



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 06:30 AM BST

PDB ID : 4A64
Title : Crystal structure of the N-terminal domain of human Cul4B at 2.57Å resolution
Authors : Vollmar, M.; Ayinampudi, V.; Cooper, C.; Guo, K.; Krojer, T.; Muniz, J.R.C.; von Delft, F.; Weigelt, J.; Arrowsmith, C.H.; Bountra, C.; Edwards, A.; Bullock, A.
Deposited on : 2011-10-31
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

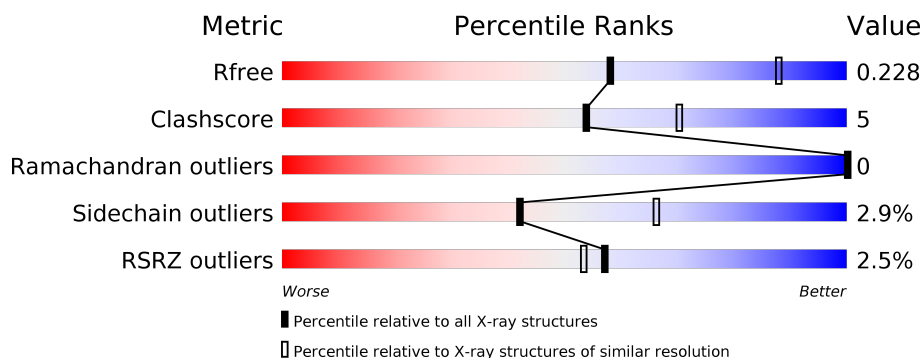
1 Overall quality at a glance ⓘ

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}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (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 on 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	354	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>••</div> </div> </div>
1	B	354	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>••</div> </div> </div>
1	C	354	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>6%</div> </div> </div>
1	D	354	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>•</div> <div>10%</div> </div> </div>

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
2	EDO	A	1537	-	-	X	-
2	EDO	B	1534	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11395 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 CULLIN-4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	4	0
			2870	1826	494	536	14			
1	B	345	Total	C	N	O	S	0	3	0
			2850	1814	484	538	14			
1	C	333	Total	C	N	O	S	0	5	0
			2764	1755	478	518	13			
1	D	320	Total	C	N	O	S	0	1	0
			2630	1667	455	496	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	SER	-	expression tag	UNP Q13620
A	187	MET	-	expression tag	UNP Q13620
A	498	ARG	VAL	engineered mutation	UNP Q13620
A	502	ASP	LEU	engineered mutation	UNP Q13620
B	186	SER	-	expression tag	UNP Q13620
B	187	MET	-	expression tag	UNP Q13620
B	498	ARG	VAL	engineered mutation	UNP Q13620
B	502	ASP	LEU	engineered mutation	UNP Q13620
C	186	SER	-	expression tag	UNP Q13620
C	187	MET	-	expression tag	UNP Q13620
C	498	ARG	VAL	engineered mutation	UNP Q13620
C	502	ASP	LEU	engineered mutation	UNP Q13620
D	186	SER	-	expression tag	UNP Q13620
D	187	MET	-	expression tag	UNP Q13620
D	498	ARG	VAL	engineered mutation	UNP Q13620
D	502	ASP	LEU	engineered mutation	UNP Q13620

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

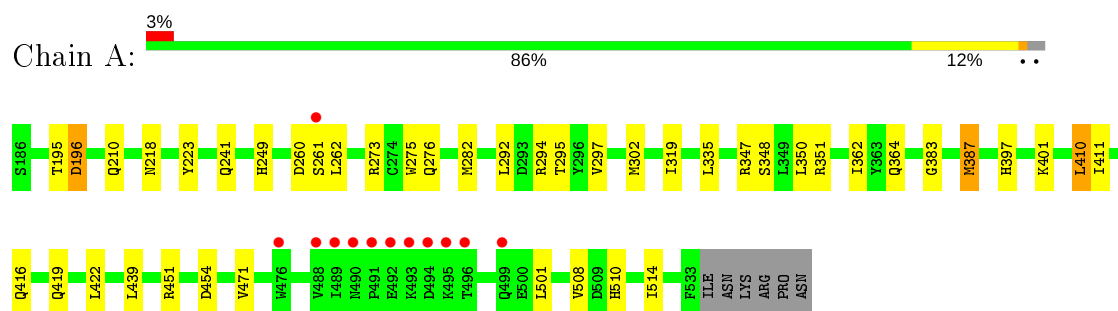
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	95	Total	O	0	0
			95	95		
3	B	58	Total	O	0	0
			58	58		
3	C	60	Total	O	0	0
			60	60		
3	D	40	Total	O	0	0
			40	40		

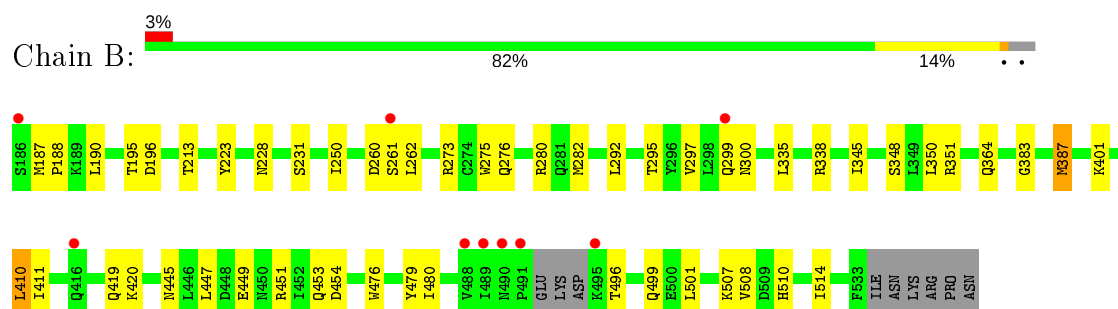
3 Residue-property plots

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.

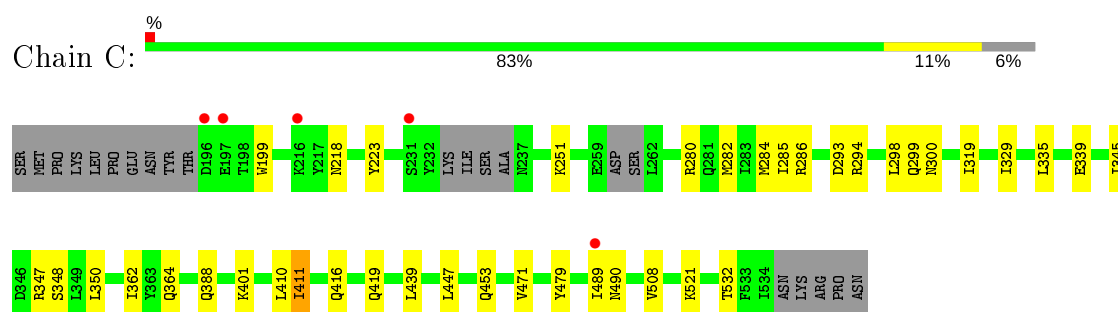
• Molecule 1: CULLIN-4B



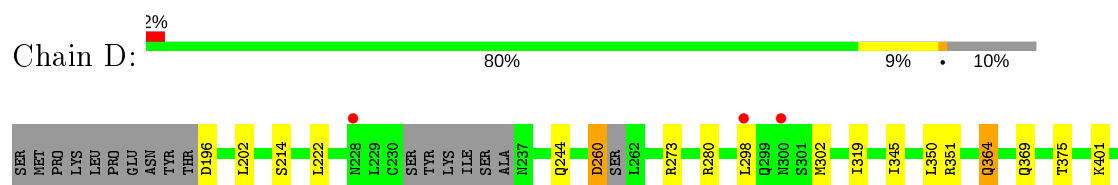
• Molecule 1: CULLIN-4B

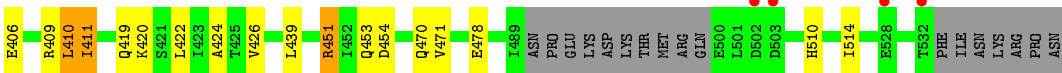


• Molecule 1: CULLIN-4B



• Molecule 1: CULLIN-4B





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.25Å 157.09Å 92.92Å 90.00° 95.71° 90.00°	Depositor
Resolution (Å)	19.74 – 2.57 19.92 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.74-2.57) 99.9 (19.92-2.57)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.56Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.184 , 0.230 0.186 , 0.228	Depositor DCC
R_{free} test set	2941 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11395	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: EDO

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	0.72	1/2928 (0.0%)	0.82	3/3948 (0.1%)
1	B	0.77	1/2904 (0.0%)	0.87	4/3916 (0.1%)
1	C	0.73	1/2819 (0.0%)	0.84	3/3797 (0.1%)
1	D	0.72	1/2669 (0.0%)	0.83	4/3594 (0.1%)
All	All	0.74	4/11320 (0.0%)	0.84	14/15255 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	369	GLN	CG-CD	5.45	1.63	1.51
1	B	275	TRP	CD2-CE2	5.12	1.47	1.41
1	C	199	TRP	CD2-CE2	5.01	1.47	1.41
1	A	275	TRP	NE1-CE2	-5.00	1.31	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	MET	CG-SD-CE	-7.58	88.07	100.20
1	C	286	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	410	LEU	CB-CG-CD2	-6.63	99.73	111.00
1	D	410	LEU	CB-CG-CD2	-6.38	100.16	111.00
1	A	273	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	D	451	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	387	MET	CG-SD-CE	-5.48	91.43	100.20
1	B	338	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	410	LEU	CB-CG-CD2	-5.29	102.01	111.00
1	D	273	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	273	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	286	ARG	CG-CD-NE	-5.19	100.91	111.80
1	C	251	LYS	CD-CE-NZ	5.17	123.59	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	409	ARG	NE-CZ-NH1	5.13	122.87	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	2870	0	2845	34	0
1	B	2850	0	2831	42	0
1	C	2764	0	2751	33	0
1	D	2630	0	2603	25	0
2	A	16	0	24	8	0
2	B	4	0	6	7	0
2	C	4	0	6	0	0
2	D	4	0	6	0	0
3	A	95	0	0	9	0
3	B	58	0	0	2	0
3	C	60	0	0	5	0
3	D	40	0	0	2	0
All	All	11395	0	11072	118	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 (118) 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:282:MET:HE2	2:B:1534:EDO:H22	1.50	0.90
1:A:351[A]:ARG:HH11	1:A:351[A]:ARG:HG2	1.40	0.84
1:A:351[B]:ARG:HD2	1:D:298:LEU:HD23	1.61	0.82
1:B:250:ILE:HG13	2:B:1534:EDO:H21	1.61	0.82
1:A:282:MET:HE1	2:A:1537:EDO:H11	1.62	0.81
1:C:282:MET:HE1	1:C:285:ILE:HD12	1.64	0.79
1:B:445[B]:ASN:ND2	1:B:449[B]:GLU:OE1	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:GLN:HG2	3:A:2025:HOH:O	1.87	0.74
1:A:282:MET:CE	2:A:1537:EDO:H11	2.18	0.73
1:C:532:THR:CG2	3:C:2055:HOH:O	2.37	0.71
1:C:532:THR:HG22	3:C:2055:HOH:O	1.91	0.70
1:B:250:ILE:CG1	2:B:1534:EDO:H21	2.23	0.68
1:D:451:ARG:NH1	1:D:454:ASP:OD2	2.26	0.68
1:B:351:ARG:HD3	1:C:298:LEU:HD23	1.76	0.67
1:A:347:ARG:H	2:A:1535:EDO:H11	1.59	0.66
1:A:351[A]:ARG:HH11	1:A:351[A]:ARG:CG	2.08	0.66
1:A:282:MET:CE	2:A:1537:EDO:C1	2.75	0.65
1:C:282:MET:CE	1:C:285:ILE:HD12	2.27	0.65
1:D:410:LEU:HD21	1:D:419:GLN:HA	1.78	0.65
1:A:276[A]:GLN:NE2	3:A:2034:HOH:O	2.26	0.64
1:A:249:HIS:HD2	3:A:2029:HOH:O	1.81	0.64
1:A:282:MET:HE2	2:A:1537:EDO:O1	1.99	0.63
1:B:451:ARG:NH1	1:B:454:ASP:OD2	2.32	0.62
1:B:351:ARG:CD	1:C:298:LEU:HD23	2.30	0.61
1:C:339:GLU:OE2	1:C:347:ARG:HD3	2.00	0.61
1:B:496:THR:CG2	1:B:499:GLN:HB3	2.29	0.61
1:C:410:LEU:HD21	1:C:419:GLN:HA	1.83	0.60
1:A:410:LEU:HD21	1:A:419:GLN:HA	1.83	0.60
1:C:439:LEU:CD1	1:C:471:VAL:HG12	2.33	0.59
1:B:282:MET:HE1	2:B:1534:EDO:H12	1.85	0.58
1:C:282:MET:HE3	3:C:2002:HOH:O	2.02	0.58
1:C:335:LEU:HD12	1:C:350:LEU:HD13	1.84	0.58
1:B:223:TYR:CE1	1:C:280:ARG:HD3	2.39	0.57
1:D:439:LEU:CD1	1:D:471:VAL:HG12	2.35	0.57
1:B:282:MET:HE2	2:B:1534:EDO:C2	2.30	0.57
1:B:496:THR:HG23	1:B:499:GLN:HB3	1.87	0.56
1:D:439:LEU:HD12	1:D:471:VAL:HG12	1.87	0.55
1:A:260:ASP:HB2	1:A:261:SER:HA	1.88	0.55
1:A:451:ARG:NH1	1:A:454:ASP:OD2	2.40	0.54
1:A:223:TYR:CE1	1:D:280:ARG:HD3	2.42	0.54
1:B:510:HIS:CE1	1:B:514:ILE:HD12	2.43	0.54
1:B:223:TYR:CZ	1:C:280:ARG:HD3	2.43	0.54
1:C:439:LEU:HD12	1:C:471:VAL:HG12	1.90	0.54
1:A:223:TYR:CZ	1:D:280:ARG:HD3	2.43	0.53
1:A:351[B]:ARG:NH1	3:A:2063:HOH:O	2.27	0.53
1:B:282:MET:CE	2:B:1534:EDO:H22	2.32	0.53
1:B:260:ASP:HA	1:B:262:LEU:H	1.75	0.52
1:B:280:ARG:HD2	1:C:223:TYR:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:HIS:HD2	3:A:2075:HOH:O	1.93	0.52
1:B:292:LEU:O	1:B:295:THR:HG22	2.10	0.52
1:B:282:MET:CE	2:B:1534:EDO:H12	2.40	0.51
1:A:351[A]:ARG:NH1	1:A:351[A]:ARG:CG	2.72	0.51
1:D:510:HIS:NE2	1:D:514:ILE:HD12	2.25	0.50
3:A:2044:HOH:O	1:D:351:ARG:NH2	2.37	0.50
1:B:410:LEU:HD21	1:B:419:GLN:HA	1.93	0.49
1:D:478:GLU:HG3	3:D:2039:HOH:O	2.11	0.49
1:C:299:GLN:O	1:C:300:ASN:HB2	2.12	0.49
1:B:420:LYS:HE3	1:D:302:MET:HE1	1.95	0.49
1:C:532:THR:HG21	3:C:2055:HOH:O	2.05	0.49
1:B:496:THR:CG2	1:B:499:GLN:CB	2.91	0.48
1:B:476:TRP:CE2	1:B:480:ILE:HD11	2.49	0.47
1:A:510:HIS:NE2	1:A:514:ILE:HD12	2.29	0.47
1:A:210:GLN:HG2	2:A:1537:EDO:H22	1.96	0.47
1:A:260:ASP:HA	1:A:262:LEU:H	1.79	0.47
1:D:364:GLN:HG3	3:D:2022:HOH:O	2.14	0.47
1:A:249:HIS:CD2	3:A:2029:HOH:O	2.63	0.46
1:A:410:LEU:HD22	1:A:422:LEU:HD23	1.97	0.46
1:D:244:GLN:HA	1:D:244:GLN:OE1	2.14	0.46
1:B:187:MET:HE3	1:B:188:PRO:HD2	1.98	0.46
1:C:319:ILE:HG21	1:C:362:ILE:HD11	1.97	0.46
1:B:195:THR:O	1:B:196:ASP:HB2	2.16	0.46
1:C:447:LEU:HD13	1:C:479:TYR:CD2	2.51	0.46
1:D:202:LEU:HD23	1:D:222:LEU:HD22	1.98	0.46
1:D:319:ILE:HG23	1:D:319:ILE:HD12	1.68	0.45
1:C:282:MET:HE1	1:C:285:ILE:CD1	2.41	0.45
3:B:2021:HOH:O	1:C:294:ARG:HD3	2.17	0.45
1:C:411:ILE:HD12	1:C:411:ILE:HA	1.65	0.45
1:A:335:LEU:HD12	1:A:350:LEU:HD13	1.99	0.45
1:B:260:ASP:CB	1:B:261:SER:HA	2.47	0.45
1:D:375:THR:HG21	1:D:422:LEU:CD1	2.47	0.45
1:A:319:ILE:HG21	1:A:362:ILE:HD11	1.98	0.45
1:C:439:LEU:HD11	1:C:471:VAL:HG12	1.99	0.45
1:C:345:ILE:HD12	1:C:350:LEU:HD22	1.98	0.44
1:A:218:ASN:HB3	3:A:2016:HOH:O	2.18	0.44
1:A:439:LEU:HD12	1:A:471:VAL:HG12	1.99	0.44
1:B:190:LEU:HD11	1:B:228:ASN:HB3	2.00	0.44
1:B:496:THR:HG22	1:B:499:GLN:HB3	1.99	0.44
1:B:496:THR:HG23	1:B:499:GLN:CB	2.46	0.44
1:B:299:GLN:O	1:D:420:LYS:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:ILE:HD12	1:D:350:LEU:HD22	1.99	0.43
1:C:489:ILE:HG22	1:C:490[B]:ASN:OD1	2.18	0.43
1:C:439:LEU:HD12	1:C:471:VAL:CG1	2.48	0.43
1:A:292:LEU:O	1:A:295:THR:HG22	2.19	0.43
1:D:260:ASP:C	1:D:260:ASP:OD1	2.57	0.43
1:A:294:ARG:HD3	3:A:2043:HOH:O	2.18	0.43
1:A:282:MET:HE2	2:A:1537:EDO:C1	2.46	0.42
1:C:411:ILE:HD11	1:D:411:ILE:HD11	2.00	0.42
1:B:447:LEU:O	1:B:507:LYS:HE2	2.19	0.42
1:A:195:THR:O	1:A:196:ASP:HB2	2.19	0.42
1:A:383:GLY:O	1:A:387:MET:HB2	2.20	0.42
1:B:300:ASN:HB3	1:D:424:ALA:HB2	2.01	0.41
1:B:213:THR:HA	1:C:218:ASN:HB2	2.03	0.41
1:B:223:TYR:CD1	1:C:280:ARG:HD3	2.54	0.41
1:B:260:ASP:HA	1:B:262:LEU:N	2.35	0.41
1:B:383:GLY:O	1:B:387:MET:HB2	2.21	0.41
1:B:335:LEU:HD12	1:B:350:LEU:HD13	2.02	0.41
1:B:231:SER:O	1:D:470:GLN:HG3	2.21	0.41
1:B:447:LEU:HD13	1:B:479:TYR:CD2	2.56	0.41
1:C:299:GLN:O	1:C:300:ASN:CB	2.68	0.41
1:C:532:THR:HG22	1:C:532:THR:O	2.21	0.41
1:B:187:MET:HE3	1:D:470:GLN:HB3	2.02	0.41
1:B:345:ILE:HD12	1:B:350:LEU:HD22	2.03	0.41
1:C:388[A]:GLN:NE2	3:C:2033:HOH:O	2.54	0.41
1:D:406:GLU:HG3	1:D:426:VAL:HG21	2.03	0.41
1:B:276[B]:GLN:NE2	3:B:2021:HOH:O	2.55	0.40
1:C:329:ILE:HG23	1:C:329:ILE:HD12	1.80	0.40
1:D:411:ILE:HD12	1:D:411:ILE:HA	1.81	0.40
1:A:282:MET:HE1	2:A:1537:EDO:C1	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	350/354 (99%)	339 (97%)	11 (3%)	0	100	100
1	B	344/354 (97%)	332 (96%)	12 (4%)	0	100	100
1	C	332/354 (94%)	324 (98%)	8 (2%)	0	100	100
1	D	313/354 (88%)	306 (98%)	7 (2%)	0	100	100
All	All	1339/1416 (95%)	1301 (97%)	38 (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	311/330 (94%)	301 (97%)	10 (3%)	39	63
1	B	313/330 (95%)	305 (97%)	8 (3%)	46	69
1	C	303/330 (92%)	293 (97%)	10 (3%)	38	61
1	D	286/330 (87%)	279 (98%)	7 (2%)	49	72
All	All	1213/1320 (92%)	1178 (97%)	35 (3%)	42	66

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	ASP
1	A	297	VAL
1	A	302	MET
1	A	348	SER
1	A	364	GLN
1	A	401	LYS
1	A	411	ILE
1	A	416	GLN
1	A	501	LEU
1	A	508	VAL
1	B	297	VAL
1	B	348	SER
1	B	364	GLN

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Mol	Chain	Res	Type
1	B	401	LYS
1	B	411	ILE
1	B	453	GLN
1	B	501	LEU
1	B	508	VAL
1	C	284	MET
1	C	293	ASP
1	C	348	SER
1	C	364	GLN
1	C	401	LYS
1	C	411	ILE
1	C	416	GLN
1	C	453	GLN
1	C	508	VAL
1	C	521	LYS
1	D	196	ASP
1	D	214	SER
1	D	260	ASP
1	D	364	GLN
1	D	401	LYS
1	D	411	ILE
1	D	453	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	A	499	GLN
1	B	384	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 monosaccharides in this entry.

5.6 Ligand geometry

7 ligands 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	$\# Z > 2$
2	EDO	C	1535	-	3,3,3	0.58	0	2,2,2	0.24	0
2	EDO	B	1534	-	3,3,3	0.58	0	2,2,2	0.65	0
2	EDO	A	1534	-	3,3,3	0.89	0	2,2,2	0.37	0
2	EDO	A	1537	-	3,3,3	0.78	0	2,2,2	1.59	0
2	EDO	A	1536	-	3,3,3	0.60	0	2,2,2	0.14	0
2	EDO	D	1533	-	3,3,3	0.51	0	2,2,2	0.45	0
2	EDO	A	1535	-	3,3,3	0.47	0	2,2,2	0.76	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
2	EDO	C	1535	-	-	0/1/1/1	-
2	EDO	B	1534	-	-	1/1/1/1	-
2	EDO	A	1534	-	-	1/1/1/1	-
2	EDO	A	1537	-	-	1/1/1/1	-
2	EDO	A	1536	-	-	1/1/1/1	-
2	EDO	D	1533	-	-	0/1/1/1	-
2	EDO	A	1535	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1534	EDO	O1-C1-C2-O2
2	A	1537	EDO	O1-C1-C2-O2
2	B	1534	EDO	O1-C1-C2-O2
2	A	1536	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1534	EDO	7	0
2	A	1537	EDO	7	0
2	A	1535	EDO	1	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	348/354 (98%)	-0.12	12 (3%) 45 41	37, 58, 103, 176	0
1	B	345/354 (97%)	-0.16	9 (2%) 56 52	37, 54, 93, 163	0
1	C	333/354 (94%)	-0.18	5 (1%) 73 71	35, 54, 94, 121	0
1	D	320/354 (90%)	-0.11	7 (2%) 62 58	36, 61, 106, 115	0
All	All	1346/1416 (95%)	-0.14	33 (2%) 57 53	35, 56, 99, 176	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	493	LYS	4.8
1	A	494	ASP	4.3
1	A	492	GLU	4.2
1	B	491	PRO	4.0
1	A	261	SER	3.9
1	A	488	VAL	3.9
1	B	490	ASN	3.8
1	A	489	ILE	3.7
1	B	489	ILE	3.6
1	B	488	VAL	3.6
1	B	261	SER	3.5
1	C	196	ASP	3.2
1	A	491	PRO	3.0
1	D	503	ASP	2.9
1	B	186	SER	2.9
1	C	231	SER	2.6
1	A	490	ASN	2.6
1	D	502	ASP	2.6
1	C	197	GLU	2.6
1	A	499	GLN	2.6
1	D	228	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	489	ILE	2.5
1	B	299	GLN	2.5
1	D	532	THR	2.5
1	B	416	GLN	2.4
1	C	216	LYS	2.3
1	A	476	TRP	2.3
1	A	495	LYS	2.2
1	D	300	ASN	2.2
1	A	496	THR	2.1
1	D	298	LEU	2.1
1	D	528	GLU	2.1
1	B	495	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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
2	EDO	A	1534	4/4	0.75	0.28	66,71,73,76	0
2	EDO	A	1536	4/4	0.86	0.19	73,77,87,89	0
2	EDO	A	1537	4/4	0.89	0.23	56,59,64,72	0
2	EDO	A	1535	4/4	0.90	0.19	47,52,57,60	0
2	EDO	C	1535	4/4	0.93	0.20	63,64,65,68	0
2	EDO	D	1533	4/4	0.94	0.18	48,53,54,54	0
2	EDO	B	1534	4/4	0.96	0.17	44,45,46,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.