



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:06 PM UTC

PDB ID : 7OP2 / pdb_00007op2
Title : Chadox1/ Chimpanzee adenovirus Y25 fiber knob protein
Authors : Rizkallah, P.J.; Baker, A.T.; Parker, A.L.; Teijeira Crespo, A.; Lipka-Lloyd, M.
Deposited on : 2021-05-28
Resolution : 1.59 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:

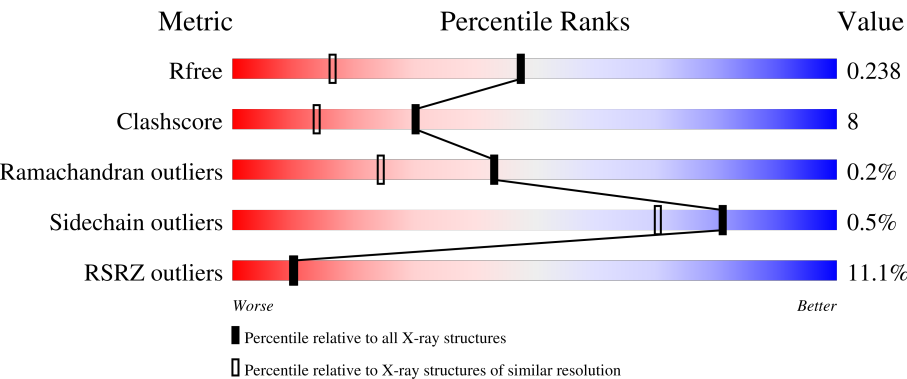
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	187	6% 88% 12%
1	B	187	12% 83% 13% ..
1	C	187	11% 84% 14% ..
1	D	187	8% 86% 13% .
1	E	187	21% 79% 18% ..

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Mol	Chain	Length	Quality of chain
1	F	187	
1	G	187	
1	H	187	
1	I	187	
1	J	187	
1	K	187	
1	L	187	

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	EDO	F	401	-	-	X	-
3	EDO	H	403	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 18792 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 Fiber.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	S	0	5	0
			1487	939	242	296	10			
1	B	181	Total	C	N	O	S	0	5	0
			1427	903	228	285	11			
1	C	184	Total	C	N	O	S	0	4	0
			1448	916	231	290	11			
1	D	187	Total	C	N	O	S	0	3	0
			1470	932	233	293	12			
1	E	187	Total	C	N	O	S	0	6	0
			1493	942	240	299	12			
1	F	187	Total	C	N	O	S	0	3	0
			1468	927	236	294	11			
1	G	187	Total	C	N	O	S	0	6	0
			1488	941	237	298	12			
1	H	181	Total	C	N	O	S	0	4	0
			1423	902	227	282	12			
1	I	187	Total	C	N	O	S	0	2	0
			1457	921	232	293	11			
1	J	187	Total	C	N	O	S	0	2	0
			1460	922	235	293	10			
1	K	182	Total	C	N	O	S	0	6	0
			1452	921	232	289	10			
1	L	179	Total	C	N	O	S	0	4	0
			1409	892	225	281	11			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

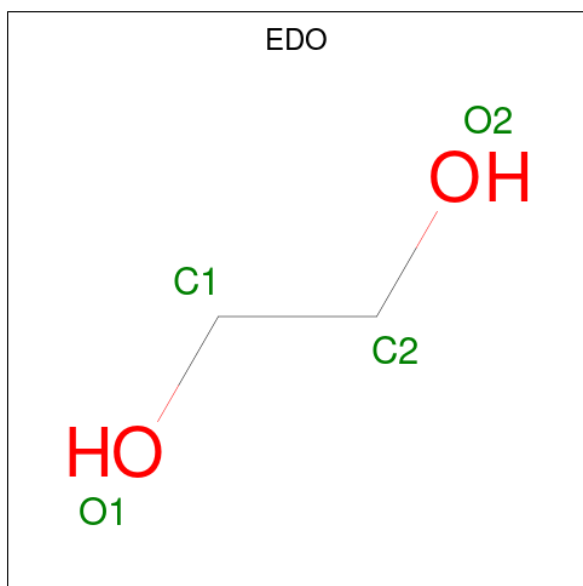
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	D	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



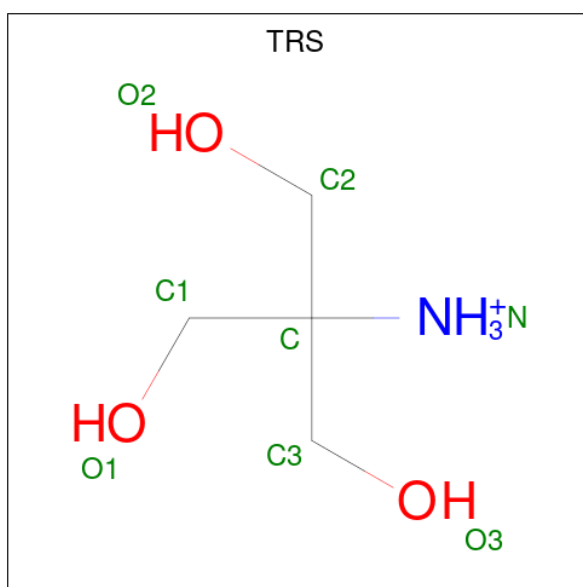
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	J	1	Total	C	O	0	0
			4	2	2		
3	J	1	Total	C	O	0	0
			4	2	2		
3	K	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			8	4	1	3		
4	D	1	Total	C	N	O	0	1
			16	8	2	6		

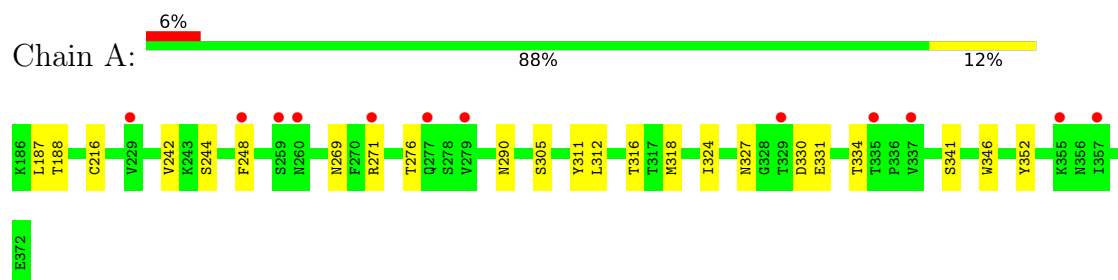
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	116	Total 116	O 116	0	0
5	B	86	Total 86	O 86	0	0
5	C	106	Total 106	O 106	0	0
5	D	115	Total 115	O 115	0	0
5	E	75	Total 75	O 75	0	0
5	F	110	Total 110	O 110	0	0
5	G	109	Total 109	O 109	0	0
5	H	78	Total 78	O 78	0	0
5	I	109	Total 109	O 109	0	0
5	J	108	Total 108	O 108	0	0
5	K	97	Total 97	O 97	0	0
5	L	97	Total 97	O 97	0	0

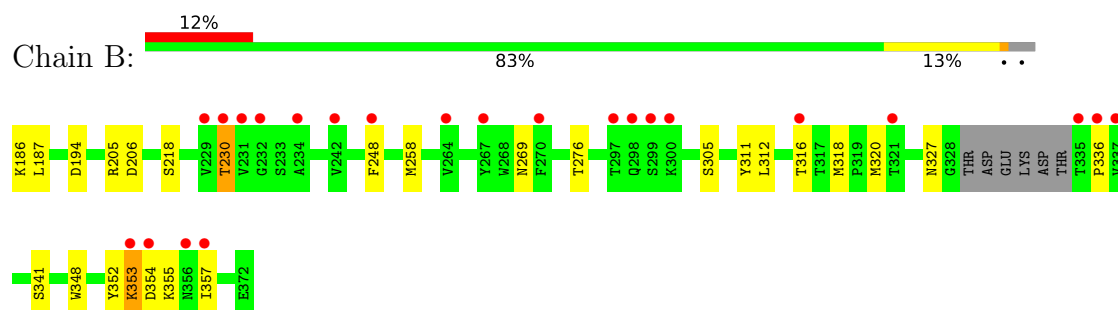
3 Residue-property plots [i](#)

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.

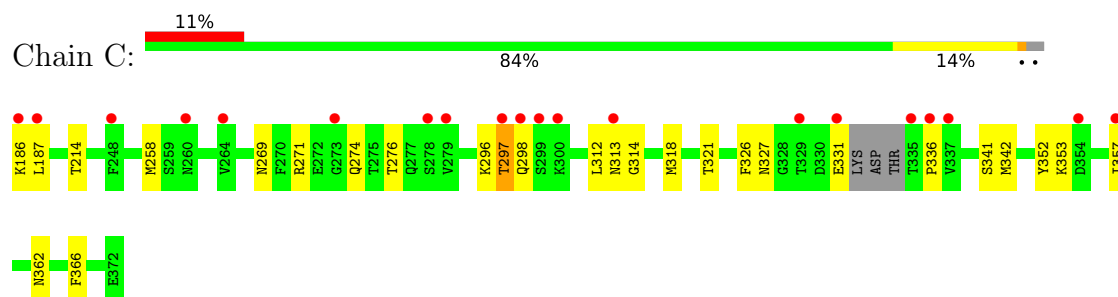
• Molecule 1: Fiber



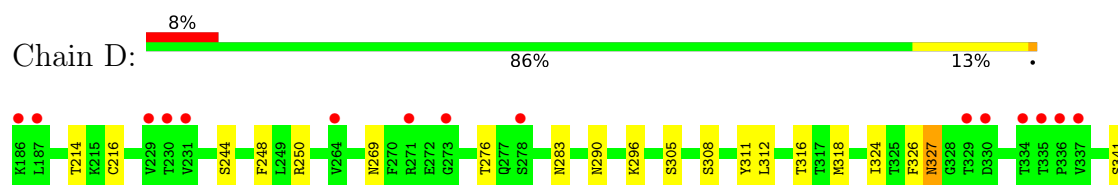
• Molecule 1: Fiber

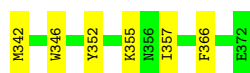


• Molecule 1: Fiber

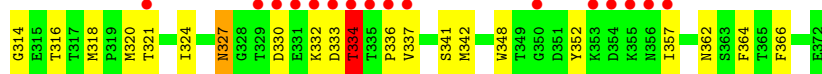
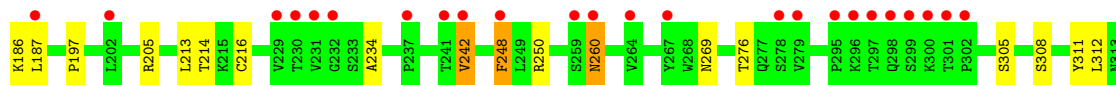
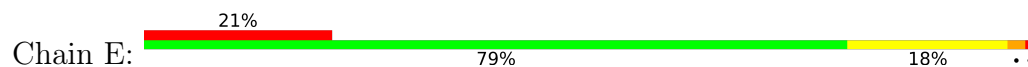


• Molecule 1: Fiber

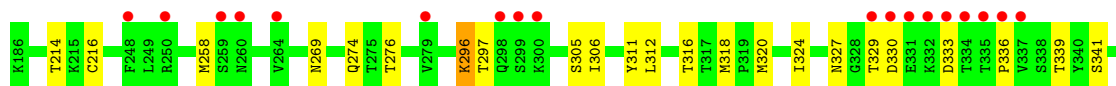
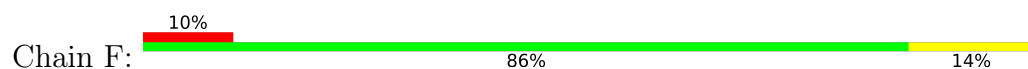




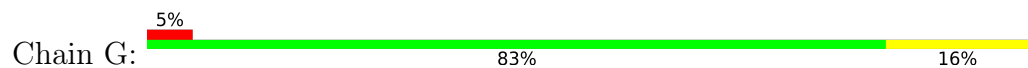
• Molecule 1: Fiber



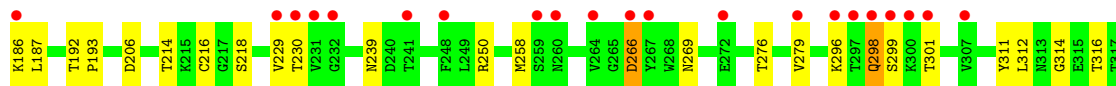
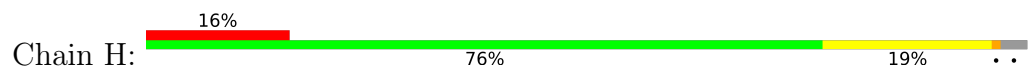
• Molecule 1: Fiber



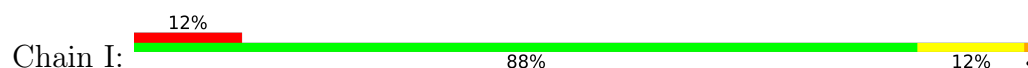
• Molecule 1: Fiber

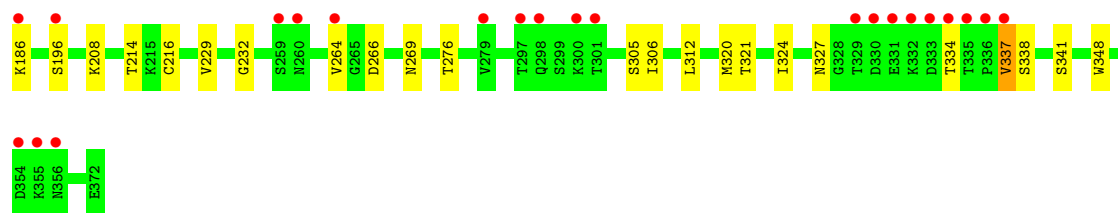


• Molecule 1: Fiber

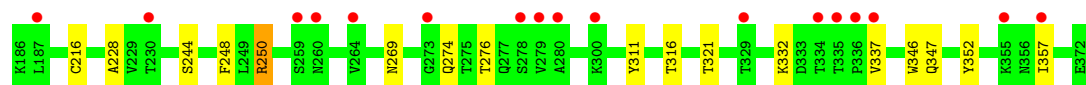
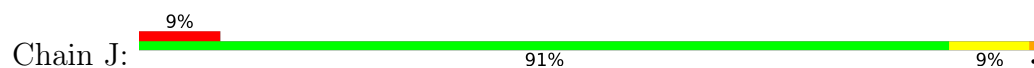


• Molecule 1: Fiber

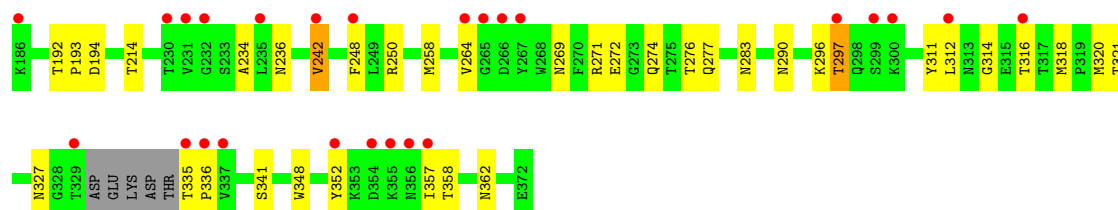
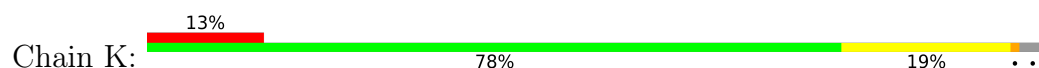




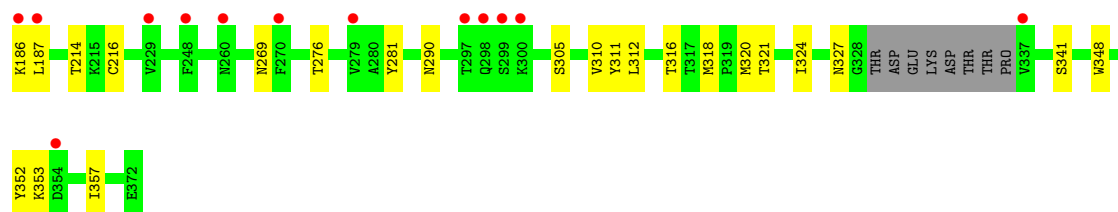
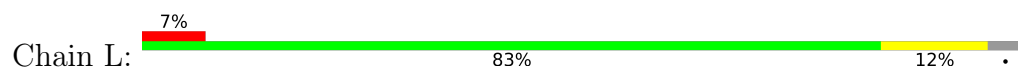
● Molecule 1: Fiber



● Molecule 1: Fiber



● Molecule 1: Fiber



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.43Å 112.26Å 98.61Å 90.00° 92.61° 90.00°	Depositor
Resolution (Å)	74.04 – 1.59 74.04 – 1.59	Depositor EDS
% Data completeness (in resolution range)	99.7 (74.04-1.59) 99.7 (74.04-1.59)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.224 , 0.244 0.219 , 0.238	Depositor DCC
R_{free} test set	14247 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.094 for h,-k,-l 0.000 for l,-k,h	Xtriage
Reported twinning fraction	0.897 for H, K, L 0.103 for -h,-k,l	Depositor
Outliers	8 of 285749 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18792	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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 21.17 % 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 7.4197e-03. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, TRS, CA

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	1.07	1/1520 (0.1%)	1.18	2/2070 (0.1%)
1	B	1.03	3/1459 (0.2%)	1.13	1/1988 (0.1%)
1	C	1.04	0/1480	1.14	0/2015
1	D	1.05	1/1504 (0.1%)	1.14	0/2050
1	E	1.03	1/1526 (0.1%)	1.16	1/2078 (0.0%)
1	F	1.04	0/1501	1.18	0/2045
1	G	1.10	2/1521 (0.1%)	1.17	1/2073 (0.0%)
1	H	1.05	1/1455 (0.1%)	1.18	4/1981 (0.2%)
1	I	1.03	0/1490	1.20	4/2031 (0.2%)
1	J	1.07	1/1493 (0.1%)	1.17	1/2035 (0.0%)
1	K	1.04	0/1485	1.16	1/2024 (0.0%)
1	L	1.02	0/1440	1.13	0/1960
All	All	1.05	10/17874 (0.1%)	1.16	15/24350 (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	E	0	3
1	F	0	1
1	G	0	1
1	I	0	1
All	All	0	6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	353	LYS	C-O	7.22	1.32	1.23
1	G	327	ASN	C-O	6.82	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	305	SER	C-O	5.61	1.31	1.23
1	H	279	VAL	C-O	5.53	1.30	1.24
1	A	187	LEU	C-O	-5.30	1.17	1.23
1	B	230	THR	N-CA	5.11	1.52	1.46
1	D	327	ASN	C-O	5.09	1.30	1.23
1	E	327	ASN	C-O	-5.05	1.17	1.23
1	J	228	ALA	C-O	5.03	1.30	1.23
1	G	260	ASN	C-O	5.01	1.31	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	283	ASN	CA-CB-CG	6.41	119.01	112.60
1	E	248	PHE	CA-CB-CG	6.14	119.94	113.80
1	G	248	PHE	CA-CB-CG	5.71	119.51	113.80
1	I	232	GLY	CA-C-O	-5.60	116.54	121.58
1	H	298	GLN	CB-CG-CD	5.48	121.91	112.60
1	A	248	PHE	CA-CB-CG	5.46	119.26	113.80
1	I	229	VAL	CA-C-O	-5.43	115.52	121.28
1	H	229	VAL	CA-C-O	-5.33	114.11	120.78
1	I	334	THR	CA-C-N	5.32	127.79	120.39
1	I	334	THR	C-N-CA	5.32	127.79	120.39
1	B	248	PHE	CA-CB-CG	5.16	118.96	113.80
1	J	250	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	A	188	THR	CA-CB-OG1	-5.10	101.95	109.60
1	H	266	ASP	CA-CB-CG	5.09	117.69	112.60
1	H	266	ASP	N-CA-C	-5.03	102.84	110.24

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	260	ASN	Mainchain
1	E	334	THR	Peptide
1	E	336	PRO	Peptide
1	F	296	LYS	Mainchain
1	G	355	LYS	Mainchain
1	I	337	VAL	Mainchain

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	1487	0	1449	20	0
1	B	1427	0	1384	29	0
1	C	1448	0	1404	27	0
1	D	1470	0	1426	32	0
1	E	1493	0	1449	42	0
1	F	1468	0	1425	30	0
1	G	1488	0	1449	28	0
1	H	1423	0	1383	34	0
1	I	1457	0	1413	19	0
1	J	1460	0	1417	12	0
1	K	1452	0	1406	29	0
1	L	1409	0	1364	23	0
2	A	1	0	0	0	0
2	D	2	0	0	0	0
2	G	1	0	0	0	0
3	A	4	0	6	0	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
3	E	4	0	6	1	0
3	F	4	0	6	8	0
3	G	16	0	24	4	0
3	H	12	0	17	4	0
3	I	8	0	12	1	0
3	J	8	0	12	0	0
3	K	4	0	6	0	0
3	L	8	0	12	1	0
4	D	24	0	36	4	0
5	A	116	0	0	0	0
5	B	86	0	0	1	0
5	C	106	0	0	1	0
5	D	115	0	0	4	0
5	E	75	0	0	0	0
5	F	110	0	0	0	0
5	G	109	0	0	4	0
5	H	78	0	0	0	0
5	I	109	0	0	2	0
5	J	108	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	97	0	0	3	0
5	L	97	0	0	0	0
All	All	18792	0	17118	293	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 8.

All (293) 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:D:318[A]:MET:HE1	1:D:357:ILE:HD13	1.15	1.14
1:A:271[B]:ARG:NH1	1:B:218[B]:SER:OG	1.85	1.09
1:E:334:THR:HG23	1:E:337:VAL:HA	1.31	1.09
1:A:331:GLU:O	1:A:334:THR:HG22	1.58	1.03
1:D:318[A]:MET:CE	1:D:357:ILE:HD13	1.93	0.98
1:B:312:LEU:HD23	1:B:318:MET:HE2	1.49	0.95
1:L:312:LEU:HD23	1:L:318:MET:HE2	1.48	0.95
1:F:318:MET:HE3	1:F:352:TYR:CD1	2.02	0.94
1:B:318:MET:HE1	1:B:357:ILE:HD13	1.49	0.93
1:F:312:LEU:HD23	1:F:318:MET:HE2	1.51	0.93
1:K:312:LEU:HD23	1:K:318:MET:HE2	1.49	0.93
1:G:312:LEU:HD23	1:G:318[A]:MET:HE2	1.51	0.93
1:H:312:LEU:HD23	1:H:318:MET:HE2	1.50	0.93
1:E:312:LEU:HD23	1:E:318:MET:HE2	1.51	0.92
1:C:312:LEU:HD23	1:C:318:MET:HE2	1.52	0.92
1:D:312:LEU:HD23	1:D:318[A]:MET:HE2	1.52	0.92
1:A:312:LEU:HD23	1:A:318:MET:HE2	1.51	0.90
1:A:271[B]:ARG:CZ	1:B:218[B]:SER:OG	2.19	0.90
1:E:364:PHE:CD2	3:F:401:EDO:H22	2.07	0.90
1:H:312:LEU:HD13	1:H:320[A]:MET:HE1	1.54	0.89
1:G:271:ARG:NH1	1:H:218[B]:SER:OG	2.05	0.89
1:C:318:MET:HE3	1:C:352:TYR:CD1	2.07	0.89
1:J:352:TYR:HB3	1:J:357:ILE:HD12	1.55	0.89
1:A:290:ASN:HD21	1:C:274:GLN:HE22	1.17	0.89
1:E:312:LEU:HD13	1:E:320[A]:MET:HE1	1.55	0.88
1:C:313:ASN:HD21	1:C:357:ILE:HG23	1.40	0.86
1:K:274:GLN:HE22	1:L:290:ASN:HD21	1.24	0.86
1:F:312:LEU:HD13	1:F:320[A]:MET:HE1	1.58	0.86
1:L:312:LEU:HD13	1:L:320[A]:MET:HE1	1.56	0.86
1:G:312:LEU:HD13	1:G:320[A]:MET:HE1	1.58	0.85
1:B:312:LEU:HD13	1:B:320[A]:MET:HE1	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:334:THR:CG2	1:E:337:VAL:HA	2.07	0.84
1:D:290:ASN:HD21	1:F:274:GLN:HE22	1.25	0.84
1:C:313:ASN:ND2	1:C:357:ILE:HG23	1.92	0.83
1:I:186:LYS:N	3:I:401:EDO:HO1	1.76	0.83
1:I:312:LEU:HD13	1:I:320[A]:MET:HE1	1.59	0.83
1:L:318:MET:HE3	1:L:352:TYR:CD1	2.14	0.82
1:K:318:MET:HE3	1:K:352:TYR:CD1	2.14	0.82
1:E:333:ASP:O	1:E:334:THR:CB	2.28	0.80
1:H:318:MET:HE3	1:H:352:TYR:CD1	2.17	0.80
1:E:318:MET:HE3	1:E:352:TYR:CD1	2.17	0.79
1:B:318:MET:HE3	1:B:352:TYR:CD1	2.17	0.78
1:B:318:MET:HE3	1:B:352:TYR:CE1	2.18	0.77
1:J:274:GLN:HE22	1:K:290:ASN:HD21	1.29	0.77
1:K:318:MET:HE3	1:K:352:TYR:CE1	2.22	0.75
1:E:318:MET:HE3	1:E:352:TYR:CE1	2.21	0.74
1:H:318:MET:HE3	1:H:352:TYR:CE1	2.22	0.74
1:A:318:MET:HE3	1:A:352:TYR:CD1	2.22	0.74
1:H:318:MET:HE1	1:H:357:ILE:HD13	1.70	0.74
1:D:318[A]:MET:HE3	1:D:352:TYR:CD1	2.23	0.73
1:D:318[A]:MET:HE3	1:D:352:TYR:CE1	2.23	0.73
1:L:318:MET:HE3	1:L:352:TYR:CE1	2.23	0.73
1:G:318[A]:MET:HE3	1:G:352:TYR:CD1	2.24	0.73
1:J:316:THR:HG21	1:K:321[A]:THR:HG21	1.68	0.73
1:G:318[A]:MET:HE3	1:G:352:TYR:CE1	2.23	0.73
1:C:342[A]:MET:CE	1:C:366:PHE:CE2	2.72	0.72
1:D:326:PHE:HE1	1:D:342[A]:MET:HE3	1.54	0.72
1:A:318:MET:HE3	1:A:352:TYR:CE1	2.25	0.71
1:F:318:MET:HE3	1:F:352:TYR:CE1	2.25	0.70
1:D:316:THR:HG21	1:E:321:THR:HG21	1.73	0.70
1:D:355:LYS:HD3	1:D:357:ILE:HD11	1.74	0.70
1:C:326:PHE:HE1	1:C:342[A]:MET:HE3	1.55	0.69
1:D:342[A]:MET:HE1	1:D:366:PHE:CE2	2.27	0.69
1:E:318:MET:HE1	1:E:357:ILE:HD13	1.75	0.69
1:D:342[A]:MET:CE	1:D:366:PHE:CE2	2.76	0.69
1:E:333:ASP:O	1:E:334:THR:OG1	2.10	0.69
1:H:298:GLN:HB3	1:H:301:THR:CG2	2.22	0.69
1:C:318:MET:HE3	1:C:352:TYR:CE1	2.28	0.69
1:C:342[A]:MET:HE1	1:C:366:PHE:CE2	2.28	0.69
1:K:318:MET:HE1	1:K:357:ILE:HD13	1.76	0.68
1:E:312:LEU:HB2	1:E:320[A]:MET:HE3	1.76	0.68
1:L:312:LEU:HB2	1:L:320[A]:MET:HE3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:320[B]:MET:HG2	1:E:348:TRP:HB3	1.76	0.68
1:G:206:ASP:HB2	1:G:230[A]:THR:CG2	2.24	0.67
1:E:334:THR:HG23	1:E:337:VAL:CA	2.19	0.67
1:F:312:LEU:HB2	1:F:320[A]:MET:HE3	1.76	0.66
1:L:318:MET:HE1	1:L:357:ILE:HD13	1.77	0.66
1:G:312:LEU:HB2	1:G:320[A]:MET:HE3	1.76	0.66
1:I:312:LEU:HB2	1:I:320[A]:MET:HE3	1.78	0.65
1:H:312:LEU:HB2	1:H:320[A]:MET:HE3	1.78	0.65
1:B:312:LEU:HB2	1:B:320[A]:MET:HE3	1.79	0.65
1:B:205:ARG:NH2	1:I:196:SER:OG	2.30	0.64
1:E:334:THR:CG2	1:E:337:VAL:HG13	2.27	0.64
1:G:320[B]:MET:HG2	1:G:348:TRP:HB3	1.80	0.64
1:G:206:ASP:HB2	1:G:230[A]:THR:HG22	1.79	0.63
4:D:404:TRS:H21	1:E:308[A]:SER:OG	1.98	0.63
1:C:342[A]:MET:CE	1:C:366:PHE:HE2	2.12	0.63
1:G:200:GLN:OE1	3:G:405:EDO:H21	1.99	0.62
1:E:311:TYR:CD2	1:E:316:THR:HA	2.34	0.62
3:H:403:EDO:H22	1:I:306:ILE:HG23	1.81	0.62
1:K:335:THR:N	1:K:336:PRO:HA	2.14	0.62
1:E:333:ASP:O	1:E:334:THR:HB	1.98	0.62
1:A:330:ASP:HB3	1:A:334:THR:HG21	1.81	0.62
1:F:258:MET:HE3	1:F:336:PRO:HG2	1.82	0.62
1:H:298:GLN:HB3	1:H:301:THR:HG21	1.81	0.61
1:K:321[A]:THR:HG23	5:K:570:HOH:O	2.00	0.61
1:E:334:THR:HG21	1:E:337:VAL:HG13	1.82	0.61
1:F:306:ILE:CG2	3:F:401:EDO:H12	2.30	0.61
1:I:320[B]:MET:HG2	1:I:348:TRP:HB3	1.81	0.61
1:H:320[B]:MET:HG2	1:H:348:TRP:HB3	1.82	0.60
1:B:320[B]:MET:HG2	1:B:348:TRP:HB3	1.83	0.60
1:D:296:LYS:HE2	5:D:589:HOH:O	2.00	0.60
1:C:318:MET:HE3	1:C:352:TYR:CG	2.37	0.60
1:D:342[A]:MET:HE1	1:D:366:PHE:CZ	2.36	0.59
1:K:320:MET:HG2	1:K:348:TRP:HB3	1.84	0.59
1:G:229[A]:VAL:HG23	5:G:545:HOH:O	2.02	0.59
1:G:269:ASN:HB3	1:G:276:THR:HB	1.85	0.58
1:K:316:THR:HG21	1:L:321:THR:HG21	1.84	0.58
1:J:269:ASN:HB3	1:J:276:THR:HB	1.86	0.58
1:A:269:ASN:HB3	1:A:276:THR:HB	1.85	0.58
1:C:342[A]:MET:HE1	1:C:366:PHE:CZ	2.39	0.58
1:D:308:SER:HB3	4:D:404:TRS:H11	1.86	0.57
1:F:312:LEU:HD23	1:F:318:MET:CE	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:269:ASN:HB3	1:L:276:THR:HB	1.86	0.57
1:A:327:ASN:HD22	1:A:341:SER:H	1.53	0.57
1:L:327:ASN:HD22	1:L:341:SER:H	1.51	0.57
1:A:216:CYS:O	1:C:214:THR:HG21	2.04	0.57
1:H:186:LYS:HG2	1:H:187:LEU:H	1.70	0.57
1:F:318:MET:HE1	1:F:357:ILE:HD13	1.87	0.57
1:I:320[A]:MET:HE2	1:I:348:TRP:CE3	2.40	0.57
1:B:194:ASP:OD2	5:B:401:HOH:O	2.18	0.56
1:C:318:MET:HE1	1:C:357:ILE:HD13	1.87	0.56
1:G:327:ASN:HD22	1:G:341:SER:H	1.53	0.56
1:B:327:ASN:HD22	1:B:341:SER:H	1.52	0.56
1:D:269:ASN:HB3	1:D:276:THR:HB	1.86	0.56
1:D:327:ASN:HD22	1:D:341:SER:H	1.54	0.56
1:K:194[A]:ASP:OD1	5:K:501:HOH:O	2.18	0.56
1:H:250:ARG:NH1	1:H:258:MET:CE	2.69	0.56
1:I:327:ASN:HD22	1:I:341:SER:H	1.53	0.56
1:F:269:ASN:HB3	1:F:276:THR:HB	1.87	0.55
1:H:364:PHE:CE2	3:H:403:EDO:H11	2.42	0.55
1:F:318:MET:HE3	1:F:352:TYR:CG	2.41	0.55
1:F:327:ASN:HD22	1:F:341:SER:H	1.54	0.55
1:K:236:ASN:ND2	1:K:358:THR:OG1	2.40	0.55
1:H:250:ARG:NH1	1:H:258:MET:HE2	2.22	0.55
1:I:337:VAL:HG22	1:I:338:SER:N	2.22	0.55
1:G:312:LEU:HB2	1:G:320[A]:MET:CE	2.37	0.55
1:B:353:LYS:O	1:B:354:ASP:HB2	2.07	0.55
1:E:312:LEU:HD23	1:E:318:MET:CE	2.32	0.55
1:G:196:SER:H	3:G:404:EDO:H21	1.71	0.55
1:I:269:ASN:HB3	1:I:276:THR:HB	1.88	0.55
1:B:318:MET:CE	1:B:357:ILE:HD13	2.27	0.55
1:D:342[A]:MET:CE	1:D:366:PHE:HE2	2.19	0.55
1:C:186:LYS:HG2	1:C:187:LEU:H	1.71	0.55
1:C:269:ASN:HB3	1:C:276:THR:HB	1.87	0.55
1:B:186:LYS:HE2	1:B:187:LEU:H	1.72	0.54
1:E:327:ASN:HD22	1:E:341:SER:H	1.54	0.54
1:A:271[B]:ARG:CD	1:B:218[B]:SER:OG	2.55	0.54
1:J:244:SER:OG	1:J:347:GLN:HG2	2.08	0.54
1:B:269:ASN:HB3	1:B:276:THR:HB	1.88	0.54
1:E:364:PHE:CE2	3:F:401:EDO:H22	2.42	0.54
1:L:312:LEU:HD23	1:L:318:MET:CE	2.32	0.54
1:C:271:ARG:HD3	5:C:561:HOH:O	2.08	0.54
1:C:327:ASN:HD22	1:C:341:SER:H	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:312:LEU:HD23	1:H:318:MET:CE	2.32	0.54
1:H:327:ASN:HD22	1:H:341:SER:H	1.55	0.53
1:C:353:LYS:HE2	1:D:283:ASN:HD22	1.73	0.53
1:K:269:ASN:HB3	1:K:276:THR:HB	1.90	0.53
1:K:312:LEU:HD23	1:K:318:MET:CE	2.31	0.53
1:A:271[B]:ARG:HH11	1:B:218[B]:SER:HG	1.55	0.53
1:C:353:LYS:HE2	1:D:283:ASN:ND2	2.24	0.53
1:A:271[B]:ARG:HD2	1:B:218[B]:SER:OG	2.09	0.53
1:J:321:THR:HG21	1:L:316:THR:HG21	1.91	0.52
1:B:316:THR:HG21	1:C:321:THR:HG21	1.91	0.52
1:E:342[A]:MET:HE2	1:E:366:PHE:CZ	2.45	0.52
1:F:339:THR:HG23	1:J:332:LYS:HB3	1.91	0.52
1:L:312:LEU:HB2	1:L:320[A]:MET:CE	2.39	0.52
1:H:316:THR:HG21	1:I:321:THR:HG21	1.92	0.51
1:B:312:LEU:HB2	1:B:320[A]:MET:CE	2.39	0.51
1:H:269:ASN:HB3	1:H:276:THR:HB	1.92	0.51
1:E:269:ASN:HB3	1:E:276:THR:HB	1.91	0.51
1:H:364:PHE:CD2	3:H:403:EDO:H11	2.46	0.51
1:C:296:LYS:O	1:C:297:THR:OG1	2.20	0.51
1:C:342[A]:MET:HE1	1:C:366:PHE:HE2	1.73	0.51
1:G:318[A]:MET:HE1	1:G:357:ILE:HG13	1.93	0.51
1:E:197:PRO:O	1:E:205[A]:ARG:HD3	2.10	0.51
1:K:327:ASN:HD22	1:K:341:SER:H	1.57	0.51
1:L:281:TYR:HA	3:L:402:EDO:H21	1.93	0.51
1:L:320[A]:MET:HE2	1:L:348:TRP:CE3	2.46	0.51
1:D:296:LYS:CE	5:D:589:HOH:O	2.56	0.50
1:E:248:PHE:CD2	1:E:330:ASP:HB3	2.46	0.50
1:I:312:LEU:HB2	1:I:320[A]:MET:CE	2.41	0.50
1:E:312:LEU:HB2	1:E:320[A]:MET:CE	2.41	0.49
1:F:306:ILE:HG23	3:F:401:EDO:C1	2.42	0.49
1:H:312:LEU:HB2	1:H:320[A]:MET:CE	2.40	0.49
1:C:312:LEU:HD23	1:C:318:MET:CE	2.33	0.49
1:D:318[A]:MET:CE	1:D:357:ILE:CD1	2.81	0.49
1:G:206:ASP:HB2	1:G:230[A]:THR:HG21	1.93	0.49
1:D:342[A]:MET:HE1	1:D:366:PHE:HE2	1.74	0.49
1:C:342[A]:MET:CE	1:C:366:PHE:CZ	2.96	0.48
1:K:274:GLN:NE2	1:L:290:ASN:HD21	2.03	0.48
1:D:214:THR:HG21	1:E:216:CYS:O	2.13	0.48
1:E:213:LEU:HD21	1:E:342[A]:MET:HE1	1.96	0.48
1:E:234:ALA:HB1	1:E:242:VAL:HG12	1.95	0.48
1:A:311:TYR:CD1	1:A:316:THR:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:320[A]:MET:HE2	1:F:348:TRP:CE3	2.49	0.47
1:E:342[A]:MET:CE	1:E:366:PHE:CZ	2.96	0.47
1:K:234:ALA:HB1	1:K:242:VAL:HG12	1.96	0.47
1:G:230[A]:THR:HG22	5:G:566:HOH:O	2.12	0.47
1:K:272:GLU:HB2	1:K:277[A]:GLN:HG2	1.97	0.47
1:L:186:LYS:HG2	1:L:187:LEU:H	1.79	0.47
1:F:297:THR:O	1:F:329:THR:CG2	2.62	0.47
1:G:214:THR:HG21	1:H:216:CYS:O	2.14	0.47
1:G:272:GLU:OE1	5:G:501:HOH:O	2.20	0.47
1:F:297:THR:O	1:F:329:THR:HG21	2.14	0.47
1:H:298:GLN:HB3	1:H:301:THR:HG23	1.96	0.47
1:F:312:LEU:HB2	1:F:320[A]:MET:CE	2.42	0.46
1:J:311:TYR:CD1	1:J:316:THR:HA	2.51	0.46
1:K:271:ARG:NH1	5:K:509:HOH:O	2.47	0.46
1:D:342[A]:MET:CE	1:D:366:PHE:CZ	2.97	0.46
1:K:335:THR:N	1:K:336:PRO:CA	2.77	0.46
1:E:334:THR:HG22	1:E:334:THR:O	2.15	0.46
1:B:312:LEU:HD23	1:B:318:MET:CE	2.32	0.46
1:F:296:LYS:O	1:J:337:VAL:CG2	2.64	0.46
4:D:405[B]:TRS:O3	5:D:501:HOH:O	2.02	0.46
1:J:216:CYS:O	1:L:214:THR:HG21	2.16	0.46
1:F:306:ILE:CG2	3:F:401:EDO:C1	2.94	0.45
1:I:208:LYS:NZ	5:I:504:HOH:O	2.49	0.45
1:K:248[B]:PHE:CD1	1:K:250:ARG:NH1	2.84	0.45
1:D:216:CYS:O	1:F:214:THR:HG21	2.15	0.45
1:G:246:ILE:HD13	5:G:557:HOH:O	2.16	0.45
1:K:296:LYS:O	1:K:297:THR:OG1	2.21	0.45
1:H:311:TYR:CD1	1:H:316:THR:HA	2.51	0.45
1:D:318[B]:MET:SD	1:D:357:ILE:HD13	2.57	0.45
1:I:186:LYS:N	5:I:502:HOH:O	2.50	0.45
1:E:186:LYS:HE2	1:E:187:LEU:H	1.81	0.45
1:D:248[B]:PHE:CD2	1:D:250:ARG:NH1	2.84	0.45
4:D:405[A]:TRS:H22	5:D:501:HOH:O	2.17	0.45
1:G:311:TYR:CD1	1:G:316:THR:HA	2.52	0.44
1:E:318:MET:HE1	1:E:357:ILE:CD1	2.45	0.44
1:E:320[A]:MET:HE2	1:E:348:TRP:CE3	2.53	0.44
1:I:264:VAL:HG12	1:I:266:ASP:OD1	2.17	0.44
1:A:271[B]:ARG:NE	1:B:218[B]:SER:OG	2.48	0.44
1:A:271[B]:ARG:NH1	1:B:218[B]:SER:HG	2.04	0.44
1:H:214:THR:HG21	1:I:216:CYS:O	2.18	0.43
1:K:318:MET:HE1	1:K:357:ILE:CD1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:ARG:NH1	1:E:260:ASN:O	2.51	0.43
1:E:364:PHE:HA	3:F:401:EDO:H11	2.00	0.43
1:J:244:SER:HA	1:J:346:TRP:O	2.19	0.43
3:E:401:EDO:H22	1:F:349:THR:HG23	2.00	0.43
1:K:192:THR:HB	1:K:193:PRO:HD2	2.01	0.43
1:K:311:TYR:CD1	1:K:316:THR:HA	2.52	0.43
1:L:310:VAL:HG23	1:L:320[B]:MET:HE3	2.01	0.43
1:D:290:ASN:HD21	1:F:274:GLN:NE2	2.05	0.43
1:F:306:ILE:HG23	3:F:401:EDO:H11	2.00	0.43
1:K:214:THR:HG21	1:L:216:CYS:O	2.18	0.43
1:K:314:GLY:HA2	1:K:362:ASN:OD1	2.19	0.43
1:B:258:MET:HE3	1:B:336:PRO:HG2	2.00	0.43
1:G:216:CYS:O	1:I:214:THR:HG21	2.19	0.43
1:D:327:ASN:ND2	1:D:341:SER:H	2.17	0.42
1:H:320[A]:MET:HE3	1:H:320[A]:MET:HB2	1.96	0.42
1:C:314:GLY:HA2	1:C:362:ASN:OD1	2.19	0.42
1:D:311:TYR:CD1	1:D:316:THR:HA	2.54	0.42
1:H:206:ASP:HA	1:H:230:THR:HG23	2.01	0.42
1:A:327:ASN:ND2	1:A:341:SER:H	2.17	0.42
1:F:306:ILE:HG21	3:F:401:EDO:H12	2.01	0.42
1:H:342[A]:MET:HE2	1:H:344:PHE:CZ	2.55	0.42
1:J:248:PHE:CE2	1:J:250:ARG:HD3	2.54	0.42
1:F:311:TYR:CD2	1:F:316:THR:HA	2.54	0.42
1:H:296:LYS:HG3	1:H:296:LYS:O	2.20	0.42
1:H:318:MET:CE	1:H:357:ILE:HD13	2.46	0.42
1:B:311:TYR:CD1	1:B:316:THR:HA	2.55	0.42
1:C:258:MET:HE3	1:C:336:PRO:HG2	2.01	0.42
3:H:403:EDO:C2	1:I:306:ILE:HG23	2.49	0.41
1:E:314:GLY:HA2	1:E:362:ASN:OD1	2.21	0.41
1:H:239:ASN:HA	1:H:353:LYS:HD3	2.03	0.41
1:I:305:SER:HA	1:I:324:ILE:O	2.20	0.41
1:E:305:SER:HA	1:E:324:ILE:O	2.20	0.41
1:H:327:ASN:ND2	1:H:341:SER:H	2.18	0.41
1:F:305:SER:HA	1:F:324:ILE:O	2.19	0.41
1:A:305:SER:HA	1:A:324:ILE:O	2.21	0.41
1:G:305:SER:HA	1:G:324:ILE:O	2.21	0.41
1:B:206:ASP:HA	1:B:230:THR:HG23	2.03	0.41
1:E:250:ARG:NH2	1:E:333:ASP:OD2	2.53	0.41
1:F:318:MET:HE1	1:F:357:ILE:CD1	2.51	0.41
1:H:299:SER:HB3	1:H:328:GLY:HA2	2.03	0.41
1:K:258:MET:HE3	1:K:336:PRO:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:305:SER:HA	1:L:324:ILE:O	2.21	0.41
1:D:305:SER:HA	1:D:324:ILE:O	2.21	0.41
1:H:192:THR:HB	1:H:193:PRO:HD2	2.03	0.41
1:H:314:GLY:HA2	1:H:362:ASN:OD1	2.21	0.41
1:L:311:TYR:CD1	1:L:316:THR:HA	2.56	0.41
1:L:327:ASN:ND2	1:L:341:SER:H	2.17	0.41
1:A:244:SER:HA	1:A:346:TRP:O	2.21	0.40
1:E:342[A]:MET:CE	1:E:366:PHE:CE2	3.04	0.40
1:G:195:PRO:HA	3:G:404:EDO:H21	2.03	0.40
1:G:327:ASN:ND2	1:G:341:SER:H	2.17	0.40
1:G:244:SER:HA	1:G:346:TRP:O	2.21	0.40
1:B:352:TYR:HA	1:B:355:LYS:HD2	2.04	0.40
1:B:352:TYR:HB3	1:B:357:ILE:HD12	2.03	0.40
1:E:214:THR:HG21	1:F:216:CYS:O	2.20	0.40
1:D:244:SER:HA	1:D:346:TRP:O	2.20	0.40
1:G:267:TYR:CG	3:G:404:EDO:H12	2.56	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	190/187 (102%)	183 (96%)	7 (4%)	0	100	100
1	B	182/187 (97%)	177 (97%)	5 (3%)	0	100	100
1	C	184/187 (98%)	175 (95%)	8 (4%)	1 (0%)	24	10
1	D	188/187 (100%)	181 (96%)	7 (4%)	0	100	100
1	E	191/187 (102%)	181 (95%)	8 (4%)	2 (1%)	12	3
1	F	188/187 (100%)	181 (96%)	7 (4%)	0	100	100
1	G	191/187 (102%)	185 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	181/187 (97%)	175 (97%)	6 (3%)	0	100	100
1	I	187/187 (100%)	180 (96%)	7 (4%)	0	100	100
1	J	187/187 (100%)	179 (96%)	8 (4%)	0	100	100
1	K	183/187 (98%)	173 (94%)	9 (5%)	1 (0%)	24	10
1	L	179/187 (96%)	173 (97%)	6 (3%)	0	100	100
All	All	2231/2244 (99%)	2143 (96%)	84 (4%)	4 (0%)	43	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	334	THR
1	K	297	THR
1	C	297	THR
1	E	332	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	170/165 (103%)	168 (99%)	2 (1%)	63	43
1	B	164/165 (99%)	164 (100%)	0	100	100
1	C	166/165 (101%)	164 (99%)	2 (1%)	63	43
1	D	168/165 (102%)	168 (100%)	0	100	100
1	E	171/165 (104%)	170 (99%)	1 (1%)	78	66
1	F	168/165 (102%)	166 (99%)	2 (1%)	63	43
1	G	171/165 (104%)	171 (100%)	0	100	100
1	H	163/165 (99%)	162 (99%)	1 (1%)	78	66
1	I	167/165 (101%)	167 (100%)	0	100	100
1	J	167/165 (101%)	167 (100%)	0	100	100
1	K	166/165 (101%)	164 (99%)	2 (1%)	63	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	161/165 (98%)	160 (99%)	1 (1%)	78	66
All	All	2002/1980 (101%)	1991 (100%)	11 (0%)	81	70

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242[A]	VAL
1	A	242[B]	VAL
1	C	298	GLN
1	C	331	GLU
1	E	242	VAL
1	F	330	ASP
1	F	333	ASP
1	H	266	ASP
1	K	242	VAL
1	K	264	VAL
1	L	353	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	ASN
1	A	327	ASN
1	A	356	ASN
1	B	219	GLN
1	B	304	ASN
1	B	327	ASN
1	B	356	ASN
1	C	274	GLN
1	C	304	ASN
1	C	313	ASN
1	C	327	ASN
1	C	356	ASN
1	D	304	ASN
1	D	309	GLN
1	D	327	ASN
1	D	356	ASN
1	E	304	ASN
1	E	309	GLN
1	E	313	ASN
1	E	327	ASN

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Mol	Chain	Res	Type
1	E	356	ASN
1	F	274	GLN
1	F	277	GLN
1	F	304	ASN
1	F	309	GLN
1	F	313	ASN
1	F	327	ASN
1	F	356	ASN
1	G	304	ASN
1	G	309	GLN
1	G	327	ASN
1	G	356	ASN
1	H	219	GLN
1	H	304	ASN
1	H	309	GLN
1	H	313	ASN
1	H	327	ASN
1	H	356	ASN
1	I	304	ASN
1	I	309	GLN
1	I	313	ASN
1	I	327	ASN
1	I	356	ASN
1	J	219	GLN
1	J	260	ASN
1	J	274	GLN
1	J	304	ASN
1	J	309	GLN
1	J	356	ASN
1	K	219	GLN
1	K	236	ASN
1	K	274	GLN
1	K	298	GLN
1	K	304	ASN
1	K	313	ASN
1	K	327	ASN
1	L	277	GLN
1	L	298	GLN
1	L	304	ASN
1	L	313	ASN
1	L	327	ASN
1	L	356	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 ⓘ

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	H	401	-	3,3,3	0.29	0	2,2,2	0.04	0
3	EDO	G	405	-	3,3,3	0.04	0	2,2,2	0.36	0
4	TRS	D	405[A]	-	7,7,7	0.35	0	9,9,9	0.44	0
3	EDO	A	402	-	3,3,3	0.23	0	2,2,2	0.14	0
3	EDO	G	403	-	3,3,3	0.26	0	2,2,2	0.19	0
3	EDO	F	401	-	3,3,3	0.81	0	2,2,2	0.25	0
3	EDO	J	402	-	3,3,3	0.41	0	2,2,2	0.31	0
3	EDO	L	401	-	3,3,3	0.29	0	2,2,2	0.22	0
3	EDO	L	402	-	3,3,3	0.28	0	2,2,2	0.11	0
3	EDO	G	402	-	3,3,3	0.23	0	2,2,2	0.31	0
3	EDO	G	404	-	3,3,3	0.36	0	2,2,2	0.35	0
4	TRS	D	405[B]	-	7,7,7	0.32	0	9,9,9	0.33	0
3	EDO	H	403	-	3,3,3	0.71	0	2,2,2	0.23	0
3	EDO	D	403	-	3,3,3	0.24	0	2,2,2	0.30	0
3	EDO	K	401	-	3,3,3	0.41	0	2,2,2	0.20	0
3	EDO	J	401	-	3,3,3	0.25	0	2,2,2	0.29	0
4	TRS	D	404	-	7,7,7	0.24	0	9,9,9	0.48	0
3	EDO	H	402	-	3,3,3	0.20	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	I	401	-	3,3,3	0.06	0	2,2,2	0.12	0
3	EDO	I	402	-	3,3,3	0.05	0	2,2,2	0.05	0
3	EDO	E	401	-	3,3,3	0.02	0	2,2,2	0.14	0
3	EDO	C	401	-	3,3,3	0.44	0	2,2,2	0.26	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	EDO	H	401	-	-	0/1/1/1	-
3	EDO	G	405	-	-	1/1/1/1	-
4	TRS	D	405[A]	-	-	6/9/9/9	-
3	EDO	A	402	-	-	0/1/1/1	-
3	EDO	G	403	-	-	0/1/1/1	-
3	EDO	F	401	-	-	0/1/1/1	-
3	EDO	J	402	-	-	0/1/1/1	-
3	EDO	L	401	-	-	0/1/1/1	-
3	EDO	L	402	-	-	1/1/1/1	-
3	EDO	G	402	-	-	0/1/1/1	-
3	EDO	G	404	-	-	1/1/1/1	-
4	TRS	D	405[B]	-	-	3/9/9/9	-
3	EDO	H	403	-	-	1/1/1/1	-
3	EDO	D	403	-	-	0/1/1/1	-
3	EDO	K	401	-	-	0/1/1/1	-
3	EDO	J	401	-	-	0/1/1/1	-
4	TRS	D	404	-	-	6/9/9/9	-
3	EDO	H	402	-	-	1/1/1/1	-
3	EDO	I	401	-	-	0/1/1/1	-
3	EDO	I	402	-	-	1/1/1/1	-
3	EDO	E	401	-	-	1/1/1/1	-
3	EDO	C	401	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	404	TRS	C1-C-C2-O2
4	D	404	TRS	C3-C-C2-O2
4	D	404	TRS	N-C-C2-O2
4	D	405[A]	TRS	C2-C-C1-O1
4	D	405[A]	TRS	C1-C-C2-O2
4	D	405[A]	TRS	N-C-C2-O2
4	D	405[B]	TRS	N-C-C3-O3
4	D	405[A]	TRS	C3-C-C1-O1
4	D	405[B]	TRS	C1-C-C3-O3
3	G	404	EDO	O1-C1-C2-O2
3	I	402	EDO	O1-C1-C2-O2
4	D	404	TRS	N-C-C3-O3
4	D	405[A]	TRS	C3-C-C2-O2
4	D	404	TRS	C1-C-C3-O3
4	D	404	TRS	C2-C-C3-O3
3	G	405	EDO	O1-C1-C2-O2
3	H	403	EDO	O1-C1-C2-O2
3	L	402	EDO	O1-C1-C2-O2
4	D	405[A]	TRS	N-C-C1-O1
4	D	405[B]	TRS	C2-C-C3-O3
3	E	401	EDO	O1-C1-C2-O2
3	H	402	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	405	EDO	1	0
4	D	405[A]	TRS	1	0
3	F	401	EDO	8	0
3	L	402	EDO	1	0
3	G	404	EDO	3	0
4	D	405[B]	TRS	1	0
3	H	403	EDO	4	0
4	D	404	TRS	2	0
3	I	401	EDO	1	0
3	E	401	EDO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	187/187 (100%)	0.55	12 (6%)	25 26	10, 22, 36, 48	5 (2%)
1	B	181/187 (96%)	1.07	23 (12%)	8 7	10, 27, 50, 84	5 (2%)
1	C	184/187 (98%)	0.79	20 (10%)	10 10	10, 25, 48, 78	4 (2%)
1	D	187/187 (100%)	0.57	15 (8%)	18 18	8, 22, 38, 55	3 (1%)
1	E	187/187 (100%)	1.24	40 (21%)	2 2	10, 28, 61, 91	6 (3%)
1	F	187/187 (100%)	0.62	19 (10%)	12 12	10, 22, 47, 85	3 (1%)
1	G	187/187 (100%)	0.39	9 (4%)	35 37	9, 20, 36, 44	6 (3%)
1	H	181/187 (96%)	1.16	30 (16%)	4 4	11, 28, 52, 82	4 (2%)
1	I	187/187 (100%)	0.71	22 (11%)	9 9	9, 23, 47, 69	2 (1%)
1	J	187/187 (100%)	0.64	17 (9%)	15 15	9, 23, 41, 59	2 (1%)
1	K	182/187 (97%)	0.94	25 (13%)	6 6	10, 24, 44, 69	6 (3%)
1	L	179/187 (95%)	0.63	13 (7%)	21 21	12, 24, 41, 58	4 (2%)
All	All	2216/2244 (98%)	0.78	245 (11%)	10 10	8, 24, 46, 91	50 (2%)

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	335	THR	6.9
1	J	336	PRO	6.7
1	K	267	TYR	6.5
1	I	336	PRO	6.4
1	B	232	GLY	6.3
1	J	337	VAL	6.3
1	F	335	THR	6.0
1	E	335	THR	5.8
1	H	336	PRO	5.8
1	E	334	THR	5.8
1	K	264	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
1	E	332	LYS	5.7
1	E	330	ASP	5.6
1	K	232	GLY	5.5
1	K	231	VAL	5.4
1	E	297	THR	5.3
1	K	335	THR	5.2
1	B	231	VAL	5.2
1	C	297	THR	5.2
1	H	231	VAL	5.2
1	B	335	THR	5.2
1	K	336	PRO	5.0
1	H	267	TYR	5.0
1	J	259	SER	5.0
1	B	336	PRO	5.0
1	H	297	THR	4.9
1	H	337	VAL	4.9
1	E	300[A]	LYS	4.9
1	E	230	THR	4.9
1	B	337	VAL	4.8
1	E	231	VAL	4.8
1	B	297	THR	4.8
1	E	333	ASP	4.8
1	C	335	THR	4.7
1	H	248	PHE	4.6
1	K	329	THR	4.5
1	A	259	SER	4.5
1	E	248	PHE	4.5
1	I	332	LYS	4.5
1	E	357	ILE	4.4
1	E	264	VAL	4.4
1	B	230	THR	4.3
1	A	335	THR	4.3
1	F	333	ASP	4.3
1	A	248	PHE	4.3
1	G	328	GLY	4.2
1	F	334	THR	4.2
1	K	248[A]	PHE	4.2
1	L	300	LYS	4.2
1	J	335	THR	4.2
1	H	264	VAL	4.2
1	K	297	THR	4.1
1	I	335	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	L	299	SER	4.1
1	I	334	THR	4.0
1	E	337	VAL	4.0
1	K	266	ASP	4.0
1	B	267	TYR	3.9
1	K	354	ASP	3.9
1	D	187	LEU	3.9
1	L	186	LYS	3.9
1	H	259	SER	3.9
1	C	336	PRO	3.9
1	E	232	GLY	3.9
1	F	337	VAL	3.9
1	I	337	VAL	3.9
1	K	337	VAL	3.8
1	H	186	LYS	3.8
1	K	355	LYS	3.8
1	E	336	PRO	3.8
1	C	298	GLN	3.8
1	F	336	PRO	3.8
1	E	267	TYR	3.8
1	H	230	THR	3.8
1	B	242	VAL	3.7
1	F	332	LYS	3.7
1	C	354	ASP	3.7
1	F	300	LYS	3.7
1	B	248	PHE	3.7
1	B	299	SER	3.7
1	J	279	VAL	3.7
1	B	357	ILE	3.6
1	H	232	GLY	3.6
1	K	230	THR	3.6
1	E	299	SER	3.6
1	K	186[A]	LYS	3.6
1	E	229	VAL	3.6
1	E	242	VAL	3.6
1	G	264	VAL	3.6
1	D	186	LYS	3.6
1	D	335	THR	3.5
1	D	230	THR	3.5
1	E	329	THR	3.5
1	F	260	ASN	3.5
1	E	260	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	K	357	ILE	3.5
1	C	299	SER	3.4
1	G	187	LEU	3.4
1	H	260	ASN	3.4
1	J	260	ASN	3.4
1	I	298	GLN	3.4
1	C	279	VAL	3.3
1	K	242	VAL	3.3
1	J	334	THR	3.3
1	C	300	LYS	3.3
1	K	356	ASN	3.3
1	G	186	LYS	3.3
1	G	329	THR	3.3
1	E	321	THR	3.2
1	H	354	ASP	3.2
1	H	298	GLN	3.2
1	E	331	GLU	3.1
1	B	298	GLN	3.1
1	I	354	ASP	3.1
1	G	334	THR	3.0
1	B	300	LYS	3.0
1	I	300	LYS	3.0
1	A	337	VAL	3.0
1	E	356	ASN	3.0
1	E	353	LYS	3.0
1	C	260	ASN	2.9
1	C	337	VAL	2.9
1	H	299	SER	2.9
1	L	337	VAL	2.9
1	I	329	THR	2.9
1	C	357	ILE	2.9
1	D	334	THR	2.9
1	H	301	THR	2.9
1	H	356	ASN	2.9
1	C	248	PHE	2.9
1	H	229	VAL	2.9
1	E	350	GLY	2.9
1	B	234	ALA	2.8
1	D	330	ASP	2.8
1	E	298	GLN	2.8
1	E	354	ASP	2.8
1	J	357	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	336	PRO	2.8
1	J	329	THR	2.7
1	F	331	GLU	2.7
1	E	355	LYS	2.7
1	F	259[A]	SER	2.7
1	J	264	VAL	2.7
1	A	260	ASN	2.7
1	C	329	THR	2.7
1	J	278	SER	2.7
1	A	271[A]	ARG	2.7
1	H	352	TYR	2.6
1	L	297	THR	2.6
1	H	355	LYS	2.6
1	F	299	SER	2.6
1	A	279	VAL	2.6
1	H	300	LYS	2.6
1	E	295	PRO	2.6
1	D	231	VAL	2.6
1	L	279	VAL	2.6
1	L	354[A]	ASP	2.6
1	H	357	ILE	2.5
1	K	352	TYR	2.5
1	F	329	THR	2.5
1	L	187	LEU	2.5
1	D	264	VAL	2.5
1	D	337	VAL	2.5
1	I	301	THR	2.5
1	E	302	PRO	2.5
1	L	248	PHE	2.5
1	B	229	VAL	2.5
1	I	279	VAL	2.5
1	I	297	THR	2.5
1	K	300	LYS	2.4
1	L	260	ASN	2.4
1	A	329	THR	2.4
1	H	338	SER	2.4
1	B	316	THR	2.4
1	J	230	THR	2.4
1	B	354	ASP	2.4
1	G	335	THR	2.4
1	K	312	LEU	2.4
1	E	259	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	265	GLY	2.4
1	H	272	GLU	2.4
1	F	298	GLN	2.3
1	C	186	LYS	2.3
1	F	330	ASP	2.3
1	L	270	PHE	2.3
1	L	298	GLN	2.3
1	D	271	ARG	2.3
1	F	264	VAL	2.3
1	I	356	ASN	2.3
1	G	248	PHE	2.3
1	I	260	ASN	2.3
1	F	279	VAL	2.3
1	D	329	THR	2.3
1	E	301	THR	2.3
1	H	266	ASP	2.3
1	K	316	THR	2.3
1	J	300	LYS	2.3
1	C	187	LEU	2.3
1	B	270	PHE	2.2
1	E	241	THR	2.2
1	G	279	VAL	2.2
1	E	202	LEU	2.2
1	I	333	ASP	2.2
1	J	280	ALA	2.2
1	F	248	PHE	2.2
1	K	299	SER	2.2
1	B	264	VAL	2.2
1	B	356	ASN	2.2
1	K	235	LEU	2.2
1	E	237	PRO	2.2
1	D	273	GLY	2.2
1	E	278	SER	2.2
1	A	277	GLN	2.2
1	E	279	VAL	2.2
1	H	279	VAL	2.2
1	I	331	GLU	2.2
1	E	296	LYS	2.2
1	A	357	ILE	2.1
1	C	278	SER	2.1
1	F	250	ARG	2.1
1	I	196	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	355	LYS	2.1
1	A	229	VAL	2.1
1	D	278	SER	2.1
1	B	321	THR	2.1
1	H	296	LYS	2.1
1	J	355	LYS	2.1
1	I	259	SER	2.1
1	D	229	VAL	2.1
1	L	229	VAL	2.1
1	H	241	THR	2.1
1	E	187	LEU	2.1
1	J	187	LEU	2.1
1	I	355	LYS	2.1
1	F	357	ILE	2.1
1	C	273	GLY	2.1
1	J	273	GLY	2.1
1	I	186	LYS	2.0
1	C	264	VAL	2.0
1	H	307	VAL	2.0
1	I	330	ASP	2.0
1	B	353	LYS	2.0
1	C	331	GLU	2.0
1	I	264	VAL	2.0
1	C	313	ASN	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
4	TRS	D	404	8/8	0.65	0.23	39,47,49,55	0
3	EDO	G	405	4/4	0.73	0.17	38,38,39,40	0
3	EDO	L	402	4/4	0.74	0.16	30,35,35,40	0
3	EDO	G	404	4/4	0.76	0.18	35,39,40,43	0
3	EDO	I	402	4/4	0.79	0.16	40,45,47,54	0
3	EDO	E	401	4/4	0.82	0.17	47,47,49,49	0
4	TRS	D	405[A]	8/8	0.83	0.13	15,19,22,22	8
4	TRS	D	405[B]	8/8	0.83	0.13	20,21,22,24	8
3	EDO	I	401	4/4	0.84	0.14	40,42,43,44	0
3	EDO	K	401	4/4	0.87	0.14	18,20,21,22	0
3	EDO	H	402	4/4	0.88	0.13	29,30,31,32	0
3	EDO	H	401	4/4	0.88	0.13	20,21,22,23	0
3	EDO	H	403	4/4	0.90	0.12	18,22,23,23	0
3	EDO	J	402	4/4	0.91	0.10	19,21,22,23	0
3	EDO	G	402	4/4	0.91	0.10	20,24,25,26	0
3	EDO	F	401	4/4	0.92	0.12	19,20,20,20	0
3	EDO	A	402	4/4	0.94	0.09	23,25,27,27	0
3	EDO	C	401	4/4	0.94	0.08	17,19,20,20	0
3	EDO	L	401	4/4	0.95	0.09	20,21,23,24	0
3	EDO	D	403	4/4	0.96	0.07	17,21,21,22	0
3	EDO	J	401	4/4	0.96	0.07	19,24,25,26	0
3	EDO	G	403	4/4	0.96	0.07	20,22,22,24	0
2	CA	G	401	1/1	0.97	0.11	32,32,32,32	0
2	CA	D	402	1/1	0.98	0.04	28,28,28,28	0
2	CA	D	401	1/1	0.98	0.04	24,24,24,24	0
2	CA	A	401	1/1	0.99	0.05	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.