



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:58 PM UTC

PDB ID : 5MKV / pdb_00005mkv
Title : Crystal Structure of Human Dihydropyrimidinease-like 2 (DPYSL2A)/Collapsin Response Mediator Protein (CRMP2) residues 13-516
Authors : Sethi, R.; Zheng, Y.; Krojer, T.; Velupillai, S.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Ahmed, A.A.; von Delft, F.
Deposited on : 2016-12-05
Resolution : 1.80 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

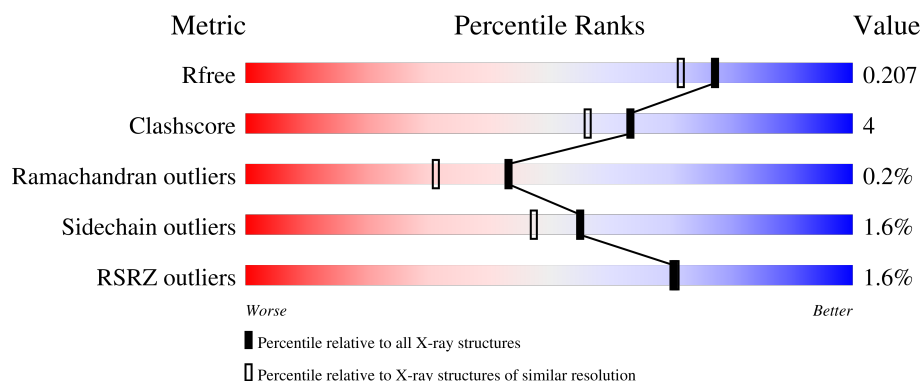
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	504	86% 10% .
1	B	504	85% 10% .
1	C	504	88% 9% ..
1	D	504	88% 8% ..

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
2	EDO	A	606	-	-	X	-
2	EDO	A	607	-	-	X	-
2	EDO	B	603	-	-	X	-
2	EDO	B	604	-	-	X	-

2 Entry composition [i](#)

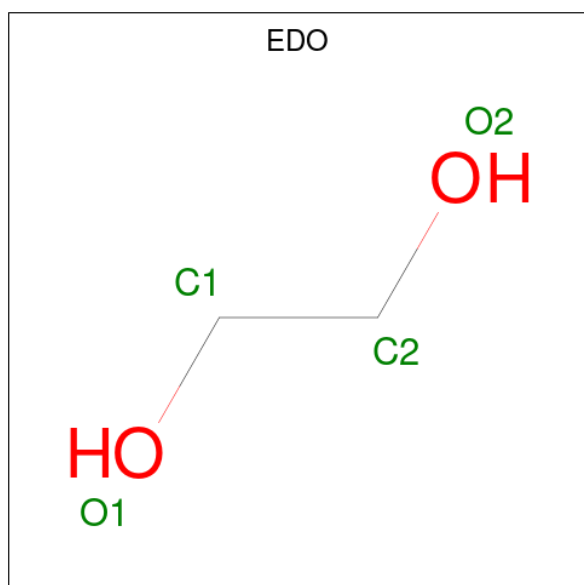
There are 3 unique types of molecules in this entry. The entry contains 15644 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dihydropyrimidinase-related protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3732	2352	638	724	18			
1	B	482	Total	C	N	O	S	0	1	0
			3704	2334	634	717	19			
1	C	493	Total	C	N	O	S	0	0	0
			3781	2382	645	735	19			
1	D	488	Total	C	N	O	S	0	0	0
			3743	2358	640	726	19			

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: 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		

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

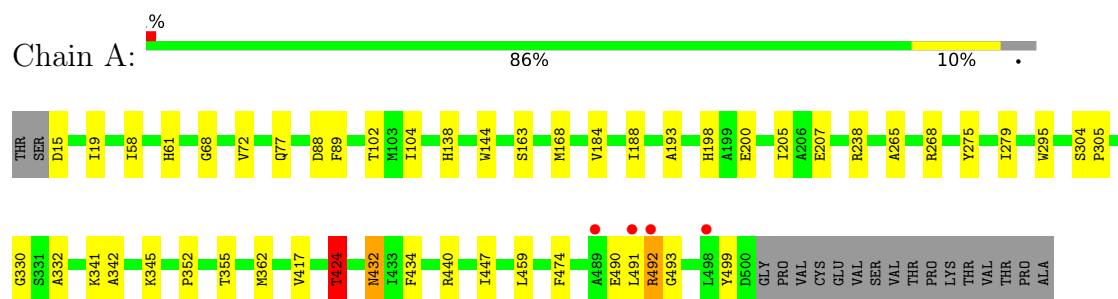
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	220	Total 220	O 220	0	0
3	B	84	Total 84	O 84	0	0
3	C	154	Total 154	O 154	0	0
3	D	138	Total 138	O 138	0	0

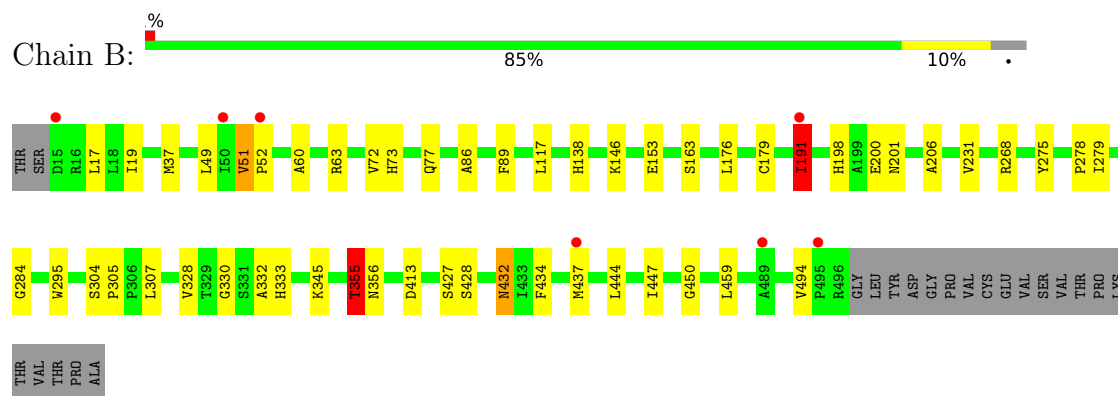
3 Residue-property plots [i](#)

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.

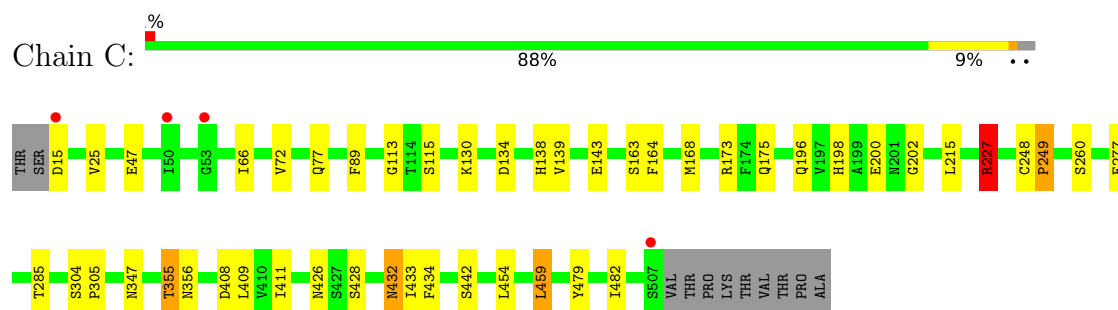
- Molecule 1: Dihydropyrimidinase-related protein 2



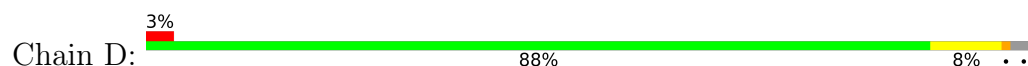
- Molecule 1: Dihydropyrimidinase-related protein 2

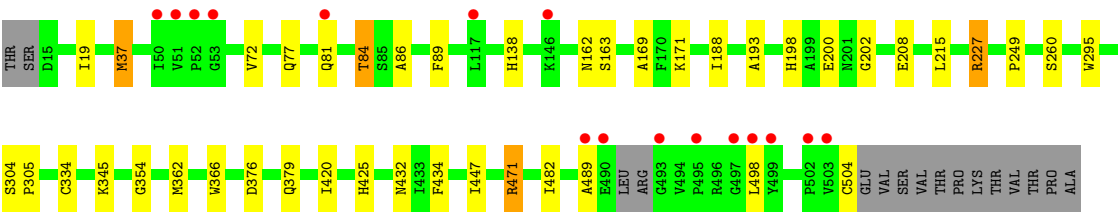


- Molecule 1: Dihydropyrimidinase-related protein 2



- Molecule 1: Dihydropyrimidinase-related protein 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.90Å 157.51Å 87.42Å 90.00° 93.61° 90.00°	Depositor
Resolution (Å)	19.87 – 1.80 19.87 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.87-1.80) 97.7 (19.87-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.167 , 0.200 0.177 , 0.207	Depositor DCC
R_{free} test set	9717 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 29.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15644	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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	1.32	9/3809 (0.2%)	1.15	10/5171 (0.2%)
1	B	1.24	3/3783 (0.1%)	1.10	3/5135 (0.1%)
1	C	1.33	12/3859 (0.3%)	1.17	7/5240 (0.1%)
1	D	1.28	5/3820 (0.1%)	1.13	10/5185 (0.2%)
All	All	1.29	29/15271 (0.2%)	1.14	30/20731 (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	C	0	1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	227	ARG	CD-NE	-11.98	1.29	1.46
1	D	227	ARG	CD-NE	-8.02	1.35	1.46
1	D	362	MET	CG-SD	-6.94	1.63	1.80
1	B	494	VAL	CA-C	6.72	1.58	1.53
1	C	248	CYS	C-O	-6.65	1.16	1.24
1	C	134	ASP	CA-C	6.45	1.60	1.52
1	A	362	MET	CG-SD	-6.44	1.64	1.80
1	C	260	SER	CB-OG	-6.43	1.29	1.42
1	A	474	PHE	CA-CB	6.34	1.58	1.52
1	A	104	ILE	C-O	6.28	1.30	1.24
1	B	206	ALA	N-CA	6.23	1.53	1.46
1	C	426	ASN	C-O	-6.19	1.15	1.24
1	B	49	LEU	CA-C	5.71	1.60	1.52
1	C	47	GLU	N-CA	5.62	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	ILE	N-CA	5.47	1.52	1.46
1	A	168	MET	SD-CE	-5.47	1.65	1.79
1	C	277	GLU	CA-C	5.40	1.58	1.52
1	C	285	THR	C-O	5.36	1.29	1.23
1	A	238	ARG	N-CA	-5.36	1.39	1.46
1	D	489	ALA	CA-C	5.35	1.59	1.52
1	A	424	THR	CB-CG2	-5.33	1.34	1.52
1	D	260	SER	N-CA	5.24	1.52	1.46
1	A	362	MET	CB-CG	5.22	1.68	1.52
1	C	249	PRO	C-O	5.17	1.29	1.23
1	A	265	ALA	N-CA	5.12	1.52	1.46
1	C	168	MET	SD-CE	-5.10	1.66	1.79
1	C	196	GLN	C-O	-5.02	1.17	1.23
1	D	471	ARG	NE-CZ	-5.01	1.27	1.33
1	C	411	ILE	CA-CB	5.00	1.59	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	227	ARG	NE-CZ-NH2	-18.50	102.55	119.20
1	D	227	ARG	NE-CZ-NH2	-14.85	105.84	119.20
1	C	227	ARG	NE-CZ-NH1	10.47	131.97	121.50
1	A	424	THR	N-CA-CB	-10.02	97.75	110.98
1	D	227	ARG	NE-CZ-NH1	8.00	129.50	121.50
1	C	227	ARG	CD-NE-CZ	7.75	135.25	124.40
1	C	442	SER	N-CA-C	6.85	114.38	108.22
1	B	86	ALA	N-CA-C	6.84	120.51	111.75
1	D	86	ALA	N-CA-C	6.75	119.47	111.71
1	A	58	ILE	CB-CA-C	-6.10	101.54	110.62
1	A	499	TYR	CA-C-N	6.04	132.57	121.70
1	A	499	TYR	C-N-CA	6.04	132.57	121.70
1	A	342	ALA	N-CA-C	5.89	119.94	112.87
1	D	227	ARG	CD-NE-CZ	5.82	132.55	124.40
1	A	424	THR	CB-CA-C	5.61	118.47	109.27
1	A	424	THR	OG1-CB-CG2	5.61	120.51	109.30
1	D	81	GLN	CA-CB-CG	5.55	125.21	114.10
1	D	227	ARG	CG-CD-NE	-5.54	99.81	112.00
1	C	227	ARG	CG-CD-NE	-5.53	99.83	112.00
1	B	355	THR	N-CA-CB	-5.44	102.81	111.62
1	D	84	THR	N-CA-CB	-5.43	101.18	111.00
1	A	362	MET	CB-CA-C	5.24	119.76	110.85
1	D	489	ALA	N-CA-C	5.23	116.69	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	227	ARG	CB-CA-C	-5.22	104.20	111.41
1	A	207	GLU	N-CA-C	5.18	116.61	111.07
1	B	191	ILE	CA-CB-CG2	5.18	119.30	110.50
1	D	208	GLU	N-CA-C	5.10	116.92	111.36
1	C	130	LYS	N-CA-C	5.07	120.33	114.04
1	A	493	GLY	N-CA-C	-5.05	101.21	113.18
1	D	227	ARG	CB-CA-C	-5.04	104.60	111.21

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	227	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	3732	0	3667	29	0
1	B	3704	0	3647	38	0
1	C	3781	0	3712	22	0
1	D	3743	0	3677	25	0
2	A	44	0	66	9	0
2	B	16	0	24	14	0
2	C	4	0	6	0	0
2	D	24	0	36	6	0
3	A	220	0	0	5	0
3	B	84	0	0	5	0
3	C	154	0	0	3	0
3	D	138	0	0	2	0
All	All	15644	0	14835	119	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 4.

All (119) 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)
2:A:606:EDO:H21	3:A:710:HOH:O	1.58	1.01
1:B:268:ARG:HE	2:B:603:EDO:C1	1.81	0.93
1:A:332:ALA:O	2:A:606:EDO:H12	1.75	0.87
1:A:77:GLN:HE21	1:A:89:PHE:H	1.27	0.80
1:A:432:ASN:HD22	1:A:434:PHE:H	1.30	0.79
1:B:138:HIS:HD2	1:B:163:SER:OG	1.65	0.78
1:D:425:HIS:HB2	2:D:606:EDO:H11	1.66	0.77
1:A:424:THR:HG21	3:A:734:HOH:O	1.85	0.76
2:B:604:EDO:H22	3:B:724:HOH:O	1.88	0.74
1:C:432:ASN:HD22	1:C:434:PHE:H	1.35	0.73
1:A:332:ALA:O	2:A:606:EDO:C1	2.37	0.73
1:C:113:GLY:N	1:C:143:GLU:OE2	2.20	0.72
1:D:77:GLN:HE21	1:D:89:PHE:H	1.37	0.71
1:A:15:ASP:N	3:A:701:HOH:O	2.23	0.70
1:C:200:GLU:OE2	1:C:227:ARG:HD3	1.92	0.69
1:C:138:HIS:HD2	1:C:163:SER:OG	1.76	0.67
1:C:355:THR:HG23	1:C:356:ASN:O	1.93	0.67
1:B:268:ARG:NE	2:B:603:EDO:O1	2.27	0.66
1:B:432:ASN:HD22	1:B:434:PHE:H	1.43	0.65
1:C:198:HIS:HD2	3:C:832:HOH:O	1.80	0.64
1:D:138:HIS:HD2	1:D:163:SER:OG	1.81	0.64
2:B:602:EDO:O1	3:B:702:HOH:O	2.15	0.63
1:A:198:HIS:HD2	3:A:892:HOH:O	1.82	0.62
1:D:366:TRP:HZ2	2:D:604:EDO:H12	1.65	0.62
1:B:17:LEU:HD23	1:B:37:MET:HE1	1.82	0.61
1:A:138:HIS:HD2	1:A:163:SER:OG	1.84	0.61
1:B:37:MET:HE1	1:B:447:ILE:HG21	1.82	0.61
1:B:198:HIS:HD2	3:B:771:HOH:O	1.82	0.61
1:D:198:HIS:HD2	3:D:827:HOH:O	1.85	0.59
1:C:347:ASN:C	1:C:347:ASN:HD22	2.11	0.58
1:B:153:GLU:CG	1:B:191:ILE:HD11	2.33	0.58
1:B:37:MET:HE3	1:B:450:GLY:HA2	1.85	0.57
1:D:200:GLU:OE2	1:D:227:ARG:HD3	2.04	0.57
1:A:198:HIS:HE1	1:A:200:GLU:OE1	1.87	0.57
1:B:17:LEU:HD23	1:B:37:MET:CE	2.35	0.56
1:B:153:GLU:HG2	1:B:191:ILE:HD11	1.86	0.56
1:B:333:HIS:HE1	2:B:604:EDO:H22	1.70	0.56
1:C:198:HIS:HE1	1:C:200:GLU:OE1	1.88	0.56
1:C:454:LEU:HD13	1:C:459:LEU:HD13	1.88	0.56
1:B:268:ARG:HE	2:B:603:EDO:H12	1.67	0.55
1:B:268:ARG:NE	2:B:603:EDO:C1	2.62	0.55
1:B:427:SER:HB2	2:B:604:EDO:H21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:603:EDO:H22	3:D:819:HOH:O	2.05	0.55
1:B:19:ILE:HD11	1:B:447:ILE:HD13	1.88	0.55
1:C:249:PRO:HB3	1:C:482:ILE:HD11	1.90	0.54
1:D:366:TRP:CZ2	2:D:604:EDO:H12	2.42	0.54
1:D:249:PRO:HB3	1:D:482:ILE:HD11	1.89	0.54
1:C:408:ASP:C	1:C:409:LEU:HD12	2.33	0.53
1:B:77:GLN:HE21	1:B:89:PHE:H	1.57	0.53
1:D:425:HIS:HB2	2:D:606:EDO:C1	2.37	0.53
1:C:479:TYR:HA	1:C:482:ILE:HD12	1.90	0.53
1:A:355:THR:OG1	2:A:606:EDO:H22	2.07	0.53
1:B:201:ASN:HB3	1:B:231:VAL:HG13	1.91	0.52
1:A:19:ILE:HD11	1:A:447:ILE:CD1	2.40	0.52
1:B:198:HIS:HE1	1:B:200:GLU:OE1	1.93	0.52
1:B:179[B]:CYS:SG	1:D:171:LYS:NZ	2.76	0.50
1:D:162:ASN:OD1	1:D:471:ARG:NH1	2.43	0.50
1:C:25:VAL:HB	1:C:66:ILE:HG22	1.94	0.50
1:C:432:ASN:ND2	1:C:434:PHE:H	2.07	0.50
1:A:432:ASN:ND2	1:A:434:PHE:H	2.03	0.50
1:A:268:ARG:HH22	2:A:607:EDO:H12	1.75	0.50
1:A:72:VAL:O	1:A:138:HIS:HE1	1.96	0.49
1:B:304:SER:HA	1:B:305:PRO:C	2.37	0.49
1:D:72:VAL:O	1:D:138:HIS:HE1	1.96	0.48
1:D:198:HIS:HE1	1:D:200:GLU:OE1	1.96	0.48
1:A:77:GLN:NE2	1:A:88:ASP:HB2	2.29	0.48
1:A:492:ARG:CB	3:C:818:HOH:O	2.62	0.48
1:C:77:GLN:HE21	1:C:89:PHE:H	1.60	0.48
1:D:376:ASP:H	1:D:379:GLN:NE2	2.12	0.47
1:A:417:VAL:HG22	1:A:440:ARG:HG3	1.97	0.47
1:C:138:HIS:CD2	1:C:163:SER:OG	2.64	0.47
1:B:279:ILE:HA	1:B:330:GLY:O	2.15	0.46
1:D:19:ILE:HD12	1:D:37:MET:HE1	1.97	0.46
1:C:72:VAL:O	1:C:138:HIS:HE1	1.98	0.46
1:B:432:ASN:ND2	1:B:434:PHE:H	2.13	0.46
1:B:60:ALA:O	1:B:63:ARG:HB2	2.15	0.45
1:B:275:TYR:CE1	2:B:603:EDO:C2	3.00	0.45
1:A:268:ARG:NH2	2:A:607:EDO:H12	2.32	0.45
1:D:420:ILE:HG21	1:D:434:PHE:HB2	1.99	0.45
1:C:139:VAL:O	1:C:164:PHE:HA	2.17	0.45
1:A:268:ARG:HH22	2:A:607:EDO:H21	1.82	0.44
1:B:37:MET:CE	1:B:447:ILE:HG21	2.48	0.44
1:A:279:ILE:HA	1:A:330:GLY:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ASP:HB2	1:B:444:LEU:HG	2.00	0.43
1:B:275:TYR:CE1	2:B:603:EDO:H22	2.53	0.43
1:A:275:TYR:HE1	2:A:607:EDO:H11	1.83	0.43
1:C:77:GLN:HG2	3:C:704:HOH:O	2.18	0.43
1:C:175:GLN:OE1	1:C:202:GLY:HA3	2.19	0.43
1:D:334:CYS:O	1:D:354:GLY:HA3	2.19	0.43
1:B:72:VAL:O	1:B:138:HIS:HE1	2.02	0.43
1:B:153:GLU:HG3	1:B:191:ILE:HD11	1.99	0.42
1:B:284:GLY:O	1:B:437:MET:HE1	2.19	0.42
1:D:295:TRP:CZ2	1:D:345:LYS:HA	2.54	0.42
1:D:304:SER:HA	1:D:305:PRO:C	2.45	0.42
1:A:355:THR:H	2:A:606:EDO:C1	2.32	0.42
1:B:355:THR:HG23	1:B:356:ASN:O	2.19	0.42
1:B:51:VAL:HG12	1:B:52:PRO:O	2.20	0.42
1:B:73:HIS:CD2	1:B:332:ALA:HA	2.55	0.42
2:B:601:EDO:C1	3:B:703:HOH:O	2.68	0.42
1:D:188:ILE:HG23	1:D:193:ALA:HB3	2.02	0.42
1:B:278:PRO:HD2	1:B:328:VAL:O	2.19	0.41
1:A:61:HIS:HE1	3:A:909:HOH:O	2.02	0.41
1:D:169:ALA:HA	1:D:202:GLY:HA3	2.02	0.41
1:B:275:TYR:CE1	2:B:603:EDO:H21	2.55	0.41
1:A:68:GLY:HA3	1:A:102:THR:OG1	2.21	0.41
1:A:295:TRP:CZ2	1:A:345:LYS:HA	2.55	0.41
2:B:604:EDO:C2	3:B:724:HOH:O	2.58	0.41
1:D:432:ASN:ND2	2:D:606:EDO:H21	2.36	0.41
1:A:304:SER:HA	1:A:305:PRO:C	2.45	0.41
1:B:295:TRP:CZ2	1:B:345:LYS:HA	2.56	0.41
1:B:268:ARG:NE	2:B:603:EDO:H12	2.33	0.41
1:D:19:ILE:HD11	1:D:447:ILE:CD1	2.51	0.41
1:D:249:PRO:HD3	1:D:482:ILE:HD13	2.03	0.41
1:A:341:LYS:HA	1:A:352:PRO:HD2	2.02	0.40
1:A:144:TRP:CE3	1:A:184:VAL:HG22	2.57	0.40
1:A:188:ILE:HG23	1:A:193:ALA:HB3	2.04	0.40
1:C:304:SER:HA	1:C:305:PRO:C	2.46	0.40
1:C:355:THR:OG1	1:C:433:ILE:HG21	2.21	0.40
1:D:376:ASP:H	1:D:379:GLN:HE21	1.70	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	484/504 (96%)	469 (97%)	13 (3%)	2 (0%)	30	19
1	B	481/504 (95%)	465 (97%)	15 (3%)	1 (0%)	43	31
1	C	491/504 (97%)	481 (98%)	10 (2%)	0	100	100
1	D	484/504 (96%)	468 (97%)	16 (3%)	0	100	100
All	All	1940/2016 (96%)	1883 (97%)	54 (3%)	3 (0%)	43	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	490	GLU
1	A	492	ARG
1	B	146	LYS

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	404/423 (96%)	400 (99%)	4 (1%)	68	64
1	B	402/423 (95%)	393 (98%)	9 (2%)	45	34
1	C	410/423 (97%)	402 (98%)	8 (2%)	48	38
1	D	406/423 (96%)	401 (99%)	5 (1%)	63	57
All	All	1622/1692 (96%)	1596 (98%)	26 (2%)	55	47

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	424	THR
1	A	432	ASN
1	A	459	LEU
1	A	491	LEU
1	B	51	VAL
1	B	117	LEU
1	B	176	LEU
1	B	191	ILE
1	B	307	LEU
1	B	355	THR
1	B	428	SER
1	B	432	ASN
1	B	459	LEU
1	C	15	ASP
1	C	115	SER
1	C	173	ARG
1	C	215	LEU
1	C	355	THR
1	C	428	SER
1	C	432	ASN
1	C	459	LEU
1	D	37	MET
1	D	84	THR
1	D	215	LEU
1	D	498	LEU
1	D	504	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	61	HIS
1	A	77	GLN
1	A	122	GLN
1	A	138	HIS
1	A	198	HIS
1	A	209	GLN
1	A	237	ASN
1	A	245	GLN
1	A	247	ASN
1	A	432	ASN
1	B	44	GLN
1	B	61	HIS

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Mol	Chain	Res	Type
1	B	77	GLN
1	B	122	GLN
1	B	138	HIS
1	B	149	GLN
1	B	198	HIS
1	B	237	ASN
1	B	245	GLN
1	B	247	ASN
1	B	432	ASN
1	C	77	GLN
1	C	122	GLN
1	C	138	HIS
1	C	149	GLN
1	C	175	GLN
1	C	198	HIS
1	C	245	GLN
1	C	247	ASN
1	C	347	ASN
1	C	432	ASN
1	C	449	GLN
1	D	29	GLN
1	D	77	GLN
1	D	122	GLN
1	D	138	HIS
1	D	198	HIS
1	D	209	GLN
1	D	210	GLN
1	D	247	ASN
1	D	379	GLN
1	D	449	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 oligosaccharides in this entry.

5.6 Ligand geometry

22 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	A	610	-	3,3,3	1.55	0	2,2,2	0.58	0
2	EDO	B	602	-	3,3,3	0.30	0	2,2,2	1.24	0
2	EDO	B	603	-	3,3,3	1.00	0	2,2,2	0.89	0
2	EDO	A	604	-	3,3,3	0.70	0	2,2,2	0.15	0
2	EDO	A	605	-	3,3,3	0.76	0	2,2,2	0.31	0
2	EDO	A	609	-	3,3,3	0.80	0	2,2,2	0.41	0
2	EDO	D	604	-	3,3,3	0.94	0	2,2,2	1.10	0
2	EDO	C	601	-	3,3,3	0.70	0	2,2,2	0.68	0
2	EDO	A	606	-	3,3,3	0.34	0	2,2,2	1.44	0
2	EDO	D	605	-	3,3,3	0.42	0	2,2,2	1.22	0
2	EDO	D	602	-	3,3,3	0.51	0	2,2,2	0.44	0
2	EDO	B	601	-	3,3,3	0.45	0	2,2,2	0.85	0
2	EDO	D	601	-	3,3,3	0.61	0	2,2,2	1.15	0
2	EDO	D	603	-	3,3,3	0.49	0	2,2,2	0.25	0
2	EDO	A	602	-	3,3,3	0.37	0	2,2,2	1.43	0
2	EDO	A	611	-	3,3,3	0.47	0	2,2,2	1.00	0
2	EDO	A	603	-	3,3,3	0.60	0	2,2,2	0.55	0
2	EDO	A	601	-	3,3,3	0.48	0	2,2,2	0.46	0
2	EDO	A	608	-	3,3,3	0.32	0	2,2,2	0.48	0
2	EDO	A	607	-	3,3,3	1.03	0	2,2,2	1.00	0
2	EDO	B	604	-	3,3,3	0.46	0	2,2,2	0.45	0
2	EDO	D	606	-	3,3,3	0.73	0	2,2,2	0.82	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	A	610	-	-	1/1/1/1	-
2	EDO	B	602	-	-	1/1/1/1	-
2	EDO	B	603	-	-	1/1/1/1	-
2	EDO	A	604	-	-	1/1/1/1	-
2	EDO	A	605	-	-	1/1/1/1	-
2	EDO	A	609	-	-	1/1/1/1	-
2	EDO	D	604	-	-	1/1/1/1	-
2	EDO	C	601	-	-	1/1/1/1	-
2	EDO	A	606	-	-	1/1/1/1	-
2	EDO	D	605	-	-	0/1/1/1	-
2	EDO	D	602	-	-	1/1/1/1	-
2	EDO	B	601	-	-	0/1/1/1	-
2	EDO	D	601	-	-	1/1/1/1	-
2	EDO	D	603	-	-	1/1/1/1	-
2	EDO	A	602	-	-	1/1/1/1	-
2	EDO	A	611	-	-	1/1/1/1	-
2	EDO	A	603	-	-	0/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
2	EDO	A	608	-	-	0/1/1/1	-
2	EDO	A	607	-	-	1/1/1/1	-
2	EDO	B	604	-	-	1/1/1/1	-
2	EDO	D	606	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	607	EDO	O1-C1-C2-O2
2	A	609	EDO	O1-C1-C2-O2
2	D	604	EDO	O1-C1-C2-O2
2	A	610	EDO	O1-C1-C2-O2
2	A	611	EDO	O1-C1-C2-O2
2	B	602	EDO	O1-C1-C2-O2
2	B	604	EDO	O1-C1-C2-O2
2	D	603	EDO	O1-C1-C2-O2
2	A	605	EDO	O1-C1-C2-O2
2	B	603	EDO	O1-C1-C2-O2
2	C	601	EDO	O1-C1-C2-O2
2	A	602	EDO	O1-C1-C2-O2
2	A	604	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	606	EDO	O1-C1-C2-O2
2	D	601	EDO	O1-C1-C2-O2
2	D	602	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	EDO	1	0
2	B	603	EDO	8	0
2	D	604	EDO	2	0
2	A	606	EDO	5	0
2	B	601	EDO	1	0
2	D	603	EDO	1	0
2	A	607	EDO	4	0
2	B	604	EDO	4	0
2	D	606	EDO	3	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	486/504 (96%)	-0.49	4 (0%)	82 83	12, 19, 36, 79	0
1	B	482/504 (95%)	-0.05	7 (1%)	72 72	16, 27, 48, 69	1 (0%)
1	C	493/504 (97%)	-0.42	4 (0%)	82 83	13, 21, 38, 65	0
1	D	488/504 (96%)	-0.21	16 (3%)	49 49	15, 24, 51, 86	0
All	All	1949/2016 (96%)	-0.30	31 (1%)	70 71	12, 23, 45, 86	1 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	491	LEU	6.6
1	D	498	LEU	3.5
1	D	490	GLU	3.4
1	C	507	SER	3.4
1	B	15	ASP	3.3
1	D	489	ALA	3.1
1	B	50	ILE	3.0
1	D	493	GLY	3.0
1	D	50	ILE	2.9
1	D	51	VAL	2.8
1	D	81	GLN	2.7
1	C	53	GLY	2.7
1	D	503	VAL	2.6
1	D	502	PRO	2.5
1	A	492	ARG	2.4
1	D	495	PRO	2.4
1	D	53	GLY	2.4
1	D	117	LEU	2.3
1	B	191	ILE	2.2
1	C	15	ASP	2.2
1	D	146	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	498	LEU	2.2
1	C	50	ILE	2.2
1	B	489	ALA	2.2
1	A	489	ALA	2.2
1	D	499	TYR	2.1
1	B	52	PRO	2.1
1	D	497	GLY	2.1
1	B	495	PRO	2.1
1	B	437	MET	2.0
1	D	52	PRO	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 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($\text{\AA}^2$)	Q<0.9
2	EDO	A	611	4/4	0.70	0.16	41,44,47,53	0
2	EDO	A	609	4/4	0.74	0.19	49,51,53,56	0
2	EDO	A	602	4/4	0.77	0.18	42,49,51,57	0
2	EDO	A	610	4/4	0.78	0.19	36,36,40,46	0
2	EDO	D	603	4/4	0.79	0.24	34,35,45,48	0
2	EDO	B	603	4/4	0.81	0.21	27,36,37,40	0
2	EDO	D	605	4/4	0.81	0.15	40,45,45,46	0
2	EDO	B	602	4/4	0.82	0.14	42,43,49,52	0
2	EDO	A	607	4/4	0.85	0.14	37,39,45,47	0
2	EDO	B	601	4/4	0.85	0.24	32,33,35,43	0
2	EDO	D	604	4/4	0.86	0.11	28,31,36,42	0
2	EDO	A	605	4/4	0.86	0.14	40,41,44,50	0
2	EDO	D	602	4/4	0.87	0.14	34,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	606	4/4	0.87	0.30	38,39,40,45	0
2	EDO	B	604	4/4	0.88	0.32	35,52,54,65	0
2	EDO	C	601	4/4	0.88	0.13	34,36,38,39	0
2	EDO	A	603	4/4	0.89	0.12	34,43,49,52	0
2	EDO	A	604	4/4	0.90	0.11	39,43,45,46	0
2	EDO	A	601	4/4	0.91	0.11	34,39,44,51	0
2	EDO	D	601	4/4	0.91	0.12	31,34,35,35	0
2	EDO	D	606	4/4	0.92	0.25	26,35,36,39	0
2	EDO	A	608	4/4	0.94	0.10	32,38,40,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.