARG	NE-CZ-NH1	-7.52	116.54	120.30
1	C	1044	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	D	405	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	A	405	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	B	716	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	B	1044	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	A	172	ASN	CB-CA-C	-7.15	96.11	110.40
1	A	783	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	1043	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	C	341	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	C	405	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	C	579	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	C	1043	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	B	-3	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	B	417	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	A	1044	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	A	845	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	A	845	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	B	290	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	C	1044	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	D	633	ILE	CB-CG1-CD1	6.20	131.25	113.90
1	D	1044	ARG	NE-CZ-NH2	6.13	123.36	120.30
1	C	550	LYS	CB-CA-C	-6.11	98.19	110.40
1	A	286	GLU	CB-CA-C	-6.08	98.25	110.40
1	A	735	ASP	CB-CG-OD1	5.95	123.66	118.30
1	B	341	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	405	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	A	810	GLU	CA-CB-CG	5.81	126.17	113.40
1	A	984	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	1104	MET	N-CA-C	-5.67	95.68	111.00
1	C	783	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	C	402	ASP	CB-CG-OD1	5.63	123.36	118.30
1	C	405	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	D	286	GLU	CB-CA-C	-5.59	99.22	110.40
1	D	533	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	677	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	B	543	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	1002	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	C	1116	ILE	CG1-CB-CG2	-5.39	99.54	111.40
1	C	545	ARG	NE-CZ-NH2	-5.36	117.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	D	845	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	783	ARG	CG-CD-NE	-5.29	100.68	111.80
1	B	33	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	D	402	ASP	CB-CG-OD1	5.23	123.00	118.30
1	A	15	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	854	ARG	CG-CD-NE	-5.17	100.95	111.80
1	B	402	ASP	CB-CG-OD1	5.16	122.94	118.30
1	D	543	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	D	1043	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	B	656	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	-3	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	B	46	GLU	CB-CA-C	-5.11	100.18	110.40
1	B	1044	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	B	15	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	1002	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	B	226	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	C	15	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	C	233	ARG	NE-CZ-NH1	5.02	122.81	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	8956	0	8931	84	0
1	B	8934	0	8899	74	0
1	C	8520	0	8510	73	0
1	D	8946	0	8906	69	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	12	1	0
3	B	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	27	0	12	3	0
3	D	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	44	0	23	0	0
5	D	44	0	23	2	0
6	A	210	0	0	3	0
6	B	243	0	0	6	0
6	C	220	0	0	5	0
6	D	246	0	0	4	0
All	All	36479	0	35340	293	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 4.

All (293) 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:B:915:VAL:HG23	6:B:1317:HOH:O	1.48	1.14
1:A:886:THR:HG22	1:A:888:GLU:OE2	1.58	1.04
1:D:690:LYS:HE2	6:D:1443:HOH:O	1.65	0.94
1:D:1078:SER:OG	1:D:1100:GLU:OE2	1.87	0.93
1:B:1010:GLN:HG3	6:B:1309:HOH:O	1.68	0.92
1:C:618:ASP:OD2	1:C:650:LYS:HE2	1.69	0.92
1:A:222:HIS:H	1:A:328:GLN:HE22	1.19	0.91
1:C:501:LYS:NZ	1:C:509:GLU:OE1	2.03	0.91
1:B:1060:LYS:HE3	1:B:1125:GLU:OE2	1.69	0.91
1:D:1078:SER:OG	1:D:1100:GLU:CG	2.19	0.90
1:B:880:MET:HA	1:B:885:LEU:CD1	2.02	0.90
1:C:677:ARG:HD3	6:C:1379:HOH:O	1.72	0.89
1:D:1060:LYS:NZ	1:D:1120:HIS:O	2.05	0.89
1:D:1078:SER:OG	1:D:1100:GLU:CD	2.18	0.81
1:B:880:MET:HA	1:B:885:LEU:HD12	1.60	0.81
1:B:405:ARG:NH2	6:B:1301:HOH:O	2.13	0.81
1:B:1076:PRO:HG3	6:B:1486:HOH:O	1.80	0.81
1:A:1078:SER:HB3	1:A:1100:GLU:OE1	1.80	0.81
1:A:618:ASP:OD2	1:A:650:LYS:HE2	1.82	0.79
1:C:1119:LEU:HD13	1:C:1134:ILE:HG12	1.63	0.79
1:A:886:THR:CG2	1:A:888:GLU:OE2	2.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:THR:CG2	1:A:888:GLU:CD	2.53	0.77
1:D:609:ASN:OD1	1:D:614:GLN:O	2.04	0.76
1:D:618:ASP:OD2	1:D:650:LYS:HE2	1.85	0.75
1:C:608:SER:HB3	1:C:647:GLN:OE1	1.86	0.75
1:D:1078:SER:OG	1:D:1100:GLU:HG3	1.85	0.74
1:C:1049:ASN:HD21	1:C:1054:GLN:HG3	1.52	0.74
1:B:1049:ASN:HD21	1:B:1054:GLN:CD	1.92	0.73
1:B:222:HIS:H	1:B:328:GLN:HE22	1.34	0.72
1:B:927:VAL:O	1:B:930:LYS:HG2	1.88	0.72
1:C:328:GLN:HA	1:C:331:ILE:HD12	1.73	0.71
1:C:984:ARG:HD2	6:C:1456:HOH:O	1.91	0.70
1:B:369:ILE:HD12	1:B:410:VAL:HG21	1.74	0.70
1:D:823:HIS:HD2	1:D:825:MET:H	1.39	0.70
1:C:369:ILE:HD12	1:C:410:VAL:HG21	1.73	0.69
1:C:608:SER:OG	1:C:609:ASN:OD1	2.09	0.69
1:A:369:ILE:HD12	1:A:410:VAL:HG21	1.74	0.69
1:C:618:ASP:OD2	1:C:650:LYS:CE	2.40	0.69
1:D:152:TYR:CE2	1:D:172:ASN:HA	2.28	0.68
1:A:886:THR:HG21	1:A:888:GLU:CD	2.12	0.68
1:B:823:HIS:HD2	1:B:825:MET:H	1.40	0.68
1:A:823:HIS:HD2	1:A:825:MET:H	1.40	0.67
1:D:369:ILE:HD12	1:D:410:VAL:HG21	1.75	0.67
1:B:908:ARG:HG2	1:B:927:VAL:HG23	1.78	0.66
1:C:908:ARG:HD3	1:C:930:LYS:HB3	1.76	0.66
1:A:886:THR:HG22	1:A:888:GLU:CD	2.13	0.66
1:B:608:SER:OG	1:B:609:ASN:OD1	2.13	0.65
1:A:886:THR:O	1:A:889:ASP:HB2	1.96	0.65
1:A:326:PRO:HB2	1:A:330:GLU:HB2	1.80	0.64
1:A:72:GLU:O	1:C:1013:LYS:NZ	2.30	0.64
1:C:823:HIS:HD2	1:C:825:MET:H	1.44	0.64
1:D:883:ASN:HB2	1:D:885:LEU:CD2	2.28	0.64
1:A:608:SER:OG	1:A:609:ASN:OD1	2.14	0.63
1:C:207:HIS:HD2	3:C:1202:ADP:O3'	1.82	0.63
1:C:745:SER:HG	5:D:1201:2BA:H2OP	1.45	0.63
1:A:168:ARG:NH1	1:A:186:GLU:OE2	2.32	0.62
1:D:885:LEU:H	1:D:885:LEU:HD23	1.63	0.62
1:B:893:ARG:HB2	1:B:896:GLU:OE1	2.00	0.61
1:C:1088:ASP:OD1	1:C:1088:ASP:N	2.33	0.61
1:A:120:LYS:HE2	1:A:199:GLU:OE2	2.01	0.60
1:C:952:ASP:OD1	1:C:956:LYS:HE2	2.01	0.60
1:C:1102:MET:O	1:C:1103:LYS:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:THR:HG22	1:A:887:GLU:N	2.16	0.60
1:C:286:GLU:OE1	3:C:1202:ADP:O1A	2.20	0.59
1:B:908:ARG:HG2	1:B:927:VAL:CG2	2.31	0.59
1:A:116:LYS:HE3	1:A:286:GLU:CG	2.33	0.59
1:C:1096:LEU:HD11	1:C:1110:ALA:HB2	1.85	0.59
1:A:952:ASP:OD1	1:A:956:LYS:HE2	2.03	0.58
1:B:293:VAL:HG23	6:B:1449:HOH:O	2.02	0.58
1:B:609:ASN:ND2	1:B:614:GLN:O	2.35	0.58
1:D:952:ASP:OD1	1:D:956:LYS:HE2	2.03	0.58
1:B:474:ASN:HD21	1:B:1051:GLN:H	1.50	0.58
1:A:474:ASN:HD21	1:A:1051:GLN:H	1.51	0.58
1:C:207:HIS:CD2	3:C:1202:ADP:O3'	2.57	0.58
1:A:167:MET:O	1:A:168:ARG:HD2	2.04	0.57
1:D:645:LEU:HD12	1:D:692:LEU:HD23	1.87	0.57
1:A:116:LYS:HE3	1:A:286:GLU:HG2	1.86	0.57
1:C:815:SER:HB3	6:D:1336:HOH:O	2.05	0.56
1:C:398:ASN:ND2	6:C:1306:HOH:O	2.38	0.56
1:C:813:ILE:HG21	1:D:803:ARG:CZ	2.35	0.56
1:D:847:ASP:OD1	1:D:850:LYS:NZ	2.32	0.56
1:D:474:ASN:HD21	1:D:1051:GLN:H	1.51	0.56
1:B:1060:LYS:CE	1:B:1125:GLU:OE2	2.49	0.56
1:C:474:ASN:HD21	1:C:1051:GLN:H	1.52	0.56
1:C:364:PRO:HG2	1:C:410:VAL:HG13	1.88	0.56
1:A:364:PRO:HG2	1:A:410:VAL:HG13	1.88	0.55
1:D:883:ASN:HB2	1:D:885:LEU:HD22	1.88	0.55
1:C:1057:VAL:O	1:C:1057:VAL:HG12	2.05	0.55
1:A:609:ASN:ND2	1:A:614:GLN:O	2.40	0.55
1:C:908:ARG:NH1	6:C:1307:HOH:O	2.40	0.54
1:B:586:TRP:CZ2	1:B:967:ILE:HD11	2.42	0.54
1:B:132:PRO:HG2	1:B:200:LYS:HD3	1.90	0.54
1:A:132:PRO:HG2	1:A:200:LYS:HD3	1.90	0.54
1:A:11:GLU:OE1	1:A:392:LYS:HE2	2.07	0.54
1:A:293:VAL:HG23	1:A:392:LYS:HE2	1.90	0.54
1:B:474:ASN:ND2	1:B:1051:GLN:H	2.05	0.54
1:C:474:ASN:ND2	1:C:1051:GLN:H	2.06	0.54
1:D:822:MET:HG2	1:D:854:ARG:HH21	1.73	0.54
1:B:364:PRO:HG2	1:B:410:VAL:HG13	1.89	0.53
1:A:888:GLU:OE2	1:A:888:GLU:N	2.32	0.53
1:D:364:PRO:HG2	1:D:410:VAL:HG13	1.89	0.53
1:C:842:LEU:HD22	1:C:845:ARG:HD3	1.91	0.53
1:D:1071:ILE:HD12	1:D:1134:ILE:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:474:ASN:ND2	1:D:1051:GLN:H	2.06	0.53
1:B:1049:ASN:HD21	1:B:1054:GLN:NE2	2.05	0.53
1:C:908:ARG:HG2	1:C:927:VAL:HG23	1.90	0.53
1:D:494:LEU:H	1:D:794:GLN:HE21	1.55	0.53
1:A:157:LYS:HE2	1:A:197:TYR:OH	2.08	0.53
1:A:813:ILE:HG21	1:B:803:ARG:CZ	2.38	0.52
1:B:880:MET:CA	1:B:885:LEU:HD12	2.36	0.52
1:D:842:LEU:HD22	1:D:845:ARG:HD3	1.92	0.52
1:A:505:ASN:HA	6:A:1429:HOH:O	2.09	0.52
1:A:612:GLY:HA3	1:A:971:MET:CE	2.39	0.52
1:D:885:LEU:N	1:D:885:LEU:HD23	2.24	0.52
1:A:474:ASN:ND2	1:A:1051:GLN:H	2.08	0.51
1:C:847:ASP:OD1	1:C:850:LYS:NZ	2.32	0.51
1:D:880:MET:O	1:D:885:LEU:HD23	2.10	0.51
1:B:167:MET:O	1:B:168:ARG:HD2	2.10	0.51
1:A:501:LYS:NZ	1:A:509:GLU:OE1	2.44	0.51
1:A:1090:VAL:HG22	1:A:1114:GLY:O	2.10	0.51
1:A:11:GLU:CD	1:A:392:LYS:HE3	2.31	0.51
1:D:341:ARG:HD3	6:D:1307:HOH:O	2.10	0.51
1:C:927:VAL:HG21	1:C:932:VAL:HG22	1.93	0.50
1:D:1080:LEU:HB2	1:D:1098:VAL:HG13	1.92	0.50
1:D:458:ARG:HH21	1:D:458:ARG:HG2	1.76	0.50
1:C:609:ASN:ND2	1:C:614:GLN:O	2.43	0.50
1:A:885:LEU:CD2	1:A:889:ASP:HB3	2.42	0.50
1:D:1077:GLY:HA3	1:D:1100:GLU:O	2.11	0.50
1:D:612:GLY:HA3	1:D:971:MET:CE	2.42	0.50
1:A:1053:VAL:O	1:A:1056:GLN:HB2	2.12	0.50
1:B:759:THR:HG21	1:B:799:TRP:CD1	2.46	0.50
1:B:612:GLY:HA3	1:B:971:MET:CE	2.42	0.50
1:B:964:HIS:O	1:B:967:ILE:HD12	2.12	0.50
1:C:886:THR:CG2	1:C:888:GLU:HG2	2.42	0.50
1:C:803:ARG:CZ	1:D:813:ILE:HG21	2.42	0.50
1:C:908:ARG:CD	1:C:930:LYS:HB3	2.42	0.50
1:D:147:ALA:O	1:D:151:GLY:HA2	2.12	0.50
1:A:109:HIS:HE1	1:A:265:VAL:O	1.95	0.50
1:A:494:LEU:H	1:A:794:GLN:HE21	1.59	0.49
1:B:880:MET:HA	1:B:885:LEU:HD13	1.92	0.49
1:D:569:TRP:CE3	1:D:633:ILE:CD1	2.95	0.49
1:A:803:ARG:CZ	1:B:813:ILE:HG21	2.43	0.49
1:A:847:ASP:OD1	1:A:850:LYS:NZ	2.32	0.49
1:B:39:VAL:H	1:B:375:ASN:ND2	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ARG:HG3	1:A:175:GLU:OE1	2.13	0.48
1:C:5:LEU:HD23	1:C:5:LEU:C	2.33	0.48
1:B:1049:ASN:ND2	1:B:1054:GLN:NE2	2.61	0.48
1:B:1101:ALA:O	1:B:1102:MET:HB2	2.12	0.48
1:D:855:LYS:O	1:D:855:LYS:HE3	2.13	0.48
1:D:109:HIS:HE1	1:D:265:VAL:O	1.96	0.48
1:D:888:GLU:O	1:D:889:ASP:C	2.48	0.48
1:B:880:MET:O	1:B:885:LEU:HD12	2.14	0.48
1:B:586:TRP:CZ2	1:B:967:ILE:CD1	2.97	0.48
1:D:120:LYS:HE2	1:D:199:GLU:OE2	2.14	0.47
1:C:126:ALA:O	1:C:260:LYS:HD3	2.14	0.47
1:C:908:ARG:HD3	1:C:930:LYS:CB	2.42	0.47
1:D:346:ASP:OD1	6:D:1301:HOH:O	2.20	0.47
1:C:109:HIS:HE1	1:C:265:VAL:O	1.97	0.47
1:B:1046:VAL:HG13	1:C:1065:THR:HB	1.97	0.47
1:A:10:GLY:HA2	6:A:1459:HOH:O	2.15	0.47
1:C:730:HIS:NE2	1:C:756:ASP:OD1	2.45	0.47
1:A:172:ASN:HB2	1:A:175:GLU:HB2	1.97	0.47
1:C:745:SER:OG	5:D:1201:2BA:O2P1	2.21	0.47
1:A:414:PHE:O	6:A:1301:HOH:O	2.21	0.47
1:B:109:HIS:HE1	1:B:265:VAL:O	1.98	0.47
1:B:886:THR:HG22	1:B:887:GLU:N	2.29	0.47
1:B:991:LEU:HD13	1:B:1011:ILE:HA	1.96	0.47
1:C:923:GLN:O	1:C:927:VAL:HG12	2.15	0.47
1:B:730:HIS:NE2	1:B:756:ASP:OD1	2.44	0.46
1:B:842:LEU:HD22	1:B:845:ARG:HD3	1.97	0.46
1:D:608:SER:OG	1:D:609:ASN:ND2	2.47	0.46
1:C:957:ILE:HD12	1:C:959:TYR:CZ	2.51	0.46
1:B:433:GLU:CD	1:B:433:GLU:H	2.18	0.46
1:C:991:LEU:HD13	1:C:1011:ILE:HA	1.96	0.46
1:D:1081:GLU:HB3	1:D:1098:VAL:HG12	1.98	0.46
1:D:886:THR:HG22	1:D:887:GLU:H	1.81	0.46
1:A:172:ASN:HB3	1:A:175:GLU:H	1.81	0.46
1:B:132:PRO:HG2	1:B:200:LYS:CD	2.46	0.46
1:C:494:LEU:H	1:C:794:GLN:HE21	1.64	0.46
1:C:886:THR:HG22	1:C:887:GLU:N	2.30	0.46
1:D:106:GLU:H	1:D:109:HIS:HD2	1.63	0.46
1:D:923:GLN:O	1:D:927:VAL:HG22	2.17	0.45
1:B:126:ALA:O	1:B:260:LYS:HD3	2.16	0.45
1:C:369:ILE:HD12	1:C:410:VAL:CG2	2.44	0.45
1:D:368:GLY:O	1:D:395:THR:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:446:ASP:OD1	1:D:446:ASP:N	2.49	0.45
1:A:269:ASN:OD1	1:A:310:GLN:HG2	2.17	0.45
1:B:618:ASP:OD2	1:B:650:LYS:HE3	2.17	0.45
1:B:842:LEU:CD2	1:B:845:ARG:HD3	2.46	0.45
1:C:221:ILE:HD11	1:C:325:LEU:HD13	1.98	0.45
1:A:886:THR:CG2	1:A:887:GLU:N	2.79	0.45
1:A:923:GLN:O	1:A:927:VAL:HG22	2.15	0.45
1:B:883:ASN:HB2	1:B:885:LEU:HD11	1.98	0.45
1:C:1085:LYS:O	1:C:1088:ASP:OD1	2.35	0.45
1:C:4:LEU:HD23	1:C:5:LEU:N	2.31	0.45
1:D:730:HIS:NE2	1:D:756:ASP:OD1	2.45	0.45
1:D:759:THR:HG21	1:D:799:TRP:CD1	2.52	0.45
1:A:462:THR:OG1	1:A:1044:ARG:NH1	2.50	0.45
1:A:922:LEU:HG	1:A:926:ILE:HD12	1.99	0.45
1:B:120:LYS:NZ	1:B:131:ILE:O	2.47	0.45
1:A:369:ILE:HD12	1:A:410:VAL:CG2	2.45	0.45
1:C:4:LEU:C	1:C:4:LEU:HD23	2.37	0.45
1:D:922:LEU:HG	1:D:926:ILE:HD12	1.99	0.45
1:A:957:ILE:HD12	1:A:959:TYR:CZ	2.52	0.44
1:C:39:VAL:H	1:C:375:ASN:ND2	2.15	0.44
1:C:250:PHE:CZ	1:C:280:ASP:HA	2.53	0.44
1:D:39:VAL:H	1:D:375:ASN:ND2	2.15	0.44
1:A:1096:LEU:HD11	1:A:1110:ALA:HB2	2.00	0.44
1:D:957:ILE:HD12	1:D:959:TYR:CZ	2.53	0.44
1:A:207:HIS:ND1	3:A:1202:ADP:O3'	2.40	0.44
1:B:586:TRP:HZ2	1:B:967:ILE:CD1	2.31	0.44
1:A:885:LEU:HD22	1:A:889:ASP:HB3	1.98	0.44
1:B:82:TYR:CZ	1:B:293:VAL:HG22	2.53	0.44
1:B:369:ILE:HD12	1:B:410:VAL:CG2	2.46	0.44
1:D:991:LEU:HD13	1:D:1011:ILE:HA	1.99	0.44
1:D:886:THR:HG22	1:D:887:GLU:N	2.33	0.44
1:A:759:THR:HG21	1:A:799:TRP:CD1	2.53	0.44
1:D:152:TYR:CD2	1:D:172:ASN:HA	2.53	0.44
1:D:569:TRP:CE3	1:D:633:ILE:HD12	2.52	0.44
1:B:221:ILE:HD11	1:B:325:LEU:HD13	2.00	0.44
1:A:1084:VAL:HG12	1:A:1085:LYS:N	2.33	0.43
1:A:39:VAL:H	1:A:375:ASN:ND2	2.16	0.43
1:D:502:THR:H	1:D:505:ASN:HD22	1.66	0.43
1:A:146:PHE:CE1	1:A:150:TYR:CD2	3.05	0.43
1:C:368:GLY:O	1:C:395:THR:HA	2.19	0.43
1:B:586:TRP:HZ2	1:B:967:ILE:HD13	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:880:MET:HA	1:D:885:LEU:CD2	2.48	0.43
1:A:1104:MET:HG2	1:A:1104:MET:H	1.63	0.43
1:A:198:VAL:HG12	1:A:199:GLU:N	2.34	0.43
1:B:161:GLY:HA2	1:B:191:PHE:CZ	2.54	0.43
1:B:368:GLY:O	1:B:395:THR:HA	2.18	0.43
1:A:578:TYR:CZ	1:A:585:PRO:HD2	2.54	0.43
1:C:116:LYS:HD3	1:C:116:LYS:HA	1.84	0.43
1:C:216:ARG:HD2	6:C:1345:HOH:O	2.18	0.43
1:B:1084:VAL:HG12	1:B:1085:LYS:N	2.34	0.43
1:D:4:LEU:HD23	1:D:4:LEU:C	2.39	0.43
1:A:221:ILE:HD11	1:A:325:LEU:HD13	2.01	0.43
1:B:269:ASN:OD1	1:B:310:GLN:HG2	2.19	0.43
1:A:701:ALA:HA	1:A:730:HIS:O	2.19	0.42
1:B:922:LEU:HG	1:B:926:ILE:HD12	2.01	0.42
1:A:1011:ILE:O	1:A:1011:ILE:CG2	2.66	0.42
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.85	0.42
1:A:368:GLY:O	1:A:395:THR:HA	2.19	0.42
1:C:269:ASN:OD1	1:C:310:GLN:HG2	2.18	0.42
1:D:612:GLY:N	1:D:971:MET:CE	2.83	0.42
1:A:250:PHE:CZ	1:A:280:ASP:HA	2.54	0.42
1:C:502:THR:H	1:C:505:ASN:HD22	1.68	0.42
1:C:608:SER:CB	1:C:647:GLN:OE1	2.64	0.42
1:D:840:VAL:HG12	1:D:840:VAL:O	2.19	0.42
1:D:890:VAL:HG13	1:D:899:PHE:CZ	2.54	0.42
1:A:730:HIS:NE2	1:A:756:ASP:OD1	2.45	0.42
1:B:1096:LEU:HD11	1:B:1110:ALA:HB2	2.00	0.42
1:C:1119:LEU:CD1	1:C:1134:ILE:HG12	2.41	0.42
1:C:922:LEU:HG	1:C:926:ILE:HD12	2.01	0.42
1:A:1011:ILE:O	1:A:1011:ILE:HG22	2.20	0.42
1:C:759:THR:HG21	1:C:799:TRP:CD1	2.55	0.42
1:A:840:VAL:O	1:A:840:VAL:HG12	2.19	0.42
1:B:106:GLU:H	1:B:109:HIS:HD2	1.68	0.42
1:B:132:PRO:HB2	1:B:200:LYS:HD2	2.02	0.42
1:B:840:VAL:HG12	1:B:840:VAL:O	2.20	0.42
1:D:269:ASN:OD1	1:D:310:GLN:HG2	2.19	0.42
1:A:165:ARG:NH1	1:A:190:ALA:HB1	2.35	0.41
1:B:4:LEU:HD23	1:B:4:LEU:C	2.41	0.41
1:C:840:VAL:O	1:C:840:VAL:HG12	2.19	0.41
1:A:1100:GLU:HA	1:A:1104:MET:O	2.20	0.41
1:C:1129:THR:O	1:C:1130:GLN:HB2	2.20	0.41
1:C:338:ILE:O	1:C:394:CYS:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ALA:O	1:A:251:ARG:HD2	2.21	0.41
1:D:880:MET:HA	1:D:885:LEU:HD21	2.02	0.41
1:A:502:THR:H	1:A:505:ASN:HD22	1.68	0.41
1:C:367:PHE:O	1:C:406:LYS:HE3	2.20	0.41
1:A:1102:MET:O	1:A:1103:LYS:HB2	2.21	0.41
1:A:153:PRO:HG2	1:A:201:TYR:CD2	2.56	0.41
1:D:157:LYS:HE2	1:D:197:TYR:OH	2.21	0.41
1:A:338:ILE:O	1:A:394:CYS:HA	2.21	0.41
1:A:775:TYR:C	1:A:775:TYR:CD1	2.94	0.41
1:D:533:ARG:HD2	1:D:533:ARG:C	2.41	0.41
1:B:957:ILE:HD12	1:B:959:TYR:CZ	2.55	0.41
1:D:1129:THR:O	1:D:1130:GLN:HB2	2.21	0.41
1:A:1071:ILE:HD12	1:A:1134:ILE:HG23	2.02	0.41
1:B:1077:GLY:HA3	1:B:1100:GLU:O	2.21	0.41
1:B:178:ASP:OD1	1:B:182:ARG:NH1	2.54	0.41
1:B:220:ILE:HD12	1:B:263:LYS:HA	2.04	0.40
1:C:993:ASP:OD2	1:C:995:PRO:HD2	2.21	0.40
1:B:1010:GLN:CG	6:B:1309:HOH:O	2.46	0.40
1:B:1013:LYS:NZ	1:D:72:GLU:O	2.55	0.40
1:B:250:PHE:CZ	1:B:280:ASP:HA	2.56	0.40
1:C:1053:VAL:O	1:C:1056:GLN:HB2	2.20	0.40
1:D:462:THR:OG1	1:D:1044:ARG:NH1	2.54	0.40
1:B:964:HIS:HA	1:B:967:ILE:HD11	2.02	0.40
1:A:457:LEU:HA	1:A:457:LEU:HD12	1.83	0.40
1:C:1077:GLY:HA3	1:C:1100:GLU:O	2.21	0.40
1:A:1129:THR:O	1:A:1130:GLN:HB2	2.21	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	1142/1145 (100%)	1114 (98%)	28 (2%)	0	100	100
1	B	1138/1145 (99%)	1110 (98%)	27 (2%)	1 (0%)	55	67
1	C	1079/1145 (94%)	1053 (98%)	25 (2%)	1 (0%)	55	67
1	D	1140/1145 (100%)	1114 (98%)	25 (2%)	1 (0%)	55	67
All	All	4499/4580 (98%)	4391 (98%)	105 (2%)	3 (0%)	55	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	269	ASN
1	D	269	ASN
1	B	269	ASN

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	955/956 (100%)	924 (97%)	31 (3%)	44	60
1	B	953/956 (100%)	928 (97%)	25 (3%)	51	69
1	C	917/956 (96%)	898 (98%)	19 (2%)	59	76
1	D	953/956 (100%)	927 (97%)	26 (3%)	50	67
All	All	3778/3824 (99%)	3677 (97%)	101 (3%)	50	67

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	165	ARG
1	A	168	ARG
1	A	171	ARG
1	A	173	ASP
1	A	186	GLU
1	A	200	LYS
1	A	263	LYS

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Mol	Chain	Res	Type
1	A	280	ASP
1	A	398	ASN
1	A	457	LEU
1	A	460	ARG
1	A	499	LYS
1	A	569	TRP
1	A	690	LYS
1	A	705	MET
1	A	832	ASN
1	A	834	LYS
1	A	854	ARG
1	A	855	LYS
1	A	884	ASP
1	A	888	GLU
1	A	893	ARG
1	A	901	GLU
1	A	929	ASP
1	A	1006	LYS
1	A	1074	THR
1	A	1102	MET
1	A	1104	MET
1	A	1107	THR
1	A	1123	LYS
1	B	135	ASN
1	B	160	LEU
1	B	182	ARG
1	B	280	ASP
1	B	489	GLU
1	B	499	LYS
1	B	542	THR
1	B	569	TRP
1	B	705	MET
1	B	832	ASN
1	B	834	LYS
1	B	870	SER
1	B	884	ASP
1	B	885	LEU
1	B	896	GLU
1	B	901	GLU
1	B	927	VAL
1	B	930	LYS
1	B	1006	LYS

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Mol	Chain	Res	Type
1	B	1010	GLN
1	B	1013	LYS
1	B	1054	GLN
1	B	1060	LYS
1	B	1119	LEU
1	B	1123	LYS
1	C	120	LYS
1	C	280	ASP
1	C	398	ASN
1	C	457	LEU
1	C	499	LYS
1	C	542	THR
1	C	569	TRP
1	C	705	MET
1	C	834	LYS
1	C	921	LYS
1	C	928	LYS
1	C	1010	GLN
1	C	1013	LYS
1	C	1088	ASP
1	C	1091	GLN
1	C	1102	MET
1	C	1104	MET
1	C	1116	ILE
1	C	1123	LYS
1	D	26	SER
1	D	120	LYS
1	D	135	ASN
1	D	157	LYS
1	D	168	ARG
1	D	182	ARG
1	D	280	ASP
1	D	446	ASP
1	D	542	THR
1	D	569	TRP
1	D	591	LYS
1	D	705	MET
1	D	727	LEU
1	D	855	LYS
1	D	884	ASP
1	D	885	LEU
1	D	888	GLU

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Mol	Chain	Res	Type
1	D	901	GLU
1	D	929	ASP
1	D	1010	GLN
1	D	1060	LYS
1	D	1074	THR
1	D	1075	MET
1	D	1078	SER
1	D	1100	GLU
1	D	1119	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	HIS
1	A	219	ASN
1	A	308	GLN
1	A	328	GLN
1	A	375	ASN
1	A	412	HIS
1	A	439	GLN
1	A	474	ASN
1	A	481	ASN
1	A	505	ASN
1	A	547	GLN
1	A	739	ASN
1	A	794	GLN
1	A	817	GLN
1	A	823	HIS
1	A	832	ASN
1	A	1010	GLN
1	A	1069	ASN
1	A	1094	GLN
1	B	109	HIS
1	B	219	ASN
1	B	308	GLN
1	B	328	GLN
1	B	375	ASN
1	B	412	HIS
1	B	439	GLN
1	B	474	ASN
1	B	481	ASN
1	B	505	ASN

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Mol	Chain	Res	Type
1	B	547	GLN
1	B	582	ASN
1	B	739	ASN
1	B	817	GLN
1	B	823	HIS
1	B	832	ASN
1	B	983	GLN
1	B	1010	GLN
1	B	1049	ASN
1	B	1054	GLN
1	B	1069	ASN
1	B	1094	GLN
1	C	109	HIS
1	C	207	HIS
1	C	219	ASN
1	C	308	GLN
1	C	375	ASN
1	C	398	ASN
1	C	412	HIS
1	C	439	GLN
1	C	474	ASN
1	C	481	ASN
1	C	505	ASN
1	C	547	GLN
1	C	739	ASN
1	C	794	GLN
1	C	823	HIS
1	C	829	GLN
1	C	832	ASN
1	C	940	HIS
1	C	1049	ASN
1	C	1094	GLN
1	D	109	HIS
1	D	177	HIS
1	D	219	ASN
1	D	308	GLN
1	D	375	ASN
1	D	412	HIS
1	D	439	GLN
1	D	474	ASN
1	D	481	ASN
1	D	505	ASN

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Mol	Chain	Res	Type
1	D	547	GLN
1	D	609	ASN
1	D	615	ASN
1	D	739	ASN
1	D	794	GLN
1	D	823	HIS
1	D	1010	GLN
1	D	1049	ASN
1	D	1054	GLN
1	D	1094	GLN
1	D	1128	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](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
3	ADP	A	1202	4	25,29,29	0.97	1 (4%)	24,45,45	1.69	1 (4%)
5	2BA	A	1204	-	44,50,50	1.25	6 (13%)	46,78,78	1.98	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	B	1202	4	25,29,29	1.23	4 (16%)	24,45,45	1.55	5 (20%)
3	ADP	C	1202	4	25,29,29	1.47	5 (20%)	24,45,45	1.95	5 (20%)
5	2BA	D	1201	-	44,50,50	1.33	7 (15%)	46,78,78	2.06	7 (15%)
3	ADP	D	1203	4	25,29,29	1.35	4 (16%)	24,45,45	1.63	3 (12%)

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
3	ADP	A	1202	4	-	0/12/32/32	0/3/3/3
5	2BA	A	1204	-	-	0/22/62/62	0/6/7/7
3	ADP	B	1202	4	-	0/12/32/32	0/3/3/3
3	ADP	C	1202	4	-	0/12/32/32	0/3/3/3
5	2BA	D	1201	-	-	0/22/62/62	0/6/7/7
3	ADP	D	1203	4	-	0/12/32/32	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1201	2BA	C2'-C1'	-3.14	1.48	1.53
5	A	1204	2BA	C2'-C1'	-2.95	1.49	1.53
5	D	1201	2BA	O4'-C1'1	-2.84	1.37	1.41
3	B	1202	ADP	C2'-C1'	-2.51	1.49	1.53
3	D	1203	ADP	C4-N3	-2.32	1.32	1.35
3	D	1203	ADP	C2'-C1'	-2.22	1.50	1.53
5	A	1204	2BA	C51-N71	-2.16	1.32	1.39
5	D	1201	2BA	C51-N71	-2.05	1.32	1.39
3	C	1202	ADP	C2-N1	2.04	1.37	1.33
5	D	1201	2BA	C81-N71	2.06	1.38	1.34
5	A	1204	2BA	C21-N11	2.07	1.37	1.33
5	D	1201	2BA	C5-C4	2.12	1.45	1.40
5	D	1201	2BA	C2-N1	2.12	1.37	1.33
5	A	1204	2BA	C2-N3	2.20	1.35	1.32
3	B	1202	ADP	C2-N1	2.36	1.38	1.33
3	D	1203	ADP	O4'-C1'	2.38	1.44	1.41
3	B	1202	ADP	C2-N3	2.39	1.36	1.32
3	A	1202	ADP	C5-C4	2.50	1.46	1.40
5	A	1204	2BA	C4-N3	2.56	1.39	1.35
3	C	1202	ADP	C2-N3	2.59	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1202	ADP	O4'-C1'	2.73	1.45	1.41
3	D	1203	ADP	C5-C4	3.00	1.47	1.40
3	B	1202	ADP	C5-C4	3.00	1.47	1.40
5	D	1201	2BA	C21-N31	3.01	1.37	1.32
5	A	1204	2BA	C51-C41	3.24	1.47	1.40
3	C	1202	ADP	PB-O3A	3.31	1.65	1.60
3	C	1202	ADP	C5-C4	3.40	1.48	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1201	2BA	N31-C21-N11	-8.32	121.61	128.86
5	A	1204	2BA	N3-C2-N1	-7.82	122.05	128.86
3	C	1202	ADP	N3-C2-N1	-7.09	122.69	128.86
5	A	1204	2BA	N31-C21-N11	-6.97	122.79	128.86
3	A	1202	ADP	N3-C2-N1	-6.86	122.89	128.86
5	D	1201	2BA	N3-C2-N1	-6.22	123.44	128.86
3	D	1203	ADP	N3-C2-N1	-4.92	124.58	128.86
3	B	1202	ADP	N3-C2-N1	-3.56	125.75	128.86
5	D	1201	2BA	C51-C61-N61	-3.34	113.66	120.47
5	A	1204	2BA	C5-C6-N6	-3.18	113.98	120.47
5	D	1201	2BA	O5'1-P1-O1P1	-3.15	96.55	109.25
3	C	1202	ADP	C1'-N9-C4	-2.98	121.49	126.64
3	B	1202	ADP	O2'-C2'-C1'	-2.76	102.97	111.61
5	D	1201	2BA	C2'1-C3'1-C4'1	-2.70	98.41	103.23
3	B	1202	ADP	C4-C5-N7	-2.68	106.82	109.41
5	A	1204	2BA	C1'-N9-C4	-2.32	122.63	126.64
3	C	1202	ADP	C4-C5-N7	-2.22	107.26	109.41
5	A	1204	2BA	C41-C51-N71	-2.04	107.44	109.41
5	D	1201	2BA	N61-C61-N11	2.06	122.85	118.77
3	C	1202	ADP	O2A-PA-O1A	2.10	123.13	112.28
3	B	1202	ADP	O3B-PB-O2B	2.20	116.50	107.61
5	A	1204	2BA	C21-N11-C61	2.23	122.67	118.77
3	B	1202	ADP	N6-C6-N1	2.35	123.43	118.77
3	C	1202	ADP	O3'-C3'-C4'	2.36	117.98	111.09
5	A	1204	2BA	N61-C61-N11	2.91	124.54	118.77
3	D	1203	ADP	O3B-PB-O1B	3.02	122.32	110.50
3	D	1203	ADP	N6-C6-N1	3.30	125.30	118.77
5	D	1201	2BA	N6-C6-N1	3.44	125.59	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1202	ADP	1	0
3	C	1202	ADP	3	0
5	D	1201	2BA	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 ⓘ

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	1144/1145 (99%)	-0.20	39 (3%)	46	53	12, 35, 79, 126	0
1	B	1142/1145 (99%)	-0.26	39 (3%)	46	53	12, 33, 78, 108	0
1	C	1083/1145 (94%)	-0.23	39 (3%)	43	50	14, 35, 77, 113	0
1	D	1144/1145 (99%)	-0.14	53 (4%)	33	40	15, 34, 82, 111	0
All	All	4513/4580 (98%)	-0.21	170 (3%)	41	48	12, 34, 80, 126	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	201	TYR	6.7
1	D	189	GLY	5.9
1	B	457	LEU	5.6
1	A	1102	MET	5.1
1	D	892	ALA	5.1
1	C	198	VAL	5.1
1	A	1057	VAL	5.0
1	D	890	VAL	5.0
1	C	197	TYR	4.8
1	A	1103	LYS	4.7
1	B	135	ASN	4.4
1	B	897	LEU	4.2
1	C	1082	ILE	4.2
1	D	929	ASP	4.1
1	B	149	THR	4.0
1	C	892	ALA	4.0
1	A	1058	VAL	4.0
1	D	1103	LYS	4.0
1	A	191	PHE	3.9
1	D	896	GLU	3.9
1	B	150	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	1081	GLU	3.9
1	A	194	GLY	3.9
1	A	885	LEU	3.8
1	D	181	ALA	3.8
1	A	881	ILE	3.8
1	A	892	ALA	3.7
1	C	1083	LEU	3.6
1	C	1123	LYS	3.6
1	B	146	PHE	3.6
1	D	187	ALA	3.5
1	B	148	LYS	3.5
1	C	202	ILE	3.5
1	B	139	ASP	3.5
1	C	131	ILE	3.4
1	C	1081	GLU	3.4
1	D	1122	VAL	3.4
1	A	163	GLY	3.4
1	D	1083	LEU	3.4
1	D	891	TYR	3.4
1	C	896	GLU	3.3
1	B	845	ARG	3.3
1	B	147	ALA	3.3
1	C	1084	VAL	3.3
1	B	1080	LEU	3.3
1	B	195	GLU	3.2
1	C	890	VAL	3.2
1	C	199	GLU	3.2
1	C	1057	VAL	3.2
1	A	1101	ALA	3.2
1	D	897	LEU	3.2
1	D	1086	ALA	3.2
1	B	151	GLY	3.2
1	B	181	ALA	3.1
1	D	881	ILE	3.1
1	B	888	GLU	3.1
1	D	139	ASP	3.1
1	B	892	ALA	3.1
1	D	1101	ALA	3.1
1	B	144	LEU	3.1
1	A	1055	ALA	3.1
1	D	178	ASP	3.0
1	C	132	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1086	ALA	3.0
1	A	187	ALA	3.0
1	D	1127	ILE	3.0
1	D	174	ALA	3.0
1	D	1126	ALA	3.0
1	C	1103	LYS	3.0
1	B	838	ALA	2.9
1	B	177	HIS	2.9
1	D	185	SER	2.9
1	C	891	TYR	2.9
1	A	1126	ALA	2.9
1	D	1104	MET	2.9
1	B	844	HIS	2.9
1	A	844	HIS	2.8
1	D	1105	GLU	2.8
1	C	1093	GLY	2.8
1	D	884	ASP	2.8
1	D	852	MET	2.8
1	B	896	GLU	2.8
1	D	841	GLY	2.7
1	C	1106	THR	2.7
1	C	1087	GLY	2.7
1	A	164	GLY	2.7
1	B	1122	VAL	2.7
1	B	842	LEU	2.7
1	D	888	GLU	2.7
1	C	456	ARG	2.7
1	A	929	ASP	2.7
1	D	840	VAL	2.7
1	D	1058	VAL	2.7
1	D	1080	LEU	2.7
1	D	1102	MET	2.6
1	A	891	TYR	2.6
1	C	946	PHE	2.6
1	B	1057	VAL	2.6
1	B	884	ASP	2.6
1	D	889	ASP	2.6
1	A	895	ASN	2.6
1	D	898	ASN	2.6
1	A	1096	LEU	2.5
1	D	1096	LEU	2.5
1	C	1085	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	142	GLY	2.5
1	A	135	ASN	2.5
1	B	1101	ALA	2.5
1	C	203	GLU	2.5
1	C	1111	PRO	2.5
1	B	1124	GLY	2.5
1	A	1122	VAL	2.5
1	D	886	THR	2.5
1	A	1105	GLU	2.5
1	C	1124	GLY	2.5
1	A	897	LEU	2.5
1	C	942	GLU	2.4
1	C	1086	ALA	2.4
1	D	844	HIS	2.4
1	A	1104	MET	2.4
1	C	1058	VAL	2.4
1	D	838	ALA	2.4
1	B	898	ASN	2.4
1	B	185	SER	2.4
1	A	946	PHE	2.4
1	B	891	TYR	2.4
1	B	895	ASN	2.4
1	D	143	ALA	2.4
1	D	893	ARG	2.4
1	C	884	ASP	2.4
1	A	1095	ALA	2.4
1	C	1116	ILE	2.3
1	C	1101	ALA	2.3
1	C	1126	ALA	2.3
1	D	931	ALA	2.3
1	B	152	TYR	2.3
1	D	894	GLY	2.3
1	A	888	GLU	2.2
1	A	898	ASN	2.2
1	D	148	LYS	2.2
1	A	842	LEU	2.2
1	C	200	LYS	2.2
1	C	898	ASN	2.2
1	C	842	LEU	2.2
1	B	885	LEU	2.2
1	A	893	ARG	2.2
1	D	1079	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	926	ILE	2.2
1	B	174	ALA	2.2
1	D	177	HIS	2.2
1	D	1095	ALA	2.1
1	D	144	LEU	2.1
1	B	615	ASN	2.1
1	C	841	GLY	2.1
1	D	1085	LYS	2.1
1	A	947	GLU	2.1
1	D	851	GLN	2.1
1	B	881	ILE	2.1
1	D	845	ARG	2.1
1	A	189	GLY	2.1
1	B	138	VAL	2.1
1	C	881	ILE	2.0
1	A	190	ALA	2.0
1	A	186	GLU	2.0
1	A	890	VAL	2.0
1	A	1100	GLU	2.0
1	A	181	ALA	2.0
1	D	180	TYR	2.0
1	B	189	GLY	2.0
1	D	1123	LYS	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, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	ADP	C	1202	27/27	0.93	0.25	0.30	59,67,73,77	0
2	MN	C	1201	1/1	0.99	0.12	0.22	45,45,45,45	0
5	2BA	A	1204	44/44	0.98	0.12	-0.40	14,19,20,22	0
3	ADP	A	1202	27/27	0.97	0.09	-0.52	35,41,59,66	0
5	2BA	D	1201	44/44	0.99	0.12	-0.69	14,18,22,25	0
2	MN	D	1202	1/1	0.98	0.14	-0.79	45,45,45,45	0
3	ADP	B	1202	27/27	0.97	0.07	-1.03	35,39,61,65	0
2	MN	B	1201	1/1	0.98	0.11	-1.16	50,50,50,50	0
3	ADP	D	1203	27/27	0.96	0.08	-1.19	34,46,56,57	0
2	MN	A	1201	1/1	0.98	0.12	-1.21	50,50,50,50	0
4	MG	B	1203	1/1	0.97	0.07	-	31,31,31,31	0
4	MG	D	1204	1/1	0.97	0.17	-	31,31,31,31	0
4	MG	C	1203	1/1	0.98	0.06	-	47,47,47,47	0
4	MG	A	1203	1/1	0.95	0.07	-	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.