



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:59 AM UTC

PDB ID : 7XZN / pdb_00007xzn
Title : Formate-tetrahydrofolate ligase from *Peptostreptococcus anaerobius*
Authors : Fang, C.L.; Zhang, Y.
Deposited on : 2022-06-03
Resolution : 2.04 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

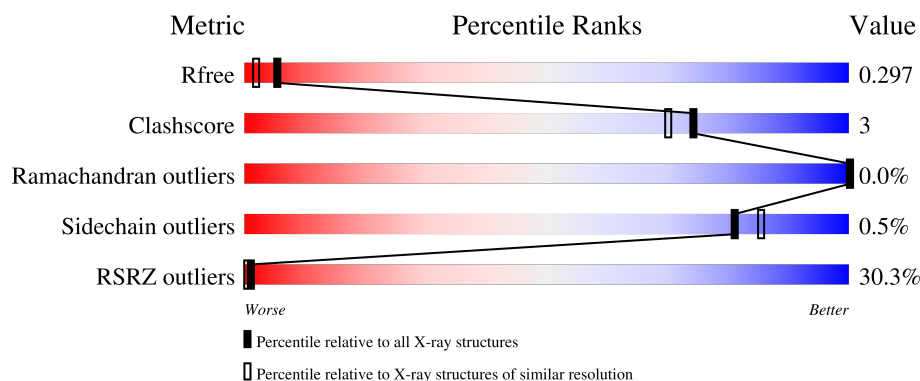
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	562	30% 91% 7%
1	B	562	34% 92% 7%
1	C	562	34% 90% 9%
1	D	562	23% 93% 6%

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
3	TAM	A	605	-	X	-	-
3	TAM	B	602	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16831 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 Formate--tetrahydrofolate ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4159	2617	717	804	21			
1	B	556	Total	C	N	O	S	0	0	0
			4162	2619	715	807	21			
1	C	556	Total	C	N	O	S	0	0	0
			4172	2625	719	807	21			
1	D	555	Total	C	N	O	S	0	0	0
			4137	2600	714	802	21			

There are 16 discrepancies between the modelled and reference sequences:

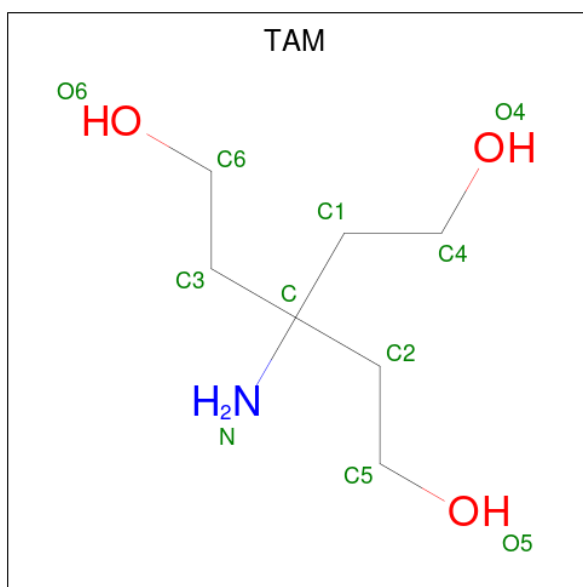
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A0A379CIH2
A	-2	SER	-	expression tag	UNP A0A379CIH2
A	-1	HIS	-	expression tag	UNP A0A379CIH2
A	0	MET	-	expression tag	UNP A0A379CIH2
B	-3	GLY	-	expression tag	UNP A0A379CIH2
B	-2	SER	-	expression tag	UNP A0A379CIH2
B	-1	HIS	-	expression tag	UNP A0A379CIH2
B	0	MET	-	expression tag	UNP A0A379CIH2
C	-3	GLY	-	expression tag	UNP A0A379CIH2
C	-2	SER	-	expression tag	UNP A0A379CIH2
C	-1	HIS	-	expression tag	UNP A0A379CIH2
C	0	MET	-	expression tag	UNP A0A379CIH2
D	-3	GLY	-	expression tag	UNP A0A379CIH2
D	-2	SER	-	expression tag	UNP A0A379CIH2
D	-1	HIS	-	expression tag	UNP A0A379CIH2
D	0	MET	-	expression tag	UNP A0A379CIH2

- 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		
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	C	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		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is TRIS(HYDROXYETHYL)AMINOMETHANE (CCD ID: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	7	1	3		
3	B	1	Total	C	N	O	0	0
			11	7	1	3		
3	C	1	Total	C	N	O	0	0
			11	7	1	3		
3	D	1	Total	C	N	O	0	0
			11	7	1	3		

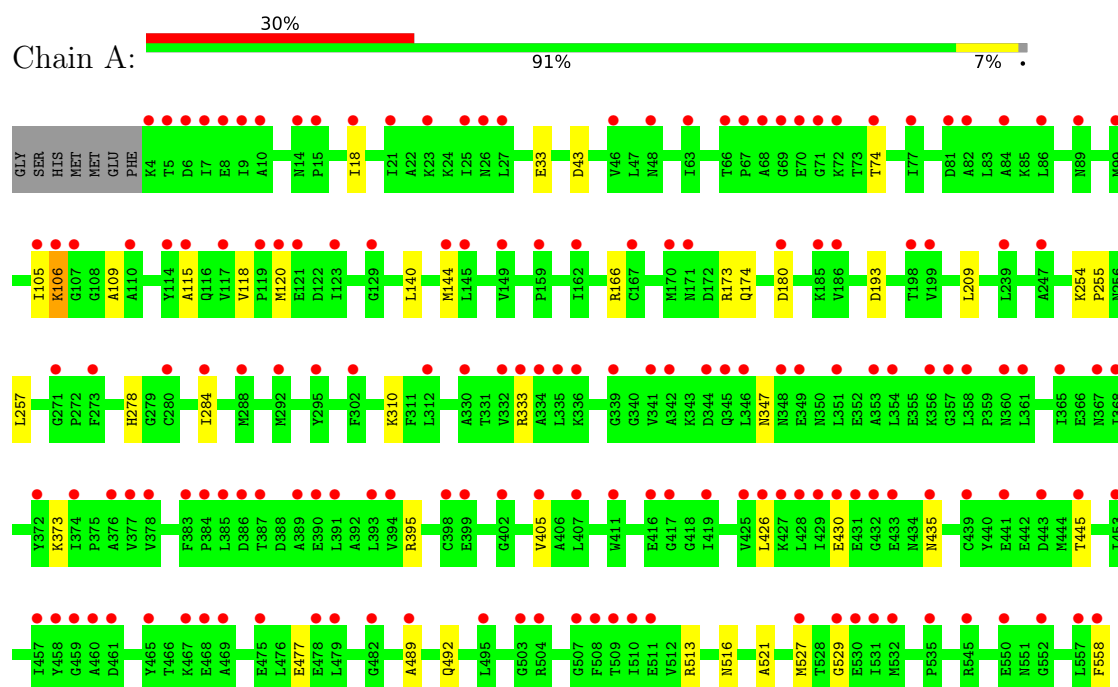
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total	O	0	0
			28	28		
4	B	36	Total	O	0	0
			36	36		
4	C	28	Total	O	0	0
			28	28		
4	D	25	Total	O	0	0
			25	25		

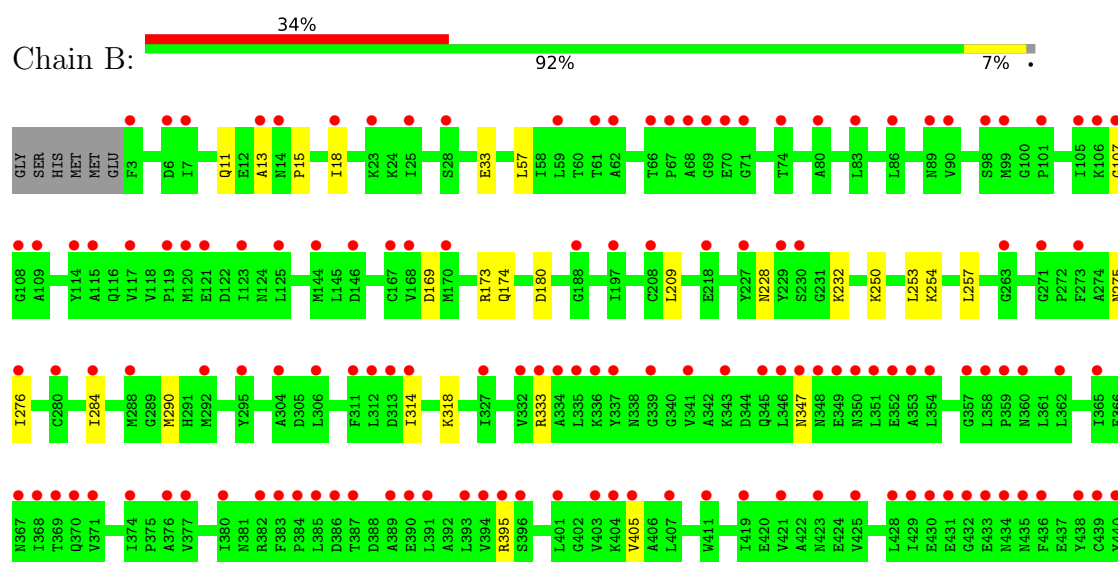
3 Residue-property plots [i](#)

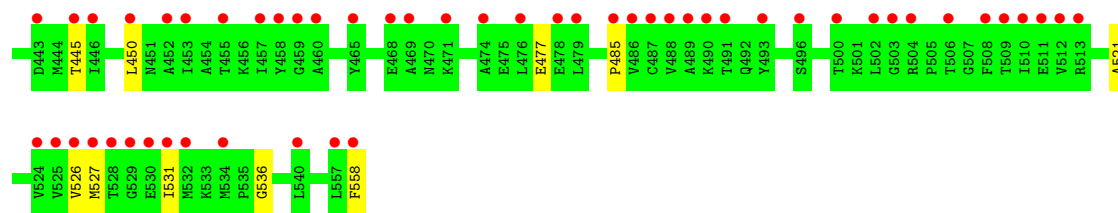
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Formate--tetrahydrofolate ligase

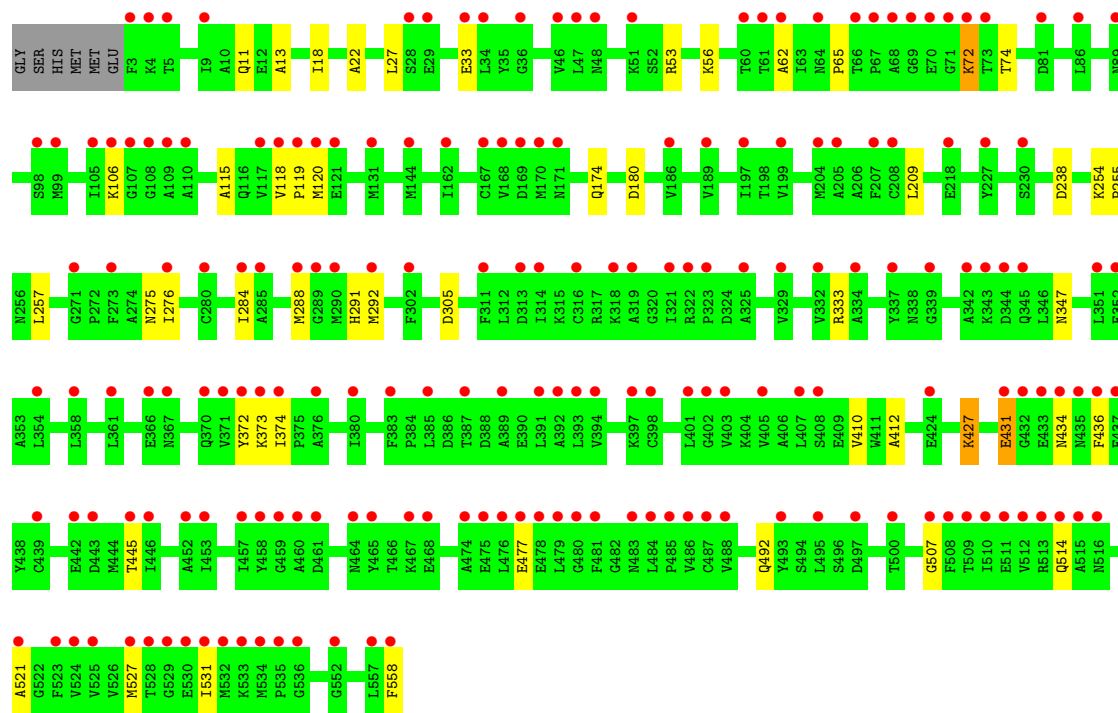
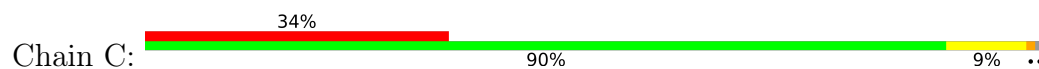


• Molecule 1: Formate--tetrahydrofolate ligase

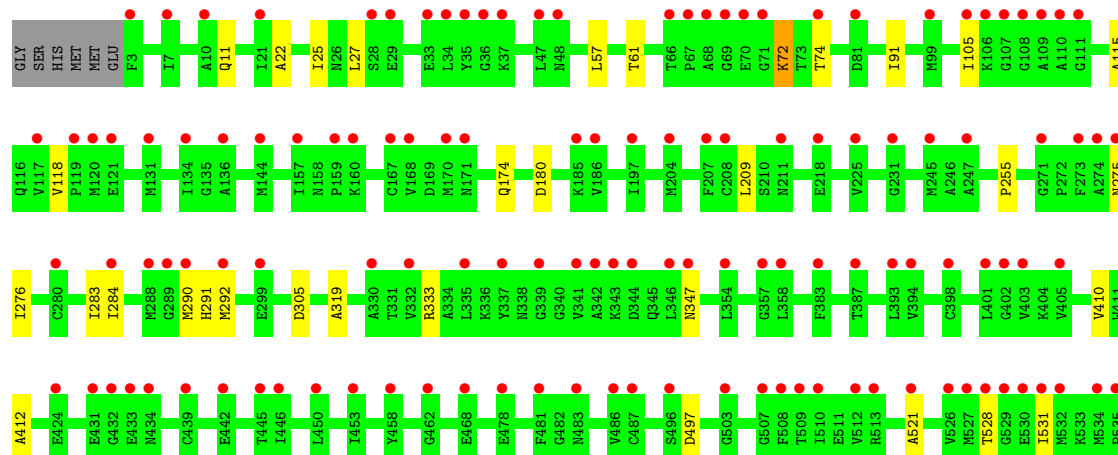
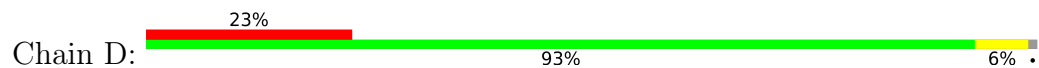




• Molecule 1: Formate--tetrahydrofolate ligase



• Molecule 1: Formate--tetrahydrofolate ligase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.87Å 116.30Å 107.38Å 90.00° 92.58° 90.00°	Depositor
Resolution (Å)	30.50 – 2.04 30.50 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.50-2.04) 99.9 (30.50-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.272 , 0.283 0.286 , 0.297	Depositor DCC
R_{free} test set	2012 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16831	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8167e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: TAM, 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	0.11	0/4218	0.30	0/5711
1	B	0.10	0/4221	0.28	0/5716
1	C	0.10	0/4232	0.29	0/5731
1	D	0.11	0/4195	0.29	0/5685
All	All	0.11	0/16866	0.29	0/22843

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	4159	0	4195	27	0
1	B	4162	0	4190	23	0
1	C	4172	0	4201	32	0
1	D	4137	0	4155	23	0
2	A	16	0	24	2	0
2	B	4	0	6	2	0
2	C	12	0	18	4	0
2	D	8	0	12	1	0
3	A	11	0	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	17	3	0
3	C	11	0	17	3	0
3	D	11	0	17	1	0
4	A	28	0	0	0	0
4	B	36	0	0	1	0
4	C	28	0	0	0	0
4	D	25	0	0	0	0
All	All	16831	0	16869	103	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 3.

All (103) 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:105:ILE:HG22	1:A:106:LYS:H	1.46	0.79
1:D:291:HIS:HD2	1:D:292:MET:HE3	1.49	0.76
1:D:11:GLN:O	3:D:603:TAM:N	2.25	0.69
1:D:57:LEU:HB2	1:D:290:MET:HE2	1.76	0.68
1:A:173:ARG:HH21	2:A:603:EDO:H21	1.59	0.68
1:D:333:ARG:NH1	1:D:347:ASN:OD1	2.27	0.67
1:C:333:ARG:NH1	1:C:347:ASN:OD1	2.32	0.62
1:A:333:ARG:NH1	1:A:347:ASN:OD1	2.33	0.62
1:C:13:ALA:O	3:C:604:TAM:H11	2.00	0.62
1:C:53:ARG:O	2:C:603:EDO:O1	2.14	0.60
1:B:57:LEU:HB2	1:B:290:MET:HE3	1.83	0.59
1:B:536:GLY:HA3	2:B:601:EDO:H21	1.85	0.59
1:C:11:GLN:O	3:C:604:TAM:N	2.36	0.58
1:A:33:GLU:OE2	1:A:254:LYS:NZ	2.34	0.58
3:B:602:TAM:N	3:B:602:TAM:O6	2.40	0.55
1:C:209:LEU:HD12	1:C:521:ALA:HB1	1.89	0.55
1:A:140:LEU:HG	1:A:144:MET:HE2	1.90	0.54
1:A:489:ALA:HB3	1:A:527:MET:HG3	1.90	0.54
1:D:412:ALA:O	2:D:601:EDO:O1	2.25	0.54
1:B:18:ILE:HD11	1:B:257:LEU:HG	1.89	0.53
1:C:65:PRO:HD2	1:C:492:GLN:O	2.08	0.53
1:A:105:ILE:HG22	1:A:106:LYS:N	2.21	0.53
1:B:169:ASP:OD2	4:B:701:HOH:O	2.19	0.52
1:A:513:ARG:CZ	1:A:529:GLY:HA2	2.40	0.51
1:B:173:ARG:HH21	2:B:601:EDO:H22	1.75	0.51
1:C:445:THR:OG1	1:C:477:GLU:OE2	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:MET:HE3	1:A:558:PHE:CZ	2.45	0.50
1:A:516:ASN:OD1	1:A:527:MET:HE1	2.12	0.50
1:A:18:ILE:HD11	1:A:257:LEU:HG	1.94	0.49
1:A:255:PRO:HG3	1:A:284:ILE:HG22	1.94	0.49
1:B:13:ALA:O	1:B:15:PRO:HD3	2.13	0.49
1:C:33:GLU:OE2	1:C:254:LYS:NZ	2.41	0.49
1:D:74:THR:HG22	1:D:410:VAL:HG23	1.94	0.49
1:C:427:LYS:O	1:C:431:GLU:HG2	2.12	0.49
1:A:395:ARG:HA	1:A:405:VAL:HG21	1.95	0.48
1:B:527:MET:HE1	1:B:531:ILE:HB	1.93	0.48
1:C:74:THR:HG23	1:C:115:ALA:HB3	1.95	0.48
1:B:445:THR:OG1	1:B:477:GLU:OE2	2.32	0.48
1:B:450:LEU:HD21	1:B:526:VAL:HG21	1.94	0.48
1:C:74:THR:HG22	1:C:410:VAL:HG23	1.96	0.47
1:C:412:ALA:O	2:C:601:EDO:O1	2.32	0.47
1:D:255:PRO:HG3	1:D:284:ILE:HG22	1.96	0.47
1:B:314:ILE:O	1:B:318:LYS:HD3	2.14	0.47
1:C:18:ILE:HD11	1:C:257:LEU:HG	1.95	0.47
3:B:602:TAM:HN1	3:B:602:TAM:H41	1.41	0.46
1:C:372:TYR:O	1:C:436:PHE:HA	2.16	0.46
1:D:292:MET:HA	1:D:292:MET:HE2	1.97	0.46
1:A:426:LEU:O	1:A:430:GLU:HG3	2.16	0.46
1:D:275:ASN:ND2	1:D:531:ILE:HD11	2.32	0.46
1:D:497:ASP:HB3	1:D:528:THR:HG21	1.99	0.45
1:B:11:GLN:O	3:B:602:TAM:H51	2.17	0.45
1:D:275:ASN:OD1	1:D:276:ILE:N	2.45	0.45
1:B:174:GLN:O	1:D:180:ASP:HB2	2.16	0.45
1:B:333:ARG:NH1	1:B:347:ASN:OD1	2.50	0.45
1:C:275:ASN:OD1	1:C:276:ILE:N	2.47	0.45
1:D:74:THR:HG23	1:D:115:ALA:HB3	1.99	0.45
1:C:120:MET:HE2	1:C:558:PHE:CE1	2.52	0.44
1:A:445:THR:OG1	1:A:477:GLU:OE2	2.35	0.44
1:D:209:LEU:HD12	1:D:521:ALA:HB1	1.99	0.44
1:C:62:ALA:HB2	1:C:72:LYS:HG3	1.98	0.44
1:A:373:LYS:HB2	1:A:435:ASN:O	2.18	0.44
1:B:228:ASN:OD1	1:B:232:LYS:N	2.45	0.44
1:B:107:GLY:O	1:B:558:PHE:HD2	2.01	0.43
1:D:72:LYS:HB2	1:D:72:LYS:HE3	1.63	0.43
1:B:33:GLU:OE2	1:B:254:LYS:NZ	2.36	0.43
1:C:56:LYS:HE2	2:C:603:EDO:O2	2.18	0.43
1:C:292:MET:HA	1:C:292:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:ILE:HG21	1:D:91:ILE:HD11	1.99	0.43
3:C:604:TAM:HN1	3:C:604:TAM:H42	1.64	0.43
1:B:253:LEU:HG	1:B:284:ILE:HD12	2.00	0.43
1:C:22:ALA:HB1	1:C:27:LEU:HB2	2.01	0.43
1:A:43:ASP:OD2	2:A:601:EDO:H21	2.18	0.43
1:A:166:ARG:NH1	1:A:193:ASP:OD2	2.51	0.43
1:A:74:THR:HG23	1:A:115:ALA:HB3	2.01	0.43
1:C:531:ILE:HD12	1:C:531:ILE:HA	1.92	0.43
1:A:492:GLN:OE1	1:A:492:GLN:N	2.51	0.42
1:B:395:ARG:HA	1:B:405:VAL:HG21	2.01	0.42
1:C:118:VAL:HG13	1:C:119:PRO:HA	2.00	0.42
1:B:275:ASN:OD1	1:B:276:ILE:N	2.47	0.42
1:C:238:ASP:HA	2:C:602:EDO:H21	2.00	0.42
1:B:250:LYS:HD2	1:D:552:GLY:O	2.20	0.42
1:A:109:ALA:HA	1:A:120:MET:SD	2.60	0.42
1:A:209:LEU:HD12	1:A:521:ALA:HB1	2.01	0.42
1:D:22:ALA:HB1	1:D:27:LEU:HB2	2.02	0.42
1:A:180:ASP:HB2	1:C:174:GLN:O	2.19	0.42
1:B:180:ASP:HB2	1:D:174:GLN:O	2.19	0.41
1:B:209:LEU:HD12	1:B:521:ALA:HB1	2.01	0.41
1:C:374:ILE:HA	1:C:434:ASN:ND2	2.34	0.41
1:C:288:MET:HE3	1:C:288:MET:HB2	1.95	0.41
1:B:318:LYS:HE2	1:B:485:PRO:HG2	2.02	0.41
1:C:514:GLN:HB3	1:C:527:MET:HB2	2.02	0.41
1:A:105:ILE:CG2	1:A:106:LYS:H	2.23	0.41
1:C:373:LYS:O	1:C:434:ASN:ND2	2.54	0.41
1:A:278:HIS:HA	1:A:310:LYS:HD3	2.03	0.41
1:D:61:THR:HA	1:D:72:LYS:HD3	2.02	0.41
1:D:528:THR:O	1:D:528:THR:HG22	2.20	0.41
1:A:174:GLN:O	1:C:180:ASP:HB2	2.20	0.41
1:C:291:HIS:ND1	1:C:292:MET:HE3	2.36	0.41
1:C:255:PRO:HG3	1:C:284:ILE:HG22	2.02	0.40
1:C:305:ASP:OD1	1:C:305:ASP:N	2.52	0.40
1:D:283:ILE:HD13	1:D:319:ALA:HB2	2.03	0.40
1:A:120:MET:HE3	1:A:558:PHE:CE2	2.56	0.40
1:D:305:ASP:OD1	1:D:305:ASP:N	2.53	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	553/562 (98%)	532 (96%)	21 (4%)	0	100	100
1	B	554/562 (99%)	535 (97%)	19 (3%)	0	100	100
1	C	554/562 (99%)	532 (96%)	21 (4%)	1 (0%)	43	37
1	D	553/562 (98%)	531 (96%)	22 (4%)	0	100	100
All	All	2214/2248 (98%)	2130 (96%)	83 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	507	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	434/447 (97%)	432 (100%)	2 (0%)	81	85
1	B	434/447 (97%)	434 (100%)	0	100	100
1	C	436/447 (98%)	432 (99%)	4 (1%)	70	75
1	D	430/447 (96%)	427 (99%)	3 (1%)	76	80
All	All	1734/1788 (97%)	1725 (100%)	9 (0%)	81	85

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	LYS
1	A	118	VAL
1	C	72	LYS
1	C	106	LYS
1	C	427	LYS
1	C	431	GLU
1	D	72	LYS
1	D	105	ILE
1	D	118	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	360	ASN
1	A	435	ASN
1	B	16	GLN
1	B	26	ASN
1	B	64	ASN
1	B	360	ASN
1	B	514	GLN
1	B	516	ASN
1	C	11	GLN
1	C	16	GLN
1	C	514	GLN
1	C	516	ASN
1	D	16	GLN
1	D	516	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

14 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$
3	TAM	D	603	-	10,10,10	0.50	0	12,12,12	1.31	1 (8%)
3	TAM	B	602	-	10,10,10	0.47	0	12,12,12	1.60	3 (25%)
2	EDO	A	603	-	3,3,3	0.43	0	2,2,2	0.35	0
2	EDO	C	603	-	3,3,3	0.39	0	2,2,2	0.48	0
2	EDO	C	602	-	3,3,3	0.42	0	2,2,2	0.34	0
2	EDO	D	602	-	3,3,3	0.43	0	2,2,2	0.35	0
3	TAM	A	605	-	10,10,10	0.52	0	12,12,12	5.39	8 (66%)
2	EDO	A	601	-	3,3,3	0.42	0	2,2,2	0.31	0
2	EDO	B	601	-	3,3,3	0.42	0	2,2,2	0.32	0
2	EDO	C	601	-	3,3,3	0.43	0	2,2,2	0.38	0
3	TAM	C	604	-	10,10,10	0.51	0	12,12,12	1.53	3 (25%)
2	EDO	A	602	-	3,3,3	0.43	0	2,2,2	0.37	0
2	EDO	D	601	-	3,3,3	0.42	0	2,2,2	0.39	0
2	EDO	A	604	-	3,3,3	0.42	0	2,2,2	0.43	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	TAM	D	603	-	-	7/12/12/12	-
3	TAM	B	602	-	-	11/12/12/12	-
2	EDO	A	603	-	-	0/1/1/1	-
2	EDO	C	603	-	-	0/1/1/1	-
2	EDO	C	602	-	-	1/1/1/1	-
2	EDO	D	602	-	-	1/1/1/1	-
3	TAM	A	605	-	-	7/12/12/12	-
2	EDO	A	601	-	-	1/1/1/1	-
2	EDO	B	601	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	C	601	-	-	0/1/1/1	-
3	TAM	C	604	-	-	6/12/12/12	-
2	EDO	A	602	-	-	0/1/1/1	-
2	EDO	D	601	-	-	0/1/1/1	-
2	EDO	A	604	-	-	0/1/1/1	-

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	605	TAM	C1-C-N	-10.21	82.58	108.22
3	A	605	TAM	C2-C-N	-9.19	85.16	108.22
3	A	605	TAM	C3-C-N	-7.30	89.89	108.22
3	A	605	TAM	C2-C-C1	5.73	120.62	110.50
3	A	605	TAM	C3-C-C1	4.95	119.23	110.50
3	A	605	TAM	C3-C-C2	4.58	118.59	110.50
3	A	605	TAM	C4-C1-C	-3.77	111.53	115.97
3	B	602	TAM	C4-C1-C	-3.40	111.96	115.97
3	A	605	TAM	C5-C2-C	-3.35	112.01	115.97
3	D	603	TAM	C5-C2-C	-3.30	112.08	115.97
3	C	604	TAM	C6-C3-C	-3.13	112.28	115.97
3	C	604	TAM	C5-C2-C	-3.03	112.39	115.97
3	B	602	TAM	C6-C3-C	-2.96	112.48	115.97
3	C	604	TAM	C4-C1-C	-2.24	113.33	115.97
3	B	602	TAM	C3-C-C2	2.13	114.27	110.50

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	605	TAM	C3-C-C1-C4
3	A	605	TAM	N-C-C1-C4
3	A	605	TAM	C1-C-C2-C5
3	A	605	TAM	N-C-C2-C5
3	A	605	TAM	C1-C-C3-C6
3	A	605	TAM	N-C-C3-C6
3	A	605	TAM	C-C1-C4-O4
3	B	602	TAM	C2-C-C1-C4
3	B	602	TAM	C3-C-C1-C4
3	B	602	TAM	N-C-C1-C4
3	B	602	TAM	C1-C-C2-C5

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Mol	Chain	Res	Type	Atoms
3	B	602	TAM	C3-C-C2-C5
3	B	602	TAM	N-C-C2-C5
3	B	602	TAM	C1-C-C3-C6
3	B	602	TAM	C2-C-C3-C6
3	B	602	TAM	N-C-C3-C6
3	C	604	TAM	C3-C-C1-C4
3	C	604	TAM	N-C-C1-C4
3	C	604	TAM	C1-C-C2-C5
3	C	604	TAM	C3-C-C2-C5
3	C	604	TAM	N-C-C2-C5
3	D	603	TAM	C2-C-C1-C4
3	D	603	TAM	C3-C-C1-C4
3	D	603	TAM	N-C-C1-C4
3	D	603	TAM	C1-C-C2-C5
3	D	603	TAM	C3-C-C2-C5
3	D	603	TAM	N-C-C2-C5
3	B	602	TAM	C-C3-C6-O6
3	C	604	TAM	C2-C-C1-C4
2	D	602	EDO	O1-C1-C2-O2
3	D	603	TAM	C-C1-C4-O4
3	B	602	TAM	C-C1-C4-O4
2	C	602	EDO	O1-C1-C2-O2
2	A	601	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	603	TAM	1	0
3	B	602	TAM	3	0
2	A	603	EDO	1	0
2	C	603	EDO	2	0
2	C	602	EDO	1	0
2	A	601	EDO	1	0
2	B	601	EDO	2	0
2	C	601	EDO	1	0
3	C	604	TAM	3	0
2	D	601	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	555/562 (98%)	1.63	166 (29%) 1 0	31, 54, 88, 102	0
1	B	556/562 (98%)	1.75	189 (33%) 1 0	32, 52, 81, 96	0
1	C	556/562 (98%)	1.68	189 (33%) 1 0	31, 50, 76, 104	0
1	D	555/562 (98%)	1.52	130 (23%) 2 1	31, 50, 78, 106	0
All	All	2222/2248 (98%)	1.65	674 (30%) 1 0	31, 52, 82, 106	0

All (674) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	68	ALA	8.0
1	D	110	ALA	7.1
1	B	105	ILE	5.8
1	C	529	GLY	5.8
1	D	105	ILE	5.7
1	A	105	ILE	5.5
1	A	430	GLU	5.4
1	D	107	GLY	5.4
1	A	144	MET	5.3
1	C	105	ILE	5.2
1	A	68	ALA	5.2
1	A	394	VAL	5.1
1	C	70	GLU	5.1
1	D	70	GLU	5.0
1	B	394	VAL	5.0
1	B	530	GLU	4.8
1	D	160	LYS	4.8
1	D	530	GLU	4.7
1	B	433	GLU	4.6
1	A	71	GLY	4.5
1	C	530	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	393	LEU	4.5
1	B	558	PHE	4.5
1	B	120	MET	4.4
1	A	432	GLY	4.4
1	B	459	GLY	4.4
1	D	527	MET	4.4
1	B	106	LYS	4.4
1	D	120	MET	4.3
1	C	110	ALA	4.3
1	C	527	MET	4.3
1	C	68	ALA	4.3
1	B	348	ASN	4.3
1	C	66	THR	4.3
1	B	332	VAL	4.3
1	A	443	ASP	4.2
1	B	529	GLY	4.2
1	A	433	GLU	4.2
1	C	343	LYS	4.1
1	B	445	THR	4.1
1	B	107	GLY	4.0
1	C	383	PHE	4.0
1	D	273	PHE	4.0
1	D	508	PHE	4.0
1	A	527	MET	4.0
1	B	346	LEU	4.0
1	D	557	LEU	4.0
1	C	373	LYS	4.0
1	B	351	LEU	4.0
1	A	341	VAL	4.0
1	D	3	PHE	4.0
1	C	284	ILE	4.0
1	A	67	PRO	3.9
1	C	458	TYR	3.9
1	B	108	GLY	3.9
1	A	119	PRO	3.9
1	A	273	PHE	3.9
1	C	487	CYS	3.9
1	B	385	LEU	3.9
1	C	532	MET	3.9
1	C	107	GLY	3.9
1	B	391	LEU	3.9
1	A	7	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	468	GLU	3.8
1	C	435	ASN	3.8
1	B	3	PHE	3.8
1	B	70	GLU	3.8
1	A	292	MET	3.8
1	B	439	CYS	3.8
1	D	68	ALA	3.8
1	B	67	PRO	3.8
1	C	433	GLU	3.8
1	D	106	LYS	3.7
1	C	371	VAL	3.7
1	C	394	VAL	3.7
1	C	3	PHE	3.7
1	A	330	ALA	3.7
1	D	108	GLY	3.7
1	A	110	ALA	3.7
1	D	532	MET	3.7
1	C	171	ASN	3.7
1	D	431	GLU	3.7
1	A	376	ALA	3.7
1	D	170	MET	3.6
1	D	462	GLY	3.6
1	C	28	SER	3.6
1	C	557	LEU	3.6
1	D	439	CYS	3.6
1	C	432	GLY	3.6
1	B	349	GLU	3.6
1	A	284	ILE	3.6
1	C	342	ALA	3.6
1	D	342	ALA	3.6
1	B	465	TYR	3.6
1	C	467	LYS	3.6
1	C	339	GLY	3.6
1	B	443	ASP	3.5
1	B	117	VAL	3.5
1	D	7	ILE	3.5
1	D	66	THR	3.5
1	B	431	GLU	3.5
1	A	332	VAL	3.5
1	A	26	ASN	3.5
1	D	383	PHE	3.5
1	B	450	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	7	ILE	3.5
1	C	531	ILE	3.5
1	C	67	PRO	3.5
1	A	354	LEU	3.5
1	C	106	LYS	3.5
1	A	393	LEU	3.4
1	B	476	LEU	3.4
1	A	439	CYS	3.4
1	D	167	CYS	3.4
1	D	513	ARG	3.4
1	B	452	ALA	3.4
1	D	531	ILE	3.4
1	A	558	PHE	3.4
1	B	527	MET	3.4
1	A	357	GLY	3.4
1	B	510	ILE	3.4
1	B	230	SER	3.3
1	D	354	LEU	3.3
1	A	530	GLU	3.3
1	C	288	MET	3.3
1	A	339	GLY	3.3
1	A	117	VAL	3.3
1	C	486	VAL	3.3
1	C	510	ILE	3.3
1	A	89	ASN	3.3
1	B	339	GLY	3.3
1	A	377	VAL	3.3
1	D	445	THR	3.2
1	C	316	CYS	3.2
1	A	69	GLY	3.2
1	A	25	ILE	3.2
1	B	557	LEU	3.2
1	B	383	PHE	3.2
1	C	445	THR	3.2
1	B	432	GLY	3.2
1	D	433	GLU	3.2
1	A	120	MET	3.2
1	A	342	ALA	3.2
1	B	429	ILE	3.2
1	A	445	THR	3.2
1	C	398	CYS	3.2
1	B	460	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	389	ALA	3.2
1	A	510	ILE	3.2
1	B	125	LEU	3.2
1	D	47	LEU	3.2
1	B	66	THR	3.2
1	B	509	THR	3.2
1	B	474	ALA	3.1
1	A	335	LEU	3.1
1	A	385	LEU	3.1
1	A	391	LEU	3.1
1	A	557	LEU	3.1
1	C	437	GLU	3.1
1	B	119	PRO	3.1
1	D	398	CYS	3.1
1	D	394	VAL	3.1
1	B	440	TYR	3.1
1	B	144	MET	3.1
1	C	120	MET	3.1
1	C	528	THR	3.1
1	D	339	GLY	3.1
1	C	434	ASN	3.1
1	B	280	CYS	3.1
1	D	109	ALA	3.1
1	A	358	LEU	3.1
1	A	428	LEU	3.1
1	B	354	LEU	3.1
1	C	34	LEU	3.1
1	C	47	LEU	3.1
1	D	144	MET	3.1
1	D	36	GLY	3.1
1	D	402	GLY	3.1
1	D	67	PRO	3.1
1	A	489	ALA	3.1
1	C	109	ALA	3.1
1	C	460	ALA	3.1
1	A	4	LYS	3.1
1	C	117	VAL	3.1
1	D	450	LEU	3.1
1	B	531	ILE	3.1
1	B	436	PHE	3.0
1	C	118	VAL	3.0
1	C	354	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	117	VAL	3.0
1	A	503	GLY	3.0
1	C	513	ARG	3.0
1	B	358	LEU	3.0
1	D	393	LEU	3.0
1	B	284	ILE	3.0
1	D	284	ILE	3.0
1	B	503	GLY	3.0
1	A	383	PHE	3.0
1	C	99	MET	3.0
1	C	474	ALA	3.0
1	B	335	LEU	3.0
1	B	401	LEU	3.0
1	C	495	LEU	3.0
1	A	478	GLU	3.0
1	C	48	ASN	3.0
1	B	387	THR	3.0
1	B	227	TYR	3.0
1	B	295	TYR	3.0
1	A	532	MET	3.0
1	B	376	ALA	2.9
1	C	511	GLU	2.9
1	A	167	CYS	2.9
1	A	356	LYS	2.9
1	C	500	THR	2.9
1	C	325	ALA	2.9
1	A	351	LEU	2.9
1	A	429	ILE	2.9
1	C	453	ILE	2.9
1	C	170	MET	2.9
1	C	345	GLN	2.9
1	C	535	PRO	2.9
1	D	292	MET	2.9
1	C	558	PHE	2.9
1	D	458	TYR	2.9
1	B	367	ASN	2.9
1	A	334	ALA	2.9
1	D	330	ALA	2.9
1	B	69	GLY	2.9
1	C	484	LEU	2.9
1	C	431	GLU	2.9
1	A	48	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	89	ASN	2.9
1	C	407	LEU	2.8
1	B	425	VAL	2.8
1	C	439	CYS	2.8
1	D	509	THR	2.8
1	A	15	PRO	2.8
1	C	468	GLU	2.8
1	A	107	GLY	2.8
1	B	532	MET	2.8
1	C	452	ALA	2.8
1	D	432	GLY	2.8
1	C	358	LEU	2.8
1	A	411	TRP	2.8
1	C	186	VAL	2.8
1	C	280	CYS	2.8
1	D	434	ASN	2.8
1	C	207	PHE	2.8
1	C	273	PHE	2.8
1	C	292	MET	2.8
1	C	313	ASP	2.8
1	C	71	GLY	2.8
1	C	61	THR	2.8
1	B	384	PRO	2.8
1	B	411	TRP	2.8
1	B	485	PRO	2.8
1	B	487	CYS	2.8
1	B	434	ASN	2.8
1	B	288	MET	2.8
1	C	534	MET	2.8
1	C	352	GLU	2.8
1	D	35	TYR	2.8
1	A	86	LEU	2.8
1	D	343	LYS	2.8
1	A	365	ILE	2.8
1	B	368	ILE	2.8
1	D	208	CYS	2.8
1	B	14	ASN	2.7
1	D	171	ASN	2.7
1	B	469	ALA	2.7
1	B	455	THR	2.7
1	B	403	VAL	2.7
1	D	487	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	129	GLY	2.7
1	A	507	GLY	2.7
1	B	271	GLY	2.7
1	D	271	GLY	2.7
1	B	508	PHE	2.7
1	C	515	ALA	2.7
1	A	361	LEU	2.7
1	A	509	THR	2.7
1	D	401	LEU	2.7
1	A	70	GLU	2.7
1	B	488	VAL	2.7
1	C	507	GLY	2.7
1	B	345	GLN	2.7
1	C	391	LEU	2.7
1	B	170	MET	2.7
1	B	511	GLU	2.7
1	D	121	GLU	2.7
1	A	405	VAL	2.7
1	B	28	SER	2.7
1	B	25	ILE	2.7
1	B	365	ILE	2.7
1	B	371	VAL	2.7
1	B	453	ILE	2.7
1	D	405	VAL	2.7
1	C	344	ASP	2.7
1	D	344	ASP	2.7
1	A	467	LYS	2.7
1	C	69	GLY	2.7
1	D	231	GLY	2.7
1	A	511	GLU	2.6
1	B	304	ALA	2.6
1	A	170	MET	2.6
1	A	372	TYR	2.6
1	B	524	VAL	2.6
1	C	51	LYS	2.6
1	C	332	VAL	2.6
1	D	21	ILE	2.6
1	D	446	ILE	2.6
1	B	395	ARG	2.6
1	A	417	GLY	2.6
1	B	357	GLY	2.6
1	B	370	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	99	MET	2.6
1	A	389	ALA	2.6
1	A	66	THR	2.6
1	B	528	THR	2.6
1	A	384	PRO	2.6
1	B	407	LEU	2.6
1	B	479	LEU	2.6
1	A	81	ASP	2.6
1	C	443	ASP	2.6
1	B	114	TYR	2.6
1	B	337	TYR	2.6
1	A	378	VAL	2.6
1	B	276	ILE	2.6
1	B	405	VAL	2.6
1	B	526	VAL	2.6
1	C	9	ILE	2.6
1	D	186	VAL	2.6
1	C	167	CYS	2.6
1	D	69	GLY	2.6
1	C	218	GLU	2.6
1	D	534	MET	2.6
1	B	74	THR	2.6
1	D	247	ALA	2.6
1	A	145	LEU	2.6
1	D	346	LEU	2.6
1	B	273	PHE	2.6
1	C	98	SER	2.6
1	C	446	ILE	2.6
1	B	478	GLU	2.6
1	C	271	GLY	2.6
1	D	503	GLY	2.6
1	D	507	GLY	2.6
1	A	99	MET	2.6
1	B	360	ASN	2.6
1	D	119	PRO	2.6
1	B	496	SER	2.6
1	C	351	LEU	2.6
1	C	393	LEU	2.6
1	D	28	SER	2.6
1	A	431	GLU	2.5
1	A	63	ILE	2.5
1	C	321	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	374	ILE	2.5
1	A	459	GLY	2.5
1	B	292	MET	2.5
1	C	131	MET	2.5
1	A	280	CYS	2.5
1	B	167	CYS	2.5
1	A	427	LYS	2.5
1	C	521	ALA	2.5
1	B	390	GLU	2.5
1	C	478	GLU	2.5
1	D	288	MET	2.5
1	A	77	ILE	2.5
1	A	425	VAL	2.5
1	B	336	LYS	2.5
1	B	458	TYR	2.5
1	A	345	GLN	2.5
1	B	115	ALA	2.5
1	D	29	GLU	2.5
1	B	86	LEU	2.5
1	A	9	ILE	2.5
1	B	327	ILE	2.5
1	B	341	VAL	2.5
1	B	374	ILE	2.5
1	D	280	CYS	2.5
1	D	81	ASP	2.5
1	C	509	THR	2.5
1	B	359	PRO	2.5
1	C	485	PRO	2.5
1	C	401	LEU	2.5
1	B	71	GLY	2.5
1	C	108	GLY	2.5
1	A	14	ASN	2.5
1	A	367	ASN	2.5
1	B	350	ASN	2.5
1	A	149	VAL	2.4
1	A	162	ILE	2.5
1	A	531	ILE	2.5
1	B	123	ILE	2.5
1	B	314	ILE	2.5
1	B	419	ILE	2.5
1	C	457	ILE	2.5
1	C	461	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	229	TYR	2.4
1	D	528	THR	2.4
1	A	460	ALA	2.4
1	B	534	MET	2.4
1	D	131	MET	2.4
1	A	479	LEU	2.4
1	A	495	LEU	2.4
1	B	513	ARG	2.4
1	A	271	GLY	2.4
1	B	188	GLY	2.4
1	D	289	GLY	2.4
1	D	481	PHE	2.4
1	C	367	ASN	2.4
1	A	457	ILE	2.4
1	D	218	GLU	2.4
1	C	488	VAL	2.4
1	D	168	VAL	2.4
1	A	159	PRO	2.4
1	A	247	ALA	2.4
1	A	469	ALA	2.4
1	B	389	ALA	2.4
1	C	533	LYS	2.4
1	A	346	LEU	2.4
1	C	481	PHE	2.4
1	C	514	GLN	2.4
1	A	386	ASP	2.4
1	C	162	ILE	2.4
1	C	329	VAL	2.4
1	D	197	ILE	2.4
1	B	99	MET	2.4
1	D	496	SER	2.4
1	B	404	LYS	2.4
1	A	114	TYR	2.4
1	C	205	ALA	2.4
1	C	392	ALA	2.4
1	B	312	LEU	2.4
1	C	385	LEU	2.4
1	D	358	LEU	2.4
1	D	468	GLU	2.4
1	D	478	GLU	2.4
1	C	552	GLY	2.4
1	D	48	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	311	PHE	2.4
1	C	436	PHE	2.4
1	A	545	ARG	2.4
1	B	486	VAL	2.4
1	D	290	MET	2.4
1	D	403	VAL	2.4
1	B	369	THR	2.4
1	D	74	THR	2.4
1	B	438	TYR	2.3
1	B	493	TYR	2.3
1	B	13	ALA	2.3
1	C	334	ALA	2.3
1	C	376	ALA	2.3
1	C	424	GLU	2.3
1	D	442	GLU	2.3
1	A	171	ASN	2.3
1	B	83	LEU	2.3
1	B	428	LEU	2.3
1	C	64	ASN	2.3
1	D	34	LEU	2.3
1	C	536	GLY	2.3
1	A	6	ASP	2.3
1	B	6	ASP	2.3
1	B	386	ASP	2.3
1	A	106	LYS	2.3
1	B	23	LYS	2.3
1	A	21	ILE	2.3
1	B	380	ILE	2.3
1	C	403	VAL	2.3
1	D	341	VAL	2.3
1	A	74	THR	2.3
1	B	121	GLU	2.3
1	C	370	GLN	2.3
1	C	227	TYR	2.3
1	C	372	TYR	2.3
1	A	529	GLY	2.3
1	B	146	ASP	2.3
1	A	72	LYS	2.3
1	C	144	MET	2.3
1	D	37	LYS	2.3
1	C	311	PHE	2.3
1	D	225	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	512	VAL	2.3
1	A	435	ASN	2.3
1	C	459	GLY	2.3
1	D	357	GLY	2.3
1	C	318	LYS	2.3
1	B	98	SER	2.3
1	C	121	GLU	2.3
1	C	230	SER	2.3
1	C	508	PHE	2.3
1	C	523	PHE	2.3
1	D	134	ILE	2.3
1	B	90	VAL	2.3
1	B	377	VAL	2.3
1	B	525	VAL	2.3
1	C	73	THR	2.3
1	C	119	PRO	2.3
1	B	347	ASN	2.3
1	A	398	CYS	2.3
1	C	208	CYS	2.3
1	A	84	ALA	2.3
1	A	461	ASP	2.3
1	C	81	ASP	2.3
1	C	497	ASP	2.3
1	D	10	ALA	2.3
1	D	136	ALA	2.3
1	D	335	LEU	2.3
1	A	18	ILE	2.2
1	A	123	ILE	2.2
1	D	453	ILE	2.2
1	D	546	ILE	2.2
1	A	535	PRO	2.2
1	B	61	THR	2.2
1	B	500	THR	2.2
1	C	60	THR	2.2
1	A	348	ASN	2.2
1	A	344	ASP	2.2
1	A	115	ALA	2.2
1	C	62	ALA	2.2
1	C	290	MET	2.2
1	D	204	MET	2.2
1	A	426	LEU	2.2
1	A	550	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	333	ARG	2.2
1	C	322	ARG	2.2
1	B	101	PRO	2.2
1	B	423	ASN	2.2
1	C	4	LYS	2.2
1	C	5	THR	2.2
1	C	276	ILE	2.2
1	C	464	ASN	2.2
1	C	483	ASN	2.2
1	B	168	VAL	2.2
1	C	46	VAL	2.2
1	C	189	VAL	2.2
1	D	332	VAL	2.2
1	D	535	PRO	2.2
1	B	313	ASP	2.2
1	D	245	MET	2.2
1	A	402	GLY	2.2
1	B	80	ALA	2.2
1	C	477	GLU	2.2
1	B	502	LEU	2.2
1	C	493	TYR	2.2
1	A	419	ILE	2.2
1	C	314	ILE	2.2
1	C	323	PRO	2.2
1	C	512	VAL	2.2
1	A	475	GLU	2.2
1	B	218	GLU	2.2
1	B	352	GLU	2.2
1	B	430	GLU	2.2
1	C	36	GLY	2.2
1	D	529	GLY	2.2
1	A	353	ALA	2.2
1	A	239	LEU	2.2
1	B	59	LEU	2.2
1	B	362	LEU	2.2
1	B	343	LYS	2.2
1	C	397	LYS	2.2
1	C	516	ASN	2.2
1	B	506	THR	2.2
1	B	457	ILE	2.1
1	C	442	GLU	2.1
1	D	111	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	334	ALA	2.1
1	B	353	ALA	2.1
1	D	274	ALA	2.1
1	D	521	ALA	2.1
1	A	407	LEU	2.1
1	A	23	LYS	2.1
1	C	72	LYS	2.1
1	D	185	LYS	2.1
1	A	465	TYR	2.1
1	C	89	ASN	2.1
1	C	465	TYR	2.1
1	D	483	ASN	2.1
1	A	349	GLU	2.1
1	A	390	GLU	2.1
1	D	424	GLU	2.1
1	D	387	THR	2.1
1	A	453	ILE	2.1
1	B	18	ILE	2.1
1	B	446	ILE	2.1
1	C	197	ILE	2.1
1	C	302	PHE	2.1
1	A	186	VAL	2.1
1	B	512	VAL	2.1
1	C	402	GLY	2.1
1	C	480	GLY	2.1
1	D	71	GLY	2.1
1	A	504	ARG	2.1
1	A	10	ALA	2.1
1	B	471	LYS	2.1
1	B	396	SER	2.1
1	C	86	LEU	2.1
1	C	479	LEU	2.1
1	A	399	GLU	2.1
1	A	441	GLU	2.1
1	B	435	ASN	2.1
1	C	475	GLU	2.1
1	D	33	GLU	2.1
1	D	299	GLU	2.1
1	D	347	ASN	2.1
1	A	295	TYR	2.1
1	A	387	THR	2.1
1	B	491	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	387	THR	2.1
1	A	368	ILE	2.1
1	A	482	GLY	2.1
1	B	197	ILE	2.1
1	C	380	ILE	2.1
1	D	157	ILE	2.1
1	D	510	ILE	2.1
1	A	302	PHE	2.1
1	C	168	VAL	2.1
1	D	526	VAL	2.1
1	A	336	LYS	2.1
1	A	82	ALA	2.1
1	B	109	ALA	2.1
1	A	27	LEU	2.1
1	C	408	SER	2.1
1	C	476	LEU	2.1
1	A	121	GLU	2.1
1	A	288	MET	2.1
1	C	33	GLU	2.1
1	C	204	MET	2.1
1	A	360	ASN	2.1
1	C	169	ASP	2.1
1	B	382	ARG	2.1
1	B	263	GLY	2.1
1	A	185	LYS	2.1
1	A	374	ILE	2.1
1	A	46	VAL	2.1
1	B	421	VAL	2.1
1	C	405	VAL	2.1
1	C	524	VAL	2.1
1	C	525	VAL	2.1
1	D	207	PHE	2.1
1	D	486	VAL	2.1
1	A	8	GLU	2.0
1	B	468	GLU	2.0
1	C	29	GLU	2.0
1	C	285	ALA	2.1
1	C	366	GLU	2.0
1	B	306	LEU	2.0
1	B	540	LEU	2.0
1	C	361	LEU	2.0
1	A	180	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	333	ARG	2.0
1	B	504	ARG	2.0
1	A	5	THR	2.0
1	A	198	THR	2.0
1	C	337	TYR	2.0
1	A	199	VAL	2.0
1	A	416	GLU	2.0
1	A	508	PHE	2.0
1	C	199	VAL	2.0
1	B	62	ALA	2.0
1	B	489	ALA	2.0
1	C	319	ALA	2.0
1	D	211	ASN	2.0
1	D	275	ASN	2.0
1	A	312	LEU	2.0
1	B	208	CYS	2.0
1	B	490	LYS	2.0
1	D	159	PRO	2.0
1	A	552	GLY	2.0
1	C	289	GLY	2.0
1	D	552	GLY	2.0
1	A	458	TYR	2.0
1	D	337	TYR	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	604	4/4	0.40	0.25	56,60,61,63	0
3	TAM	B	602	11/11	0.52	0.28	61,70,76,77	0
3	TAM	C	604	11/11	0.59	0.25	57,71,75,81	0
2	EDO	C	603	4/4	0.61	0.21	55,56,59,60	0
2	EDO	A	602	4/4	0.62	0.24	47,51,51,52	0
3	TAM	D	603	11/11	0.62	0.23	69,74,81,81	0
3	TAM	A	605	11/11	0.64	0.19	75,78,82,83	0
2	EDO	D	602	4/4	0.65	0.24	43,57,60,61	0
2	EDO	A	601	4/4	0.67	0.18	50,52,55,57	0
2	EDO	D	601	4/4	0.74	0.22	39,40,50,55	0
2	EDO	C	601	4/4	0.75	0.21	33,38,45,54	0
2	EDO	C	602	4/4	0.77	0.23	33,42,51,53	0
2	EDO	B	601	4/4	0.78	0.21	35,48,52,58	0
2	EDO	A	603	4/4	0.85	0.16	35,47,51,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.