



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 05:41 PM UTC

PDB ID : 8AXC / pdb_00008axc
Title : Crystal structure of mouse Ces2c
Authors : Eisner, H.; Riegler-Berket, L.; Rodriguez Gamez, C.; Sagmeister, T.; Chalhoub, G.; Darnhofer, B.; Panikkaveetil Jawaharlal, J.; Birner-Gruenberger, R.; Pavkov-Keller, T.; Haemmerle, G.; Schoiswohl, G.; Oberer, M.
Deposited on : 2022-08-31
Resolution : 2.12 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

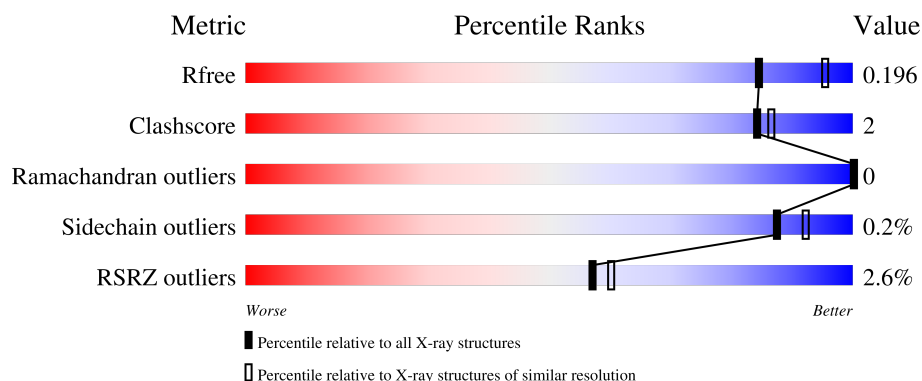
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	561	 2% 88% 5% 5%
1	B	561	 2% 89% 5% 5%
1	C	561	 2% 84% 5% 10%
1	D	561	 3% 87% 5% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33638 atoms, of which 15628 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.

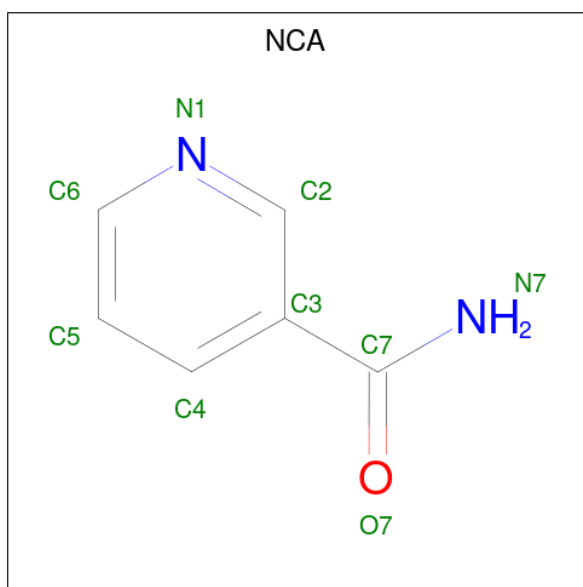
- Molecule 1 is a protein called Acylcarnitine hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	516	Total	C	H	N	O	S	0	10	0
			7969	2609	3883	697	748	32			
1	B	532	Total	C	H	N	O	S	0	16	0
			8277	2702	4037	726	776	36			
1	C	503	Total	C	H	N	O	S	0	14	0
			7798	2560	3790	682	737	29			
1	D	518	Total	C	H	N	O	S	0	8	0
			7990	2617	3894	699	750	30			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 3 is NICOTINAMIDE (CCD ID: NCA) (formula: C₆H₆N₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			13	6	4	2	1		
3	A	1	Total	C	H	N	O	0	0
			13	6	4	2	1		
3	B	1	Total	C	H	N	O	0	0
			13	6	4	2	1		
3	B	1	Total	C	H	N	O	0	0
			13	6	4	2	1		
3	C	1	Total	C	H	N	O	0	0
			13	6	4	2	1		
3	D	1	Total	C	H	N	O	0	0
			13	6	4	2	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		

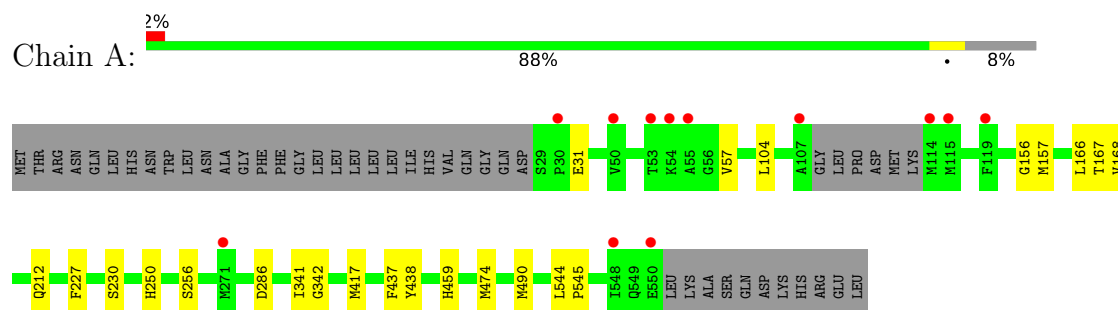
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	383	Total	O	0	0
			383	383		
5	B	417	Total	O	0	0
			417	417		
5	C	336	Total	O	0	0
			336	336		
5	D	381	Total	O	0	0
			381	381		

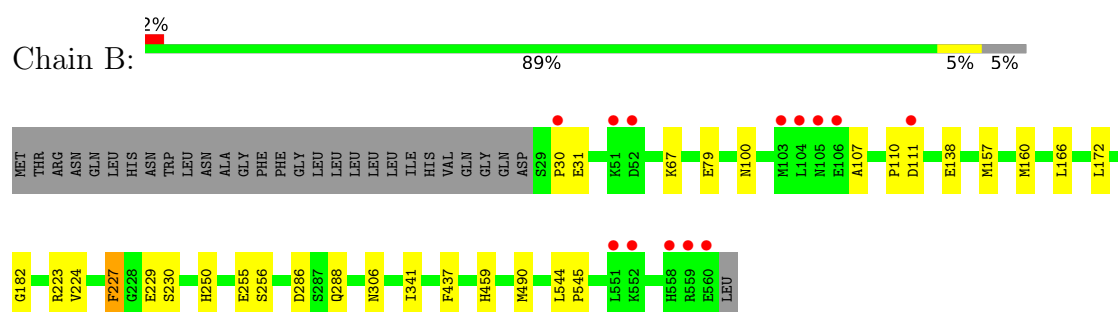
3 Residue-property plots [i](#)

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.

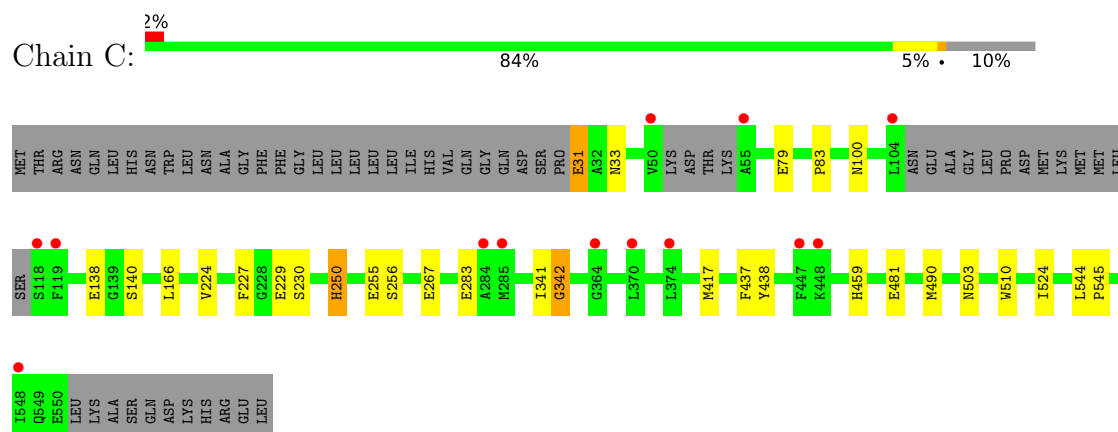
- Molecule 1: Acylcarnitine hydrolase



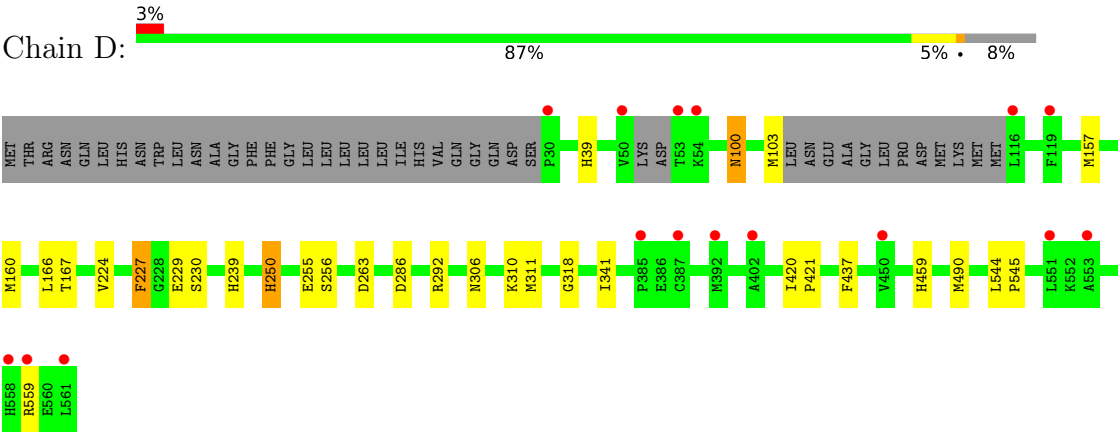
- Molecule 1: Acylcarnitine hydrolase



- Molecule 1: Acylcarnitine hydrolase



- Molecule 1: Acylcarnitine hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.05Å 143.59Å 183.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.05 – 2.12 49.05 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.05-2.12) 99.0 (49.05-2.12)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.163 , 0.196 0.163 , 0.196	Depositor DCC
R_{free} test set	7406 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33638	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NCA, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.05	2/4235 (0.0%)	1.24	5/5755 (0.1%)
1	B	1.06	1/4396 (0.0%)	1.25	3/5968 (0.1%)
1	C	1.04	3/4160 (0.1%)	1.22	4/5656 (0.1%)
1	D	1.06	3/4228 (0.1%)	1.23	6/5742 (0.1%)
All	All	1.05	9/17019 (0.1%)	1.24	18/23121 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	GLY	C-O	6.21	1.29	1.23
1	C	459	HIS	CE1-NE2	5.99	1.38	1.32
1	D	39	HIS	CE1-NE2	5.97	1.38	1.32
1	A	459	HIS	CE1-NE2	5.63	1.38	1.32
1	B	459	HIS	CE1-NE2	5.46	1.38	1.32
1	D	459	HIS	CE1-NE2	5.42	1.38	1.32
1	C	83	PRO	C-O	-5.19	1.17	1.23
1	C	342	GLY	C-O	5.16	1.28	1.23
1	D	239	HIS	CE1-NE2	5.16	1.37	1.32

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	PHE	CA-CB-CG	6.93	120.73	113.80
1	A	227	PHE	CA-CB-CG	6.90	120.70	113.80
1	D	227	PHE	CA-CB-CG	6.58	120.38	113.80
1	C	227	PHE	CA-CB-CG	6.47	120.27	113.80
1	A	167	THR	N-CA-CB	6.20	119.00	110.01
1	D	167	THR	N-CA-CB	5.99	118.69	110.01
1	D	100	ASN	CB-CA-C	5.88	120.50	110.81
1	C	31	GLU	CB-CA-C	5.63	120.79	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	PRO	CA-C-N	5.38	128.98	121.02
1	B	30	PRO	C-N-CA	5.38	128.98	121.02
1	A	250[A]	HIS	CA-CB-CG	5.36	119.16	113.80
1	A	250[B]	HIS	CA-CB-CG	5.36	119.16	113.80
1	D	292	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	C	250[A]	HIS	CA-CB-CG	-5.22	108.58	113.80
1	C	250[B]	HIS	CA-CB-CG	-5.22	108.58	113.80
1	D	250[A]	HIS	CA-CB-CG	-5.18	108.62	113.80
1	D	250[B]	HIS	CA-CB-CG	-5.18	108.62	113.80
1	A	286	ASP	CA-CB-CG	5.13	117.73	112.60

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	4086	3883	3967	15	0
1	B	4240	4037	4139	27	0
1	C	4008	3790	3874	26	0
1	D	4096	3894	3981	19	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	18	8	12	0	0
3	B	18	8	12	0	0
3	C	9	4	6	0	0
3	D	9	4	6	0	0
4	C	5	0	0	0	0
5	A	383	0	0	3	0
5	B	417	0	0	3	0
5	C	336	0	0	4	0
5	D	381	0	0	1	0
All	All	18010	15628	15997	75	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 2.

All (75) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100[A]:ASN:OD1	5:B:701:HOH:O	1.73	1.04
1:B:31:GLU:OE2	5:B:702:HOH:O	1.80	0.99
1:C:283[B]:GLU:H	1:C:283[B]:GLU:CD	1.70	0.98
1:B:286:ASP:OD2	1:D:286[B]:ASP:OD2	1.82	0.95
1:B:79:GLU:OE1	1:C:79[B]:GLU:OE1	1.90	0.89
1:B:288[B]:GLN:NE2	1:D:286[B]:ASP:OD2	2.07	0.88
1:B:79:GLU:OE1	1:C:79[B]:GLU:CD	2.17	0.86
1:B:286:ASP:OD1	1:B:288[B]:GLN:NE2	2.11	0.84
1:C:503:ASN:HD21	1:C:510:TRP:H	1.32	0.76
1:C:100[A]:ASN:OD1	5:C:701:HOH:O	2.05	0.74
1:A:57:VAL:CG2	1:A:168:VAL:HG13	2.21	0.70
1:D:100:ASN:OD1	5:D:702:HOH:O	2.08	0.70
1:B:286:ASP:OD2	1:D:286[B]:ASP:CG	2.35	0.69
1:C:283[B]:GLU:HG3	5:C:718:HOH:O	1.93	0.68
1:B:224:VAL:H	1:B:250[A]:HIS:HD2	1.42	0.67
1:B:223:ARG:HD3	1:B:250[B]:HIS:CE1	2.31	0.66
1:D:224:VAL:H	1:D:250[A]:HIS:HD2	1.42	0.66
1:C:224:VAL:H	1:C:250[A]:HIS:HD2	1.44	0.64
1:B:107:ALA:O	5:B:703:HOH:O	2.17	0.59
1:C:138:GLU:OE1	5:C:702:HOH:O	2.17	0.58
1:A:57:VAL:CG2	1:A:168:VAL:CG1	2.83	0.56
1:B:286:ASP:CG	1:D:286[B]:ASP:OD2	2.49	0.56
1:A:57:VAL:HG22	1:A:168:VAL:HG13	1.88	0.55
1:B:223:ARG:CD	1:B:250[B]:HIS:CE1	2.90	0.54
1:C:283[B]:GLU:CD	1:C:283[B]:GLU:N	2.51	0.53
1:C:503:ASN:ND2	1:C:510:TRP:H	2.04	0.53
1:C:166:LEU:HA	1:C:490:MET:CE	2.39	0.53
1:B:79:GLU:CD	1:C:79[B]:GLU:OE1	2.52	0.52
1:A:31:GLU:OE1	5:A:701:HOH:O	2.19	0.51
1:B:182:GLY:HA3	1:B:306:ASN:HD21	1.76	0.51
1:B:166:LEU:HA	1:B:490:MET:CE	2.41	0.51
1:A:166:LEU:HA	1:A:490:MET:CE	2.42	0.49
1:D:166:LEU:HA	1:D:490:MET:CE	2.43	0.49
1:C:417:MET:HG2	5:C:886:HOH:O	2.11	0.49
1:D:100:ASN:ND2	1:D:306:ASN:HD22	2.09	0.49
1:B:79:GLU:CD	1:C:79[B]:GLU:CD	2.80	0.49
1:A:104:LEU:HD21	1:A:157:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:MET:H	1:D:160:MET:HE2	1.79	0.48
1:C:267[B]:GLU:CD	1:C:267[B]:GLU:H	2.22	0.47
1:B:67:LYS:NZ	1:C:79[B]:GLU:OE2	2.41	0.46
1:B:79:GLU:OE1	1:C:79[B]:GLU:OE2	2.32	0.46
1:B:110:PRO:O	1:B:111:ASP:HB2	2.16	0.46
1:A:417:MET:HG2	5:A:916:HOH:O	2.15	0.45
1:A:474:MET:HE2	5:A:1043:HOH:O	2.16	0.45
1:D:544:LEU:HB3	1:D:545:PRO:HD3	1.99	0.45
1:A:104:LEU:HD21	1:A:157:MET:HE1	1.98	0.45
1:A:57:VAL:HG23	1:A:168:VAL:CG1	2.47	0.45
1:D:341:ILE:O	1:D:437:PHE:HA	2.15	0.45
1:B:341:ILE:O	1:B:437:PHE:HA	2.17	0.45
1:D:103:MET:HE1	1:D:310:LYS:O	2.18	0.44
1:D:224:VAL:H	1:D:250[A]:HIS:CD2	2.30	0.44
1:C:140:SER:O	1:D:559:ARG:HD3	2.17	0.44
1:B:229:GLU:HA	1:B:255:GLU:O	2.18	0.44
1:A:341:ILE:O	1:A:437:PHE:HA	2.17	0.43
1:C:341:ILE:O	1:C:437:PHE:HA	2.19	0.43
1:B:157:MET:H	1:B:160[B]:MET:HE2	1.82	0.43
1:A:544:LEU:HB3	1:A:545:PRO:HD3	1.99	0.42
1:D:263:ASP:HB3	1:D:311:MET:SD	2.58	0.42
1:D:420:ILE:HB	1:D:421:PRO:HD3	2.00	0.42
1:B:286:ASP:CG	1:B:288[B]:GLN:NE2	2.75	0.42
1:C:229:GLU:HA	1:C:255:GLU:O	2.19	0.42
1:D:229:GLU:HA	1:D:255:GLU:O	2.19	0.42
1:B:230:SER:HA	1:B:256:SER:O	2.20	0.41
1:A:230:SER:HA	1:A:256:SER:O	2.20	0.41
1:A:342:GLY:HA3	1:A:438:TYR:CE2	2.56	0.41
1:C:342:GLY:HA3	1:C:438:TYR:CE2	2.55	0.41
1:D:230:SER:HA	1:D:256:SER:O	2.20	0.41
1:B:172:LEU:HD12	1:B:172:LEU:C	2.46	0.41
1:B:544:LEU:HB3	1:B:545:PRO:HD3	2.02	0.41
1:C:544:LEU:HB3	1:C:545:PRO:HD3	2.02	0.41
1:C:230:SER:HA	1:C:256:SER:O	2.20	0.41
1:C:481[B]:GLU:HB3	1:C:524:ILE:HG23	2.03	0.41
1:A:212[B]:GLN:HE22	1:D:318:GLY:C	2.28	0.41
1:C:166:LEU:HA	1:C:490:MET:HE3	2.01	0.41
1:C:31:GLU:HG3	1:C:33:ASN:H	1.85	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/561 (93%)	507 (97%)	15 (3%)	0	100	100
1	B	546/561 (97%)	531 (97%)	15 (3%)	0	100	100
1	C	511/561 (91%)	498 (98%)	13 (2%)	0	100	100
1	D	520/561 (93%)	507 (98%)	13 (2%)	0	100	100
All	All	2099/2244 (94%)	2043 (97%)	56 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	444/474 (94%)	444 (100%)	0	100	100
1	B	462/474 (98%)	460 (100%)	2 (0%)	84	89
1	C	434/474 (92%)	434 (100%)	0	100	100
1	D	444/474 (94%)	443 (100%)	1 (0%)	87	92
All	All	1784/1896 (94%)	1781 (100%)	3 (0%)	87	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	138	GLU
1	B	227	PHE
1	D	227	PHE

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	211	GLN
1	A	288	GLN
1	A	424	GLN
1	A	518	GLN
1	B	141	ASN
1	B	306	ASN
1	B	403	GLN
1	B	424	GLN
1	B	499	HIS
1	C	169	ASN
1	C	288	GLN
1	C	424	GLN
1	C	499	HIS
1	C	503	ASN
1	C	515	HIS
1	C	546	GLN
1	D	44	GLN
1	D	100	ASN
1	D	141	ASN
1	D	169	ASN
1	D	424	GLN
1	D	454	HIS
1	D	499	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	NCA	D	602	-	9,9,9	0.23	0	11,11,11	0.39	0
3	NCA	B	602	-	9,9,9	0.20	0	11,11,11	0.35	0
3	NCA	C	603	-	9,9,9	0.23	0	11,11,11	0.37	0
4	SO4	C	601	-	4,4,4	0.32	0	6,6,6	0.27	0
3	NCA	B	603	-	9,9,9	0.30	0	11,11,11	0.38	0
3	NCA	A	602	-	9,9,9	0.22	0	11,11,11	0.39	0
3	NCA	A	603	-	9,9,9	0.22	0	11,11,11	0.52	0

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	NCA	D	602	-	-	0/4/4/4	0/1/1/1
3	NCA	B	602	-	-	0/4/4/4	0/1/1/1
3	NCA	C	603	-	-	0/4/4/4	0/1/1/1
3	NCA	B	603	-	-	0/4/4/4	0/1/1/1
3	NCA	A	602	-	-	0/4/4/4	0/1/1/1
3	NCA	A	603	-	-	0/4/4/4	0/1/1/1

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	516/561 (91%)	-0.36	12 (2%) 61 64	10, 29, 64, 114	10 (1%)
1	B	532/561 (94%)	-0.35	13 (2%) 59 62	12, 27, 69, 123	16 (3%)
1	C	503/561 (89%)	-0.23	13 (2%) 57 60	10, 28, 77, 109	14 (2%)
1	D	518/561 (92%)	-0.23	16 (3%) 51 54	11, 28, 77, 116	8 (1%)
All	All	2069/2244 (92%)	-0.29	54 (2%) 57 60	10, 28, 73, 123	48 (2%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	LEU	7.2
1	C	104	LEU	5.3
1	A	114	MET	5.1
1	D	116	LEU	4.9
1	D	50	VAL	4.5
1	D	561	LEU	4.2
1	C	55	ALA	4.2
1	C	50	VAL	4.1
1	B	558	HIS	3.8
1	B	51	LYS	3.8
1	D	53	THR	3.7
1	B	103	MET	3.5
1	D	558	HIS	3.5
1	D	551	LEU	3.4
1	B	559	ARG	3.1
1	D	559	ARG	3.1
1	A	119	PHE	3.0
1	A	55	ALA	3.0
1	C	118	SER	3.0
1	B	30	PRO	2.9
1	B	551	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	450	VAL	2.9
1	D	387	CYS	2.8
1	C	285	MET	2.8
1	A	107	ALA	2.6
1	B	106	GLU	2.6
1	A	54	LYS	2.6
1	D	119	PHE	2.5
1	A	115	MET	2.5
1	A	50	VAL	2.4
1	A	548	ILE	2.4
1	B	105	ASN	2.4
1	A	30	PRO	2.4
1	D	385	PRO	2.4
1	C	284[A]	ALA	2.3
1	D	402	ALA	2.3
1	D	553	ALA	2.3
1	C	448	LYS	2.3
1	A	550	GLU	2.3
1	B	560	GLU	2.3
1	B	552	LYS	2.3
1	C	548	ILE	2.2
1	D	392	MET	2.2
1	A	53	THR	2.2
1	D	30	PRO	2.2
1	B	52	ASP	2.2
1	B	111	ASP	2.2
1	C	119	PHE	2.1
1	A	271	MET	2.1
1	C	364	GLY	2.1
1	C	447	PHE	2.1
1	D	54	LYS	2.0
1	C	370	LEU	2.0
1	C	374	LEU	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 ⓘ

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(Å ²)	Q<0.9
3	NCA	A	603	9/9	0.84	0.18	45,47,56,56	13
3	NCA	C	603	9/9	0.91	0.10	30,39,42,43	0
3	NCA	B	603	9/9	0.92	0.09	36,39,49,52	13
3	NCA	A	602	9/9	0.93	0.09	29,35,38,38	0
3	NCA	B	602	9/9	0.94	0.07	22,29,33,33	0
3	NCA	D	602	9/9	0.95	0.08	23,31,36,36	0
4	SO4	C	601	5/5	0.96	0.07	34,36,44,44	5
2	CL	D	601	1/1	0.99	0.03	26,26,26,26	0
2	CL	A	601	1/1	0.99	0.03	25,25,25,25	0
2	CL	B	601	1/1	0.99	0.03	26,26,26,26	0
2	CL	C	602	1/1	0.99	0.03	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.