



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:07 AM UTC

PDB ID : 5X6X / pdb_00005x6x
Title : Crystal structure of the capping enzyme P5 from Rice Dwarf Virus
Authors : Nakamichi, Y.; Higashiura, A.; Nakagawa, A.
Deposited on : 2017-02-23
Resolution : 2.10 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

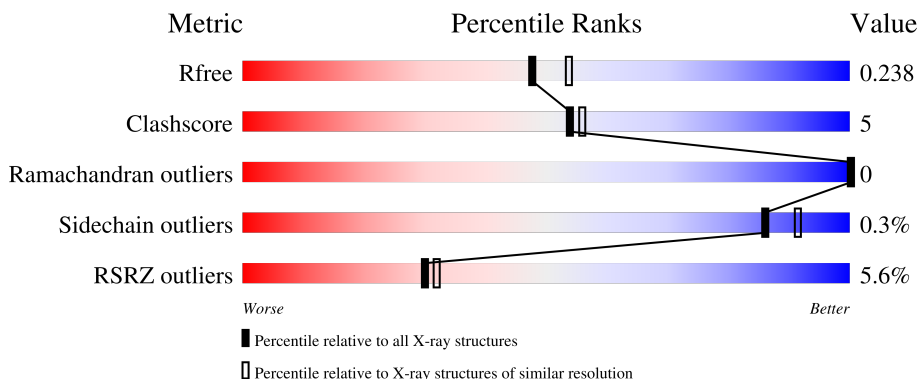
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	804	0% 87% 9% .
1	B	804	3% 87% 10% .
1	C	804	2% 86% 11% .
1	D	804	14% 84% 13% .

2 Entry composition [i](#)

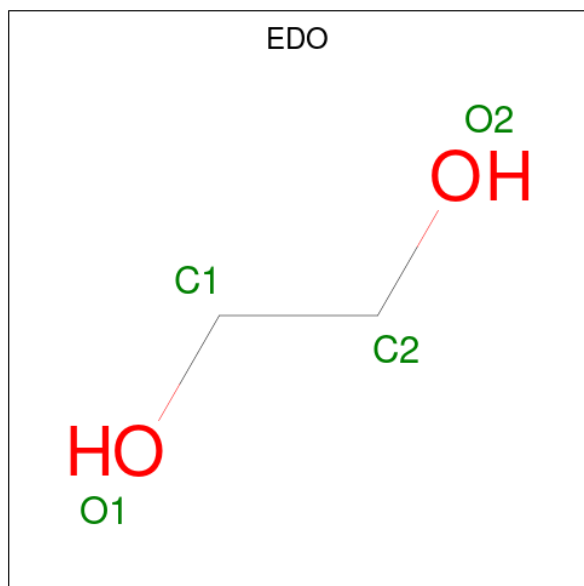
There are 3 unique types of molecules in this entry. The entry contains 26049 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 mRNA capping enzyme P5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	779	Total	C	N	O	S	0	0	0
			6193	3990	1026	1140	37			
1	A	776	Total	C	N	O	S	0	1	0
			6186	3987	1029	1132	38			
1	B	778	Total	C	N	O	S	0	0	0
			6185	3986	1024	1138	37			
1	D	778	Total	C	N	O	S	0	4	0
			6223	4010	1031	1144	38			

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

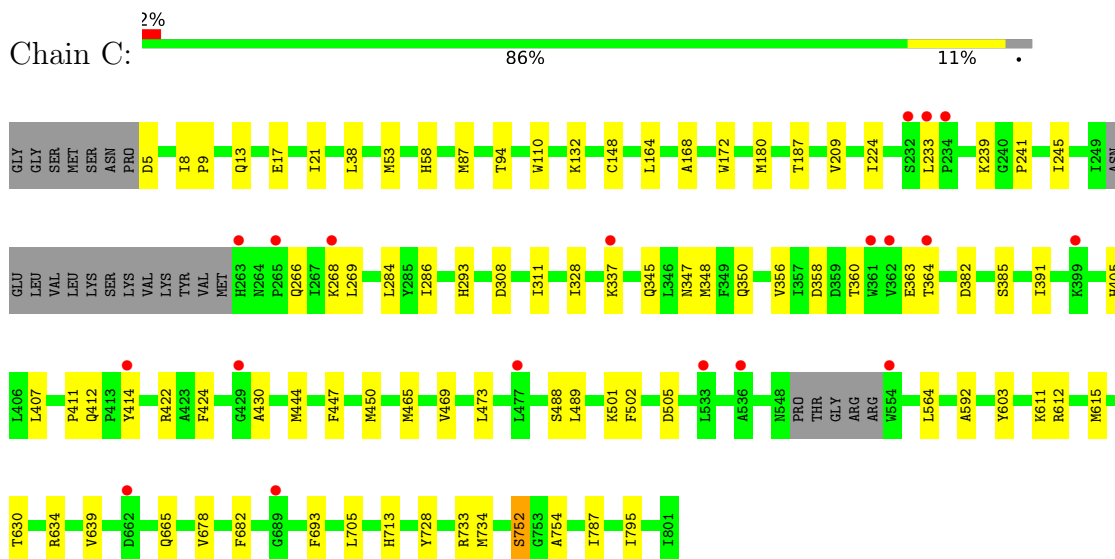
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	312	Total O 312 312	0	0
3	A	349	Total O 349 349	0	0
3	B	270	Total O 270 270	0	0
3	D	307	Total O 307 307	0	0

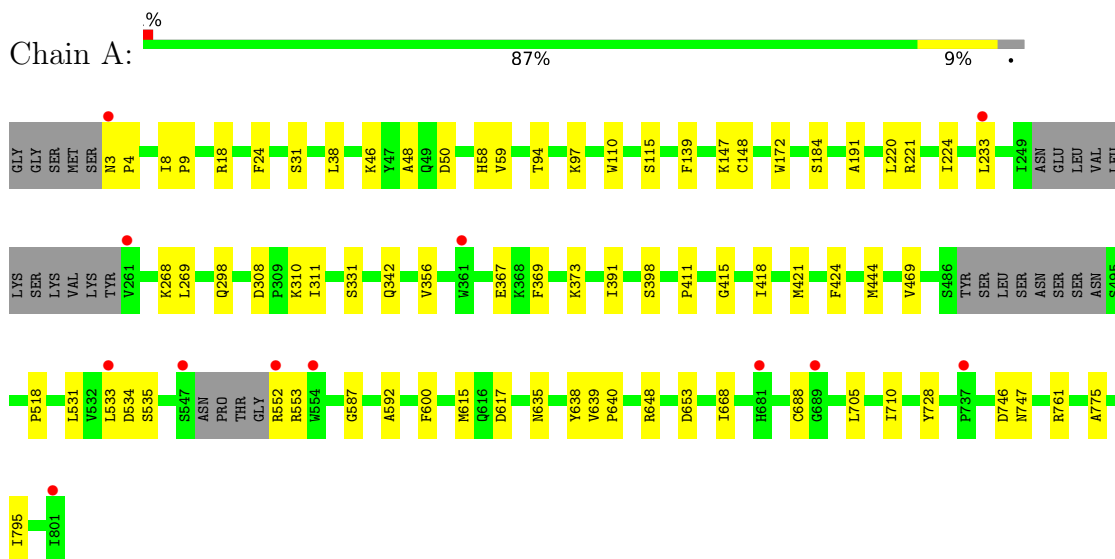
3 Residue-property plots [i](#)

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.

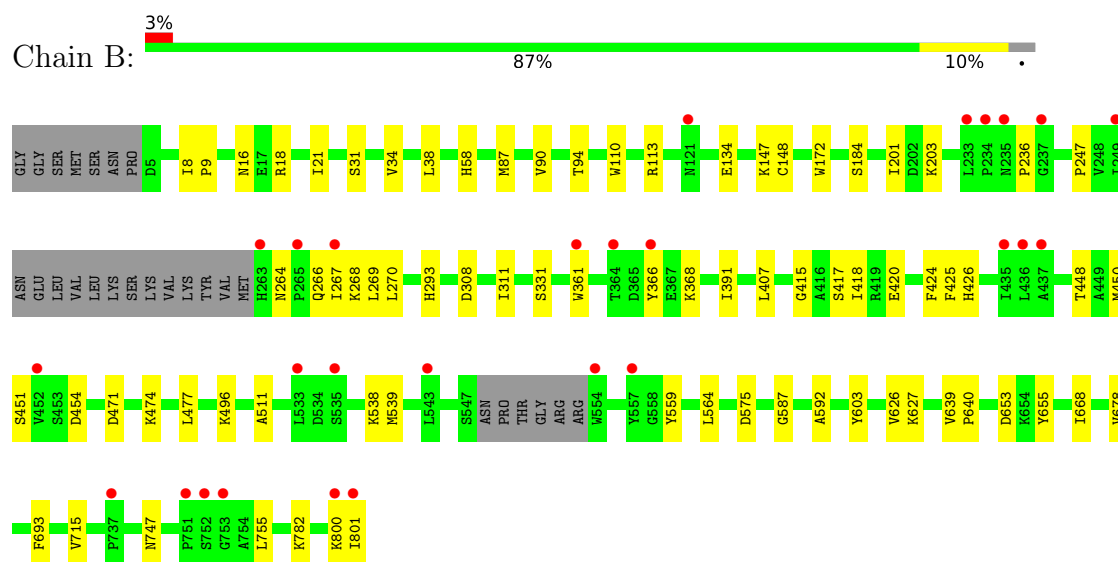
- Molecule 1: mRNA capping enzyme P5



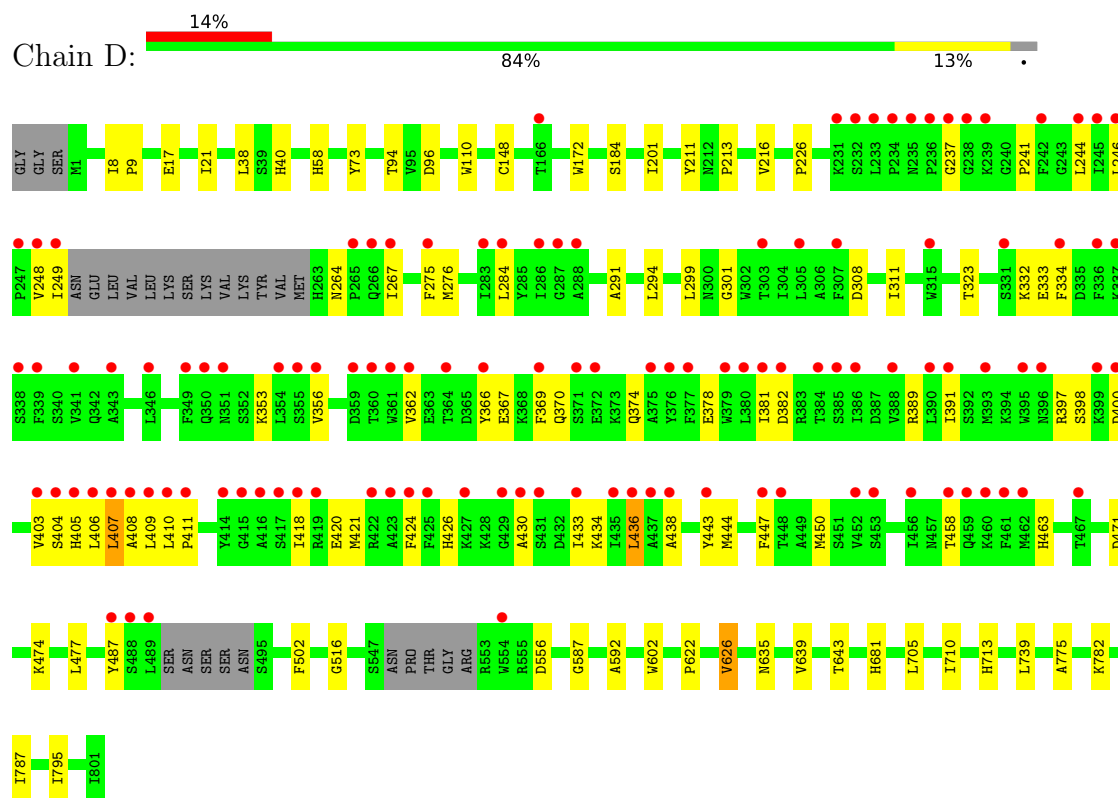
- Molecule 1: mRNA capping enzyme P5



- Molecule 1: mRNA capping enzyme P5



• Molecule 1: mRNA capping enzyme P5



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	77.23Å 83.85Å 143.25Å 103.41° 102.47° 95.37°	Depositor
Resolution (Å)	44.50 – 2.10 44.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (44.50-2.10) 98.4 (44.50-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.10Å)	Xtriage
Refinement program	PHENIX (dev_2614: ???)	Depositor
R, R_{free}	0.188 , 0.237 0.189 , 0.238	Depositor DCC
R_{free} test set	9494 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26049	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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	0.33	0/6335	0.50	0/8594
1	B	0.32	0/6335	0.49	0/8597
1	C	0.35	0/6343	0.50	0/8608
1	D	0.33	0/6373	0.50	0/8645
All	All	0.33	0/25386	0.50	0/34444

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	6186	0	6190	54	0
1	B	6185	0	6179	54	0
1	C	6193	0	6185	69	0
1	D	6223	0	6218	75	0
2	A	12	0	18	4	0
2	C	8	0	12	3	0
2	D	4	0	6	0	0
3	A	349	0	0	4	0
3	B	270	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	312	0	0	2	0
3	D	307	0	0	2	0
All	All	26049	0	24808	241	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 (241) 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:411:PRO:HB3	1:A:444:MET:HE1	1.64	0.78
1:C:268:LYS:HD2	1:C:414:TYR:HB2	1.66	0.77
1:D:367:GLU:OE2	1:D:397:ARG:HD2	1.84	0.77
1:C:734:MET:HE2	1:C:754:ALA:HB2	1.66	0.77
1:D:447:PHE:HA	1:D:450:MET:HE3	1.69	0.74
1:D:411:PRO:HG2	1:D:458:THR:HG21	1.71	0.72
1:A:533:LEU:HD13	1:A:535:SER:H	1.56	0.70
1:A:615:MET:HE2	1:A:615:MET:HA	1.72	0.70
1:C:233:LEU:HD22	1:C:469:VAL:HG21	1.73	0.70
1:D:418:ILE:HG22	1:D:420:GLU:H	1.56	0.70
1:A:233:LEU:HG	1:A:469:VAL:HG21	1.73	0.69
1:C:308:ASP:HB3	1:C:311:ILE:HG13	1.76	0.68
1:B:538:LYS:HD3	1:B:539:MET:N	2.09	0.68
1:D:411:PRO:HB3	1:D:444:MET:HE1	1.75	0.67
1:A:615:MET:HE3	1:A:728:TYR:HE2	1.60	0.67
1:A:3:ASN:HB3	1:A:4:PRO:HD3	1.78	0.66
1:A:533:LEU:HD22	1:A:534:ASP:H	1.60	0.66
1:B:538:LYS:HD3	1:B:539:MET:H	1.61	0.66
1:C:615:MET:HE3	1:C:728:TYR:CE2	2.32	0.64
1:A:615:MET:HE3	1:A:728:TYR:CE2	2.34	0.62
1:C:239:LYS:HB2	1:C:245:ILE:HB	1.82	0.61
1:D:241:PRO:HD3	1:D:430:ALA:HB2	1.84	0.60
1:D:367:GLU:OE1	1:D:398:SER:N	2.31	0.60
1:C:615:MET:HE3	1:C:728:TYR:HE2	1.66	0.60
1:B:450:MET:HE2	1:B:454:ASP:HB3	1.84	0.60
1:C:87:MET:HE3	1:D:635:ASN:HD21	1.68	0.59
1:C:615:MET:HE2	1:C:615:MET:HA	1.85	0.59
1:D:406:LEU:HD21	1:D:433:ILE:HG22	1.84	0.58
1:D:291:ALA:HB1	1:D:294:LEU:HD12	1.84	0.58
1:A:552:ARG:HG3	1:A:553:ARG:H	1.69	0.58
1:C:284:LEU:HB3	1:C:356:VAL:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:418:ILE:HD12	1:D:418:ILE:H	1.70	0.57
1:D:400:ASP:HB3	1:D:434:LYS:HD2	1.87	0.56
1:D:362:VAL:HG23	1:D:366:TYR:HA	1.87	0.56
1:D:713:HIS:HA	1:D:787:ILE:HD13	1.86	0.56
1:D:391:ILE:O	1:D:424:PHE:HA	2.05	0.56
1:C:38:LEU:O	1:C:94:THR:HA	2.06	0.56
1:A:421:MET:HE3	1:A:444:MET:HE3	1.88	0.56
1:C:328:ILE:HG13	1:C:348:MET:HE1	1.87	0.56
1:C:268:LYS:HD3	1:C:414:TYR:C	2.30	0.55
1:D:353:LYS:HB3	1:D:389:ARG:HD3	1.88	0.55
1:A:184:SER:OG	1:A:587:GLY:HA3	2.07	0.55
1:C:209:VAL:HG11	1:C:489:LEU:HD13	1.88	0.55
1:B:16:ASN:HA	1:B:782:LYS:HE2	1.89	0.55
1:A:191:ALA:HA	1:A:224:ILE:HD11	1.89	0.55
1:C:268:LYS:CD	1:C:414:TYR:HB2	2.34	0.55
1:D:381:ILE:HG23	1:D:405:HIS:HD2	1.71	0.55
1:D:201:ILE:HG21	1:D:301:GLY:HA3	1.89	0.55
1:B:38:LEU:O	1:B:94:THR:HA	2.07	0.54
1:C:268:LYS:HZ1	1:C:422:ARG:HH12	1.55	0.54
1:C:268:LYS:NZ	1:C:422:ARG:HH22	2.05	0.54
1:B:800:LYS:O	1:B:801:ILE:CG1	2.56	0.54
1:A:617:ASP:C	2:A:901:EDO:H22	2.33	0.54
1:D:332:LYS:HG2	1:D:333:GLU:O	2.06	0.54
1:A:18:ARG:HH12	1:B:21:ILE:HB	1.73	0.54
1:D:374:GLN:CD	1:D:403:VAL:HG12	2.34	0.53
1:B:368:LYS:NZ	3:B:905:HOH:O	2.37	0.52
1:C:564:LEU:HD13	1:C:603:TYR:CZ	2.44	0.52
1:D:9:PRO:HB3	1:D:639:VAL:HG22	1.90	0.52
1:C:268:LYS:HE3	1:C:412:GLN:HB3	1.92	0.52
1:C:705:LEU:HD11	1:C:795:ILE:HD13	1.91	0.52
1:D:8:ILE:HA	1:D:9:PRO:C	2.35	0.52
1:C:444:MET:HE2	1:C:444:MET:HA	1.92	0.52
1:C:110:TRP:CD1	1:C:148:CYS:HA	2.45	0.52
1:C:363:GLU:HG2	1:C:364:THR:HG23	1.91	0.51
1:B:800:LYS:O	1:B:801:ILE:HG12	2.11	0.51
1:D:308:ASP:HB3	1:D:311:ILE:HG13	1.92	0.51
1:C:132:LYS:HE3	3:C:1280:HOH:O	2.10	0.51
1:D:275:PHE:CE1	1:D:276:MET:HE2	2.45	0.51
1:A:18:ARG:NH1	1:B:21:ILE:HB	2.26	0.51
1:B:184:SER:OG	1:B:587:GLY:HA3	2.11	0.51
1:B:268:LYS:HG2	1:B:269:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:TRP:CZ2	1:D:592:ALA:HB2	2.46	0.51
1:C:164:LEU:N	3:C:1002:HOH:O	2.35	0.51
1:A:268:LYS:HG3	1:A:269:LEU:HD12	1.92	0.50
1:B:496:LYS:HG3	1:B:559:TYR:CZ	2.46	0.50
1:C:172:TRP:CZ2	1:C:592:ALA:HB2	2.46	0.50
1:B:415:GLY:O	1:B:418:ILE:HG13	2.11	0.50
1:D:356:VAL:HB	1:D:391:ILE:HG23	1.93	0.50
1:C:8:ILE:HA	1:C:9:PRO:C	2.36	0.50
1:C:168:ALA:HB1	1:D:643:THR:HG23	1.93	0.50
1:B:451:SER:OG	1:B:454:ASP:OD2	2.30	0.50
1:B:9:PRO:HB3	1:B:639:VAL:HG22	1.93	0.50
1:D:378:GLU:HG2	1:D:404:SER:HB2	1.92	0.50
1:D:374:GLN:NE2	1:D:403:VAL:HG12	2.27	0.50
1:C:363:GLU:OE1	1:C:363:GLU:N	2.44	0.50
1:B:172:TRP:CZ2	1:B:592:ALA:HB2	2.47	0.50
1:B:471:ASP:HB3	1:B:474:LYS:HG2	1.94	0.49
1:D:710:ILE:HD11	1:D:775:ALA:HA	1.94	0.49
1:D:38:LEU:O	1:D:94:THR:HA	2.12	0.49
1:D:362:VAL:CG2	1:D:366:TYR:HA	2.42	0.49
1:C:17:GLU:O	1:C:21:ILE:HG12	2.12	0.49
1:A:38:LEU:O	1:A:94:THR:HA	2.12	0.49
1:B:16:ASN:OD1	1:B:18:ARG:HB3	2.13	0.48
1:B:266:GLN:HB3	1:B:293:HIS:HB2	1.94	0.48
1:A:746:ASP:HB3	2:A:901:EDO:H11	1.94	0.48
1:D:622:PRO:O	1:D:626:VAL:HG22	2.13	0.48
1:C:53:MET:HE1	1:D:73:TYR:CE2	2.49	0.48
1:A:172:TRP:CZ2	1:A:592:ALA:HB2	2.49	0.48
1:C:473:LEU:HD13	1:C:502:PHE:HB2	1.95	0.48
1:A:8:ILE:HA	1:A:9:PRO:C	2.37	0.48
1:B:361:TRP:CD1	1:B:366:TYR:CZ	3.02	0.48
1:C:734:MET:HE1	1:C:752:SER:O	2.13	0.48
1:A:308:ASP:O	1:A:331:SER:HA	2.13	0.48
1:B:31:SER:O	1:B:147:LYS:HE3	2.13	0.48
1:D:471:ASP:HB3	1:D:474:LYS:HD3	1.96	0.48
1:B:236:PRO:HB2	1:B:247:PRO:HB3	1.96	0.48
1:D:382:ASP:HB3	1:D:405:HIS:CD2	2.48	0.48
1:B:538:LYS:HA	1:B:538:LYS:HE2	1.96	0.48
1:A:747:ASN:ND2	2:A:901:EDO:H21	2.30	0.47
1:C:9:PRO:HB3	1:C:639:VAL:HG22	1.96	0.47
1:B:391:ILE:HB	1:B:425:PHE:HB2	1.95	0.47
1:B:564:LEU:HD13	1:B:603:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:SER:OG	1:D:587:GLY:HA3	2.15	0.47
1:C:209:VAL:HG12	1:C:488:SER:HB2	1.97	0.47
1:A:415:GLY:O	1:A:418:ILE:HG13	2.15	0.47
1:A:18:ARG:NH1	1:B:18:ARG:HA	2.30	0.46
1:D:436:LEU:HD11	1:D:438:ALA:HB3	1.97	0.46
1:C:241:PRO:HD3	1:C:430:ALA:HB2	1.98	0.46
1:B:8:ILE:HA	1:B:9:PRO:C	2.40	0.46
1:C:266:GLN:H	1:C:266:GLN:HG2	1.55	0.46
1:A:221:ARG:O	1:A:298:GLN:HG3	2.16	0.46
1:D:367:GLU:OE2	1:D:397:ARG:HA	2.15	0.46
1:D:211:TYR:OH	1:D:463:HIS:ND1	2.35	0.46
1:B:264:ASN:HB3	1:B:267:ILE:HB	1.97	0.46
1:D:366:TYR:O	1:D:370:GLN:HG3	2.15	0.46
1:D:17:GLU:OE1	1:D:782:LYS:HE3	2.16	0.45
1:D:400:ASP:OD2	1:D:436:LEU:HD23	2.17	0.45
1:D:406:LEU:HD21	1:D:433:ILE:CG2	2.47	0.45
1:B:418:ILE:HD13	1:B:420:GLU:HG3	1.97	0.45
1:D:381:ILE:HG23	1:D:405:HIS:CD2	2.50	0.45
1:D:17:GLU:O	1:D:21:ILE:HG12	2.17	0.45
1:D:362:VAL:HG21	1:D:369:PHE:HB3	1.99	0.45
1:A:367:GLU:OE2	1:A:398:SER:OG	2.24	0.45
1:C:286:ILE:HG22	1:C:360:THR:CG2	2.46	0.45
1:C:634:ARG:HE	2:C:901:EDO:C2	2.30	0.45
1:A:688:CYS:O	1:A:761:ARG:NH1	2.50	0.45
1:D:299:LEU:HB2	1:D:323:THR:HB	1.99	0.45
1:D:249:ILE:HG21	1:D:450:MET:HE1	1.98	0.45
1:D:264:ASN:HB2	1:D:267:ILE:HB	1.98	0.45
1:C:268:LYS:CE	1:C:412:GLN:HB3	2.46	0.45
1:A:110:TRP:CD1	1:A:148:CYS:HA	2.52	0.45
1:A:139:PHE:HA	1:B:640:PRO:HB3	1.99	0.45
1:D:244:LEU:HB3	1:D:408:ALA:HB2	1.98	0.45
1:A:638:TYR:O	1:A:640:PRO:HD3	2.17	0.44
1:C:356:VAL:HB	1:C:391:ILE:HG12	2.00	0.44
1:A:391:ILE:O	1:A:424:PHE:HA	2.16	0.44
1:D:237:GLY:HA3	1:D:248:VAL:HG13	1.99	0.44
1:A:369:PHE:CZ	1:A:373:LYS:HD3	2.53	0.44
1:B:308:ASP:HB3	1:B:311:ILE:HG13	2.00	0.44
1:D:477:LEU:HD11	1:D:502:PHE:CE1	2.53	0.44
1:B:110:TRP:CD1	1:B:148:CYS:HA	2.52	0.44
1:D:705:LEU:HD11	1:D:795:ILE:HD13	2.00	0.44
1:C:350:GLN:HE22	1:C:385:SER:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:678:VAL:HG21	1:C:693:PHE:HB3	2.00	0.44
1:B:267:ILE:HA	1:B:270:LEU:HB2	2.00	0.44
1:B:269:LEU:HD23	1:B:293:HIS:CE1	2.53	0.44
1:D:211:TYR:CE2	1:D:213:PRO:HG3	2.52	0.44
1:C:187:THR:HG23	1:C:224:ILE:HD11	1.99	0.43
1:A:31:SER:O	1:A:147:LYS:HE3	2.18	0.43
1:A:311:ILE:O	1:A:331:SER:HB3	2.17	0.43
1:A:97:LYS:NZ	3:A:1019:HOH:O	2.50	0.43
1:B:678:VAL:HG21	1:B:693:PHE:HB3	2.01	0.43
1:A:24:PHE:CG	1:A:531:LEU:HD22	2.53	0.43
1:A:653:ASP:HB2	1:A:668:ILE:HG13	1.99	0.43
1:B:113:ARG:HD3	1:B:575:ASP:OD2	2.18	0.43
1:C:5:ASP:N	1:C:13:GLN:HE21	2.16	0.43
1:A:9:PRO:HB3	1:A:639:VAL:HG22	2.00	0.43
1:D:366:TYR:CD1	1:D:367:GLU:HG2	2.53	0.43
1:D:406:LEU:O	1:D:406:LEU:HG	2.18	0.43
1:D:516:GLY:HA3	1:D:602:TRP:CE3	2.52	0.43
1:A:648:ARG:HB2	3:A:1002:HOH:O	2.18	0.43
1:D:110:TRP:CD1	1:D:148:CYS:HA	2.54	0.43
1:D:407:LEU:HD23	1:D:426:HIS:CG	2.53	0.43
1:C:269:LEU:HB3	1:C:293:HIS:CE1	2.54	0.43
1:C:391:ILE:O	1:C:424:PHE:HA	2.19	0.43
1:C:345:GLN:C	1:C:347:ASN:H	2.27	0.43
1:A:342[A]:GLN:NE2	3:A:1024:HOH:O	2.52	0.43
1:B:417:SER:HA	1:B:448:THR:HG22	1.99	0.43
1:C:501:LYS:HE2	1:C:505:ASP:OD1	2.18	0.43
1:A:705:LEU:HD11	1:A:795:ILE:HD13	2.00	0.43
1:B:308:ASP:O	1:B:331:SER:HA	2.19	0.42
1:B:391:ILE:O	1:B:424:PHE:HA	2.19	0.42
1:D:739:LEU:HD23	1:D:739:LEU:HA	1.94	0.42
1:C:286:ILE:HG22	1:C:360:THR:HG23	2.02	0.42
1:D:409:LEU:HD21	1:D:421:MET:SD	2.59	0.42
1:A:518:PRO:HD3	1:A:600:PHE:CE2	2.54	0.42
1:B:34:VAL:HB	1:B:90:VAL:HG22	2.01	0.42
1:D:410:LEU:HD12	1:D:424:PHE:CE1	2.54	0.42
1:C:58:HIS:CE1	1:D:58:HIS:CE1	3.08	0.42
1:C:630:THR:CG2	2:C:901:EDO:H22	2.49	0.42
1:C:665:GLN:NE2	1:C:682:PHE:HB3	2.34	0.42
1:A:710:ILE:HD11	1:A:775:ALA:HA	2.01	0.42
1:C:447:PHE:HA	1:C:450:MET:HE2	2.01	0.42
1:C:286:ILE:HB	1:C:358:ASP:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:HIS:HB3	3:D:1261:HOH:O	2.19	0.42
1:D:216:VAL:HA	1:D:226:PRO:HG3	2.01	0.42
1:B:203:LYS:HD2	1:B:203:LYS:HA	1.82	0.42
1:D:477:LEU:HD23	1:D:477:LEU:HA	1.88	0.42
1:A:46:LYS:NZ	1:A:50:ASP:OD2	2.52	0.42
1:D:267:ILE:HD12	1:D:267:ILE:HA	1.88	0.42
1:D:367:GLU:OE2	1:D:397:ARG:CD	2.63	0.42
1:C:407:LEU:HD23	1:C:465:MET:HE3	2.02	0.42
1:A:356:VAL:HB	1:A:391:ILE:HG23	2.01	0.42
1:C:268:LYS:CE	1:C:422:ARG:HH22	2.33	0.41
1:C:268:LYS:HE2	1:C:414:TYR:H	1.84	0.41
1:C:337:LYS:HD2	1:A:269:LEU:HD13	2.02	0.41
1:A:310:LYS:NZ	3:A:1022:HOH:O	2.51	0.41
1:C:180:MET:HE2	1:C:180:MET:HB2	1.78	0.41
1:A:115:SER:OG	1:A:147:LYS:HD3	2.21	0.41
1:B:407:LEU:HB2	1:B:426:HIS:HB3	2.02	0.41
1:B:626:VAL:HG23	1:B:627:LYS:HG2	2.02	0.41
1:D:382:ASP:HB3	1:D:405:HIS:NE2	2.35	0.41
1:D:418:ILE:HG21	1:D:420:GLU:HG2	2.03	0.41
1:C:350:GLN:NE2	1:C:385:SER:HB2	2.36	0.41
1:B:653:ASP:HB2	1:B:668:ILE:HG13	2.03	0.41
1:D:284:LEU:HD21	1:D:334:PHE:CE1	2.56	0.41
1:C:268:LYS:HE3	1:C:422:ARG:HH22	1.86	0.41
1:C:411:PRO:HB3	1:C:444:MET:HE1	2.01	0.41
1:C:634:ARG:HE	2:C:901:EDO:H21	1.85	0.41
1:C:713:HIS:HA	1:C:787:ILE:HD13	2.03	0.41
1:A:58:HIS:CE1	1:B:58:HIS:CE1	3.09	0.41
1:A:220:LEU:HD13	1:A:220:LEU:HA	1.85	0.41
1:C:382:ASP:OD2	1:C:405:HIS:NE2	2.50	0.41
1:C:611:LYS:HG2	1:C:612:ARG:HG2	2.02	0.41
1:B:311:ILE:O	1:B:331:SER:HB3	2.20	0.41
1:D:487:TYR:HE2	1:D:556:ASP:HB2	1.84	0.41
1:A:48:ALA:CB	1:A:59:VAL:HG11	2.51	0.40
1:A:552:ARG:HD3	1:A:552:ARG:HA	1.89	0.40
1:A:444:MET:HG3	2:A:903:EDO:H21	2.03	0.40
1:B:471:ASP:HB3	1:B:474:LYS:CG	2.51	0.40
1:B:747:ASN:HB2	1:B:755:LEU:HD11	2.02	0.40
1:C:172:TRP:HZ2	1:C:592:ALA:HB2	1.83	0.40
1:C:615:MET:HE1	1:C:733:ARG:HB2	2.04	0.40
1:B:201:ILE:HG12	3:B:1126:HOH:O	2.21	0.40
1:B:477:LEU:HB3	1:B:511:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:TYR:HB2	3:B:1164:HOH:O	2.20	0.40
1:A:635:ASN:HD21	1:B:87:MET:HE3	1.86	0.40
1:D:246:LEU:HD22	1:D:443:TYR:CG	2.57	0.40
1:D:681:HIS:HB2	3:D:1013:HOH:O	2.20	0.40
1:B:267:ILE:HA	1:B:267:ILE:HD12	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	769/804 (96%)	752 (98%)	17 (2%)	0	100	100
1	B	772/804 (96%)	750 (97%)	22 (3%)	0	100	100
1	C	773/804 (96%)	755 (98%)	18 (2%)	0	100	100
1	D	774/804 (96%)	752 (97%)	22 (3%)	0	100	100
All	All	3088/3216 (96%)	3009 (97%)	79 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	687/711 (97%)	687 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	688/711 (97%)	686 (100%)	2 (0%)	86	91
1	C	689/711 (97%)	688 (100%)	1 (0%)	88	93
1	D	692/711 (97%)	687 (99%)	5 (1%)	76	83
All	All	2756/2844 (97%)	2748 (100%)	8 (0%)	86	91

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	752	SER
1	B	134	GLU
1	B	715	VAL
1	D	96[A]	ASP
1	D	96[B]	ASP
1	D	407	LEU
1	D	436	LEU
1	D	626	VAL

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

Mol	Chain	Res	Type
1	C	88	GLN
1	C	167	ASN
1	C	350	GLN
1	C	351	ASN
1	C	597	ASN
1	C	747	ASN
1	A	88	GLN
1	A	298	GLN
1	A	347	ASN
1	A	459	GLN
1	A	597	ASN
1	A	781	ASN
1	B	88	GLN
1	B	167	ASN
1	B	300	ASN
1	B	374	GLN
1	B	412	GLN
1	B	610	HIS
1	D	13	GLN
1	D	88	GLN

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Mol	Chain	Res	Type
1	D	374	GLN
1	D	405	HIS
1	D	747	ASN

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 ⓘ

6 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	903	-	3,3,3	0.43	0	2,2,2	0.41	0
2	EDO	A	901	-	3,3,3	0.35	0	2,2,2	0.32	0
2	EDO	C	901	-	3,3,3	0.47	0	2,2,2	0.42	0
2	EDO	D	901	-	3,3,3	0.64	0	2,2,2	0.15	0
2	EDO	C	902	-	3,3,3	0.53	0	2,2,2	0.07	0
2	EDO	A	902	-	3,3,3	0.41	0	2,2,2	0.50	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	903	-	-	0/1/1/1	-
2	EDO	A	901	-	-	0/1/1/1	-
2	EDO	C	901	-	-	0/1/1/1	-
2	EDO	D	901	-	-	0/1/1/1	-
2	EDO	C	902	-	-	1/1/1/1	-
2	EDO	A	902	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	902	EDO	O1-C1-C2-O2
2	A	902	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	903	EDO	1	0
2	A	901	EDO	3	0
2	C	901	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	776/804 (96%)	-0.04	12 (1%) 72 74	16, 32, 51, 76	1 (0%)
1	B	778/804 (96%)	0.20	27 (3%) 47 49	21, 36, 62, 79	0
1	C	779/804 (96%)	0.09	19 (2%) 59 62	17, 33, 55, 76	0
1	D	778/804 (96%)	0.50	116 (14%) 5 5	11, 34, 80, 94	4 (0%)
All	All	3111/3216 (96%)	0.19	174 (5%) 30 32	11, 34, 65, 94	5 (0%)

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	415	GLY	5.1
1	D	409	LEU	5.0
1	D	406	LEU	4.8
1	D	407	LEU	4.8
1	D	361	TRP	4.7
1	D	249	ILE	4.5
1	D	339	PHE	4.4
1	D	424	PHE	4.4
1	D	461	PHE	4.2
1	D	430	ALA	4.2
1	D	418	ILE	4.1
1	D	411	PRO	4.0
1	D	244	LEU	4.0
1	C	233	LEU	4.0
1	D	377	PHE	4.0
1	D	362	VAL	3.9
1	D	239	LYS	3.9
1	D	336	PHE	3.9
1	C	265	PRO	3.8
1	D	384	THR	3.8
1	D	307	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	554	TRP	3.7
1	D	233	LEU	3.7
1	A	261	VAL	3.6
1	A	533	LEU	3.6
1	D	489	LEU	3.6
1	D	364	THR	3.5
1	D	234	PRO	3.4
1	C	689	GLY	3.4
1	D	338	SER	3.4
1	D	436	LEU	3.4
1	D	334	PHE	3.4
1	D	395	TRP	3.3
1	D	265	PRO	3.3
1	D	458	THR	3.2
1	D	375	ALA	3.2
1	D	266	GLN	3.2
1	D	245	ILE	3.2
1	D	366	TYR	3.2
1	D	433	ILE	3.2
1	D	408	ALA	3.1
1	D	356	VAL	3.1
1	D	379	TRP	3.1
1	D	467	THR	3.1
1	B	361	TRP	3.0
1	D	376	TYR	3.0
1	D	429	GLY	3.0
1	D	487	TYR	3.0
1	B	801	ILE	3.0
1	D	360	THR	3.0
1	D	448	THR	3.0
1	D	350	GLN	3.0
1	A	801	ILE	3.0
1	B	364	THR	3.0
1	D	346	LEU	2.9
1	D	380	LEU	2.9
1	D	452	VAL	2.9
1	D	242	PHE	2.9
1	D	284	LEU	2.9
1	D	405	HIS	2.9
1	D	443	TYR	2.9
1	B	233	LEU	2.9
1	D	236	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	369	PHE	2.9
1	D	287	GLY	2.9
1	D	400	ASP	2.8
1	D	435	ILE	2.8
1	D	416	ALA	2.8
1	B	265	PRO	2.8
1	D	456	ILE	2.8
1	D	337	LYS	2.8
1	D	275	PHE	2.8
1	D	386	ILE	2.8
1	D	404	SER	2.8
1	D	488	SER	2.8
1	D	438	ALA	2.8
1	D	267	ILE	2.8
1	D	417	SER	2.7
1	D	399	LYS	2.7
1	D	422	ARG	2.7
1	D	372	GLU	2.7
1	D	396	ASN	2.7
1	D	341	VAL	2.7
1	D	403	VAL	2.7
1	D	283	ILE	2.7
1	D	371	SER	2.7
1	D	390	LEU	2.7
1	D	355	SER	2.7
1	D	391	ILE	2.7
1	B	263	HIS	2.6
1	D	382	ASP	2.6
1	D	388	VAL	2.6
1	C	232	SER	2.6
1	C	554	TRP	2.6
1	D	431	SER	2.6
1	D	381	ILE	2.5
1	D	393	MET	2.5
1	A	3	ASN	2.5
1	D	305	LEU	2.5
1	D	425	PHE	2.5
1	D	248	VAL	2.5
1	D	247	PRO	2.5
1	C	263	HIS	2.5
1	D	246	LEU	2.5
1	D	349	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	238	GLY	2.5
1	B	737	PRO	2.4
1	C	536	ALA	2.4
1	D	354	LEU	2.4
1	D	410	LEU	2.4
1	D	459	GLN	2.4
1	D	359	ASP	2.4
1	D	453	SER	2.4
1	D	437	ALA	2.4
1	C	414	TYR	2.4
1	A	681	HIS	2.4
1	B	753	GLY	2.4
1	D	237	GLY	2.4
1	B	452	VAL	2.4
1	B	435	ILE	2.3
1	B	437	ALA	2.3
1	C	429	GLY	2.3
1	B	235	ASN	2.3
1	A	554	TRP	2.3
1	D	427	LYS	2.3
1	D	286	ILE	2.3
1	C	362	VAL	2.3
1	D	343	ALA	2.3
1	A	547	SER	2.2
1	C	234	PRO	2.2
1	A	552	ARG	2.2
1	D	414	TYR	2.2
1	B	751	PRO	2.2
1	D	460	LYS	2.2
1	D	423	ALA	2.2
1	B	557	TYR	2.2
1	D	331	SER	2.2
1	D	315	TRP	2.2
1	B	249	ILE	2.2
1	B	267	ILE	2.2
1	D	462	MET	2.2
1	B	533	LEU	2.2
1	D	235	ASN	2.2
1	B	234	PRO	2.1
1	C	477	LEU	2.1
1	A	233	LEU	2.1
1	D	303	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	361	TRP	2.1
1	D	447	PHE	2.1
1	B	436	LEU	2.1
1	B	752	SER	2.1
1	D	385	SER	2.1
1	B	121	ASN	2.1
1	C	364	THR	2.1
1	A	737	PRO	2.1
1	D	288	ALA	2.1
1	D	232	SER	2.1
1	D	419	ARG	2.1
1	B	237	GLY	2.1
1	C	399	LYS	2.1
1	C	533	LEU	2.0
1	C	662	ASP	2.0
1	C	268	LYS	2.0
1	C	337	LYS	2.0
1	B	366	TYR	2.0
1	D	231	LYS	2.0
1	B	535	SER	2.0
1	A	361	TRP	2.0
1	D	554	TRP	2.0
1	D	351	ASN	2.0
1	B	543	LEU	2.0
1	B	800	LYS	2.0
1	D	166	THR	2.0
1	A	689	GLY	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(Å ²)	Q<0.9
2	EDO	A	902	4/4	0.83	0.23	31,37,39,45	0
2	EDO	D	901	4/4	0.87	0.12	31,31,33,36	0
2	EDO	C	901	4/4	0.88	0.12	31,33,37,40	0
2	EDO	C	902	4/4	0.88	0.11	33,35,39,40	0
2	EDO	A	901	4/4	0.93	0.19	30,31,35,36	0
2	EDO	A	903	4/4	0.94	0.10	40,41,42,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.