



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2025 – 09:10 am GMT

PDB ID : 9S3L / pdb_00009s3l
Title : ClxA from Clostridium cavendishii (apo)
Authors : Ascham, A.; Grogan, G.
Deposited on : 2025-07-24
Resolution : 2.57 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

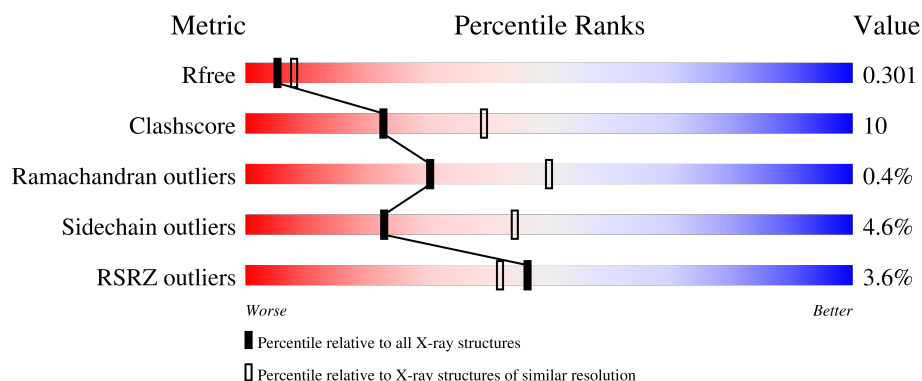
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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}	164625	4456 (2.60-2.56)
Clashscore	180529	4905 (2.60-2.56)
Ramachandran outliers	177936	4847 (2.60-2.56)
Sidechain outliers	177891	4847 (2.60-2.56)
RSRZ outliers	164620	4456 (2.60-2.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	401	<div> <div>4%</div> <div>72%</div> <div>25%</div> <div>.</div> </div>
1	B	401	<div> <div>4%</div> <div>73%</div> <div>25%</div> <div>..</div> </div>
1	C	401	<div> <div>3%</div> <div>73%</div> <div>24%</div> <div>.</div> </div>
1	D	401	<div> <div>3%</div> <div>76%</div> <div>23%</div> <div>..</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12198 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 Phenylacetate-CoA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3046	1961	500	571	14			
1	B	398	Total	C	N	O	S	0	0	0
			3029	1942	497	576	14			
1	C	399	Total	C	N	O	S	0	0	0
			3033	1951	499	569	14			
1	D	398	Total	C	N	O	S	0	0	0
			3005	1931	494	566	14			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	D	1	Total	Mg	0	0
			1	1		

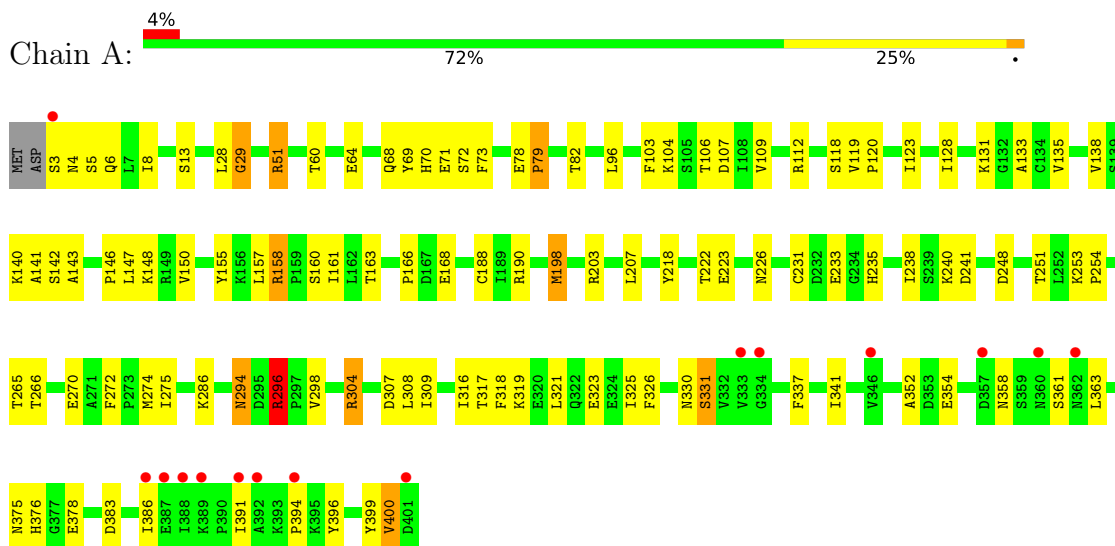
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total 23	O 23	0	0
4	B	22	Total 22	O 22	0	0
4	C	18	Total 18	O 18	0	0
4	D	15	Total 15	O 15	0	0

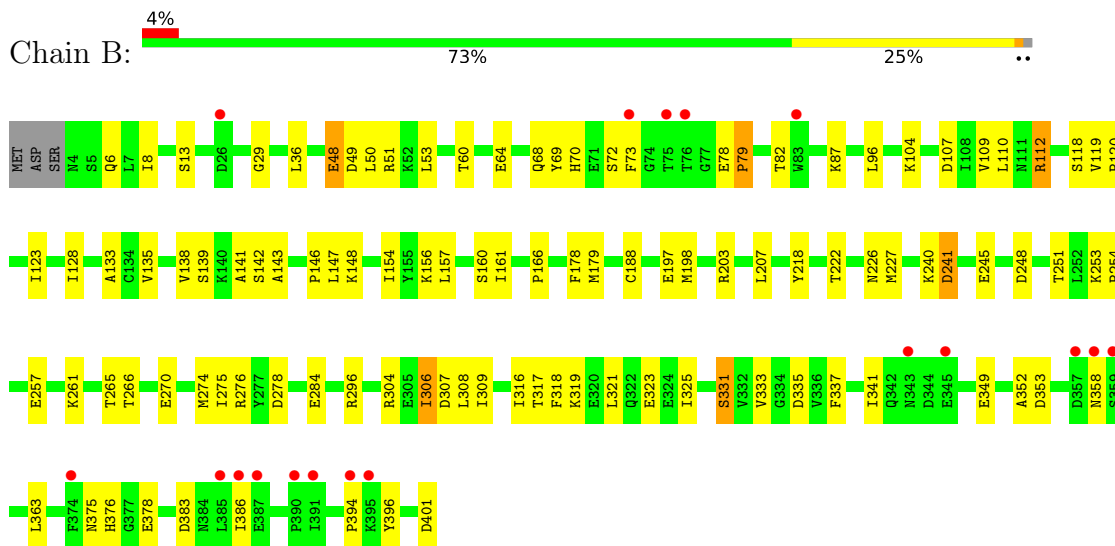
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

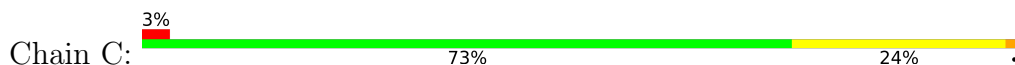
• Molecule 1: Phenylacetate-CoA ligase

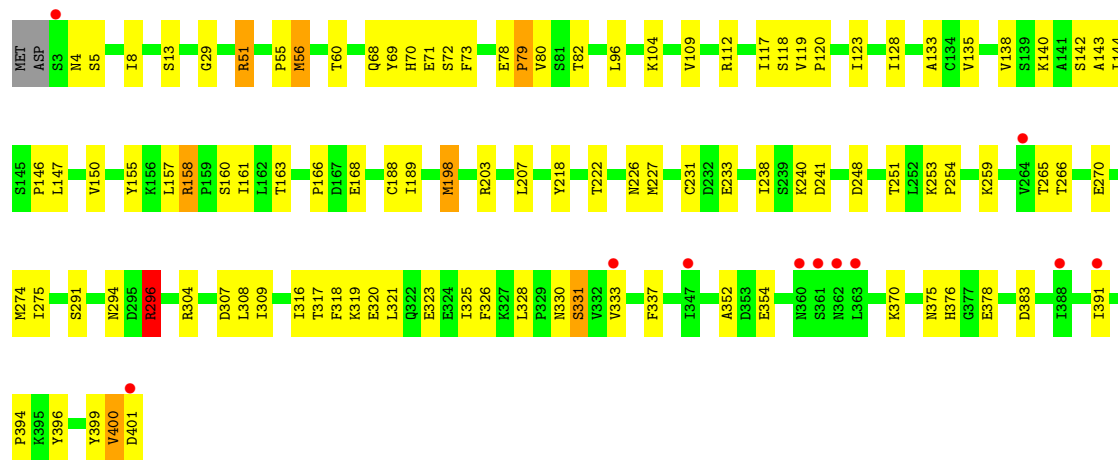


• Molecule 1: Phenylacetate-CoA ligase

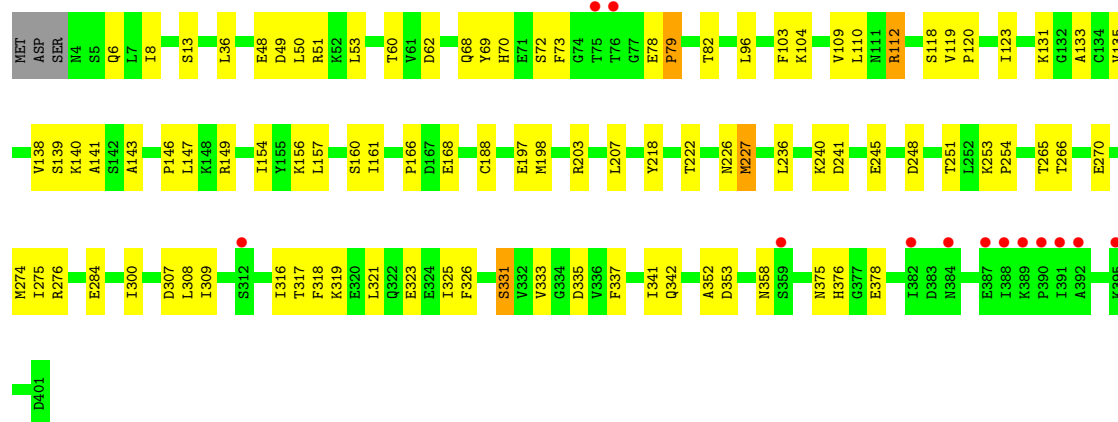
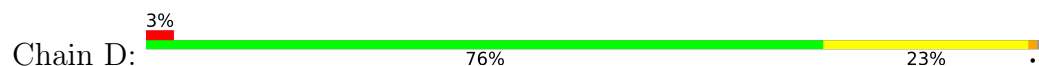


• Molecule 1: Phenylacetate-CoA ligase





● Molecule 1: Phenylacetate-CoA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.94Å 79.97Å 81.77Å 90.26° 95.58° 103.50°	Depositor
Resolution (Å)	40.71 – 2.57 40.71 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.71-2.57) 99.2 (40.71-2.57)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.265 , 0.301 0.267 , 0.301	Depositor DCC
R_{free} test set	2740 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	1.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12198	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

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	0.56	0/3102	1.10	5/4208 (0.1%)
1	B	0.56	0/3085	1.09	3/4185 (0.1%)
1	C	0.56	0/3089	1.09	5/4192 (0.1%)
1	D	0.55	0/3061	1.07	2/4157 (0.0%)
All	All	0.56	0/12337	1.09	15/16742 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	3
All	All	0	6

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ARG	CG-CD-NE	-9.34	91.45	112.00
1	C	296	ARG	CG-CD-NE	-9.07	92.05	112.00
1	C	79	PRO	N-CA-CB	-6.43	96.50	103.25
1	A	79	PRO	N-CA-CB	-6.11	96.83	103.25
1	A	73	PHE	CA-CB-CG	6.09	119.89	113.80
1	B	73	PHE	CA-CB-CG	6.07	119.86	113.80
1	C	73	PHE	CA-CB-CG	6.06	119.86	113.80
1	A	235	HIS	CA-CB-CG	6.03	119.83	113.80
1	B	79	PRO	N-CA-CB	-5.76	97.20	103.25
1	D	73	PHE	CA-CB-CG	5.76	119.56	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	79	PRO	N-CA-CB	-5.69	97.27	103.25
1	C	56	MET	CG-SD-CE	5.57	113.16	100.90
1	A	383	ASP	CA-CB-CG	5.20	117.80	112.60
1	C	383	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	241	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	ARG	Sidechain
1	A	304	ARG	Sidechain
1	A	51	ARG	Sidechain
1	C	203	ARG	Sidechain
1	C	304	ARG	Sidechain
1	C	51	ARG	Sidechain

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	3046	0	3001	74	1
1	B	3029	0	2945	70	0
1	C	3033	0	2973	65	0
1	D	3005	0	2915	62	1
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	B	2	0	0	0	0
3	D	1	0	0	0	0
4	A	23	0	0	2	0
4	B	22	0	0	0	0
4	C	18	0	0	3	0
4	D	15	0	0	2	0
All	All	12198	0	11834	247	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 10.

All (247) 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:223:GLU:OE1	4:A:601:HOH:O	1.60	1.16
1:D:118:SER:OG	1:D:120:PRO:HD2	1.72	0.90
1:B:118:SER:OG	1:B:120:PRO:HD2	1.72	0.89
1:A:118:SER:OG	1:A:120:PRO:HD2	1.72	0.89
1:D:70:HIS:CG	1:D:119:VAL:HG22	2.08	0.89
1:C:118:SER:OG	1:C:120:PRO:HD2	1.73	0.89
1:B:70:HIS:CG	1:B:119:VAL:HG22	2.08	0.88
1:A:309:ILE:HG23	1:A:341:ILE:HD11	1.61	0.81
1:A:71:GLU:OE2	1:B:156:LYS:NZ	2.15	0.79
1:A:158:ARG:NH1	1:A:158:ARG:HG2	2.00	0.77
1:C:158:ARG:NH1	1:C:158:ARG:HG2	2.00	0.76
1:C:400:VAL:O	1:C:401:ASP:C	2.30	0.73
1:C:60:THR:OG1	1:C:270:GLU:O	2.07	0.72
1:A:60:THR:OG1	1:A:270:GLU:O	2.07	0.72
1:D:70:HIS:CD2	1:D:119:VAL:HG22	2.25	0.72
1:B:60:THR:OG1	1:B:270:GLU:O	2.08	0.71
1:B:70:HIS:CD2	1:B:119:VAL:HG22	2.24	0.71
1:D:60:THR:OG1	1:D:270:GLU:O	2.08	0.71
1:B:118:SER:HG	1:B:120:PRO:HD2	1.59	0.67
1:B:70:HIS:CG	1:B:119:VAL:CG2	2.79	0.64
1:C:56:MET:HB2	4:C:609:HOH:O	1.98	0.63
1:A:286:LYS:HB2	1:A:298:VAL:CG2	2.28	0.63
1:D:70:HIS:CG	1:D:119:VAL:CG2	2.80	0.63
1:D:104:LYS:O	1:D:133:ALA:HB2	2.00	0.62
1:A:158:ARG:HG2	1:A:158:ARG:HH11	1.63	0.62
1:A:399:TYR:CE1	1:B:341:ILE:HD13	2.35	0.62
1:C:399:TYR:CE1	1:D:341:ILE:HD13	2.35	0.62
1:C:80:VAL:O	4:C:601:HOH:O	2.16	0.60
1:C:158:ARG:HG2	1:C:158:ARG:HH11	1.64	0.60
1:A:304:ARG:HG3	4:A:611:HOH:O	2.01	0.60
1:B:394:PRO:HB2	1:B:396:TYR:CE1	2.37	0.59
1:C:104:LYS:O	1:C:133:ALA:HB2	2.01	0.59
1:C:394:PRO:HB2	1:C:396:TYR:CE1	2.37	0.59
1:B:70:HIS:ND1	1:B:119:VAL:HG22	2.18	0.59
1:D:143:ALA:O	1:D:146:PRO:HD3	2.03	0.59
1:B:143:ALA:O	1:B:146:PRO:HD3	2.03	0.58
1:A:265:THR:HA	1:A:274:MET:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:THR:HA	1:D:274:MET:O	2.04	0.58
1:A:143:ALA:O	1:A:146:PRO:HD3	2.03	0.58
1:C:240:LYS:HE3	1:C:241:ASP:OD1	2.03	0.58
1:B:70:HIS:CE1	1:B:119:VAL:HG22	2.39	0.57
1:B:240:LYS:HE3	1:B:241:ASP:OD1	2.04	0.57
1:D:70:HIS:CE1	1:D:119:VAL:HG22	2.39	0.57
1:A:394:PRO:HB2	1:A:396:TYR:CE1	2.38	0.57
1:C:143:ALA:O	1:C:146:PRO:HD3	2.04	0.57
1:A:286:LYS:HB2	1:A:298:VAL:HG23	1.84	0.57
1:B:265:THR:HA	1:B:274:MET:O	2.03	0.57
1:A:69:TYR:CE2	1:B:157:LEU:HD21	2.38	0.57
1:D:70:HIS:ND1	1:D:119:VAL:HG22	2.19	0.57
1:C:157:LEU:HD21	1:D:69:TYR:CE2	2.40	0.57
1:C:238:ILE:O	1:C:296:ARG:HG3	2.04	0.56
1:C:265:THR:HA	1:C:274:MET:O	2.04	0.56
1:B:353:ASP:OD1	1:B:376:HIS:NE2	2.32	0.56
1:D:140:LYS:HE2	1:D:168:GLU:CD	2.31	0.56
1:C:140:LYS:HE2	1:C:168:GLU:CD	2.30	0.56
1:A:140:LYS:HE2	1:A:168:GLU:CD	2.30	0.56
1:C:155:TYR:O	1:C:158:ARG:NH1	2.39	0.56
1:A:240:LYS:HE3	1:A:241:ASP:OD1	2.05	0.55
1:A:112:ARG:HB3	1:A:163:THR:O	2.07	0.55
1:D:118:SER:HG	1:D:120:PRO:HD2	1.70	0.55
1:C:109:VAL:HG22	1:C:161:ILE:HB	1.89	0.55
1:D:353:ASP:OD1	1:D:376:HIS:NE2	2.33	0.55
1:A:238:ILE:O	1:A:296:ARG:HG3	2.07	0.55
1:A:148:LYS:HE3	1:A:386:ILE:HB	1.89	0.54
1:A:375:ASN:HB2	1:A:378:GLU:CD	2.32	0.54
1:C:112:ARG:HB3	1:C:163:THR:O	2.07	0.54
1:D:319:LYS:O	1:D:323:GLU:HG2	2.07	0.54
1:A:109:VAL:HG22	1:A:161:ILE:HB	1.89	0.54
1:A:155:TYR:O	1:A:158:ARG:NH1	2.40	0.54
1:C:319:LYS:O	1:C:323:GLU:HG2	2.07	0.54
1:A:319:LYS:O	1:A:323:GLU:HG2	2.07	0.54
1:B:128:ILE:HG23	1:B:133:ALA:HB3	1.90	0.54
1:A:396:TYR:OH	1:B:203:ARG:NH2	2.40	0.53
1:C:70:HIS:CE1	1:C:119:VAL:HG23	2.43	0.53
1:D:109:VAL:HG22	1:D:161:ILE:HB	1.91	0.53
1:C:375:ASN:HB2	1:C:378:GLU:CD	2.33	0.53
1:D:160:SER:HA	1:D:188:CYS:O	2.09	0.53
1:A:141:ALA:O	1:B:142:SER:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:SER:HA	1:B:188:CYS:O	2.09	0.53
1:A:70:HIS:CE1	1:A:119:VAL:HG23	2.44	0.53
1:A:157:LEU:HD21	1:B:69:TYR:CE2	2.44	0.53
1:B:265:THR:HG23	1:B:275:ILE:HA	1.92	0.52
1:D:265:THR:HG23	1:D:275:ILE:HA	1.92	0.52
1:B:109:VAL:HG22	1:B:161:ILE:HB	1.91	0.52
1:C:158:ARG:HH11	1:C:158:ARG:CG	2.23	0.52
1:D:240:LYS:HE3	1:D:241:ASP:OD1	2.09	0.52
1:A:160:SER:HA	1:A:188:CYS:O	2.10	0.52
1:B:319:LYS:O	1:B:323:GLU:HG2	2.09	0.52
1:A:358:ASN:HA	1:A:361:SER:HB3	1.91	0.52
1:D:50:LEU:O	1:D:53:LEU:HB2	2.10	0.52
1:C:160:SER:HA	1:C:188:CYS:O	2.10	0.52
1:C:142:SER:HA	1:D:141:ALA:O	2.10	0.51
1:A:138:VAL:HG11	1:A:150:VAL:HG22	1.90	0.51
1:B:8:ILE:HD11	1:B:36:LEU:CD1	2.41	0.51
1:B:261:LYS:NZ	1:B:278:ASP:OD2	2.36	0.51
1:C:69:TYR:CE2	1:D:157:LEU:HD21	2.46	0.51
1:B:253:LYS:O	1:B:254:PRO:C	2.54	0.51
1:A:106:THR:HG22	1:B:64:GLU:HG3	1.93	0.51
1:B:112:ARG:HD3	1:B:139:SER:O	2.11	0.51
1:C:144:ILE:HA	1:C:391:ILE:HD11	1.94	0.50
1:A:265:THR:HG23	1:A:275:ILE:HA	1.93	0.50
1:D:266:THR:HG23	1:D:274:MET:HB2	1.94	0.50
1:A:307:ASP:O	1:A:318:PHE:HB2	2.12	0.50
1:D:218:TYR:HB3	1:D:226:ASN:HD21	1.76	0.50
1:B:50:LEU:O	1:B:53:LEU:HB2	2.12	0.50
1:A:198:MET:HE1	1:A:319:LYS:HA	1.94	0.50
1:A:266:THR:HG23	1:A:274:MET:HB2	1.94	0.49
1:A:68:GLN:OE1	1:B:135:VAL:HB	2.12	0.49
1:A:158:ARG:HH11	1:A:158:ARG:CG	2.21	0.49
1:A:218:TYR:HB3	1:A:226:ASN:HD21	1.78	0.49
1:C:266:THR:HG23	1:C:274:MET:HB2	1.94	0.49
1:D:307:ASP:O	1:D:318:PHE:HB2	2.12	0.49
1:B:266:THR:HG23	1:B:274:MET:HB2	1.95	0.49
1:C:307:ASP:O	1:C:318:PHE:HB2	2.13	0.49
1:C:400:VAL:HG13	1:D:342:GLN:CB	2.43	0.49
1:C:51:ARG:NE	1:C:78:GLU:O	2.44	0.49
1:B:308:LEU:HD23	1:B:317:THR:HA	1.95	0.49
1:D:253:LYS:O	1:D:254:PRO:C	2.56	0.49
1:A:4:ASN:O	1:A:8:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:VAL:CG2	1:A:400:VAL:O	2.60	0.48
1:D:112:ARG:HD3	1:D:139:SER:O	2.13	0.48
1:A:135:VAL:HB	1:B:68:GLN:OE1	2.13	0.48
1:A:104:LYS:O	1:A:133:ALA:HB2	2.13	0.48
1:C:138:VAL:HG11	1:C:150:VAL:HG22	1.95	0.48
1:B:96:LEU:HD11	1:B:123:ILE:HG13	1.96	0.48
1:C:265:THR:HG23	1:C:275:ILE:HA	1.95	0.48
1:A:326:PHE:HZ	1:A:337:PHE:CE2	2.31	0.48
1:B:110:LEU:HD13	1:B:154:ILE:HG12	1.93	0.48
1:C:253:LYS:O	1:C:254:PRO:C	2.56	0.48
1:A:253:LYS:O	1:A:254:PRO:C	2.56	0.48
1:B:218:TYR:HB3	1:B:226:ASN:HD21	1.78	0.48
1:C:231:CYS:SG	1:C:233:GLU:HB2	2.54	0.48
1:B:307:ASP:O	1:B:318:PHE:HB2	2.14	0.48
1:C:71:GLU:OE2	1:D:156:LYS:NZ	2.46	0.48
1:A:51:ARG:NE	1:A:78:GLU:O	2.46	0.48
1:D:110:LEU:HD13	1:D:154:ILE:CG1	2.44	0.48
1:A:3:SER:CB	1:A:6:GLN:HG3	2.44	0.48
1:D:82:THR:HG21	1:D:222:THR:O	2.13	0.48
1:B:104:LYS:O	1:B:133:ALA:HB2	2.14	0.47
1:B:148:LYS:HG3	1:B:179:MET:SD	2.54	0.47
1:B:82:THR:HG21	1:B:222:THR:O	2.15	0.47
1:C:119:VAL:HG22	1:C:123:ILE:HG23	1.96	0.47
1:C:218:TYR:HB3	1:C:226:ASN:HD21	1.78	0.47
1:D:110:LEU:HD13	1:D:154:ILE:HG12	1.96	0.47
1:D:308:LEU:HD23	1:D:317:THR:HA	1.96	0.47
1:A:82:THR:HG21	1:A:222:THR:O	2.14	0.47
1:B:245:GLU:OE2	1:B:276:ARG:NH1	2.48	0.47
1:A:128:ILE:HG23	1:A:133:ALA:HB3	1.95	0.47
1:C:82:THR:HG21	1:C:222:THR:O	2.14	0.47
1:C:326:PHE:HZ	1:C:337:PHE:CE2	2.32	0.47
1:A:142:SER:HA	1:B:141:ALA:O	2.14	0.47
1:C:96:LEU:HD11	1:C:123:ILE:HG13	1.97	0.47
1:D:166:PRO:HB3	1:D:207:LEU:HD11	1.96	0.47
1:B:110:LEU:HD13	1:B:154:ILE:CG1	2.44	0.47
1:C:198:MET:HE1	1:C:319:LYS:HA	1.97	0.47
1:C:4:ASN:O	1:C:8:ILE:HG13	2.15	0.47
1:D:245:GLU:OE2	1:D:276:ARG:NH1	2.48	0.47
1:A:119:VAL:HG22	1:A:123:ILE:HG23	1.97	0.46
1:D:8:ILE:HD11	1:D:36:LEU:CD1	2.44	0.46
1:C:71:GLU:OE1	1:D:149:ARG:NH2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:ASP:HA	1:D:300:ILE:HD12	1.97	0.46
1:B:104:LYS:O	1:B:107:ASP:HB2	2.16	0.46
1:D:248:ASP:HB3	1:D:251:THR:OG1	2.16	0.46
1:A:308:LEU:HD23	1:A:317:THR:HA	1.97	0.46
1:A:309:ILE:HB	1:A:316:ILE:CG1	2.46	0.46
1:D:96:LEU:HD11	1:D:123:ILE:HG13	1.98	0.45
1:B:309:ILE:HB	1:B:316:ILE:CG1	2.47	0.45
1:C:248:ASP:HB3	1:C:251:THR:OG1	2.16	0.45
1:C:309:ILE:HB	1:C:316:ILE:CG1	2.46	0.45
1:B:248:ASP:HB3	1:B:251:THR:OG1	2.17	0.45
1:C:166:PRO:HB3	1:C:207:LEU:HD11	1.99	0.45
1:C:328:LEU:HB2	1:C:333:VAL:HG21	1.99	0.45
1:A:96:LEU:HD11	1:A:123:ILE:HG13	1.99	0.45
1:C:396:TYR:OH	1:D:203:ARG:NH2	2.50	0.45
1:D:309:ILE:HB	1:D:316:ILE:CG1	2.46	0.44
1:C:119:VAL:N	1:C:120:PRO:CD	2.81	0.44
1:D:236:LEU:HG	4:D:609:HOH:O	2.17	0.44
1:A:119:VAL:N	1:A:120:PRO:CD	2.81	0.44
1:B:321:LEU:O	1:B:325:ILE:HG12	2.17	0.44
1:C:308:LEU:HD23	1:C:317:THR:HA	1.99	0.44
1:C:68:GLN:OE1	1:D:135:VAL:HB	2.17	0.44
1:D:326:PHE:HZ	1:D:337:PHE:CE2	2.36	0.44
1:D:119:VAL:N	1:D:120:PRO:CD	2.81	0.43
1:B:119:VAL:N	1:B:120:PRO:CD	2.81	0.43
1:D:103:PHE:HB2	1:D:131:LYS:HG3	1.99	0.43
1:A:331:SER:O	1:A:352:ALA:HB1	2.18	0.43
1:B:325:ILE:HG22	1:B:333:VAL:HG11	2.00	0.43
1:C:331:SER:O	1:C:352:ALA:HB1	2.18	0.43
1:B:112:ARG:HH21	1:B:147:LEU:HD23	1.82	0.43
1:D:49:ASP:O	1:D:53:LEU:HD13	2.18	0.43
1:A:248:ASP:HB3	1:A:251:THR:OG1	2.18	0.43
1:B:166:PRO:HB3	1:B:207:LEU:HD11	2.01	0.43
1:D:321:LEU:O	1:D:325:ILE:HG12	2.18	0.43
1:B:178:PHE:CE2	1:B:386:ILE:HG21	2.53	0.43
1:D:112:ARG:HH21	1:D:147:LEU:HD23	1.84	0.43
1:A:103:PHE:HB2	1:A:131:LYS:HG3	2.00	0.42
1:A:321:LEU:O	1:A:325:ILE:HG12	2.19	0.42
1:C:321:LEU:O	1:C:325:ILE:HG12	2.18	0.42
1:C:259:LYS:NZ	1:C:320:GLU:OE2	2.46	0.42
1:D:331:SER:O	1:D:352:ALA:HB1	2.19	0.42
1:B:270:GLU:O	1:B:270:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:ILE:HG22	1:D:333:VAL:HG11	2.01	0.42
1:A:112:ARG:HH21	1:A:147:LEU:HD23	1.84	0.42
1:A:294:ASN:HD22	1:A:296:ARG:H	1.67	0.42
1:B:178:PHE:CD2	1:B:386:ILE:HG21	2.55	0.42
1:B:296:ARG:HA	1:B:296:ARG:HD2	1.88	0.42
1:C:112:ARG:HH21	1:C:147:LEU:HD23	1.84	0.42
1:C:309:ILE:HB	1:C:316:ILE:HG12	2.01	0.42
1:A:69:TYR:CE2	1:B:157:LEU:CD2	3.03	0.42
1:B:51:ARG:NE	1:B:78:GLU:O	2.49	0.42
1:B:331:SER:O	1:B:352:ALA:HB1	2.19	0.42
1:D:48:GLU:HB2	4:D:605:HOH:O	2.19	0.42
1:C:118:SER:HG	1:C:120:PRO:HD2	1.79	0.41
1:A:238:ILE:O	1:A:296:ARG:CG	2.68	0.41
1:C:238:ILE:O	1:C:296:ARG:CG	2.68	0.41
1:A:375:ASN:O	1:A:376:HIS:C	2.63	0.41
1:D:309:ILE:HB	1:D:316:ILE:HG12	2.01	0.41
1:A:309:ILE:HB	1:A:316:ILE:HG12	2.02	0.41
1:B:337:PHE:HA	1:B:349:GLU:O	2.20	0.41
1:C:135:VAL:HB	1:D:68:GLN:OE1	2.19	0.41
1:A:231:CYS:SG	1:A:233:GLU:HB2	2.60	0.41
1:C:189:ILE:HB	4:C:602:HOH:O	2.19	0.41
1:D:51:ARG:NE	1:D:78:GLU:O	2.47	0.41
1:C:55:PRO:HG2	1:D:156:LYS:HG2	2.02	0.41
1:C:128:ILE:HG23	1:C:133:ALA:HB3	2.02	0.41
1:D:198:MET:SD	1:D:198:MET:C	3.04	0.41
1:A:69:TYR:CZ	1:B:157:LEU:HD21	2.56	0.41
1:B:49:ASP:O	1:B:53:LEU:HD13	2.21	0.41
1:B:198:MET:C	1:B:198:MET:SD	3.04	0.41
1:B:335:ASP:OD1	1:B:335:ASP:N	2.54	0.41
1:D:375:ASN:O	1:D:376:HIS:C	2.64	0.41
1:A:28:LEU:O	1:A:29:GLY:C	2.64	0.41
1:B:309:ILE:HB	1:B:316:ILE:HG12	2.02	0.41
1:D:227:MET:HE2	1:D:227:MET:HB2	1.98	0.41
1:B:8:ILE:HD11	1:B:36:LEU:HD12	2.03	0.40
1:C:375:ASN:O	1:C:376:HIS:C	2.64	0.40
1:A:69:TYR:CD1	1:A:70:HIS:N	2.90	0.40
1:A:166:PRO:HB3	1:A:207:LEU:HD11	2.03	0.40
1:A:198:MET:C	1:A:198:MET:SD	3.04	0.40
1:B:48:GLU:CD	1:B:48:GLU:H	2.29	0.40
1:B:304:ARG:HD2	1:B:306:ILE:HD11	2.03	0.40
1:B:375:ASN:O	1:B:376:HIS:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ASP:OD2	1:A:190:ARG:NH2	2.53	0.40
1:A:272:PHE:CE2	1:A:274:MET:HE1	2.56	0.40
1:D:119:VAL:H	1:D:120:PRO:CD	2.35	0.40
1:A:400:VAL:O	1:A:400:VAL:HG23	2.21	0.40
1:C:69:TYR:CD1	1:C:70:HIS:N	2.90	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)
1:A:330:ASN:CB	1:D:62:ASP:OD1[1_655]	2.17	0.03

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	397/401 (99%)	369 (93%)	27 (7%)	1 (0%)	37	57
1	B	396/401 (99%)	368 (93%)	26 (7%)	2 (0%)	25	45
1	C	397/401 (99%)	369 (93%)	26 (6%)	2 (0%)	25	45
1	D	396/401 (99%)	368 (93%)	27 (7%)	1 (0%)	37	57
All	All	1586/1604 (99%)	1474 (93%)	106 (7%)	6 (0%)	30	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	358	ASN
1	B	358	ASN
1	A	29	GLY
1	B	29	GLY
1	C	117	ILE

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Mol	Chain	Res	Type
1	C	29	GLY

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	319/356 (90%)	305 (96%)	14 (4%)	24	46
1	B	315/356 (88%)	298 (95%)	17 (5%)	18	37
1	C	316/356 (89%)	301 (95%)	15 (5%)	22	43
1	D	309/356 (87%)	297 (96%)	12 (4%)	27	51
All	All	1259/1424 (88%)	1201 (95%)	58 (5%)	23	44

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	13	SER
1	A	64	GLU
1	A	72	SER
1	A	79	PRO
1	A	158	ARG
1	A	198	MET
1	A	294	ASN
1	A	296	ARG
1	A	331	SER
1	A	354	GLU
1	A	363	LEU
1	A	391	ILE
1	A	400	VAL
1	B	6	GLN
1	B	13	SER
1	B	48	GLU
1	B	72	SER
1	B	79	PRO
1	B	87	LYS

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Mol	Chain	Res	Type
1	B	112	ARG
1	B	138	VAL
1	B	197	GLU
1	B	227	MET
1	B	257	GLU
1	B	284	GLU
1	B	306	ILE
1	B	331	SER
1	B	363	LEU
1	B	378	GLU
1	B	383	ASP
1	C	5	SER
1	C	13	SER
1	C	72	SER
1	C	79	PRO
1	C	158	ARG
1	C	198	MET
1	C	227	MET
1	C	291	SER
1	C	294	ASN
1	C	296	ARG
1	C	330	ASN
1	C	331	SER
1	C	354	GLU
1	C	370	LYS
1	C	400	VAL
1	D	6	GLN
1	D	13	SER
1	D	72	SER
1	D	79	PRO
1	D	112	ARG
1	D	138	VAL
1	D	197	GLU
1	D	227	MET
1	D	284	GLU
1	D	331	SER
1	D	335	ASP
1	D	378	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	HIS
1	A	126	ASN
1	A	129	HIS
1	A	226	ASN
1	A	294	ASN
1	A	381	ASN
1	B	16	GLN
1	B	126	ASN
1	B	226	ASN
1	B	375	ASN
1	B	384	ASN
1	C	122	HIS
1	C	126	ASN
1	C	129	HIS
1	C	226	ASN
1	C	294	ASN
1	C	322	GLN
1	C	330	ASN
1	D	16	GLN
1	D	122	HIS
1	D	126	ASN
1	D	226	ASN
1	D	375	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	399/401 (99%)	0.36	15 (3%) 44 40	19, 41, 73, 117	0
1	B	398/401 (99%)	0.36	18 (4%) 39 34	19, 39, 84, 122	0
1	C	399/401 (99%)	0.33	11 (2%) 55 50	17, 39, 75, 123	0
1	D	398/401 (99%)	0.36	13 (3%) 49 45	18, 40, 84, 116	0
All	All	1594/1604 (99%)	0.35	57 (3%) 46 42	17, 40, 79, 123	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	390	PRO	4.3
1	B	357	ASP	4.2
1	A	389	LYS	3.8
1	A	334	GLY	3.8
1	D	392	ALA	3.6
1	C	361	SER	3.5
1	C	333	VAL	3.5
1	B	359	SER	3.4
1	D	359	SER	3.3
1	B	391	ILE	3.1
1	C	391	ILE	3.1
1	C	401	ASP	3.1
1	A	387	GLU	3.1
1	C	362	ASN	3.0
1	D	388	ILE	3.0
1	B	73	PHE	2.9
1	D	75	THR	2.9
1	C	264	VAL	2.8
1	D	382	ILE	2.8
1	B	345	GLU	2.8
1	D	390	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	387	GLU	2.7
1	A	388	ILE	2.6
1	B	75	THR	2.6
1	C	363	LEU	2.6
1	A	333	VAL	2.6
1	A	386	ILE	2.6
1	B	386	ILE	2.6
1	D	389	LYS	2.5
1	C	360	ASN	2.5
1	C	388	ILE	2.5
1	A	360	ASN	2.5
1	D	384	ASN	2.5
1	A	392	ALA	2.4
1	B	76	THR	2.4
1	D	391	ILE	2.4
1	A	3	SER	2.4
1	B	385	LEU	2.3
1	C	3	SER	2.3
1	B	358	ASN	2.3
1	D	395	LYS	2.3
1	B	83	TRP	2.3
1	B	374	PHE	2.2
1	A	401	ASP	2.2
1	A	362	ASN	2.2
1	A	391	ILE	2.2
1	A	394	PRO	2.1
1	B	26	ASP	2.1
1	A	346	VAL	2.1
1	D	76	THR	2.1
1	A	357	ASP	2.1
1	B	394	PRO	2.1
1	B	395	LYS	2.1
1	B	387	GLU	2.0
1	B	343	ASN	2.0
1	D	312	SER	2.0
1	C	347	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	B	502	1/1	0.93	0.17	30,30,30,30	0
3	MG	D	502	1/1	0.94	0.09	30,30,30,30	0
3	MG	B	503	1/1	0.96	0.04	30,30,30,30	0
2	ZN	C	501	1/1	0.98	0.04	56,56,56,56	0
2	ZN	B	501	1/1	0.99	0.03	35,35,35,35	0
2	ZN	A	501	1/1	0.99	0.03	58,58,58,58	0
2	ZN	D	501	1/1	0.99	0.04	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.