



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:42 PM GMT

PDB ID : 4MFD
Title : Structure of the carboxyl transferase domain from *Rhizobium etli* pyruvate carboxylase with oxalate
Authors : Lietzan, A.D.; St. Maurice, M.
Deposited on : 2013-08-27
Resolution : 2.55 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 (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

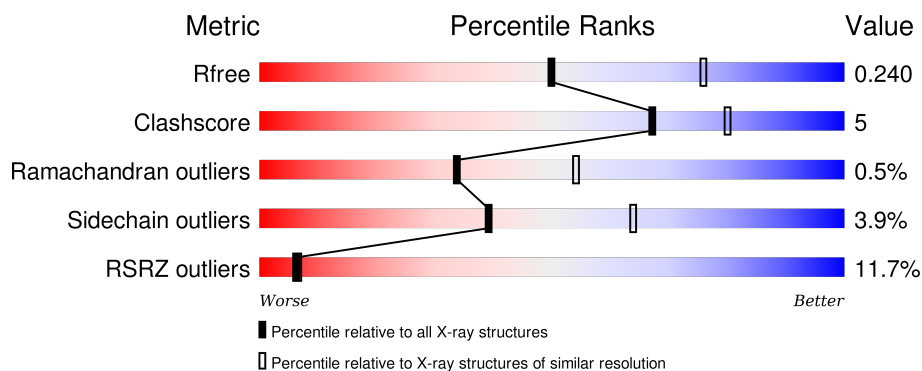
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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	632	
1	B	632	
1	C	632	
1	D	632	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	C	1104	-	-	X	-
6	GOL	B	1105	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18052 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	597	Total	C	N	O	S	0	1	0
			4557	2897	764	873	23			
1	B	597	Total	C	N	O	S	0	1	0
			4522	2878	759	862	23			
1	C	596	Total	C	N	O	S	0	1	0
			4368	2767	741	837	23			
1	D	597	Total	C	N	O	S	0	1	0
			4367	2752	746	846	23			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	MET	-	EXPRESSION TAG	UNP Q2K340
A	437	GLY	-	EXPRESSION TAG	UNP Q2K340
A	438	SER	-	EXPRESSION TAG	UNP Q2K340
A	439	SER	-	EXPRESSION TAG	UNP Q2K340
A	440	HIS	-	EXPRESSION TAG	UNP Q2K340
A	441	HIS	-	EXPRESSION TAG	UNP Q2K340
A	442	HIS	-	EXPRESSION TAG	UNP Q2K340
A	443	HIS	-	EXPRESSION TAG	UNP Q2K340
A	444	HIS	-	EXPRESSION TAG	UNP Q2K340
A	445	HIS	-	EXPRESSION TAG	UNP Q2K340
A	446	HIS	-	EXPRESSION TAG	UNP Q2K340
A	447	HIS	-	EXPRESSION TAG	UNP Q2K340
A	448	ASP	-	EXPRESSION TAG	UNP Q2K340
A	449	TYR	-	EXPRESSION TAG	UNP Q2K340
A	450	ASP	-	EXPRESSION TAG	UNP Q2K340
A	451	ILE	-	EXPRESSION TAG	UNP Q2K340
A	452	PRO	-	EXPRESSION TAG	UNP Q2K340
A	453	THR	-	EXPRESSION TAG	UNP Q2K340
A	454	SER	-	EXPRESSION TAG	UNP Q2K340
A	455	GLU	-	EXPRESSION TAG	UNP Q2K340
A	456	ASN	-	EXPRESSION TAG	UNP Q2K340

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Chain	Residue	Modelled	Actual	Comment	Reference
A	457	LEU	-	EXPRESSION TAG	UNP Q2K340
A	458	TYR	-	EXPRESSION TAG	UNP Q2K340
A	459	PHE	-	EXPRESSION TAG	UNP Q2K340
A	460	GLN	-	EXPRESSION TAG	UNP Q2K340
A	461	GLY	-	EXPRESSION TAG	UNP Q2K340
A	462	LEU	-	EXPRESSION TAG	UNP Q2K340
A	463	LEU	-	EXPRESSION TAG	UNP Q2K340
A	464	HIS	-	EXPRESSION TAG	UNP Q2K340
B	436	MET	-	EXPRESSION TAG	UNP Q2K340
B	437	GLY	-	EXPRESSION TAG	UNP Q2K340
B	438	SER	-	EXPRESSION TAG	UNP Q2K340
B	439	SER	-	EXPRESSION TAG	UNP Q2K340
B	440	HIS	-	EXPRESSION TAG	UNP Q2K340
B	441	HIS	-	EXPRESSION TAG	UNP Q2K340
B	442	HIS	-	EXPRESSION TAG	UNP Q2K340
B	443	HIS	-	EXPRESSION TAG	UNP Q2K340
B	444	HIS	-	EXPRESSION TAG	UNP Q2K340
B	445	HIS	-	EXPRESSION TAG	UNP Q2K340
B	446	HIS	-	EXPRESSION TAG	UNP Q2K340
B	447	HIS	-	EXPRESSION TAG	UNP Q2K340
B	448	ASP	-	EXPRESSION TAG	UNP Q2K340
B	449	TYR	-	EXPRESSION TAG	UNP Q2K340
B	450	ASP	-	EXPRESSION TAG	UNP Q2K340
B	451	ILE	-	EXPRESSION TAG	UNP Q2K340
B	452	PRO	-	EXPRESSION TAG	UNP Q2K340
B	453	THR	-	EXPRESSION TAG	UNP Q2K340
B	454	SER	-	EXPRESSION TAG	UNP Q2K340
B	455	GLU	-	EXPRESSION TAG	UNP Q2K340
B	456	ASN	-	EXPRESSION TAG	UNP Q2K340
B	457	LEU	-	EXPRESSION TAG	UNP Q2K340
B	458	TYR	-	EXPRESSION TAG	UNP Q2K340
B	459	PHE	-	EXPRESSION TAG	UNP Q2K340
B	460	GLN	-	EXPRESSION TAG	UNP Q2K340
B	461	GLY	-	EXPRESSION TAG	UNP Q2K340
B	462	LEU	-	EXPRESSION TAG	UNP Q2K340
B	463	LEU	-	EXPRESSION TAG	UNP Q2K340
B	464	HIS	-	EXPRESSION TAG	UNP Q2K340
C	436	MET	-	EXPRESSION TAG	UNP Q2K340
C	437	GLY	-	EXPRESSION TAG	UNP Q2K340
C	438	SER	-	EXPRESSION TAG	UNP Q2K340
C	439	SER	-	EXPRESSION TAG	UNP Q2K340
C	440	HIS	-	EXPRESSION TAG	UNP Q2K340

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Chain	Residue	Modelled	Actual	Comment	Reference
C	441	HIS	-	EXPRESSION TAG	UNP Q2K340
C	442	HIS	-	EXPRESSION TAG	UNP Q2K340
C	443	HIS	-	EXPRESSION TAG	UNP Q2K340
C	444	HIS	-	EXPRESSION TAG	UNP Q2K340
C	445	HIS	-	EXPRESSION TAG	UNP Q2K340
C	446	HIS	-	EXPRESSION TAG	UNP Q2K340
C	447	HIS	-	EXPRESSION TAG	UNP Q2K340
C	448	ASP	-	EXPRESSION TAG	UNP Q2K340
C	449	TYR	-	EXPRESSION TAG	UNP Q2K340
C	450	ASP	-	EXPRESSION TAG	UNP Q2K340
C	451	ILE	-	EXPRESSION TAG	UNP Q2K340
C	452	PRO	-	EXPRESSION TAG	UNP Q2K340
C	453	THR	-	EXPRESSION TAG	UNP Q2K340
C	454	SER	-	EXPRESSION TAG	UNP Q2K340
C	455	GLU	-	EXPRESSION TAG	UNP Q2K340
C	456	ASN	-	EXPRESSION TAG	UNP Q2K340
C	457	LEU	-	EXPRESSION TAG	UNP Q2K340
C	458	TYR	-	EXPRESSION TAG	UNP Q2K340
C	459	PHE	-	EXPRESSION TAG	UNP Q2K340
C	460	GLN	-	EXPRESSION TAG	UNP Q2K340
C	461	GLY	-	EXPRESSION TAG	UNP Q2K340
C	462	LEU	-	EXPRESSION TAG	UNP Q2K340
C	463	LEU	-	EXPRESSION TAG	UNP Q2K340
C	464	HIS	-	EXPRESSION TAG	UNP Q2K340
D	436	MET	-	EXPRESSION TAG	UNP Q2K340
D	437	GLY	-	EXPRESSION TAG	UNP Q2K340
D	438	SER	-	EXPRESSION TAG	UNP Q2K340
D	439	SER	-	EXPRESSION TAG	UNP Q2K340
D	440	HIS	-	EXPRESSION TAG	UNP Q2K340
D	441	HIS	-	EXPRESSION TAG	UNP Q2K340
D	442	HIS	-	EXPRESSION TAG	UNP Q2K340
D	443	HIS	-	EXPRESSION TAG	UNP Q2K340
D	444	HIS	-	EXPRESSION TAG	UNP Q2K340
D	445	HIS	-	EXPRESSION TAG	UNP Q2K340
D	446	HIS	-	EXPRESSION TAG	UNP Q2K340
D	447	HIS	-	EXPRESSION TAG	UNP Q2K340
D	448	ASP	-	EXPRESSION TAG	UNP Q2K340
D	449	TYR	-	EXPRESSION TAG	UNP Q2K340
D	450	ASP	-	EXPRESSION TAG	UNP Q2K340
D	451	ILE	-	EXPRESSION TAG	UNP Q2K340
D	452	PRO	-	EXPRESSION TAG	UNP Q2K340
D	453	THR	-	EXPRESSION TAG	UNP Q2K340

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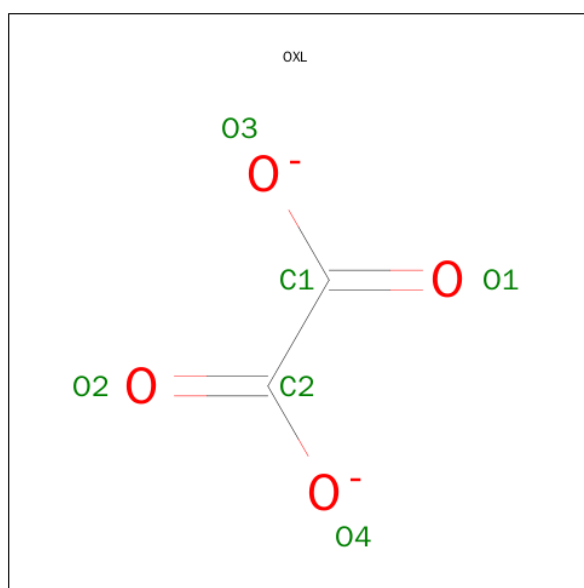
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Chain	Residue	Modelled	Actual	Comment	Reference
D	454	SER	-	EXPRESSION TAG	UNP Q2K340
D	455	GLU	-	EXPRESSION TAG	UNP Q2K340
D	456	ASN	-	EXPRESSION TAG	UNP Q2K340
D	457	LEU	-	EXPRESSION TAG	UNP Q2K340
D	458	TYR	-	EXPRESSION TAG	UNP Q2K340
D	459	PHE	-	EXPRESSION TAG	UNP Q2K340
D	460	GLN	-	EXPRESSION TAG	UNP Q2K340
D	461	GLY	-	EXPRESSION TAG	UNP Q2K340
D	462	LEU	-	EXPRESSION TAG	UNP Q2K340
D	463	LEU	-	EXPRESSION TAG	UNP Q2K340
D	464	HIS	-	EXPRESSION TAG	UNP Q2K340

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C₂O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 2 4	0	0
3	B	1	Total C O 6 2 4	0	0
3	C	1	Total C O 6 2 4	0	0
3	D	1	Total C O 6 2 4	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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0
5	A	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

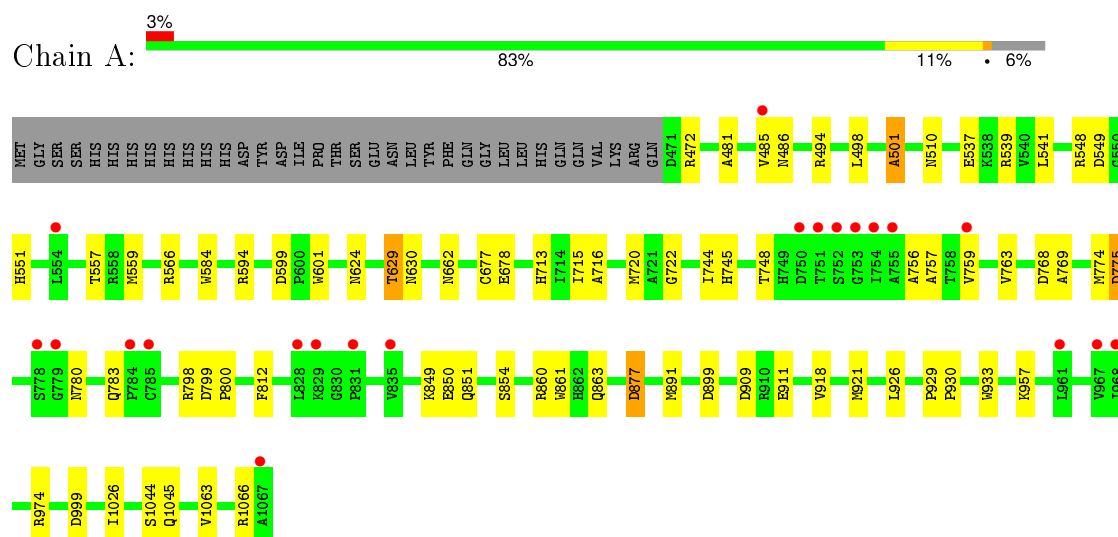
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	87	Total	O	0	0
			87	87		
7	B	46	Total	O	0	0
			46	46		
7	C	34	Total	O	0	0
			34	34		
7	D	23	Total	O	0	0
			23	23		

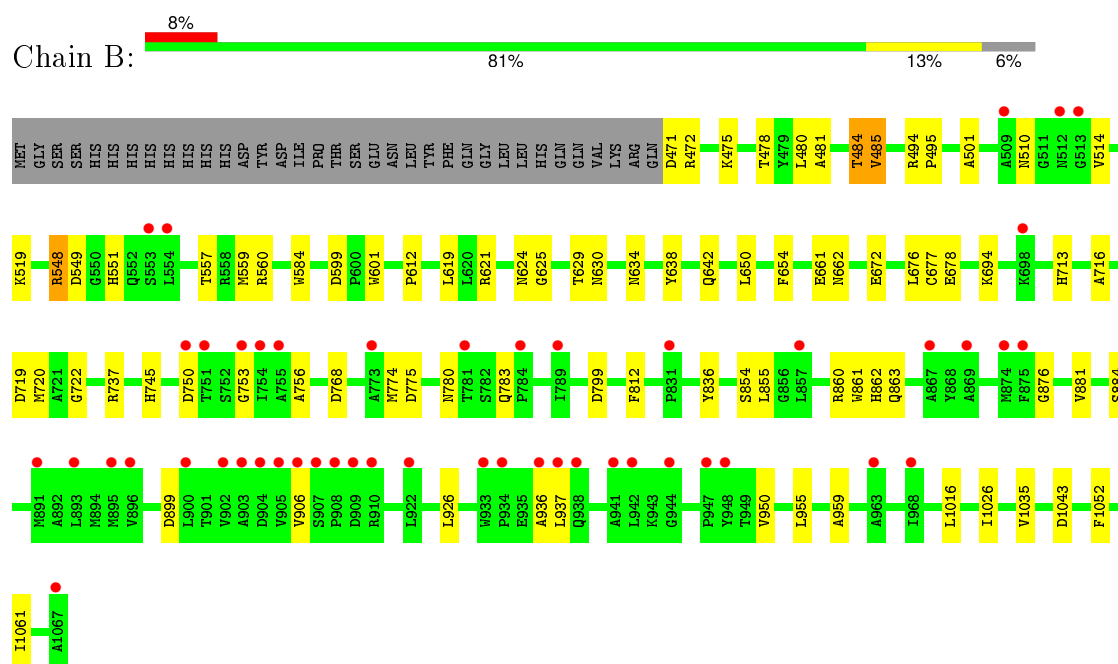
3 Residue-property plots [i](#)

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: PYRUVATE CARBOXYLASE



• Molecule 1: PYRUVATE CARBOXYLASE



• Molecule 1: PYRUVATE CARBOXYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.66Å 157.37Å 244.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.26 – 2.55 48.22 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.26-2.55) 99.4 (48.22-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.23 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.193 , 0.240 0.199 , 0.240	Depositor DCC
R_{free} test set	5406 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 108307 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18052	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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, 0.375 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: GOL, ZN, CL, MG, OXL, KCX

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	0.88	2/4644 (0.0%)	0.93	9/6314 (0.1%)
1	B	0.68	0/4609	0.79	3/6274 (0.0%)
1	C	0.78	3/4453 (0.1%)	0.85	9/6079 (0.1%)
1	D	0.55	1/4453 (0.0%)	0.69	1/6078 (0.0%)
All	All	0.73	6/18159 (0.0%)	0.82	22/24745 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	791	GLU	CD-OE2	5.42	1.31	1.25
1	D	800	PRO	N-CD	5.25	1.55	1.47
1	C	788	SER	CB-OG	-5.13	1.35	1.42
1	C	1048	VAL	C-O	5.07	1.32	1.23
1	A	911	GLU	CD-OE2	5.06	1.31	1.25
1	A	877	ASP	N-CA	5.01	1.56	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	775	ASP	CB-CG-OD1	8.88	126.30	118.30
1	A	594	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	C	633	ASP	CB-CG-OD2	7.17	124.75	118.30
1	C	544	ASP	CB-CG-OD1	7.01	124.61	118.30
1	C	696	ASP	CB-CG-OD1	6.74	124.36	118.30
1	B	719	ASP	CB-CG-OD1	6.24	123.92	118.30
1	C	539	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	C	809	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	929	PRO	C-N-CD	5.96	140.91	128.40
1	C	791	GLU	OE1-CD-OE2	5.95	130.44	123.30
1	A	974	ARG	NE-CZ-NH1	5.94	123.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	594	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	A	798	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	C	539	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	D	799	ASP	C-N-CD	5.52	139.99	128.40
1	A	768	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	A	921	MET	CG-SD-CE	5.41	108.86	100.20
1	A	798	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	560	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	C	535	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	750	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	539	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4557	0	4449	44	0
1	B	4522	0	4382	45	0
1	C	4368	0	4069	53	0
1	D	4367	0	4013	33	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	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	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	1	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	2	0
5	D	1	0	0	0	0
6	A	6	0	8	0	0
6	B	6	0	8	4	0
7	A	87	0	0	3	0
7	B	46	0	0	1	0
7	C	34	0	0	2	0
7	D	23	0	0	1	0
All	All	18052	0	16929	167	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 5.

All (167) 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:C:486:ASN:OD1	1:C:1066:ARG:HG3	1.34	1.28
1:C:931:SER:OG	1:C:932:GLY:O	1.85	0.93
1:B:480:LEU:O	1:B:484:THR:OG1	1.86	0.92
1:D:500:ASN:HD22	1:D:500:ASN:H	1.21	0.88
1:C:485:VAL:HG23	1:C:486:ASN:ND2	1.89	0.88
1:A:677:CYS:H	1:A:713:HIS:HD2	1.26	0.84
1:D:1026:ILE:O	1:D:1026:ILE:HD12	1.78	0.82
1:A:481:ALA:O	1:A:485:VAL:HG12	1.80	0.81
1:A:630:ASN:HD21	1:A:662:ASN:HD21	1.32	0.77
1:C:486:ASN:OD1	1:C:1066:ARG:CG	2.26	0.73
1:A:485:VAL:HG11	1:A:1063:VAL:HG21	1.70	0.73
1:A:472:ARG:HB3	1:A:1026:ILE:CD1	2.21	0.71
1:C:481:ALA:O	1:C:485:VAL:HG22	1.92	0.69
1:B:549:ASP:HB3	1:B:783:GLN:HE22	1.58	0.68
1:A:485:VAL:HG11	1:A:1063:VAL:CG2	2.25	0.67
1:A:624:ASN:HD22	1:A:629:THR:C	1.99	0.66
1:A:549:ASP:HB3	1:A:783:GLN:HE22	1.60	0.65
1:A:780:ASN:HA	7:A:1270:HOH:O	1.97	0.64
1:C:677:CYS:H	1:C:713:HIS:HD2	1.44	0.64
1:B:484:THR:HG23	1:B:1016:LEU:H	1.62	0.63
1:C:989:LYS:N	5:C:1104:CL:CL	2.68	0.63
1:D:838:HIS:O	1:D:839:GLU:HB2	1.97	0.62
1:C:486:ASN:N	1:C:486:ASN:HD22	1.97	0.62
1:B:677:CYS:H	1:B:713:HIS:HD2	1.46	0.62
1:B:630:ASN:HD21	1:B:662:ASN:HD21	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:GLU:O	1:C:494:ARG:NH2	2.32	0.62
1:C:942:LEU:O	1:C:943:LYS:C	2.37	0.61
1:A:799:ASP:OD1	1:A:800:PRO:HD2	2.00	0.60
1:C:559:MET:O	7:C:1225:HOH:O	2.16	0.60
1:C:633:ASP:OD1	1:C:951:ARG:NH1	2.34	0.60
1:B:780:ASN:N	6:B:1105:GOL:O1	2.29	0.60
1:C:485:VAL:HG23	1:C:486:ASN:HD22	1.65	0.59
1:C:485:VAL:C	1:C:486:ASN:HD22	2.05	0.59
1:D:630:ASN:HD21	1:D:662:ASN:HD21	1.48	0.59
1:C:577:ASN:HB2	7:C:1230:HOH:O	2.03	0.59
1:D:500:ASN:N	1:D:500:ASN:HD22	1.97	0.59
1:C:677:CYS:H	1:C:713:HIS:CD2	2.20	0.59
1:A:677:CYS:H	1:A:713:HIS:CD2	2.13	0.58
1:A:757:ALA:HA	1:C:757:ALA:HB2	1.85	0.58
1:A:851:GLN:O	1:A:854:SER:HB3	2.04	0.57
1:A:1045:GLN:OE1	1:A:1045:GLN:HA	2.05	0.57
1:B:619:LEU:HD11	1:B:654:PHE:CD2	2.39	0.57
1:C:624:ASN:ND2	1:C:630:ASN:OD1	2.38	0.57
1:B:481:ALA:O	1:B:485:VAL:HG13	2.05	0.56
1:D:500:ASN:ND2	1:D:500:ASN:H	1.97	0.56
1:B:599:ASP:OD1	1:B:601:TRP:N	2.38	0.56
1:A:757:ALA:CA	1:C:757:ALA:HB2	2.36	0.55
1:A:930:PRO:HD3	7:A:1242:HOH:O	2.06	0.54
1:A:891[B]:MET:HE1	1:A:918:VAL:HG11	1.90	0.54
1:A:485:VAL:CG1	1:A:1063:VAL:HG21	2.35	0.54
1:C:549:ASP:HB3	1:C:783:GLN:HE22	1.73	0.54
1:B:753:GLY:HA2	6:B:1105:GOL:H12	1.88	0.54
1:A:485:VAL:HG22	1:A:485:VAL:O	2.08	0.54
1:D:549:ASP:HB3	1:D:783:GLN:HE22	1.72	0.53
1:A:860:ARG:O	1:A:861:TRP:C	2.44	0.53
1:B:860:ARG:O	1:B:863:GLN:N	2.39	0.53
1:B:471:ASP:OD2	1:B:475:LYS:HE3	2.09	0.53
1:A:722:GLY:HA2	1:A:748:THR:OG1	2.10	0.52
1:B:881:VAL:O	1:B:884:SER:N	2.42	0.52
1:C:763:VAL:HA	1:C:767:VAL:HG12	1.91	0.52
1:D:835:VAL:HA	1:D:838:HIS:CE1	2.44	0.52
1:D:1026:ILE:C	1:D:1026:ILE:HD12	2.26	0.52
1:D:1063:VAL:HB	1:D:1064:PRO:HD2	1.92	0.51
1:D:597:THR:O	1:D:597:THR:HG22	2.09	0.51
1:D:881:VAL:H	1:D:884:SER:HG	1.57	0.51
1:A:677:CYS:N	1:A:713:HIS:HD2	2.01	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:777:LEU:HD21	1:C:818:ARG:HD2	1.93	0.50
1:A:486:ASN:HD21	1:A:1066:ARG:H	1.58	0.50
1:C:777:LEU:CD2	1:C:818:ARG:HD2	2.42	0.50
1:C:697:LEU:O	1:C:698:LYS:C	2.50	0.50
1:C:699:TYR:HE2	1:C:700:TYR:CE1	2.30	0.50
1:B:836:TYR:CD2	1:D:791:GLU:HG2	2.47	0.50
1:C:942:LEU:O	1:C:945:GLU:N	2.45	0.50
1:B:950:VAL:CG2	1:B:955:LEU:HD11	2.42	0.49
1:C:630:ASN:HD21	1:C:662:ASN:HD21	1.59	0.49
1:A:849:LYS:HE2	7:A:1276:HOH:O	2.12	0.49
1:B:780:ASN:H	6:B:1105:GOL:HO1	1.58	0.49
1:A:548:ARG:HD2	1:A:548:ARG:C	2.33	0.49
1:A:1045:GLN:CA	1:A:1045:GLN:OE1	2.61	0.49
1:C:539:ARG:HG3	1:C:539:ARG:O	2.12	0.49
1:B:494:ARG:HB3	1:B:495:PRO:CD	2.42	0.49
1:D:1025:ASP:OD2	1:D:1031:THR:HG22	2.12	0.49
1:C:1048:VAL:O	1:C:1062:LYS:HA	2.13	0.49
1:D:845:PHE:CD2	1:D:845:PHE:C	2.86	0.48
1:C:1043:ASP:C	1:C:1043:ASP:OD1	2.51	0.48
1:A:498:LEU:O	1:A:501:ALA:HB2	2.14	0.48
1:C:656:CYS:HA	1:C:881:VAL:CG1	2.43	0.48
1:B:722:GLY:HA3	7:B:1224:HOH:O	2.13	0.47
1:B:694:LYS:NZ	1:B:876:GLY:O	2.47	0.47
1:B:478:THR:HA	1:B:1061:ILE:HG21	1.96	0.47
1:C:698:LYS:O	1:C:702:ASN:N	2.48	0.47
1:D:535:ARG:HD3	1:D:741:GLY:O	2.15	0.47
1:C:990:VAL:HG23	5:C:1104:CL:CL	2.52	0.47
1:C:963:ALA:O	1:C:967:VAL:HG23	2.14	0.47
1:B:812:PHE:HE1	1:D:862:HIS:CD2	2.33	0.47
1:A:929:PRO:HD3	1:A:933:TRP:CZ2	2.50	0.46
1:A:849:LYS:HA	1:A:861:TRP:CZ3	2.50	0.46
1:B:650:LEU:HA	1:B:676:LEU:HB2	1.98	0.46
1:D:1023:PHE:CE1	1:D:1033:VAL:HG22	2.51	0.46
1:C:1036:ASN:OD1	1:C:1036:ASN:C	2.53	0.46
1:C:838:HIS:O	1:C:839:GLU:HB2	2.15	0.46
1:C:677:CYS:N	1:C:713:HIS:HD2	2.13	0.45
1:D:951:ARG:O	1:D:954:SER:OG	2.23	0.45
1:A:860:ARG:HG2	1:A:863:GLN:NE2	2.32	0.45
1:C:494:ARG:HB3	1:C:495:PRO:CD	2.47	0.45
1:D:718:KCX:CX	7:D:1223:HOH:O	2.64	0.45
1:C:699:TYR:CE2	1:C:700:TYR:CE1	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:737:ARG:NH2	1:B:768:ASP:OD1	2.50	0.45
1:B:1035:VAL:O	1:B:1052:PHE:HA	2.17	0.45
1:B:551:HIS:CE1	1:B:559:MET:HB3	2.52	0.45
1:D:678:GLU:HA	1:D:714:ILE:O	2.17	0.45
1:B:634:ASN:HD21	1:B:959:ALA:N	2.15	0.44
1:B:677:CYS:H	1:B:713:HIS:CD2	2.32	0.44
1:A:551:HIS:CE1	1:A:559:MET:HB3	2.53	0.44
1:A:812:PHE:HE1	1:C:862:HIS:CD2	2.35	0.44
1:C:472:ARG:CD	1:C:1026:ILE:HD11	2.48	0.44
1:B:519:LYS:HG2	1:B:612:PRO:O	2.18	0.44
1:A:812:PHE:CE1	1:C:862:HIS:CD2	3.06	0.43
1:A:716:ALA:HA	1:A:745:HIS:O	2.18	0.43
1:D:1026:ILE:HG22	1:D:1032:LEU:HG	1.99	0.43
1:D:548:ARG:C	1:D:548:ARG:HD2	2.39	0.43
1:A:486:ASN:ND2	1:A:1066:ARG:H	2.17	0.43
1:B:1043:ASP:C	1:B:1043:ASP:OD1	2.57	0.43
1:B:799:ASP:OD1	1:B:799:ASP:C	2.57	0.43
1:D:694:LYS:NZ	1:D:876:GLY:O	2.52	0.43
1:D:527:PRO:HB2	1:D:713:HIS:CD2	2.54	0.43
1:D:844:GLN:O	1:D:846:THR:N	2.52	0.43
1:D:1048:VAL:O	1:D:1062:LYS:HA	2.19	0.43
1:C:478:THR:HA	1:C:1061:ILE:HG21	2.01	0.43
1:A:678:GLU:OE1	1:A:745:HIS:ND1	2.45	0.42
1:D:988:PRO:O	1:D:992:THR:OG1	2.35	0.42
1:D:574:ALA:HB1	1:D:806:TRP:CG	2.54	0.42
1:A:599:ASP:OD1	1:A:601:TRP:N	2.48	0.42
1:C:552:GLN:HG3	1:C:557:THR:OG1	2.20	0.42
1:B:936:ALA:O	1:B:937:LEU:C	2.54	0.42
1:C:696:ASP:O	1:C:699:TYR:HB3	2.20	0.42
1:B:624:ASN:HD22	1:B:629:THR:C	2.23	0.42
1:A:756:ALA:CB	1:C:754:ILE:HG22	2.49	0.42
1:B:630:ASN:ND2	1:B:662:ASN:HD21	2.13	0.42
1:B:753:GLY:HA2	6:B:1105:GOL:C1	2.50	0.42
1:B:774:MET:O	1:B:775:ASP:C	2.58	0.42
1:A:541:LEU:O	1:A:769:ALA:HA	2.19	0.42
1:A:715:ILE:HB	1:A:744:ILE:HD13	2.02	0.42
1:C:486:ASN:N	1:C:486:ASN:ND2	2.66	0.42
1:A:774:MET:O	1:A:775:ASP:C	2.57	0.42
1:B:494:ARG:CB	1:B:495:PRO:CD	2.98	0.41
1:A:929:PRO:HD3	1:A:933:TRP:CE2	2.55	0.41
1:C:987:TYR:HB3	1:C:990:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:667:MET:HG2	1:D:677:CYS:SG	2.61	0.41
1:B:716:ALA:HA	1:B:745:HIS:O	2.20	0.41
1:C:472:ARG:HG2	1:C:1026:ILE:HD11	2.03	0.41
1:B:472:ARG:CB	1:B:1026:ILE:HD11	2.51	0.41
1:A:759:VAL:O	1:A:763:VAL:HG23	2.20	0.41
1:B:650:LEU:HD23	1:B:650:LEU:C	2.41	0.41
1:B:678:GLU:OE1	1:B:745:HIS:ND1	2.48	0.41
1:A:549:ASP:HB3	1:A:783:GLN:NE2	2.31	0.41
1:B:621:ARG:HB2	1:B:625:GLY:O	2.20	0.41
1:C:793:LEU:HD23	1:C:793:LEU:HA	1.80	0.41
1:D:898:GLN:O	1:D:899:ASP:C	2.59	0.41
1:B:548:ARG:HD2	1:B:548:ARG:C	2.42	0.40
1:C:965:ARG:HA	1:C:981:PHE:CE1	2.56	0.40
1:B:756:ALA:CB	1:D:754:ILE:HG22	2.51	0.40
1:D:987:TYR:HB3	1:D:990:VAL:HB	2.03	0.40
1:C:485:VAL:CG2	1:C:486:ASN:ND2	2.72	0.40
1:B:860:ARG:O	1:B:862:HIS:N	2.54	0.40
1:B:638:TYR:O	1:B:642:GLN:HG2	2.21	0.40
1:C:686:ASP:C	1:C:686:ASP:OD1	2.59	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	595/632 (94%)	577 (97%)	16 (3%)	2 (0%)	46 66
1	B	595/632 (94%)	570 (96%)	22 (4%)	3 (0%)	34 54
1	C	592/632 (94%)	557 (94%)	32 (5%)	3 (0%)	34 54
1	D	595/632 (94%)	566 (95%)	25 (4%)	4 (1%)	26 44
All	All	2377/2528 (94%)	2270 (96%)	95 (4%)	12 (0%)	34 54

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	501	ALA
1	D	845	PHE
1	D	1028	LYS
1	A	501	ALA
1	B	501	ALA
1	C	877	ASP
1	C	943	LYS
1	C	1028	LYS
1	A	877	ASP
1	B	861	TRP
1	D	844	GLN
1	B	906	VAL

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	467/519 (90%)	452 (97%)	15 (3%)	46	72
1	B	456/519 (88%)	442 (97%)	14 (3%)	47	73
1	C	417/519 (80%)	394 (94%)	23 (6%)	27	46
1	D	411/519 (79%)	395 (96%)	16 (4%)	39	64
All	All	1751/2076 (84%)	1683 (96%)	68 (4%)	39	64

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	494	ARG
1	A	510	ASN
1	A	537	GLU
1	A	557	THR
1	A	566	ARG
1	A	584	TRP
1	A	629	THR
1	A	720	MET

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Mol	Chain	Res	Type
1	A	850	GLU
1	A	899	ASP
1	A	909	ASP
1	A	926	LEU
1	A	957	LYS
1	A	999	ASP
1	A	1044	SER
1	B	484	THR
1	B	485	VAL
1	B	510	ASN
1	B	514	VAL
1	B	548	ARG
1	B	557	THR
1	B	584	TRP
1	B	661	GLU
1	B	672	GLU
1	B	720	MET
1	B	854	SER
1	B	855	LEU
1	B	899	ASP
1	B	926	LEU
1	C	486	ASN
1	C	514	VAL
1	C	521	LEU
1	C	558	ARG
1	C	566	ARG
1	C	577	ASN
1	C	584	TRP
1	C	629	THR
1	C	687	ILE
1	C	690	SER
1	C	706	GLU
1	C	720	MET
1	C	734	LYS
1	C	775	ASP
1	C	794	SER
1	C	797	GLU
1	C	826	SER
1	C	897	SER
1	C	998	SER
1	C	1000	THR
1	C	1031	THR

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Mol	Chain	Res	Type
1	C	1042	THR
1	C	1066	ARG
1	D	494	ARG
1	D	500	ASN
1	D	557	THR
1	D	566	ARG
1	D	584	TRP
1	D	629	THR
1	D	720	MET
1	D	794	SER
1	D	850	GLU
1	D	897	SER
1	D	998	SER
1	D	1026	ILE
1	D	1031	THR
1	D	1037	GLN
1	D	1039	VAL
1	D	1063	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	486	ASN
1	A	510	ASN
1	A	577	ASN
1	A	624	ASN
1	A	630	ASN
1	A	713	HIS
1	A	783	GLN
1	A	863	GLN
1	B	512	ASN
1	B	577	ASN
1	B	624	ASN
1	B	630	ASN
1	B	713	HIS
1	B	783	GLN
1	B	820	GLN
1	C	486	ASN
1	C	577	ASN
1	C	624	ASN
1	C	630	ASN
1	C	642	GLN

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Mol	Chain	Res	Type
1	C	702	ASN
1	C	713	HIS
1	C	783	GLN
1	C	1057	GLN
1	D	486	ASN
1	D	500	ASN
1	D	577	ASN
1	D	624	ASN
1	D	630	ASN
1	D	713	HIS
1	D	783	GLN
1	D	863	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	KCX	A	718	1,2	7,11,12	1.11	0	7,12,14	2.84	3 (42%)
1	KCX	B	718	1,2	7,11,12	0.71	0	7,12,14	2.14	1 (14%)
1	KCX	C	718	1,2	7,11,12	0.95	1 (14%)	7,12,14	1.63	2 (28%)
1	KCX	D	718	1,2	7,11,12	0.67	0	7,12,14	1.92	1 (14%)

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
1	KCX	A	718	1,2	-	0/6/10/12	0/0/0/0
1	KCX	B	718	1,2	-	0/6/10/12	0/0/0/0
1	KCX	C	718	1,2	-	0/6/10/12	0/0/0/0
1	KCX	D	718	1,2	-	0/6/10/12	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	718	KCX	CB-CA	2.02	1.55	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	718	KCX	CD-CE-NZ	2.08	117.10	111.46
1	A	718	KCX	CD-CG-CB	2.32	121.90	113.66
1	C	718	KCX	CE-NZ-CX	2.69	126.54	123.49
1	A	718	KCX	CD-CE-NZ	3.27	120.30	111.46
1	D	718	KCX	CE-NZ-CX	4.14	128.18	123.49
1	B	718	KCX	CE-NZ-CX	4.69	128.80	123.49
1	A	718	KCX	CE-NZ-CX	6.02	130.31	123.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	718	KCX	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 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	OXL	A	1102	-	0,5,5	0.00	-	0,6,6	0.00	-
6	GOL	A	1105	-	5,5,5	0.39	0	5,5,5	0.92	0
3	OXL	B	1102	-	0,5,5	0.00	-	0,6,6	0.00	-
6	GOL	B	1105	-	5,5,5	0.45	0	5,5,5	1.08	1 (20%)
3	OXL	C	1102	-	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	D	1102	-	0,5,5	0.00	-	0,6,6	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
3	OXL	A	1102	-	-	0/0/4/4	0/0/0/0
6	GOL	A	1105	-	-	0/4/4/4	0/0/0/0
3	OXL	B	1102	-	-	0/0/4/4	0/0/0/0
6	GOL	B	1105	-	-	0/4/4/4	0/0/0/0
3	OXL	C	1102	-	-	0/0/4/4	0/0/0/0
3	OXL	D	1102	-	-	0/0/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1105	GOL	C3-C2-C1	-2.03	103.17	111.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1105	GOL	4	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	596/632 (94%)	0.07	21 (3%) 48 54	29, 50, 82, 122	9 (1%)
1	B	596/632 (94%)	0.34	49 (8%) 14 16	44, 64, 109, 153	7 (1%)
1	C	595/632 (94%)	0.93	109 (18%) 2 2	35, 96, 183, 235	4 (0%)
1	D	596/632 (94%)	0.77	99 (16%) 2 2	51, 93, 142, 166	6 (1%)
All	All	2383/2528 (94%)	0.53	278 (11%) 6 6	29, 70, 150, 235	26 (1%)

All (278) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	896	VAL	8.8
1	C	934	PRO	8.6
1	D	875	PHE	6.5
1	C	907	SER	6.1
1	C	933	TRP	6.0
1	D	906	VAL	5.9
1	D	914	PHE	5.6
1	D	981	PHE	5.5
1	D	944	GLY	5.5
1	D	961	LEU	5.4
1	B	937	LEU	5.3
1	B	909	ASP	5.3
1	C	905	VAL	5.3
1	D	907	SER	5.2
1	A	968	ILE	5.1
1	C	1050	VAL	5.1
1	C	912	VAL	5.0
1	D	1036	ASN	5.0
1	B	906	VAL	5.0
1	D	972	LEU	4.7
1	C	509	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	906	VAL	4.5
1	D	1067	ALA	4.5
1	D	947	PRO	4.5
1	C	894	MET	4.4
1	B	902	VAL	4.4
1	C	1001	TYR	4.4
1	D	1019	GLY	4.4
1	B	933	TRP	4.4
1	D	903	ALA	4.4
1	B	908	PRO	4.4
1	C	914	PHE	4.3
1	B	874	MET	4.3
1	D	896	VAL	4.2
1	C	903	ALA	4.2
1	D	895	MET	4.2
1	B	867	ALA	4.2
1	D	1044	SER	4.1
1	D	1046	GLY	4.1
1	C	900	LEU	4.0
1	D	898	GLN	4.0
1	C	891[A]	MET	4.0
1	C	512	ASN	4.0
1	B	891[A]	MET	4.0
1	C	947	PRO	3.9
1	C	485	VAL	3.9
1	C	874	MET	3.9
1	D	902	VAL	3.9
1	B	895	MET	3.9
1	D	974	ARG	3.9
1	C	779	GLY	3.9
1	D	1052	PHE	3.9
1	B	900	LEU	3.8
1	C	922	LEU	3.8
1	C	1067	ALA	3.8
1	C	1039	VAL	3.8
1	D	479	TYR	3.8
1	D	891[A]	MET	3.7
1	D	984	TYR	3.7
1	D	1050	VAL	3.7
1	D	1001	TYR	3.7
1	D	933	TRP	3.7
1	C	981	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	485	VAL	3.7
1	D	941	ALA	3.6
1	C	950	VAL	3.6
1	C	1046	GLY	3.6
1	C	1040	SER	3.6
1	C	1048	VAL	3.6
1	B	893	LEU	3.6
1	B	963	ALA	3.6
1	C	1036	ASN	3.6
1	D	478	THR	3.5
1	D	894	MET	3.5
1	D	973	GLU	3.5
1	C	892	ALA	3.5
1	D	501	ALA	3.5
1	D	1014	TYR	3.5
1	B	904	ASP	3.4
1	D	923	LYS	3.4
1	D	908	PRO	3.4
1	B	907	SER	3.4
1	D	905	VAL	3.4
1	C	476	LEU	3.4
1	C	1044	SER	3.4
1	B	934	PRO	3.4
1	C	897	SER	3.4
1	D	950	VAL	3.3
1	B	905	VAL	3.3
1	D	1040	SER	3.3
1	A	785	CYS	3.3
1	B	942	LEU	3.3
1	C	953	GLY	3.3
1	D	525	LEU	3.3
1	B	948	TYR	3.3
1	C	908	PRO	3.3
1	D	1041	ALA	3.3
1	D	904	ASP	3.2
1	C	973	GLU	3.2
1	A	835	VAL	3.2
1	D	948	TYR	3.2
1	C	781	THR	3.2
1	D	911	GLU	3.2
1	C	910	ARG	3.2
1	D	874	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	944	GLY	3.1
1	A	750	ASP	3.1
1	D	1042	THR	3.1
1	D	1061	ILE	3.1
1	D	960	ASP	3.1
1	C	511	GLY	3.1
1	C	1047	MET	3.1
1	C	1052	PHE	3.1
1	C	510	ASN	3.1
1	B	896	VAL	3.1
1	C	483	VAL	3.0
1	B	784	PRO	3.0
1	D	1039	VAL	3.0
1	B	751	THR	3.0
1	C	923	LYS	2.9
1	B	875	PHE	2.9
1	C	875	PHE	2.9
1	D	631	TYR	2.9
1	A	784	PRO	2.9
1	D	979	PHE	2.9
1	B	781	THR	2.9
1	B	941	ALA	2.9
1	C	481	ALA	2.9
1	C	963	ALA	2.9
1	D	936	ALA	2.9
1	B	755	ALA	2.9
1	C	1041	ALA	2.9
1	C	831	PRO	2.9
1	C	1066	ARG	2.8
1	D	912	VAL	2.8
1	C	556	ALA	2.8
1	C	1057	GLN	2.8
1	A	778	SER	2.8
1	C	634	ASN	2.8
1	D	1063	VAL	2.8
1	A	755	ALA	2.8
1	A	752	SER	2.8
1	D	897	SER	2.8
1	C	546	THR	2.8
1	C	753	GLY	2.8
1	C	1043	ASP	2.7
1	C	477	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	974	ARG	2.7
1	D	1037	GLN	2.7
1	C	1000	THR	2.7
1	B	869	ALA	2.7
1	C	780	ASN	2.7
1	C	1018	ASP	2.7
1	B	698	LYS	2.7
1	D	942	LEU	2.7
1	D	1048	VAL	2.7
1	C	486	ASN	2.7
1	C	909	ASP	2.7
1	D	943	LYS	2.7
1	D	951	ARG	2.7
1	B	1067	ALA	2.6
1	B	512	ASN	2.6
1	C	936	ALA	2.6
1	C	754	ILE	2.6
1	C	873	GLN	2.6
1	C	976	VAL	2.6
1	D	483	VAL	2.6
1	A	779	GLY	2.6
1	D	1049	THR	2.6
1	C	587	ALA	2.6
1	C	911	GLU	2.6
1	A	753	GLY	2.6
1	B	753	GLY	2.6
1	D	638	TYR	2.6
1	D	499	GLU	2.6
1	D	909	ASP	2.5
1	C	921	MET	2.5
1	D	901	THR	2.5
1	D	963	ALA	2.5
1	C	895	MET	2.5
1	C	1019	GLY	2.5
1	A	751	THR	2.5
1	D	962	ASP	2.5
1	C	751	THR	2.5
1	D	1038	ALA	2.5
1	D	946	LYS	2.5
1	C	1064	PRO	2.4
1	C	1016	LEU	2.4
1	D	753	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	899	ASP	2.4
1	D	922	LEU	2.4
1	B	903	ALA	2.4
1	D	641	ARG	2.4
1	C	828	LEU	2.4
1	D	967	VAL	2.4
1	B	910	ARG	2.4
1	D	1003	PRO	2.4
1	A	828	LEU	2.4
1	B	554	LEU	2.4
1	C	1035	VAL	2.4
1	D	749	HIS	2.4
1	D	857	LEU	2.3
1	D	1047	MET	2.3
1	C	785	CYS	2.3
1	B	553	SER	2.3
1	C	901	THR	2.3
1	B	773	ALA	2.3
1	C	773	ALA	2.3
1	C	1034	ILE	2.3
1	C	1038	ALA	2.3
1	A	554	LEU	2.3
1	C	965	ARG	2.3
1	B	936	ALA	2.3
1	D	781	THR	2.3
1	C	513	GLY	2.3
1	B	831	PRO	2.3
1	C	478	THR	2.3
1	C	924	GLY	2.3
1	B	922	LEU	2.3
1	C	843	GLY	2.3
1	D	919	VAL	2.3
1	C	553	SER	2.2
1	A	961	LEU	2.2
1	C	776	ALA	2.2
1	D	755	ALA	2.2
1	B	944	GLY	2.2
1	C	1054	LEU	2.2
1	C	1049	THR	2.2
1	C	856	GLY	2.2
1	D	910	ARG	2.2
1	C	554	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	949	THR	2.2
1	A	967	VAL	2.2
1	D	784	PRO	2.2
1	C	1061	ILE	2.2
1	D	1043	ASP	2.2
1	B	947	PRO	2.2
1	B	509	ALA	2.2
1	D	1018	ASP	2.2
1	D	675	LYS	2.2
1	C	902	VAL	2.2
1	C	962	ASP	2.2
1	C	631	TYR	2.2
1	D	550	GLY	2.2
1	D	642	GLN	2.2
1	C	777	LEU	2.2
1	D	480	LEU	2.2
1	C	557	THR	2.2
1	D	500	ASN	2.2
1	C	550	GLY	2.1
1	D	976	VAL	2.1
1	C	774	MET	2.1
1	A	754	ILE	2.1
1	B	857	LEU	2.1
1	B	513	GLY	2.1
1	B	750	ASP	2.1
1	D	754	ILE	2.1
1	A	759	VAL	2.1
1	B	938	GLN	2.1
1	D	667	MET	2.1
1	A	831	PRO	2.1
1	C	904	ASP	2.1
1	B	754	ILE	2.1
1	C	984	TYR	2.1
1	A	829	LYS	2.1
1	C	970	LYS	2.1
1	C	979	PHE	2.1
1	D	938	GLN	2.0
1	B	789	ILE	2.0
1	D	476	LEU	2.0
1	D	553	SER	2.0
1	A	1067	ALA	2.0
1	B	968	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	915	PRO	2.0
1	D	959	ALA	2.0
1	D	975	GLU	2.0
1	C	752	SER	2.0
1	C	937	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	KCX	B	718	12/13	0.99	0.22	-	49,54,55,59	0
1	KCX	A	718	12/13	0.98	0.22	-	33,37,42,44	0
1	KCX	D	718	12/13	0.97	0.22	-	71,75,79,80	0
1	KCX	C	718	12/13	0.93	0.23	-	65,73,85,90	0

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(Å ²)	Q<0.9
4	MG	C	1103	1/1	0.81	0.23	1.47	44,44,44,44	0
6	GOL	A	1105	6/6	0.96	0.37	1.29	49,53,54,57	0
4	MG	D	1103	1/1	0.86	0.18	0.43	66,66,66,66	0
6	GOL	B	1105	6/6	0.94	0.28	0.35	55,59,66,73	0
3	OXL	C	1102	6/6	0.90	0.21	-0.76	63,74,78,80	0
3	OXL	A	1102	6/6	0.98	0.16	-0.89	40,48,53,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	OXL	B	1102	6/6	0.96	0.14	-0.95	47,54,57,63	0
3	OXL	D	1102	6/6	0.91	0.16	-0.99	66,72,74,76	0
4	MG	A	1103	1/1	0.82	0.10	-1.16	49,49,49,49	0
2	ZN	A	1101	1/1	0.99	0.15	-2.20	37,37,37,37	1
2	ZN	C	1101	1/1	0.96	0.17	-2.45	58,58,58,58	1
2	ZN	D	1101	1/1	0.94	0.12	-4.04	56,56,56,56	1
4	MG	B	1103	1/1	0.81	0.07	-5.96	51,51,51,51	0
2	ZN	B	1101	1/1	0.98	0.17	-	42,42,42,42	1
5	CL	A	1104	1/1	0.97	0.06	-	56,56,56,56	0
5	CL	B	1104	1/1	0.87	0.18	-	67,67,67,67	0
5	CL	C	1104	1/1	0.85	0.09	-	78,78,78,78	0
5	CL	D	1104	1/1	0.95	0.09	-	104,104,104,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.