



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:19 PM GMT

PDB ID : 4L80
Title : Crystal Structure of Chloroflexus aurantiacus malyl-CoA lyase in complex with magnesium, oxalate, and propionyl-CoA
Authors : Zarzycki, J.; Kerfeld, C.A.
Deposited on : 2013-06-15
Resolution : 2.01 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

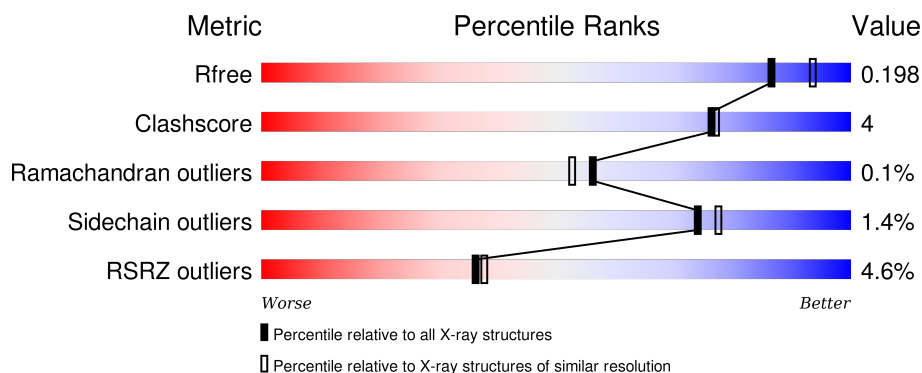
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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.



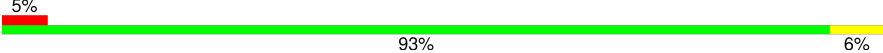
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 $\leq 5\%$. 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	348	<div> <div>6%</div> <div>88%</div> <div>11%</div> </div>
1	B	348	<div> <div>2%</div> <div>90%</div> <div>9%</div> </div>
1	C	348	<div> <div>4%</div> <div>92%</div> <div>7%</div> </div>
1	D	348	<div> <div>6%</div> <div>92%</div> <div>7%</div> </div>
1	E	348	<div> <div>5%</div> <div>88%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	348	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a red segment at the beginning labeled '5%', a green segment in the middle labeled '93%', and a yellow segment at the end labeled '6%'.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	B	402	-	-	X	-

2 Entry composition [i](#)

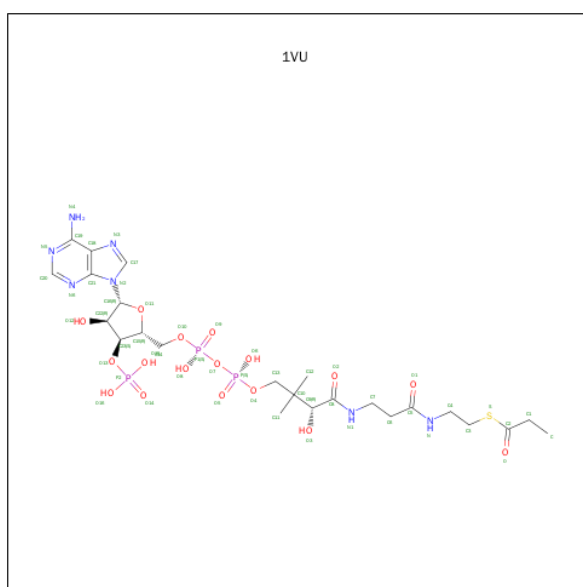
There are 6 unique types of molecules in this entry. The entry contains 18197 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HpcH/HpaI aldolase.

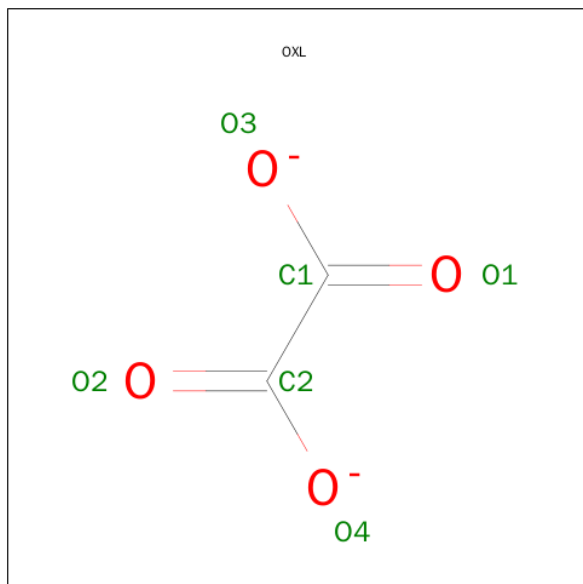
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2683	1722	470	478	13			
1	B	347	Total	C	N	O	S	0	1	0
			2701	1734	472	482	13			
1	C	347	Total	C	N	O	S	0	1	0
			2701	1734	472	482	13			
1	D	344	Total	C	N	O	S	0	1	0
			2679	1722	468	476	13			
1	E	344	Total	C	N	O	S	0	1	0
			2679	1722	468	476	13			
1	F	347	Total	C	N	O	S	0	0	0
			2695	1730	472	480	13			

- Molecule 2 is PROPIONYL COENZYME A (three-letter code: 1VU) (formula: $C_{24}H_{40}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			52	24	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			52	24	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			52	24	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			52	24	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			52	24	7	17	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			52	24	7	17	3	1		

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).

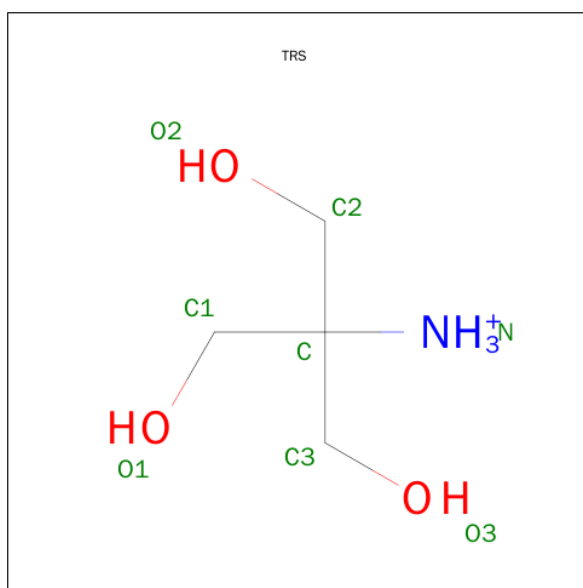


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		
3	B	1	Total	C	O	0	0
			6	2	4		
3	C	1	Total	C	O	0	0
			6	2	4		
3	D	1	Total	C	O	0	0
			6	2	4		
3	E	1	Total	C	O	0	0
			6	2	4		
3	F	1	Total	C	O	0	0
			6	2	4		

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

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

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 8 4 1 3	0	0
5	D	1	Total C N O 8 4 1 3	0	0

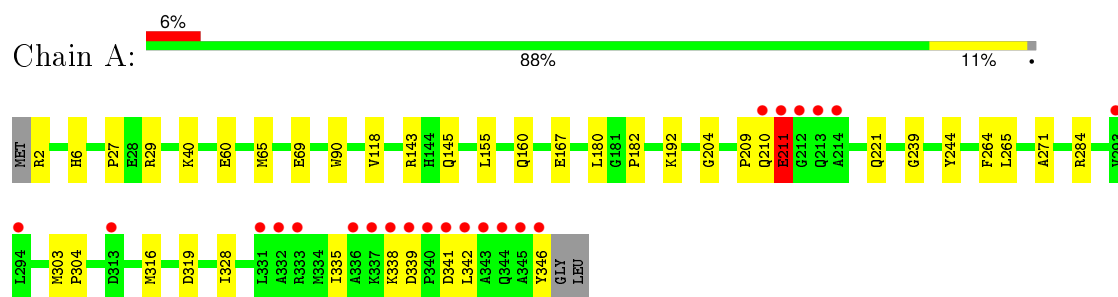
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	278	Total 278	O 278	0	0
6	B	260	Total 260	O 260	0	0
6	C	342	Total 342	O 342	0	0
6	D	286	Total 286	O 286	0	0
6	E	279	Total 279	O 279	0	0
6	F	244	Total 244	O 244	0	0

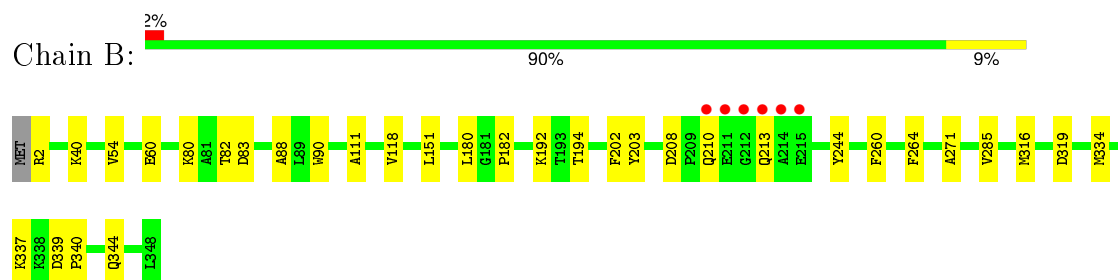
3 Residue-property plots

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.

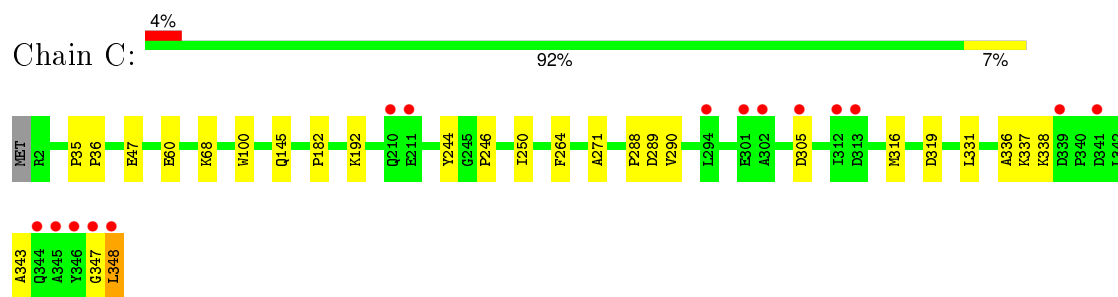
- Molecule 1: HpCh/HpaI aldolase



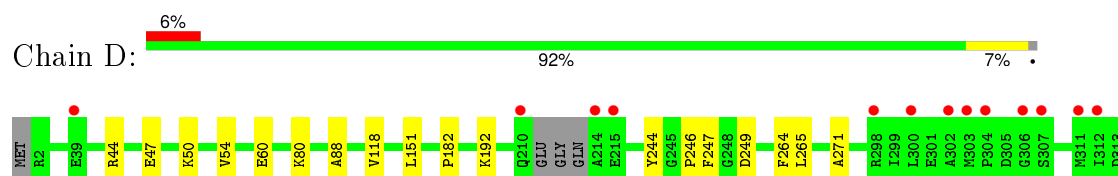
- Molecule 1: HpCh/HpaI aldolase

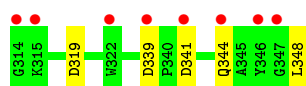


- Molecule 1: HpCh/HpaI aldolase

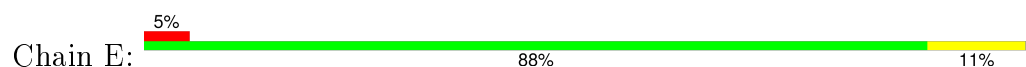


- Molecule 1: HpCh/HpaI aldolase





- Molecule 1: HpcH/HpaI aldolase



- Molecule 1: HpcH/HpaI aldolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	102.15Å 102.15Å 204.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.93 – 2.01 37.93 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.1 (37.93-2.01) 98.5 (37.93-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1303)	Depositor
R, R_{free}	0.172 , 0.201 0.168 , 0.198	Depositor DCC
R_{free} test set	1979 reflections (1.47%)	DCC
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.0	EDS
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 136815 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18197	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: OXL, 1VU, TRS, MG

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	0.28	0/2750	0.45	0/3737
1	B	0.25	0/2771	0.42	0/3765
1	C	0.24	0/2771	0.43	0/3765
1	D	0.28	0/2748	0.44	0/3733
1	E	0.24	0/2748	0.44	1/3733 (0.0%)
1	F	0.23	0/2762	0.41	0/3753
All	All	0.25	0/16550	0.43	1/22486 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	155	LEU	CB-CG-CD1	5.61	120.53	111.00

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	2683	0	2689	32	0
1	B	2701	0	2709	22	0
1	C	2701	0	2709	19	0
1	D	2679	0	2691	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2679	0	2691	28	0
1	F	2695	0	2703	14	0
2	A	52	0	38	4	0
2	B	52	0	38	4	0
2	C	52	0	38	2	0
2	D	52	0	38	2	0
2	E	52	0	38	5	0
2	F	52	0	38	2	0
3	A	6	0	0	1	0
3	B	6	0	0	2	0
3	C	6	0	0	1	0
3	D	6	0	0	0	0
3	E	6	0	0	1	0
3	F	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
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	8	0	12	0	0
5	D	8	0	12	0	0
6	A	278	0	0	9	1
6	B	260	0	0	3	0
6	C	342	0	0	9	1
6	D	286	0	0	7	0
6	E	279	0	0	5	0
6	F	244	0	0	5	0
All	All	18197	0	16444	126	1

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 (126) 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:210:GLN:O	1:A:211:GLU:HB3	1.54	1.05
1:A:209:PRO:O	6:A:626:HOH:O	1.82	0.97
2:C:401:1VU:O16	6:C:717:HOH:O	1.87	0.92
1:E:44:ARG:NH1	2:E:401:1VU:N6	2.25	0.84
1:A:2:ARG:N	6:A:729:HOH:O	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:1VU:O9	6:D:783:HOH:O	1.98	0.82
1:B:316:MET:SD	6:B:710:HOH:O	2.37	0.81
1:F:87:THR:OG1	6:F:695:HOH:O	1.98	0.81
1:C:47:GLU:OE1	6:C:699:HOH:O	1.98	0.81
1:E:297:LYS:NZ	1:E:346:TYR:O	2.13	0.81
1:E:339:ASP:OD2	6:E:665:HOH:O	2.04	0.75
1:A:27:PRO:HG2	1:A:338:LYS:HD3	1.68	0.75
1:C:305:ASP:OD2	6:C:817:HOH:O	2.05	0.75
1:D:47:GLU:OE2	6:D:750:HOH:O	2.04	0.74
1:C:145:GLN:NE2	6:C:802:HOH:O	1.96	0.74
1:D:339:ASP:OD2	6:D:566:HOH:O	2.06	0.72
1:A:210:GLN:O	1:A:211:GLU:CB	2.36	0.69
1:C:305:ASP:OD2	6:C:839:HOH:O	2.10	0.69
1:C:347:GLY:O	6:C:786:HOH:O	2.11	0.69
1:E:51:GLN:NE2	6:E:727:HOH:O	2.26	0.68
1:A:65:MET:SD	6:C:829:HOH:O	2.51	0.67
1:D:249:ASP:OD2	6:D:641:HOH:O	2.12	0.67
1:D:80:LYS:NZ	6:D:758:HOH:O	2.22	0.65
1:A:145:GLN:NE2	6:A:558:HOH:O	2.30	0.64
1:A:265:LEU:HD12	1:B:203:TYR:HB2	1.80	0.64
2:B:401:1VU:H36	3:B:402:OXL:C1	2.29	0.62
1:E:44:ARG:HH12	2:E:401:1VU:H6	1.64	0.62
1:A:143:ARG:NH2	6:A:527:HOH:O	2.32	0.62
1:A:265:LEU:HD11	1:B:202:PHE:HB2	1.82	0.62
1:F:346:TYR:HB3	1:F:348:LEU:HD23	1.82	0.60
1:F:2:ARG:N	6:F:710:HOH:O	2.33	0.60
2:A:401:1VU:H31	1:C:316:MET:CE	2.16	0.59
1:D:50:LYS:NZ	6:D:745:HOH:O	2.38	0.56
1:C:337:LYS:HD3	1:C:348:LEU:HD11	1.88	0.56
1:C:288:PRO:HG3	1:C:331:LEU:HD23	1.88	0.56
1:A:160:GLN:NE2	6:A:520:HOH:O	2.38	0.56
1:E:316:MET:CE	2:F:401:1VU:H31	2.19	0.55
1:A:211:GLU:O	1:A:211:GLU:HG3	2.05	0.55
2:A:401:1VU:H31	1:C:316:MET:HE2	1.69	0.55
1:D:341:ASP:O	1:D:344:GLN:NE2	2.41	0.54
1:F:290:VAL:HG22	6:F:680:HOH:O	2.07	0.54
1:E:341:ASP:N	1:E:341:ASP:OD1	2.39	0.53
1:E:44:ARG:NH1	2:E:401:1VU:H6	2.23	0.53
1:B:80:LYS:HE3	1:B:111:ALA:HB1	1.91	0.52
1:B:82:THR:HG22	1:B:83:ASP:N	2.24	0.52
1:E:305:ASP:OD2	6:E:656:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:ARG:HG3	6:E:774:HOH:O	2.10	0.52
1:D:182:PRO:HD2	1:D:246:PRO:HD2	1.92	0.52
1:A:167:GLU:HG2	6:A:698:HOH:O	2.09	0.51
2:B:401:1VU:H36	3:B:402:OXL:C2	2.41	0.51
1:A:342:LEU:HD23	1:A:346:TYR:CE1	2.46	0.51
1:D:247:PHE:CE2	1:D:249:ASP:HB3	2.47	0.50
1:A:341:ASP:N	1:A:341:ASP:OD1	2.43	0.50
1:C:289:ASP:OD2	1:C:290:VAL:N	2.45	0.50
1:E:182:PRO:HD2	1:E:246:PRO:HD2	1.94	0.49
1:E:160:GLN:NE2	6:E:514:HOH:O	2.30	0.49
1:A:284:ARG:NH1	6:A:657:HOH:O	2.37	0.49
1:C:336:ALA:HB1	1:C:343:ALA:HA	1.95	0.49
1:A:40:LYS:HE2	2:A:401:1VU:O12	2.12	0.48
1:C:338:LYS:NZ	6:C:753:HOH:O	2.46	0.48
1:B:40:LYS:NZ	6:B:748:HOH:O	2.38	0.48
1:D:192:LYS:HG3	1:F:264:PHE:CZ	2.49	0.48
1:E:38:VAL:HG12	1:E:40:LYS:HG2	1.95	0.48
1:A:29:ARG:HD3	1:A:335:ILE:HD13	1.94	0.48
1:D:265:LEU:HD21	1:E:202:PHE:HB2	1.95	0.48
1:A:264:PHE:CZ	1:B:192:LYS:HG3	2.49	0.48
1:A:316:MET:SD	2:B:401:1VU:H30	2.54	0.47
1:E:303:MET:HB2	1:E:322:TRP:HD1	1.79	0.47
2:A:401:1VU:H36	3:A:402:OXL:C2	2.45	0.47
1:A:180:LEU:O	1:A:182:PRO:HD3	2.15	0.47
2:E:401:1VU:H21	2:E:401:1VU:O2	2.15	0.47
1:E:196:VAL:HB	1:E:248:GLY:HA3	1.97	0.47
1:A:244:TYR:O	1:A:271:ALA:HA	2.14	0.46
2:D:401:1VU:H31	1:F:316:MET:CE	2.28	0.46
1:A:192:LYS:HG3	1:C:264:PHE:CZ	2.51	0.46
1:F:81:ALA:HB2	6:F:604:HOH:O	2.15	0.46
1:B:180:LEU:O	1:B:182:PRO:HD3	2.16	0.46
1:B:2:ARG:O	1:E:2:ARG:NH2	2.46	0.46
2:B:401:1VU:O2	2:B:401:1VU:H21	2.15	0.46
1:B:264:PHE:CZ	1:C:192:LYS:HG3	2.51	0.45
1:D:44:ARG:NH1	6:D:761:HOH:O	2.30	0.45
1:E:260:PHE:HB3	1:E:285:VAL:HG11	1.99	0.45
2:E:401:1VU:H36	3:E:402:OXL:C2	2.47	0.45
1:A:239:GLY:HA2	6:A:718:HOH:O	2.17	0.44
1:B:244:TYR:O	1:B:271:ALA:HA	2.17	0.44
1:C:244:TYR:O	1:C:271:ALA:HA	2.17	0.44
1:D:118:VAL:HG22	1:D:151:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:PRO:HD2	1:C:246:PRO:HD2	1.99	0.44
1:E:316:MET:HE3	2:F:401:1VU:H31	1.81	0.44
1:E:10:LYS:HE2	1:E:10:LYS:HB3	1.74	0.44
1:B:54:VAL:HG22	1:B:88:ALA:HB3	2.00	0.43
1:D:244:TYR:O	1:D:271:ALA:HA	2.18	0.43
1:D:264:PHE:CZ	1:E:192:LYS:HG3	2.53	0.43
1:A:6:HIS:HB2	6:A:753:HOH:O	2.18	0.43
1:E:117:ASP:HA	1:E:148:LYS:HZ1	1.82	0.43
1:F:204:GLY:HA2	1:F:221:GLN:HG2	1.99	0.43
1:E:264:PHE:CZ	1:F:192:LYS:HG3	2.53	0.43
1:F:46:PRO:O	1:F:50:LYS:HG2	2.19	0.43
1:E:54:VAL:HG22	1:E:88:ALA:HB3	2.01	0.43
1:E:244:TYR:O	1:E:271:ALA:HA	2.19	0.43
1:A:339:ASP:HB3	1:A:342:LEU:HD13	2.01	0.43
1:B:337:LYS:HD2	1:B:337:LYS:N	2.33	0.43
1:B:260:PHE:HB3	1:B:285:VAL:HG11	2.00	0.42
1:B:118:VAL:HG22	1:B:151:LEU:HB2	2.01	0.42
1:E:298:ARG:NH2	1:E:313:ASP:OD2	2.52	0.42
1:F:244:TYR:O	1:F:271:ALA:HA	2.19	0.42
1:A:303:MET:HA	1:A:304:PRO:HD2	1.85	0.42
2:C:401:1VU:H36	3:C:402:OXL:C1	2.49	0.42
1:B:208:ASP:O	1:B:210:GLN:NE2	2.53	0.42
1:B:316:MET:HE3	1:C:250:ILE:HD11	2.02	0.42
1:A:328:ILE:HD12	1:B:194:THR:HG23	2.02	0.42
1:B:339:ASP:HA	1:B:340:PRO:HD2	1.80	0.42
1:B:90:TRP:CD1	1:B:118:VAL:HB	2.55	0.41
1:F:2:ARG:N	6:F:719:HOH:O	2.52	0.41
1:D:54:VAL:HG22	1:D:88:ALA:HB3	2.02	0.41
1:E:339:ASP:HA	1:E:340:PRO:HD2	1.91	0.41
1:A:90:TRP:CD1	1:A:118:VAL:HB	2.56	0.41
1:C:35:PRO:HA	1:C:36:PRO:HD3	1.80	0.41
1:A:2:ARG:NH2	1:F:2:ARG:O	2.53	0.41
1:B:340:PRO:O	1:B:344:GLN:HG2	2.21	0.41
1:E:68:LYS:HG3	1:E:100:TRP:CE2	2.56	0.41
1:F:180:LEU:O	1:F:182:PRO:HD3	2.21	0.40
1:A:204:GLY:HA2	1:A:221:GLN:HG2	2.03	0.40
1:A:65:MET:HG3	6:C:839:HOH:O	2.21	0.40
1:C:68:LYS:HG3	1:C:100:TRP:CE2	2.57	0.40
1:B:334:MET:HG3	6:B:646:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:539:HOH:O	6:C:521:HOH:O[4_555]	1.85	0.35

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	343/348 (99%)	332 (97%)	10 (3%)	1 (0%)	46	41
1	B	346/348 (99%)	333 (96%)	13 (4%)	0	100	100
1	C	346/348 (99%)	334 (96%)	12 (4%)	0	100	100
1	D	341/348 (98%)	328 (96%)	13 (4%)	0	100	100
1	E	341/348 (98%)	329 (96%)	12 (4%)	0	100	100
1	F	345/348 (99%)	334 (97%)	10 (3%)	1 (0%)	46	41
All	All	2062/2088 (99%)	1990 (96%)	70 (3%)	2 (0%)	56	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	GLU
1	F	338	LYS

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	275/277 (99%)	270 (98%)	5 (2%)	66	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	277/277 (100%)	274 (99%)	3 (1%)	80	83
1	C	277/277 (100%)	274 (99%)	3 (1%)	80	83
1	D	275/277 (99%)	272 (99%)	3 (1%)	80	83
1	E	275/277 (99%)	272 (99%)	3 (1%)	80	83
1	F	276/277 (100%)	270 (98%)	6 (2%)	60	62
All	All	1655/1662 (100%)	1632 (99%)	23 (1%)	74	77

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLU
1	A	69	GLU
1	A	155	LEU
1	A	211	GLU
1	A	319	ASP
1	B	60	GLU
1	B	213	GLN
1	B	319	ASP
1	C	60	GLU
1	C	319	ASP
1	C	348	LEU
1	D	60	GLU
1	D	319	ASP
1	D	348	LEU
1	E	60	GLU
1	E	155	LEU
1	E	319	ASP
1	F	60	GLU
1	F	155	LEU
1	F	215	GLU
1	F	265	LEU
1	F	290	VAL
1	F	319	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	220	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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$
2	1VU	A	401	-	44,54,54	1.37	6 (13%)	55,80,80	2.37	11 (20%)
3	OXL	A	402	4	0,5,5	0.00	-	0,6,6	0.00	-
5	TRS	A	404	-	7,7,7	1.01	0	9,9,9	0.63	0
2	1VU	B	401	-	44,54,54	1.37	7 (15%)	55,80,80	2.48	7 (12%)
3	OXL	B	402	4	0,5,5	0.00	-	0,6,6	0.00	-
2	1VU	C	401	-	44,54,54	1.48	7 (15%)	55,80,80	2.10	5 (9%)
3	OXL	C	402	4	0,5,5	0.00	-	0,6,6	0.00	-
2	1VU	D	401	-	44,54,54	1.50	7 (15%)	55,80,80	2.09	8 (14%)
3	OXL	D	402	4	0,5,5	0.00	-	0,6,6	0.00	-
5	TRS	D	404	-	7,7,7	0.98	0	9,9,9	0.76	0
2	1VU	E	401	-	44,54,54	1.41	5 (11%)	55,80,80	2.14	13 (23%)
3	OXL	E	402	4	0,5,5	0.00	-	0,6,6	0.00	-
2	1VU	F	401	-	44,54,54	1.49	8 (18%)	55,80,80	2.08	7 (12%)
3	OXL	F	402	4	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
2	1VU	A	401	-	-	1/48/69/69	0/3/3/3
3	OXL	A	402	4	-	0/0/4/4	0/0/0/0
5	TRS	A	404	-	-	0/9/9/9	0/0/0/0
2	1VU	B	401	-	-	0/48/69/69	0/3/3/3
3	OXL	B	402	4	-	0/0/4/4	0/0/0/0
2	1VU	C	401	-	-	1/48/69/69	0/3/3/3
3	OXL	C	402	4	-	0/0/4/4	0/0/0/0
2	1VU	D	401	-	-	1/48/69/69	0/3/3/3
3	OXL	D	402	4	-	0/0/4/4	0/0/0/0
5	TRS	D	404	-	-	0/9/9/9	0/0/0/0
2	1VU	E	401	-	-	1/48/69/69	0/3/3/3
3	OXL	E	402	4	-	0/0/4/4	0/0/0/0
2	1VU	F	401	-	-	1/48/69/69	0/3/3/3
3	OXL	F	402	4	-	0/0/4/4	0/0/0/0

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	1VU	C2-S	-4.89	1.66	1.76
2	A	401	1VU	C2-S	-4.38	1.67	1.76
2	D	401	1VU	C2-S	-4.38	1.67	1.76
2	F	401	1VU	C2-S	-4.07	1.67	1.76
2	D	401	1VU	C21-N6	-3.36	1.30	1.35
2	B	401	1VU	P1-O8	-3.33	1.40	1.54
2	C	401	1VU	C2-S	-3.21	1.69	1.76
2	C	401	1VU	P2-O14	-3.19	1.40	1.51
2	C	401	1VU	O1-C5	-3.08	1.16	1.23
2	A	401	1VU	O1-C5	-3.02	1.16	1.23
2	D	401	1VU	O1-C5	-2.96	1.17	1.23
2	B	401	1VU	C2-S	-2.91	1.70	1.76
2	C	401	1VU	P1-O8	-2.85	1.42	1.54
2	C	401	1VU	O2-C8	-2.81	1.17	1.23
2	A	401	1VU	P1-O8	-2.72	1.43	1.54
2	F	401	1VU	P2-O14	-2.68	1.42	1.51
2	D	401	1VU	P1-O8	-2.66	1.43	1.54
2	F	401	1VU	O2-C8	-2.65	1.18	1.23
2	C	401	1VU	P-O5	-2.59	1.41	1.51
2	F	401	1VU	O1-C5	-2.58	1.17	1.23
2	B	401	1VU	O2-C8	-2.50	1.18	1.23
2	B	401	1VU	P2-O14	-2.45	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	1VU	P1-O8	-2.45	1.44	1.54
2	D	401	1VU	O2-C8	-2.35	1.18	1.23
2	E	401	1VU	O1-C5	-2.34	1.18	1.23
2	E	401	1VU	P1-O8	-2.34	1.45	1.54
2	A	401	1VU	P-O5	-2.32	1.42	1.51
2	D	401	1VU	P-O5	-2.28	1.42	1.51
2	F	401	1VU	C18-N3	-2.25	1.31	1.39
2	C	401	1VU	C18-N3	-2.21	1.31	1.39
2	B	401	1VU	P-O5	-2.20	1.43	1.51
2	A	401	1VU	P2-O14	-2.20	1.43	1.51
2	A	401	1VU	C18-N3	-2.17	1.32	1.39
2	F	401	1VU	C3-S	-2.16	1.72	1.81
2	E	401	1VU	O2-C8	-2.12	1.19	1.23
2	B	401	1VU	C18-C21	-2.11	1.35	1.40
2	D	401	1VU	C18-N3	-2.08	1.32	1.39
2	B	401	1VU	O1-C5	-2.02	1.19	1.23
2	E	401	1VU	P1-O9	2.43	1.60	1.51
2	F	401	1VU	C1-C2	2.85	1.54	1.50

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	1VU	N6-C20-N5	-11.56	120.04	128.89
2	A	401	1VU	N6-C20-N5	-10.48	120.87	128.89
2	E	401	1VU	N6-C20-N5	-10.22	121.07	128.89
2	D	401	1VU	N6-C20-N5	-8.82	122.14	128.89
2	C	401	1VU	O-C2-C1	-8.02	115.85	123.70
2	B	401	1VU	O-C2-C1	-7.68	116.18	123.70
2	F	401	1VU	N6-C20-N5	-6.81	123.68	128.89
2	F	401	1VU	P1-O7-P	-6.50	114.49	132.73
2	C	401	1VU	N6-C20-N5	-6.33	124.05	128.89
2	A	401	1VU	O-C2-C1	-6.06	117.77	123.70
2	F	401	1VU	O-C2-C1	-5.62	118.19	123.70
2	D	401	1VU	O-C2-C1	-5.20	118.61	123.70
2	E	401	1VU	O-C2-S	-4.14	119.55	122.83
2	D	401	1VU	C21-C18-N3	-3.86	105.93	109.48
2	C	401	1VU	P1-O7-P	-3.80	122.06	132.73
2	A	401	1VU	P1-O7-P	-3.72	122.29	132.73
2	B	401	1VU	C21-C18-N3	-3.50	106.26	109.48
2	F	401	1VU	C21-C18-N3	-3.44	106.32	109.48
2	E	401	1VU	C22-C16-N2	-3.20	109.40	114.29
2	A	401	1VU	C21-C18-N3	-3.17	106.57	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	1VU	C11-C10-C13	-2.74	104.95	108.50
2	E	401	1VU	P1-O7-P	-2.69	125.17	132.73
2	D	401	1VU	C16-N2-C21	-2.65	122.95	126.94
2	C	401	1VU	C21-C18-N3	-2.62	107.07	109.48
2	E	401	1VU	C21-C18-N3	-2.53	107.15	109.48
2	E	401	1VU	P2-O13-C23	-2.51	115.54	121.56
2	A	401	1VU	C11-C10-C9	-2.42	104.93	109.34
2	A	401	1VU	C16-N2-C21	-2.37	123.36	126.94
2	D	401	1VU	P1-O7-P	-2.32	126.20	132.73
2	B	401	1VU	C6-C5-N	-2.19	112.66	116.46
2	E	401	1VU	C7-C6-C5	-2.17	108.73	112.31
2	B	401	1VU	P1-O7-P	-2.15	126.69	132.73
2	F	401	1VU	C3-C4-N	-2.08	108.19	112.36
2	A	401	1VU	C12-C10-C13	-2.04	105.86	108.50
2	E	401	1VU	C3-S-C2	2.02	109.28	102.09
2	F	401	1VU	C3-S-C2	2.06	109.44	102.09
2	A	401	1VU	C7-N1-C8	2.07	126.63	122.53
2	E	401	1VU	O6-P-O7	2.19	115.04	105.09
2	E	401	1VU	O4-P-O5	2.23	118.28	109.62
2	D	401	1VU	O6-P-O7	2.26	115.35	105.09
2	A	401	1VU	C11-C10-C13	2.44	111.66	108.50
2	E	401	1VU	C23-C22-C16	2.48	105.92	99.98
2	D	401	1VU	C7-N1-C8	2.65	127.77	122.53
2	B	401	1VU	C4-N-C5	3.47	129.62	122.79
2	A	401	1VU	P2-O13-C23	3.91	130.94	121.56
2	E	401	1VU	C1-C2-S	5.55	118.34	113.36
2	D	401	1VU	C1-C2-S	6.89	119.56	113.36
2	F	401	1VU	C1-C2-S	7.57	120.17	113.36
2	A	401	1VU	C1-C2-S	7.81	120.39	113.36
2	B	401	1VU	C1-C2-S	8.46	120.97	113.36
2	C	401	1VU	C1-C2-S	8.64	121.13	113.36

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	1VU	O-C2-C1-C
2	E	401	1VU	O-C2-C1-C
2	A	401	1VU	O-C2-C1-C
2	C	401	1VU	O-C2-C1-C
2	F	401	1VU	O-C2-C1-C

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	1VU	4	0
3	A	402	OXL	1	0
2	B	401	1VU	4	0
3	B	402	OXL	2	0
2	C	401	1VU	2	0
3	C	402	OXL	1	0
2	D	401	1VU	2	0
2	E	401	1VU	5	0
3	E	402	OXL	1	0
2	F	401	1VU	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	345/348 (99%)	0.19	22 (6%)	23 24	13, 22, 52, 84	0
1	B	347/348 (99%)	-0.05	6 (1%)	73 73	15, 26, 46, 87	0
1	C	347/348 (99%)	-0.05	15 (4%)	39 40	11, 20, 51, 71	0
1	D	344/348 (98%)	0.12	21 (6%)	25 26	12, 25, 50, 68	0
1	E	344/348 (98%)	-0.01	16 (4%)	35 37	12, 24, 47, 73	0
1	F	347/348 (99%)	0.15	16 (4%)	36 38	15, 27, 51, 66	0
All	All	2074/2088 (99%)	0.06	96 (4%)	36 38	11, 24, 50, 87	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	GLY	9.5
1	A	213	GLN	6.1
1	A	344	GLN	6.1
1	A	345	ALA	6.0
1	B	212	GLY	5.9
1	A	342	LEU	5.7
1	A	346	TYR	5.6
1	C	348	LEU	5.6
1	B	213	GLN	5.5
1	E	343	ALA	5.4
1	A	343	ALA	5.1
1	B	211	GLU	5.1
1	E	340	PRO	4.6
1	B	214	ALA	4.6
1	E	344	GLN	4.5
1	A	340	PRO	4.4
1	A	211	GLU	4.2
1	A	341	ASP	4.2
1	D	210	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	347	GLY	4.1
1	D	214	ALA	4.1
1	C	339	ASP	3.9
1	B	210	GLN	3.9
1	E	348	LEU	3.9
1	D	344	GLN	3.9
1	A	294	LEU	3.8
1	A	333	ARG	3.7
1	A	214	ALA	3.7
1	F	340	PRO	3.7
1	E	345	ALA	3.7
1	A	336	ALA	3.6
1	C	341	ASP	3.4
1	C	294	LEU	3.4
1	E	347	GLY	3.4
1	E	346	TYR	3.4
1	F	343	ALA	3.3
1	B	215	GLU	3.3
1	A	210	GLN	3.3
1	F	214	ALA	3.2
1	D	304	PRO	3.2
1	F	345	ALA	3.2
1	E	294	LEU	3.2
1	D	302	ALA	3.1
1	A	338	LYS	3.0
1	D	315	LYS	2.9
1	D	300	LEU	2.9
1	C	312	ILE	2.9
1	D	307	SER	2.8
1	C	210	GLN	2.8
1	C	345	ALA	2.7
1	C	347	GLY	2.7
1	C	211	GLU	2.7
1	D	312	ILE	2.7
1	D	322	TRP	2.7
1	E	210	GLN	2.7
1	F	213	GLN	2.7
1	A	313	ASP	2.7
1	D	298	ARG	2.6
1	F	348	LEU	2.6
1	F	314	GLY	2.5
1	A	293	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	311	MET	2.5
1	F	313	ASP	2.5
1	C	346	TYR	2.5
1	C	301	GLU	2.5
1	A	331	LEU	2.5
1	A	332	ALA	2.4
1	F	310	ALA	2.4
1	D	311	MET	2.4
1	F	344	GLN	2.4
1	D	341	ASP	2.4
1	E	295	PHE	2.4
1	A	339	ASP	2.4
1	E	339	ASP	2.3
1	F	339	ASP	2.3
1	E	303	MET	2.3
1	E	336	ALA	2.3
1	D	306	GLY	2.3
1	D	314	GLY	2.3
1	F	81	ALA	2.3
1	C	344	GLN	2.2
1	D	215	GLU	2.2
1	D	39	GLU	2.2
1	C	302	ALA	2.2
1	C	313	ASP	2.2
1	F	298	ARG	2.2
1	D	339	ASP	2.2
1	E	39	GLU	2.2
1	E	215	GLU	2.2
1	D	346	TYR	2.1
1	F	346	TYR	2.1
1	A	337	LYS	2.1
1	F	347	GLY	2.1
1	E	313	ASP	2.0
1	C	305	ASP	2.0
1	D	303	MET	2.0

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

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(Å ²)	Q<0.9
5	TRS	D	404	8/8	0.98	0.14	1.80	16,19,21,22	0
5	TRS	A	404	8/8	0.98	0.15	1.33	14,16,17,17	0
3	OXL	B	402	6/6	0.94	0.16	0.78	22,23,28,36	0
2	1VU	E	401	52/52	0.85	0.18	0.72	19,40,61,72	52
2	1VU	D	401	52/52	0.88	0.15	0.35	26,39,60,65	0
2	1VU	F	401	52/52	0.87	0.14	0.27	23,38,55,63	52
2	1VU	A	401	52/52	0.90	0.14	0.19	21,36,48,55	52
3	OXL	A	402	6/6	0.95	0.13	0.07	19,22,24,30	0
2	1VU	B	401	52/52	0.92	0.12	-0.13	26,37,53,55	52
2	1VU	C	401	52/52	0.94	0.10	-0.31	16,26,45,49	0
3	OXL	E	402	6/6	0.95	0.11	-0.35	19,22,26,27	6
3	OXL	C	402	6/6	0.96	0.10	-0.63	16,18,24,28	0
3	OXL	F	402	6/6	0.96	0.11	-0.68	18,20,27,28	0
3	OXL	D	402	6/6	0.96	0.10	-1.04	22,22,27,31	0
4	MG	F	403	1/1	0.96	0.06	-2.00	24,24,24,24	0
4	MG	C	403	1/1	0.98	0.05	-2.13	15,15,15,15	0
4	MG	D	403	1/1	0.95	0.06	-2.26	24,24,24,24	0
4	MG	A	403	1/1	0.99	0.07	-2.47	21,21,21,21	0
4	MG	B	403	1/1	0.96	0.04	-2.58	26,26,26,26	0
4	MG	E	403	1/1	0.98	0.04	-2.90	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.