



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:20 PM GMT

PDB ID : 3QVI
Title : Crystal structure of KNI-10395 bound histo-aspartic protease (HAP) from Plasmodium falciparum
Authors : Bhaumik, P.; Gustchina, A.; Wlodawer, A.
Deposited on : 2011-02-25
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

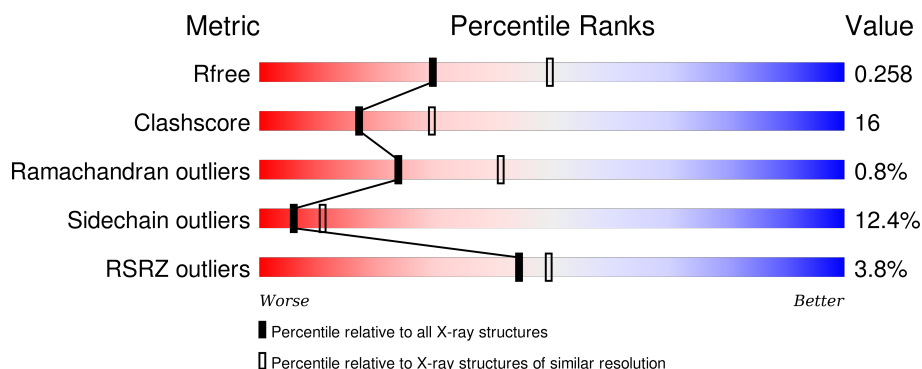
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	451	 8% 47% 19% 5% 28%
1	B	451	 2% 48% 22% • 27%
1	C	451	 2% 48% 22% • 27%
1	D	451	 1% 47% 20% • 27%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	K95	C	330	-	-	-	X
3	EDO	A	331	-	-	X	X
3	EDO	B	329	-	-	X	X
3	EDO	C	331	-	-	X	X
3	EDO	C	333	-	-	-	X
3	EDO	C	334	-	-	-	X
3	EDO	D	330	-	-	X	X
3	EDO	D	332	-	-	X	X
3	EDO	D	333	-	-	-	X
4	PG4	A	333	-	-	-	X
4	PG4	A	334	-	-	-	X
4	PG4	A	335	-	-	-	X
4	PG4	D	334	-	-	-	X
6	PG5	B	330	-	-	X	X

2 Entry composition [i](#)

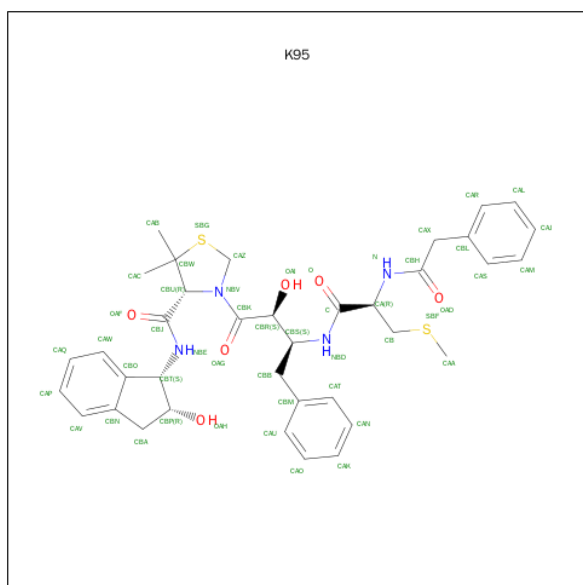
There are 8 unique types of molecules in this entry. The entry contains 11285 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Histo-aspartic protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	7	0
			2599	1683	400	508	8			
1	B	327	Total	C	N	O	S	0	6	0
			2638	1711	408	511	8			
1	C	327	Total	C	N	O	S	0	4	0
			2630	1704	407	511	8			
1	D	327	Total	C	N	O	S	0	9	0
			2655	1726	410	511	8			

- Molecule 2 is (4R)-N-[(1S,2R)-2-HYDROXY-2,3-DIHYDRO-1H-INDEN-1-YL]-3-[(2S,3S)-2-HYDROXY-3-[[S-METHYL-N-(PHENYLACETYL)-L-CYSTEINYL]AMINO]-4-PHENYLBUTANOYL]-5,5-DIMETHYL-1,3-THIAZOLIDINE-4-CARBOXAMIDE (three-letter code: K95) (formula: C₃₇H₄₄N₄O₆S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			49	37	4	6	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			49	37	4	6	2		
2	C	1	Total	C	N	O	S	0	0
			49	37	4	6	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



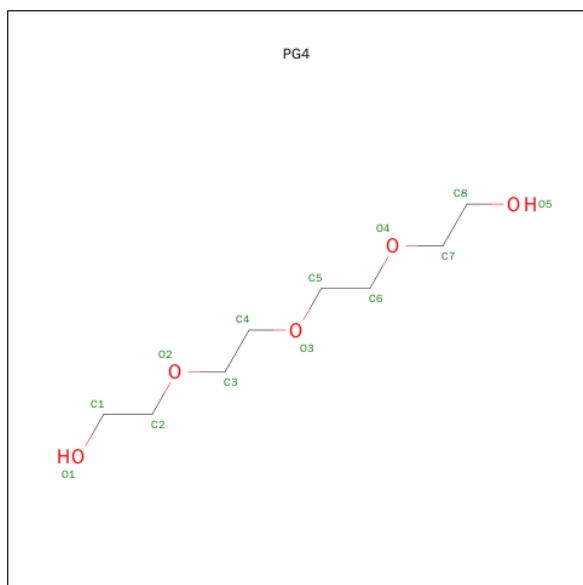
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

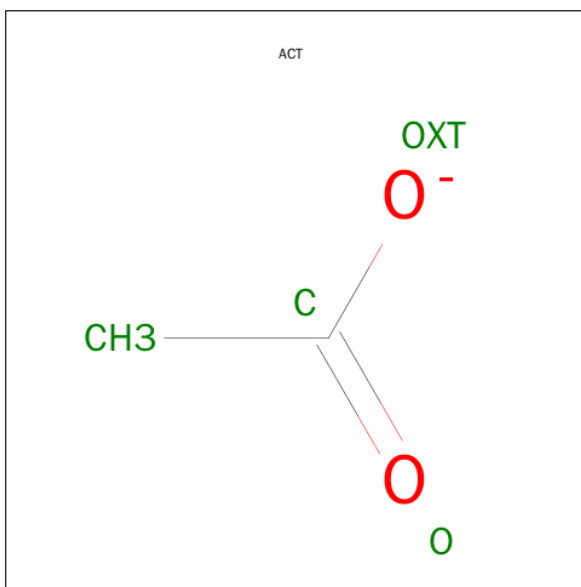
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



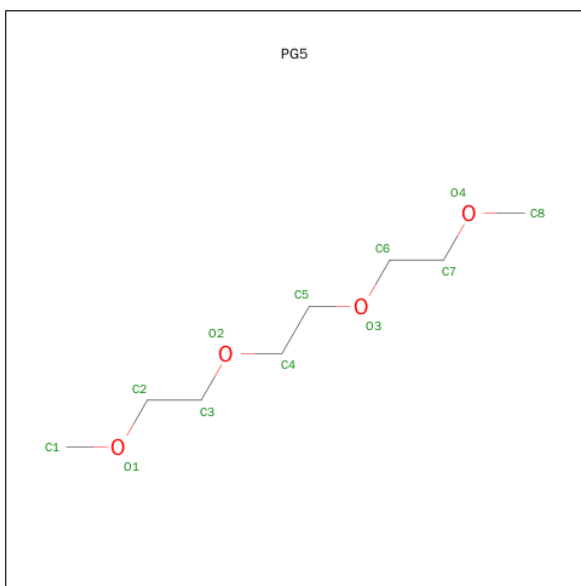
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY)]-ETHANE (three-letter code: PG5) (formula: C₈H₁₈O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			12	8	4		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total 1	Na 1	0	0

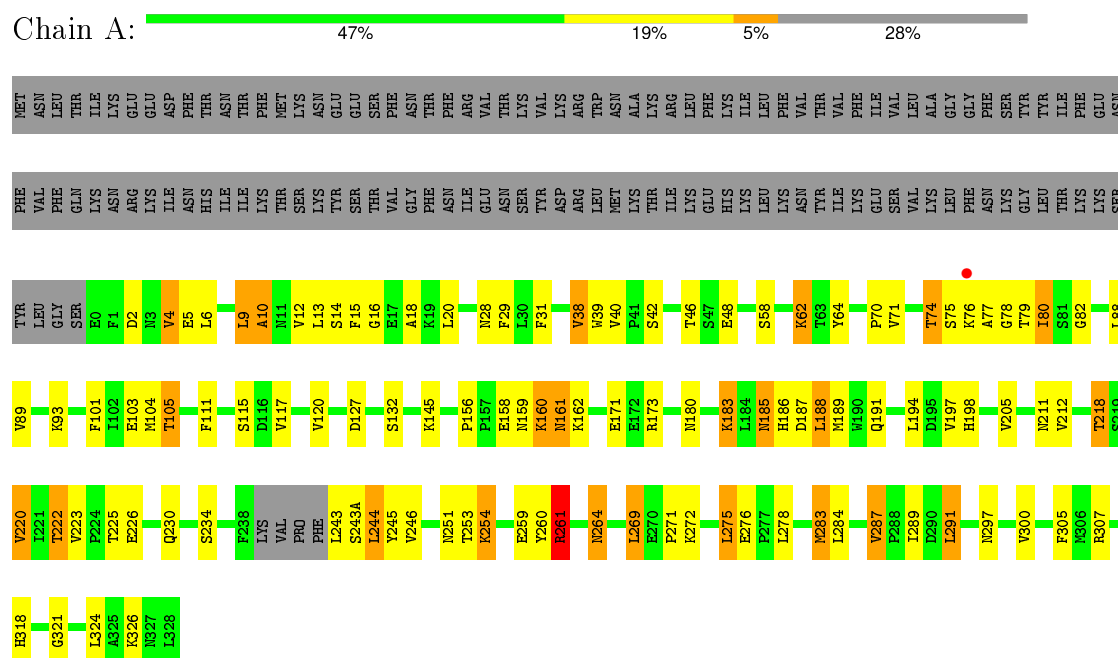
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	138	Total 138	O 138	0	0
8	B	95	Total 95	O 95	0	0
8	C	128	Total 128	O 128	0	0
8	D	147	Total 147	O 147	0	0

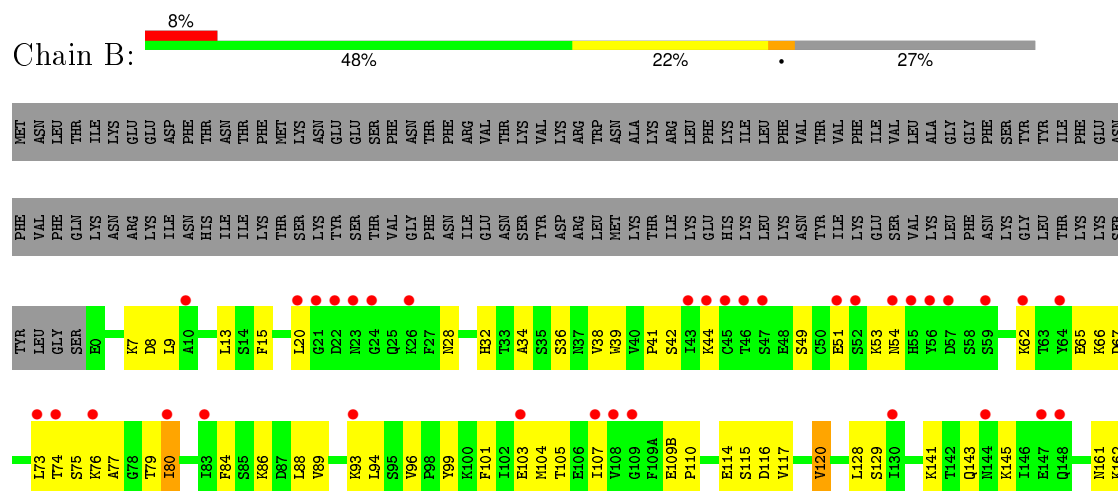
3 Residue-property plots

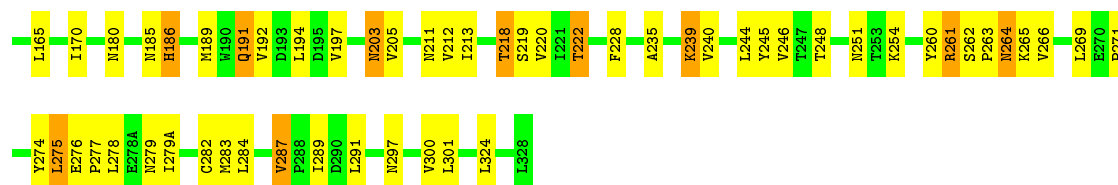
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Histo-aspartic protease

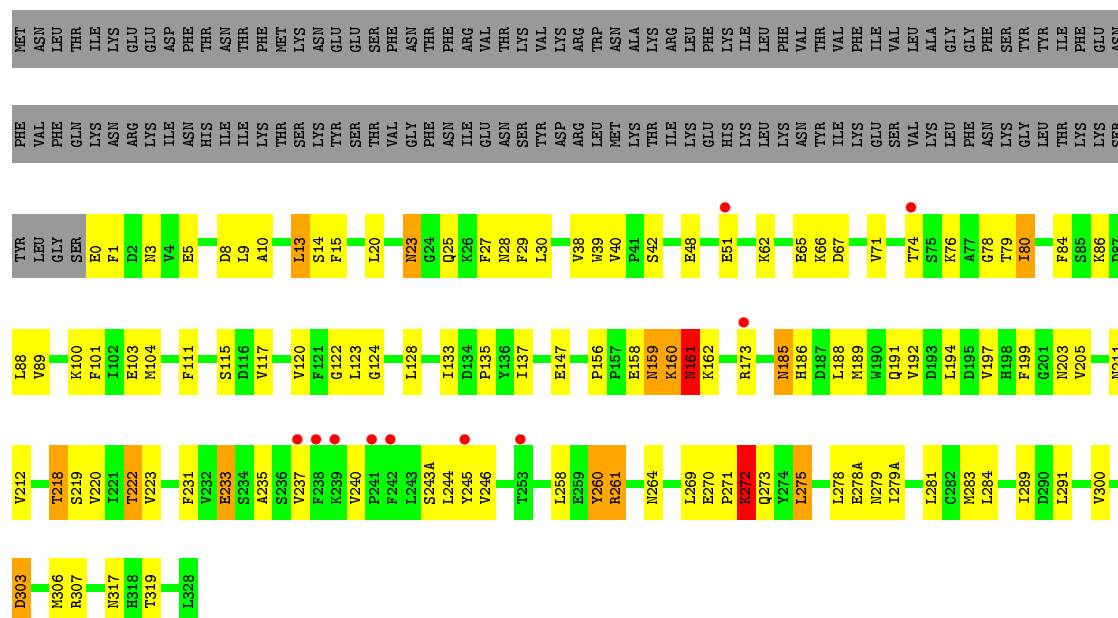


- Molecule 1: Histo-aspartic protease

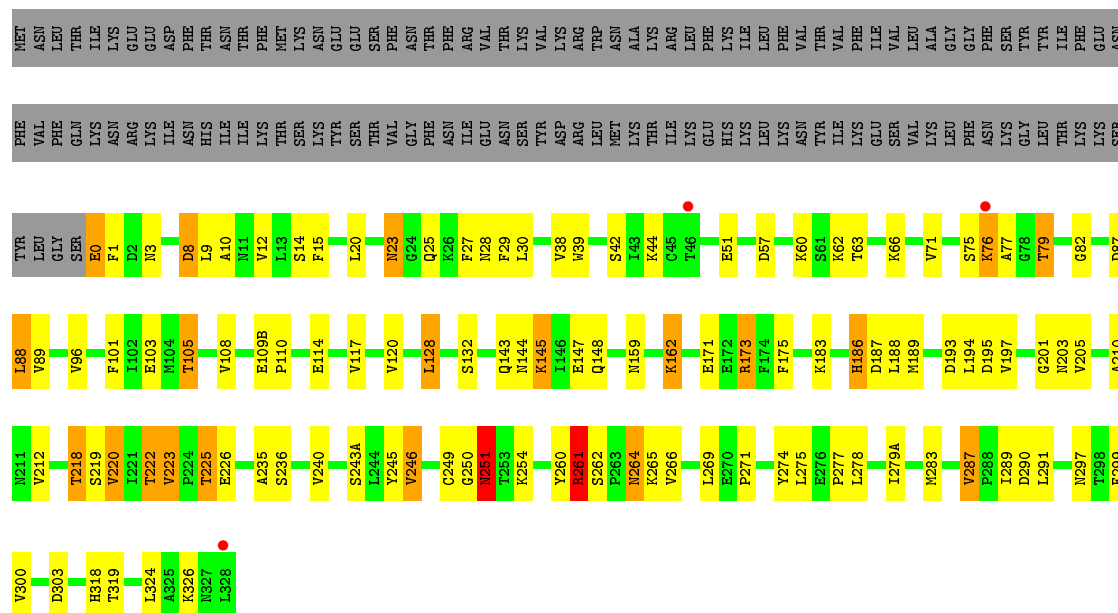




• Molecule 1: Histo-aspartic protease



• Molecule 1: Histo-aspartic protease



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.43Å 90.51Å 192.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.72 – 2.50 39.73 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.72-2.50) 100.0 (39.73-2.50)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.175 , 0.252 0.188 , 0.258	Depositor DCC
R_{free} test set	2712 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.9	EDS
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 54222 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11285	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, EDO, PG4, PG5, ACT, K95

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	0.90	0/2682	0.94	3/3639 (0.1%)
1	B	0.78	0/2722	0.86	1/3693 (0.0%)
1	C	0.91	1/2704 (0.0%)	0.94	9/3668 (0.2%)
1	D	0.93	2/2748 (0.1%)	0.93	1/3725 (0.0%)
All	All	0.88	3/10856 (0.0%)	0.92	14/14725 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	249	CYS	CB-SG	5.70	1.92	1.82
1	D	173	ARG	CG-CD	5.31	1.65	1.51
1	C	260	TYR	CD1-CE1	5.03	1.46	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	261	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	C	261	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	C	13	LEU	CB-CG-CD2	-7.34	98.53	111.00
1	A	261	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	C	9	LEU	CA-CB-CG	6.55	130.37	115.30
1	A	261	ARG	NE-CZ-NH2	-6.30	117.15	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	LEU	CA-CB-CG	5.67	128.35	115.30
1	C	284	LEU	CB-CG-CD2	-5.64	101.41	111.00
1	C	258	LEU	CA-CB-CG	5.63	128.25	115.30
1	B	261	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	D	261	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	C	303	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	C	13	LEU	CA-CB-CG	5.20	127.25	115.30
1	C	258	LEU	CB-CG-CD1	5.19	119.82	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	159	ASN	Peptide

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	2599	0	2560	90	0
1	B	2638	0	2602	96	1
1	C	2630	0	2588	89	0
1	D	2655	0	2639	96	0
2	A	49	0	44	3	0
2	C	98	0	88	6	0
3	A	12	0	18	4	0
3	B	4	0	6	5	0
3	C	16	0	24	4	0
3	D	16	0	24	13	0
4	A	33	0	44	5	0
4	D	10	0	13	4	0
5	A	4	0	3	0	0
6	B	12	0	18	7	0
7	D	1	0	0	0	0
8	A	138	0	0	19	2
8	B	95	0	0	14	1
8	C	128	0	0	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	147	0	0	19	0
All	All	11285	0	10671	349	2

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 16.

All (349) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:330:K95:CAZ	3:D:332:EDO:H21	1.57	1.31
1:D:186[B]:HIS:HE1	8:D:610:HOH:O	1.06	1.28
2:C:330:K95:HAZ	3:D:332:EDO:C2	1.79	1.11
1:C:278:LEU:O	1:D:218:THR:HG22	1.55	1.06
1:B:235:ALA:HB1	1:B:240:VAL:CG1	1.92	1.00
1:D:44[B]:LYS:HE2	8:D:724:HOH:O	1.60	0.99
1:A:5:GLU:OE2	1:B:162:LYS:HE3	1.63	0.98
1:D:51:GLU:HG3	8:D:638:HOH:O	1.61	0.98
1:B:51:GLU:HG3	8:B:648:HOH:O	1.63	0.97
1:C:13:LEU:HB3	8:C:744:HOH:O	1.64	0.97
1:D:171:GLU:OE2	8:D:579:HOH:O	1.86	0.93
1:A:291:LEU:HG	2:A:329:K95:HAAA	1.54	0.89
1:A:171:GLU:HG2	8:B:378:HOH:O	1.73	0.87
1:A:222:THR:CG2	8:A:355:HOH:O	2.23	0.85
1:B:219:SER:HB2	8:B:350:HOH:O	1.76	0.85
1:C:191:GLN:HE21	1:C:211:ASN:HD21	1.22	0.84
2:C:330:K95:HAZ	3:D:332:EDO:H21	0.86	0.83
1:A:218:THR:HG22	1:B:278:LEU:O	1.78	0.82
1:D:186[B]:HIS:CE1	8:D:610:HOH:O	1.94	0.81
1:B:186[B]:HIS:HE1	8:B:731:HOH:O	1.64	0.80
1:C:80:ILE:HD11	1:C:104:MET:HG2	1.62	0.80
1:A:183:LYS:HD2	8:A:398:HOH:O	1.81	0.80
1:A:183:LYS:HE3	4:A:335:PG4:H71	1.64	0.79
1:C:222:THR:CG2	8:C:351:HOH:O	2.30	0.79
1:A:307:ARG:HD3	8:A:378:HOH:O	1.82	0.79
1:C:222:THR:HG23	8:C:351:HOH:O	1.82	0.78
3:A:331:EDO:H22	6:B:330:PG5:H11	1.66	0.78
1:B:39:TRP:CD1	1:B:120:VAL:HG22	2.19	0.77
1:B:235:ALA:HB1	1:B:240:VAL:HG11	1.63	0.77
1:D:23:ASN:HD21	1:D:25:GLN:HE21	1.31	0.77
1:D:110:PRO:O	1:D:114[B]:GLU:HG2	1.84	0.76
1:C:1:PHE:O	1:C:3[A]:ASN:ND2	2.17	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63[B]:THR:HG23	1:D:87:ASP:OD1	1.85	0.76
1:D:222:THR:HG23	8:D:337:HOH:O	1.84	0.76
1:A:159:ASN:OD1	8:A:345:HOH:O	2.02	0.76
1:A:222:THR:HG23	8:A:355:HOH:O	1.84	0.75
1:A:77:ALA:C	8:A:576:HOH:O	2.25	0.75
1:B:264:ASN:OD1	1:D:203:ASN:ND2	2.20	0.74
1:D:63[B]:THR:HG21	1:D:88:LEU:HD22	1.68	0.73
1:B:32:HIS:CD2	1:B:34:ALA:H	2.07	0.73
1:A:12:VAL:O	1:A:13:LEU:HD23	1.88	0.73
1:D:264:ASN:ND2	8:D:391:HOH:O	2.21	0.72
1:D:42:SER:HB2	1:D:103:GLU:HB3	1.70	0.72
1:A:278:LEU:HD11	1:A:283:MET:HG3	1.70	0.72
1:A:272:LYS:HD2	1:B:109(B):GLU:O	1.90	0.71
2:C:330:K95:CAZ	3:D:332:EDO:C2	2.52	0.71
1:A:185:ASN:HD22	1:A:186:HIS:N	1.89	0.70
1:B:266:VAL:HG21	1:D:266:VAL:HG21	1.73	0.70
1:D:235:ALA:HB1	1:D:240:VAL:CG1	2.20	0.70
1:C:23:ASN:HD22	1:C:23:ASN:H	1.39	0.70
1:C:240:VAL:HB	8:C:366:HOH:O	1.92	0.69
1:C:65:GLU:OE2	1:C:86:LYS:HD3	1.92	0.69
3:A:331:EDO:H22	6:B:330:PG5:C1	2.22	0.69
1:C:10:ALA:HA	1:D:8:ASP:OD2	1.92	0.68
1:D:23:ASN:H	1:D:23:ASN:HD22	1.41	0.68
1:A:186:HIS:CD2	1:A:188:LEU:HD22	2.29	0.68
2:C:330:K95:HAZA	3:D:332:EDO:H21	1.68	0.68
1:B:39:TRP:HD1	1:B:120:VAL:HG22	1.56	0.68
1:A:80:ILE:HD13	1:A:104:MET:SD	2.33	0.68
1:C:74:THR:HG22	1:C:79:THR:OG1	1.94	0.67
1:C:135:PRO:HB3	3:C:331:EDO:H11	1.76	0.67
1:A:291:LEU:CG	2:A:329:K95:HAAA	2.25	0.66
1:B:191:GLN:HE21	1:B:211:ASN:HD21	1.43	0.66
1:B:114:GLU:HG3	8:B:343:HOH:O	1.95	0.66
1:C:191:GLN:NE2	1:C:211:ASN:HD21	1.93	0.66
1:D:289:ILE:HD12	8:D:413:HOH:O	1.96	0.66
1:C:115:SER:OG	1:C:117:VAL:HG12	1.95	0.66
1:C:272:LYS:HD3	1:C:273:GLN:NE2	2.10	0.66
1:C:278(A):GLU:OE1	8:C:556:HOH:O	2.15	0.65
1:C:188:LEU:O	8:C:780:HOH:O	2.13	0.65
1:B:279:ASN:HA	3:B:329:EDO:H12	1.79	0.65
1:C:13:LEU:HD23	8:C:744:HOH:O	1.96	0.65
1:C:15:PHE:CE1	1:C:28:ASN:HB3	2.32	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LEU:HD23	1:B:289:ILE:HD11	1.79	0.64
1:C:303:ASP:HB3	1:C:307:ARG:NH2	2.13	0.64
1:D:277:PRO:HG3	3:D:330:EDO:H22	1.80	0.64
3:A:331:EDO:C2	6:B:330:PG5:H11	2.28	0.64
1:B:277:PRO:HG3	3:B:329:EDO:H11	1.79	0.64
1:A:183:LYS:CE	4:A:335:PG4:H71	2.28	0.63
1:C:279(A):ILE:HG22	1:D:30[A]:LEU:HD23	1.80	0.63
1:C:245:TYR:CD2	1:D:245:TYR:HE1	2.15	0.63
1:A:289:ILE:HD13	1:B:246:VAL:HG21	1.80	0.63
1:B:32:HIS:HD2	1:B:34:ALA:H	1.46	0.63
1:A:48:GLU:HG3	8:A:805:HOH:O	1.98	0.62
1:D:222:THR:CG2	8:D:337:HOH:O	2.46	0.62
1:A:194:LEU:HD13	1:A:260:TYR:HB3	1.82	0.62
1:C:245:TYR:HB2	8:D:704:HOH:O	1.99	0.62
1:D:75:SER:O	1:D:77:ALA:N	2.33	0.62
3:D:330:EDO:H12	8:D:557:HOH:O	2.00	0.61
1:A:80:ILE:HD11	1:A:104:MET:HG2	1.82	0.61
1:D:39:TRP:HE1	3:D:332:EDO:HO1	1.48	0.61
1:B:222:THR:HB	1:B:300:VAL:HB	1.81	0.61
1:A:38:VAL:HG22	1:A:101:PHE:HB3	1.83	0.61
1:B:75:SER:C	1:B:77:ALA:H	2.04	0.60
8:A:383:HOH:O	3:B:329:EDO:H21	2.00	0.60
1:A:10:ALA:HB3	1:B:116:ASP:OD2	2.01	0.60
1:C:156:PRO:HB3	1:C:161:ASN:HB3	1.84	0.60
1:B:185:ASN:HD21	1:B:211:ASN:HD22	1.48	0.60
1:B:235:ALA:HB1	1:B:240:VAL:HG12	1.82	0.60
1:B:42:SER:HB2	1:B:103:GLU:HB3	1.83	0.60
1:C:185:ASN:HD22	1:C:186:HIS:N	2.00	0.60
1:A:145:LYS:NZ	4:A:334:PG4:O2	2.31	0.59
1:A:78:GLY:N	8:A:576:HOH:O	2.35	0.59
1:A:278:LEU:CD2	1:B:289:ILE:HD11	2.33	0.59
1:D:265:LYS:HD2	8:D:385:HOH:O	2.02	0.59
1:B:235:ALA:CB	1:B:240:VAL:CG1	2.76	0.59
1:C:13:LEU:HD12	1:C:15:PHE:HB2	1.84	0.59
1:B:180:ASN:ND2	1:B:265:LYS:HG2	2.18	0.59
1:C:218:THR:HG22	1:D:278:LEU:O	2.02	0.59
1:D:14:SER:O	1:D:30[A]:LEU:HD12	2.03	0.59
1:A:156:PRO:HB3	1:A:161:ASN:HB3	1.85	0.58
1:C:185:ASN:HD22	1:C:185:ASN:C	2.07	0.58
1:D:243(A):SER:OG	1:D:246:VAL:HG13	2.04	0.58
1:B:222:THR:HG23	8:B:344:HOH:O	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186[B]:HIS:CE1	8:B:731:HOH:O	2.48	0.58
1:B:220:VAL:HG11	1:B:287:VAL:CG1	2.34	0.58
1:B:235:ALA:CB	1:B:240:VAL:HG11	2.33	0.58
1:A:160:LYS:O	1:A:161:ASN:HB2	2.03	0.57
1:B:248[B]:THR:HG22	1:B:251:ASN:N	2.19	0.57
1:B:220:VAL:HG11	1:B:287:VAL:HG13	1.87	0.57
1:A:82:GLY:HA2	1:A:105:THR:HB	1.86	0.57
1:B:271:PRO:HA	1:B:274:TYR:CE1	2.40	0.57
1:B:110:PRO:O	1:B:114:GLU:HB2	2.04	0.57
1:D:109(B):GLU:OE2	1:D:109(B):GLU:HA	2.04	0.57
1:C:42:SER:HB2	1:C:103:GLU:HB3	1.87	0.57
1:C:13:LEU:HD12	1:C:15:PHE:CB	2.35	0.56
1:A:74:THR:HG23	1:A:79:THR:OG1	2.06	0.56
1:D:271:PRO:HA	1:D:274:TYR:CZ	2.41	0.56
1:A:16:GLY:HA2	1:B:7:LYS:HD3	1.87	0.56
1:C:245:TYR:CD2	1:D:245:TYR:CE1	2.93	0.55
1:A:185:ASN:HD22	1:A:186:HIS:H	1.54	0.55
1:C:111:PHE:HB3	3:D:330:EDO:H11	1.89	0.55
1:A:15:PHE:HE1	1:A:28:ASN:HB3	1.70	0.55
1:D:251:ASN:HD22	1:D:254:LYS:H	1.54	0.55
1:D:82:GLY:HA2	1:D:105:THR:HB	1.88	0.55
1:A:2:ASP:OD1	1:B:94:LEU:HD12	2.06	0.55
1:B:222:THR:CG2	8:B:344:HOH:O	2.54	0.55
1:C:122:GLY:O	3:C:331:EDO:H21	2.06	0.55
1:B:248[B]:THR:HG22	1:B:251:ASN:H	1.71	0.55
1:B:276[B]:GLU:OE2	6:B:330:PG5:H83	2.07	0.54
1:A:62:LYS:HE3	8:A:786:HOH:O	2.07	0.54
1:C:14:SER:HB2	8:C:376:HOH:O	2.07	0.54
1:C:120:VAL:HG12	1:D:279(A):ILE:HD13	1.89	0.54
1:B:74:THR:HG22	1:B:79:THR:HG23	1.89	0.54
1:B:96:VAL:CG2	1:B:143:GLN:HG3	2.36	0.54
1:B:275:LEU:HG	1:B:282:CYS:HB3	1.88	0.54
1:D:38:VAL:HG22	1:D:101:PHE:CB	2.38	0.54
1:A:289:ILE:HD13	1:B:246:VAL:CG2	2.38	0.54
1:B:235:ALA:O	1:B:240:VAL:HG12	2.08	0.53
1:B:80:ILE:HD13	1:B:107:ILE:HG12	1.91	0.53
1:D:57:ASP:OD2	1:D:60:LYS:HE2	2.09	0.53
1:C:15:PHE:HE1	1:C:28:ASN:HB3	1.71	0.53
1:A:275:LEU:CD1	1:A:284:LEU:HD12	2.39	0.53
1:A:264[A]:ASN:ND2	8:A:390:HOH:O	2.41	0.53
1:A:18:ALA:HB3	1:A:29:PHE:CE1	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:THR:HB	1:D:290:ASP:OD2	2.09	0.53
1:C:218:THR:CG2	1:D:278:LEU:O	2.57	0.53
1:C:128:LEU:HD23	8:C:372:HOH:O	2.09	0.52
1:A:4:VAL:HG13	1:B:165:LEU:HB3	1.92	0.52
1:C:128:LEU:HD13	1:C:188:LEU:HD12	1.90	0.52
1:C:279:ASN:ND2	8:C:385:HOH:O	2.42	0.52
1:C:67:ASP:HB3	1:C:84:PHE:O	2.08	0.52
1:D:251:ASN:ND2	1:D:254:LYS:H	2.07	0.52
1:B:115:SER:OG	1:B:117:VAL:HG12	2.09	0.52
1:C:222:THR:HB	1:C:300:VAL:HB	1.92	0.52
1:A:15:PHE:CE1	1:A:28:ASN:HB3	2.44	0.52
1:C:80:ILE:HD13	1:C:104:MET:SD	2.49	0.52
1:C:14:SER:O	1:C:30:LEU:HD12	2.10	0.52
1:C:80:ILE:CD1	1:C:104:MET:HG2	2.37	0.52
1:A:318:HIS:HD2	8:A:366:HOH:O	1.93	0.52
1:D:15:PHE:CE1	1:D:28:ASN:HB3	2.44	0.51
1:B:9:LEU:HB2	8:B:792:HOH:O	2.10	0.51
1:A:20:LEU:HD22	1:A:89:VAL:HG22	1.92	0.51
1:D:145:LYS:NZ	8:D:868:HOH:O	2.44	0.51
1:C:289:ILE:HD13	1:D:246:VAL:HG21	1.92	0.51
1:D:183:LYS:HA	1:D:319:THR:HG22	1.93	0.51
1:D:318:HIS:HE1	8:D:641:HOH:O	1.93	0.51
1:A:159:ASN:O	1:A:160:LYS:C	2.49	0.51
1:B:277:PRO:CG	3:B:329:EDO:H11	2.40	0.51
1:B:262:SER:HB2	1:B:263:PRO:HD2	1.93	0.51
1:D:262:SER:HA	4:D:334:PG4:H31	1.93	0.51
1:D:1:PHE:O	1:D:3:ASN:ND2	2.44	0.51
1:A:38:VAL:HG22	1:A:101:PHE:CB	2.41	0.50
1:A:18:ALA:HB3	1:A:29:PHE:CD1	2.46	0.50
1:B:228:PHE:CZ	1:B:244:LEU:HD11	2.47	0.50
1:D:277:PRO:CG	3:D:330:EDO:H22	2.40	0.50
1:A:189:MET:HE3	8:A:361:HOH:O	2.12	0.50
1:C:192:VAL:HG12	1:C:194:LEU:HG	1.94	0.50
1:C:48:GLU:HA	1:C:51:GLU:HG2	1.93	0.50
1:A:291:LEU:HG	2:A:329:K95:CAA	2.36	0.49
1:B:203:ASN:ND2	1:D:264:ASN:OD1	2.45	0.49
1:A:80:ILE:CD1	1:A:104:MET:HG2	2.42	0.49
1:C:124:GLY:N	3:C:331:EDO:H12	2.27	0.49
1:C:189:MET:HA	8:C:780:HOH:O	2.12	0.49
1:A:111:PHE:HB3	3:B:329:EDO:H22	1.94	0.49
1:A:259:GLU:OE2	1:A:261:ARG:NH1	2.39	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ASN:HD21	1:C:25:GLN:HE21	1.60	0.49
1:D:20:LEU:HD22	1:D:89:VAL:HG22	1.92	0.49
1:B:192:VAL:HG12	1:B:194:LEU:HG	1.93	0.49
8:C:354:HOH:O	1:D:171:GLU:CG	2.59	0.49
1:B:191:GLN:HB3	1:B:213:ILE:HG12	1.94	0.49
1:C:39:TRP:HD1	1:C:120:VAL:HG22	1.77	0.49
1:D:148:GLN:NE2	8:D:751:HOH:O	2.41	0.49
1:C:278:LEU:O	1:D:218:THR:CG2	2.44	0.49
1:D:38:VAL:HG22	1:D:101:PHE:HB3	1.93	0.49
1:C:194:LEU:HD13	1:C:260:TYR:HB3	1.94	0.49
1:B:41:PRO:HB2	1:B:54:ASN:O	2.12	0.48
1:C:235:ALA:O	1:C:240:VAL:HG12	2.13	0.48
1:D:226:GLU:OE2	3:D:331:EDO:O2	2.29	0.48
1:D:76:LYS:HE2	1:D:76:LYS:HA	1.94	0.48
1:B:220:VAL:CG1	1:B:287:VAL:HG13	2.43	0.48
1:A:278:LEU:O	1:B:218:THR:HG23	2.14	0.48
1:D:220:VAL:CG1	1:D:287:VAL:HG13	2.44	0.48
1:A:278:LEU:HD23	1:B:289:ILE:CD1	2.43	0.48
1:A:158:GLU:HG2	8:B:343:HOH:O	2.12	0.48
1:C:233:GLU:O	1:C:237:VAL:HG23	2.13	0.48
1:A:191:GLN:HB2	1:A:211:ASN:HD21	1.77	0.48
1:D:235:ALA:HB1	1:D:240:VAL:HG13	1.94	0.48
1:A:39:TRP:HD1	1:A:120:VAL:HG22	1.79	0.48
1:C:306:MET:SD	8:C:396:HOH:O	2.61	0.48
1:B:42:SER:HB3	1:B:104:MET:O	2.14	0.48
1:D:79:THR:HG23	1:D:108:VAL:HB	1.95	0.48
1:A:6:LEU:HA	1:B:15:PHE:O	2.14	0.47
1:A:220:VAL:HG13	1:A:287:VAL:HG13	1.96	0.47
1:A:222:THR:HG22	8:A:355:HOH:O	2.03	0.47
1:A:78:GLY:CA	8:A:576:HOH:O	2.63	0.47
1:B:262:SER:HB2	1:B:263:PRO:CD	2.45	0.47
1:C:173:ARG:HH11	1:C:173:ARG:HB3	1.79	0.47
1:D:15:PHE:HE1	1:D:28:ASN:HB3	1.80	0.47
1:A:189:MET:CE	8:A:361:HOH:O	2.63	0.47
1:C:20:LEU:HD22	1:C:89:VAL:HG22	1.95	0.47
1:C:30:LEU:HD23	1:D:279(A):ILE:HG22	1.97	0.47
1:D:223:VAL:HG22	1:D:299:PHE:CE2	2.50	0.47
1:A:269:LEU:HD11	1:A:305:PHE:HA	1.96	0.47
1:C:158:GLU:HG2	1:D:114[B]:GLU:OE2	2.14	0.47
1:B:67:ASP:HB3	1:B:84:PHE:O	2.15	0.47
1:D:173:ARG:NE	8:D:402:HOH:O	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:SER:OG	1:A:117:VAL:HG12	2.15	0.47
1:A:271:PRO:O	1:A:275:LEU:HB2	2.14	0.46
1:D:222:THR:HB	1:D:300:VAL:HB	1.97	0.46
1:B:245:TYR:O	1:B:283:MET:HA	2.15	0.46
1:D:219:SER:HA	1:D:303:ASP:HB2	1.98	0.46
1:C:39:TRP:CD1	1:C:120:VAL:HG22	2.51	0.46
1:D:128:LEU:HA	1:D:128:LEU:HD12	1.69	0.46
3:A:331:EDO:H11	6:B:330:PG5:H82	1.97	0.46
1:C:272:LYS:HG2	1:D:110:PRO:HG3	1.97	0.46
1:C:74:THR:HA	1:C:78:GLY:O	2.16	0.46
1:B:128:LEU:HD22	1:B:189:MET:HG3	1.97	0.46
1:D:0:GLU:HG3	1:D:1:PHE:N	2.30	0.46
1:A:159:ASN:HD22	1:A:160:LYS:H	1.63	0.46
1:D:220:VAL:HG11	1:D:287:VAL:HG13	1.99	0.45
1:B:44:LYS:NZ	8:B:506:HOH:O	2.47	0.45
1:D:9:LEU:HB2	8:D:809:HOH:O	2.17	0.45
1:A:127:ASP:OD2	1:A:187[B]:ASP:OD1	2.34	0.45
1:B:220:VAL:CG1	1:B:287:VAL:CG1	2.95	0.45
1:B:20:LEU:HD22	1:B:89:VAL:HG22	1.97	0.45
1:D:235:ALA:CB	1:D:240:VAL:CG1	2.92	0.45
1:A:187[A]:ASP:OD1	1:A:318:HIS:HD2	2.00	0.45
1:C:5:GLU:OE2	1:D:162:LYS:HD3	2.16	0.45
1:C:38:VAL:HG22	1:C:101:PHE:HB2	1.99	0.45
1:A:58:SER:HB2	1:A:64:TYR:CD1	2.52	0.45
1:C:278:LEU:HD22	1:C:283:MET:HE2	1.99	0.45
1:A:42:SER:HB2	1:A:103:GLU:HB3	1.98	0.45
1:D:194:LEU:HD13	1:D:260:TYR:HB3	1.99	0.45
1:A:243(A):SER:CA	1:A:244:LEU:HB3	2.47	0.45
8:C:803:HOH:O	1:D:8:ASP:HB2	2.15	0.44
1:B:75:SER:C	1:B:77:ALA:N	2.70	0.44
1:B:36:SER:CB	1:B:129:SER:HB3	2.47	0.44
1:D:27:PHE:HB2	1:D:29:PHE:CE1	2.52	0.44
1:A:120:VAL:HG12	1:B:279(A):ILE:HD13	1.99	0.44
1:B:189:MET:HB2	1:B:191:GLN:HG2	1.99	0.44
1:C:135:PRO:CB	3:C:331:EDO:H11	2.47	0.44
1:B:36:SER:HB2	1:B:129:SER:HB3	2.00	0.44
1:C:80:ILE:HD11	1:C:104:MET:CG	2.42	0.44
1:C:289:ILE:HD13	1:D:246:VAL:CG2	2.47	0.44
1:A:180:ASN:HB3	8:A:775:HOH:O	2.17	0.44
1:D:12:VAL:H	1:D:159:ASN:ND2	2.16	0.44
1:C:111:PHE:CB	3:D:330:EDO:H11	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:LEU:HD13	1:B:101:PHE:CZ	2.52	0.43
1:A:70:PRO:HB2	4:A:333:PG4:H11	2.00	0.43
1:B:65:GLU:OE2	1:B:86:LYS:HD3	2.17	0.43
1:D:8:ASP:N	1:D:8:ASP:OD1	2.51	0.43
1:B:15:PHE:CE1	1:B:28:ASN:HB3	2.52	0.43
1:B:38:VAL:HG22	1:B:101:PHE:CB	2.48	0.43
1:B:38:VAL:HG22	1:B:101:PHE:HB3	2.00	0.43
1:B:162:LYS:HA	1:B:162:LYS:HD2	1.68	0.43
1:C:317:ASN:O	1:C:319:THR:HG23	2.19	0.43
1:A:222:THR:HB	1:A:300:VAL:HB	2.00	0.43
1:A:160:LYS:NZ	1:A:160:LYS:HA	2.34	0.43
1:D:187:ASP:OD1	1:D:318:HIS:HD2	2.00	0.43
1:A:58:SER:HB2	1:A:64:TYR:CG	2.54	0.43
1:A:173:ARG:O	1:A:326:LYS:HE3	2.18	0.43
1:D:44[B]:LYS:HD3	1:D:44[B]:LYS:HA	1.73	0.43
1:A:187[A]:ASP:OD1	1:A:318:HIS:CD2	2.71	0.43
1:C:199:PHE:CE2	1:C:231:PHE:CZ	3.07	0.43
1:A:198:HIS:HB3	8:A:766:HOH:O	2.18	0.43
3:D:330:EDO:C2	8:D:762:HOH:O	2.66	0.43
1:D:189:MET:CE	8:D:344:HOH:O	2.66	0.43
1:D:271:PRO:HA	1:D:274:TYR:CE1	2.55	0.42
1:A:39:TRP:CD1	1:A:120:VAL:HG22	2.54	0.42
1:B:271:PRO:HA	1:B:274:TYR:CZ	2.54	0.42
1:B:260:TYR:CZ	1:B:301:LEU:HD21	2.54	0.42
1:B:141:LYS:HD3	8:B:743:HOH:O	2.19	0.42
1:B:185:ASN:OD1	1:B:186[B]:HIS:ND1	2.52	0.42
1:D:193:ASP:HA	1:D:210:ALA:O	2.19	0.42
1:C:100[B]:LYS:HE3	1:C:133:ILE:HG12	2.01	0.42
1:C:281:LEU:HD21	2:C:330:K95:HAS	2.01	0.42
1:C:8:ASP:OD2	8:C:803:HOH:O	2.21	0.42
1:C:245:TYR:CE2	1:D:245:TYR:CE1	3.07	0.42
1:D:262:SER:CA	4:D:334:PG4:H31	2.49	0.42
1:D:38:VAL:HG22	1:D:101:PHE:HB2	2.02	0.42
8:C:354:HOH:O	1:D:171:GLU:HG2	2.18	0.42
6:B:330:PG5:H32	8:B:350:HOH:O	2.19	0.42
1:B:185:ASN:HD21	1:B:211:ASN:ND2	2.17	0.42
1:C:271:PRO:O	1:C:275:LEU:HB2	2.20	0.42
1:A:180:ASN:O	1:A:321:GLY:HA2	2.20	0.41
1:B:170:ILE:HA	8:B:345:HOH:O	2.20	0.41
1:D:175:PHE:C	1:D:326[B]:LYS:HE3	2.40	0.41
1:D:110:PRO:HB2	1:D:114[B]:GLU:CG	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:SER:HA	1:C:303:ASP:HB2	2.01	0.41
1:C:123:LEU:HD22	1:C:137:ILE:HD12	2.03	0.41
1:C:0:GLU:HB2	8:C:354:HOH:O	2.20	0.41
1:C:80:ILE:CD1	1:C:104:MET:CG	2.98	0.41
1:C:27:PHE:HB2	1:C:29:PHE:CE1	2.56	0.41
1:B:264:ASN:HB2	1:D:201:GLY:O	2.19	0.41
1:D:261:ARG:O	4:D:334:PG4:H31	2.19	0.41
1:B:240:VAL:O	1:B:240:VAL:HG13	2.21	0.41
1:A:226:GLU:OE2	1:A:230:GLN:NE2	2.53	0.41
1:B:235:ALA:CA	1:B:240:VAL:HG12	2.51	0.41
1:A:80:ILE:CD1	1:A:104:MET:CG	2.99	0.41
1:B:191:GLN:NE2	1:B:211:ASN:HD21	2.15	0.41
1:D:250:GLY:O	1:D:251:ASN:C	2.59	0.41
1:B:89:VAL:HG21	1:B:99:TYR:HB3	2.03	0.41
1:A:276:GLU:CB	6:B:330:PG5:H51	2.51	0.41
1:A:16:GLY:HA3	1:A:31:PHE:HE1	1.86	0.41
1:D:195:ASP:OD2	4:D:334:PG4:H21	2.21	0.41
1:C:279(A):ILE:CG2	1:D:30[A]:LEU:HD23	2.46	0.40
4:A:333:PG4:H71	4:A:333:PG4:H51	1.92	0.40
1:B:228:PHE:CE2	1:B:244:LEU:HD11	2.56	0.40
1:B:240:VAL:HG23	1:B:254:LYS:HB2	2.03	0.40
1:C:128:LEU:HD12	1:C:128:LEU:HA	1.95	0.40
1:B:94:LEU:HD22	1:B:145:LYS:HB3	2.02	0.40
1:B:53:LYS:NZ	1:B:115:SER:O	2.54	0.40
1:C:278:LEU:HD22	1:C:283:MET:CE	2.51	0.40
1:A:318:HIS:CD2	8:A:366:HOH:O	2.71	0.40
1:D:143:GLN:O	1:D:144:ASN:HB2	2.21	0.40
1:A:9:LEU:HD13	1:A:9:LEU:HA	1.62	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:873:HOH:O	8:B:874:HOH:O[4_445]	1.65	0.55
1:B:239:LYS:CE	8:A:397:HOH:O[4_545]	1.82	0.38

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	326/451 (72%)	308 (94%)	15 (5%)	3 (1%)	21	37
1	B	331/451 (73%)	313 (95%)	17 (5%)	1 (0%)	46	68
1	C	329/451 (73%)	312 (95%)	14 (4%)	3 (1%)	21	37
1	D	334/451 (74%)	323 (97%)	8 (2%)	3 (1%)	21	37
All	All	1320/1804 (73%)	1256 (95%)	54 (4%)	10 (1%)	24	41

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	ASN
1	C	160	LYS
1	C	161	ASN
1	C	272	LYS
1	D	76	LYS
1	A	254	LYS
1	A	10	ALA
1	B	49	SER
1	D	10	ALA
1	D	251	ASN

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	300/414 (72%)	252 (84%)	48 (16%)	3	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	303/414 (73%)	272 (90%)	31 (10%)	9	17
1	C	301/414 (73%)	268 (89%)	33 (11%)	8	14
1	D	306/414 (74%)	265 (87%)	41 (13%)	5	9
All	All	1210/1656 (73%)	1057 (87%)	153 (13%)	6	10

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	9	LEU
1	A	14	SER
1	A	38	VAL
1	A	40	VAL
1	A	46	THR
1	A	62	LYS
1	A	71	VAL
1	A	74	THR
1	A	75	SER
1	A	76	LYS
1	A	80	ILE
1	A	88	LEU
1	A	93	LYS
1	A	105	THR
1	A	132[A]	SER
1	A	132[B]	SER
1	A	160	LYS
1	A	162	LYS
1	A	183	LYS
1	A	185	ASN
1	A	188	LEU
1	A	197	VAL
1	A	205	VAL
1	A	212	VAL
1	A	218	THR
1	A	220	VAL
1	A	222	THR
1	A	223	VAL
1	A	225[A]	THR
1	A	225[B]	THR
1	A	234	SER
1	A	243	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	245	TYR
1	A	246	VAL
1	A	251	ASN
1	A	253	THR
1	A	254	LYS
1	A	261	ARG
1	A	264[A]	ASN
1	A	264[B]	ASN
1	A	269	LEU
1	A	275	LEU
1	A	283	MET
1	A	287	VAL
1	A	291	LEU
1	A	297	ASN
1	A	324	LEU
1	B	8	ASP
1	B	13	LEU
1	B	62	LYS
1	B	66	LYS
1	B	73	LEU
1	B	76	LYS
1	B	80	ILE
1	B	88	LEU
1	B	93	LYS
1	B	105	THR
1	B	120	VAL
1	B	161	ASN
1	B	186[A]	HIS
1	B	186[B]	HIS
1	B	191	GLN
1	B	197	VAL
1	B	203	ASN
1	B	205	VAL
1	B	212	VAL
1	B	218	THR
1	B	222	THR
1	B	239	LYS
1	B	261	ARG
1	B	264	ASN
1	B	269	LEU
1	B	275	LEU
1	B	284	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	287	VAL
1	B	291	LEU
1	B	297	ASN
1	B	324	LEU
1	C	23	ASN
1	C	40	VAL
1	C	62	LYS
1	C	66	LYS
1	C	71	VAL
1	C	76	LYS
1	C	80	ILE
1	C	88	LEU
1	C	147	GLU
1	C	159	ASN
1	C	160	LYS
1	C	161	ASN
1	C	162	LYS
1	C	185	ASN
1	C	197	VAL
1	C	203	ASN
1	C	205	VAL
1	C	212	VAL
1	C	218	THR
1	C	220	VAL
1	C	222	THR
1	C	223	VAL
1	C	233	GLU
1	C	243(A)	SER
1	C	244	LEU
1	C	246	VAL
1	C	261	ARG
1	C	264	ASN
1	C	269	LEU
1	C	270	GLU
1	C	272	LYS
1	C	275	LEU
1	C	291	LEU
1	D	0	GLU
1	D	8	ASP
1	D	23	ASN
1	D	62	LYS
1	D	66	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	71	VAL
1	D	79	THR
1	D	88	LEU
1	D	96	VAL
1	D	105	THR
1	D	117	VAL
1	D	120	VAL
1	D	128	LEU
1	D	132	SER
1	D	145	LYS
1	D	147	GLU
1	D	162	LYS
1	D	186[A]	HIS
1	D	186[B]	HIS
1	D	188	LEU
1	D	197	VAL
1	D	205	VAL
1	D	212	VAL
1	D	218	THR
1	D	220	VAL
1	D	222	THR
1	D	223	VAL
1	D	225	THR
1	D	236[A]	SER
1	D	236[B]	SER
1	D	246	VAL
1	D	251	ASN
1	D	261	ARG
1	D	264	ASN
1	D	269	LEU
1	D	275	LEU
1	D	283	MET
1	D	287	VAL
1	D	291	LEU
1	D	297	ASN
1	D	324	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	159	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	185	ASN
1	A	191	GLN
1	A	198	HIS
1	A	203	ASN
1	A	211	ASN
1	A	251	ASN
1	A	317	ASN
1	A	318	HIS
1	B	32	HIS
1	B	55	HIS
1	B	148	GLN
1	B	161	ASN
1	B	198	HIS
1	B	203	ASN
1	B	211	ASN
1	B	264	ASN
1	B	318	HIS
1	C	23	ASN
1	C	148	GLN
1	C	159	ASN
1	C	185	ASN
1	C	191	GLN
1	C	203	ASN
1	C	211	ASN
1	C	264	ASN
1	C	279	ASN
1	C	317	ASN
1	C	318	HIS
1	D	23	ASN
1	D	148	GLN
1	D	159	ASN
1	D	203	ASN
1	D	251	ASN
1	D	264	ASN
1	D	318	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 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	$\# Z > 2$
2	K95	A	329	-	53,53,53	1.88	11 (20%)	68,75,75	2.09	13 (19%)
3	EDO	A	330	-	3,3,3	0.54	0	2,2,2	0.37	0
3	EDO	A	331	-	3,3,3	0.61	0	2,2,2	0.30	0
3	EDO	A	332	-	3,3,3	0.59	0	2,2,2	0.38	0
4	PG4	A	333	-	12,12,12	0.69	0	11,11,11	0.53	0
4	PG4	A	334	-	9,9,12	0.63	0	8,8,11	0.46	0
4	PG4	A	335	-	9,9,12	0.51	0	8,8,11	0.60	0
5	ACT	A	336	-	1,3,3	1.72	0	0,3,3	0.00	-
3	EDO	B	329	-	3,3,3	0.43	0	2,2,2	0.43	0
6	PG5	B	330	-	11,11,11	0.57	0	10,10,10	0.34	0
2	K95	C	329	-	53,53,53	1.75	8 (15%)	68,75,75	1.30	8 (11%)
2	K95	C	330	-	53,53,53	2.02	9 (16%)	68,75,75	1.33	9 (13%)
3	EDO	C	331	-	3,3,3	0.27	0	2,2,2	0.35	0
3	EDO	C	332	-	3,3,3	0.35	0	2,2,2	0.78	0
3	EDO	C	333	-	3,3,3	0.54	0	2,2,2	0.33	0
3	EDO	C	334	-	3,3,3	0.45	0	2,2,2	0.55	0
3	EDO	D	330	-	3,3,3	0.55	0	2,2,2	0.15	0
3	EDO	D	331	-	3,3,3	0.33	0	2,2,2	0.75	0
3	EDO	D	332	-	3,3,3	0.46	0	2,2,2	0.47	0
3	EDO	D	333	-	3,3,3	0.26	0	2,2,2	1.12	0
4	PG4	D	334	-	9,9,12	0.50	0	8,8,11	0.59	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	K95	A	329	-	-	0/43/71/71	0/5/5/5
3	EDO	A	330	-	-	0/1/1/1	0/0/0/0
3	EDO	A	331	-	-	0/1/1/1	0/0/0/0
3	EDO	A	332	-	-	0/1/1/1	0/0/0/0
4	PG4	A	333	-	-	0/10/10/10	0/0/0/0
4	PG4	A	334	-	-	0/7/7/10	0/0/0/0
4	PG4	A	335	-	-	0/7/7/10	0/0/0/0
5	ACT	A	336	-	-	0/0/0/0	0/0/0/0
3	EDO	B	329	-	-	0/1/1/1	0/0/0/0
6	PG5	B	330	-	-	0/9/9/9	0/0/0/0
2	K95	C	329	-	-	0/43/71/71	0/5/5/5
2	K95	C	330	-	-	0/43/71/71	0/5/5/5
3	EDO	C	331	-	-	0/1/1/1	0/0/0/0
3	EDO	C	332	-	-	0/1/1/1	0/0/0/0
3	EDO	C	333	-	-	0/1/1/1	0/0/0/0
3	EDO	C	334	-	-	0/1/1/1	0/0/0/0
3	EDO	D	330	-	-	0/1/1/1	0/0/0/0
3	EDO	D	331	-	-	0/1/1/1	0/0/0/0
3	EDO	D	332	-	-	0/1/1/1	0/0/0/0
3	EDO	D	333	-	-	0/1/1/1	0/0/0/0
4	PG4	D	334	-	-	0/7/7/10	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	329	K95	CBW-SBG	-2.84	1.79	1.85
2	C	329	K95	CBU-CBJ	2.02	1.56	1.52
2	C	330	K95	CBS-NBD	2.02	1.49	1.46
2	A	329	K95	CBP-CBT	2.08	1.57	1.55
2	A	329	K95	CAL-CAJ	2.09	1.43	1.38
2	C	330	K95	CBT-NBE	2.20	1.50	1.46
2	A	329	K95	CBA-CBN	2.22	1.54	1.50
2	A	329	K95	CAM-CAJ	2.25	1.43	1.38
2	A	329	K95	CBR-CBS	2.29	1.57	1.54
2	A	329	K95	CAR-CBL	2.34	1.43	1.38
2	C	330	K95	CAX-CBH	2.38	1.57	1.51
2	C	329	K95	CBA-CBN	2.53	1.55	1.50
2	C	329	K95	OAI-CBR	2.58	1.47	1.42
2	C	330	K95	CBA-CBN	2.68	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	329	K95	CB-SBF	2.70	1.83	1.80
2	C	330	K95	CBB-CBM	2.90	1.58	1.51
2	C	329	K95	CBR-CBK	3.24	1.56	1.53
2	A	329	K95	CBU-CBJ	3.57	1.58	1.52
2	A	329	K95	CB-SBF	3.75	1.84	1.80
2	A	329	K95	CBO-CBT	3.82	1.55	1.51
2	C	330	K95	CB-SBF	4.13	1.85	1.80
2	C	330	K95	CBU-CBJ	4.30	1.60	1.52
2	C	329	K95	CBR-CBS	4.41	1.59	1.54
2	C	329	K95	CBO-CBT	4.68	1.56	1.51
2	C	330	K95	CBO-CBT	5.52	1.57	1.51
2	C	329	K95	CBU-NBV	7.10	1.51	1.46
2	C	330	K95	CBU-NBV	8.23	1.52	1.46
2	A	329	K95	CBU-NBV	8.90	1.52	1.46

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	329	K95	CAA-SBF-CB	-12.15	81.46	101.21
2	A	329	K95	CBO-CBT-NBE	-3.87	108.98	114.36
2	A	329	K95	CAX-CBH-N	-3.77	109.92	115.96
2	C	330	K95	CBO-CBT-NBE	-3.17	109.96	114.36
2	C	329	K95	CBO-CBT-NBE	-3.10	110.05	114.36
2	A	329	K95	SBG-CAZ-NBV	-2.95	100.82	105.26
2	A	329	K95	CBU-CBW-SBG	-2.92	99.16	104.13
2	C	329	K95	OAG-CBK-NBV	-2.56	117.01	121.41
2	A	329	K95	CAX-CBL-CAR	-2.51	117.09	120.86
2	C	330	K95	CBU-CBW-SBG	-2.48	99.91	104.13
2	A	329	K95	CBN-CBO-CBT	-2.45	108.52	110.39
2	C	329	K95	CB-CA-N	-2.28	105.21	110.83
2	A	329	K95	C-CA-N	-2.26	104.89	111.26
2	C	330	K95	CBJ-CBU-NBV	-2.25	106.86	112.60
2	A	329	K95	CBA-CBN-CBO	-2.18	108.42	110.98
2	A	329	K95	CB-CA-N	-2.16	105.52	110.83
2	C	330	K95	CAC-CBW-CAB	-2.13	107.48	110.88
2	C	330	K95	CBN-CBA-CBP	2.07	105.54	103.38
2	C	329	K95	CAZ-SBG-CBW	2.09	101.54	95.30
2	C	329	K95	CBN-CBA-CBP	2.10	105.56	103.38
2	C	330	K95	CBW-CBU-NBV	2.10	109.59	106.44
2	C	329	K95	CBW-CBU-NBV	2.12	109.62	106.44
2	C	329	K95	OAI-CBR-CBS	2.19	114.90	108.57
2	A	329	K95	OAH-CBP-CBT	2.32	116.83	110.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	330	K95	CBW-CBU-CBJ	2.76	118.97	113.28
2	A	329	K95	CAS-CBL-CAR	2.76	122.56	118.13
2	A	329	K95	CAB-CBW-CBU	2.85	117.95	111.56
2	C	330	K95	CBB-CBS-NBD	3.55	114.03	110.14
2	C	330	K95	OAI-CBR-CBK	4.72	116.01	108.53
2	C	329	K95	CAA-SBF-CB	4.82	109.05	101.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	329	K95	3	0
3	A	331	EDO	4	0
4	A	333	PG4	2	0
4	A	334	PG4	1	0
4	A	335	PG4	2	0
3	B	329	EDO	5	0
6	B	330	PG5	7	0
2	C	330	K95	6	0
3	C	331	EDO	4	0
3	D	330	EDO	6	0
3	D	331	EDO	1	0
3	D	332	EDO	6	0
4	D	334	PG4	4	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	323/451 (71%)	-0.17	1 (0%) 94 95	19, 34, 61, 95	0
1	B	327/451 (72%)	0.34	35 (10%) 8 8	21, 55, 85, 97	0
1	C	327/451 (72%)	-0.12	10 (3%) 52 57	20, 36, 64, 94	0
1	D	327/451 (72%)	-0.20	3 (0%) 85 88	19, 30, 52, 84	0
All	All	1304/1804 (72%)	-0.04	49 (3%) 44 49	19, 36, 77, 97	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	59	SER	3.4
1	B	46	THR	3.4
1	B	22	ASP	3.4
1	C	253	THR	3.3
1	B	130	ILE	3.3
1	B	21	GLY	3.1
1	B	74	THR	3.0
1	B	20	LEU	2.9
1	B	80	ILE	2.9
1	A	76	LYS	2.8
1	B	93	LYS	2.8
1	B	57	ASP	2.8
1	C	51	GLU	2.8
1	C	242	PHE	2.7
1	B	108	VAL	2.7
1	C	245	TYR	2.7
1	B	52	SER	2.6
1	C	238	PHE	2.6
1	B	45	CYS	2.6
1	B	73	LEU	2.5
1	B	10	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	47	SER	2.5
1	B	107	ILE	2.5
1	B	51	GLU	2.5
1	B	24	GLY	2.5
1	B	23	ASN	2.4
1	B	148	GLN	2.4
1	B	103	GLU	2.4
1	B	109	GLY	2.4
1	C	241	PRO	2.4
1	B	62	LYS	2.4
1	C	74	THR	2.3
1	B	26	LYS	2.3
1	B	147	GLU	2.3
1	B	76	LYS	2.3
1	C	173	ARG	2.3
1	B	55	HIS	2.3
1	B	144[A]	ASN	2.2
1	C	237	VAL	2.2
1	B	54	ASN	2.2
1	B	44	LYS	2.2
1	C	239	LYS	2.2
1	D	328	LEU	2.1
1	B	64	TYR	2.1
1	D	46	THR	2.1
1	D	76	LYS	2.1
1	B	56	TYR	2.1
1	B	83	ILE	2.1
1	B	43	ILE	2.1

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 carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	EDO	C	331	4/4	0.97	0.33	14.79	31,32,34,36	0
3	EDO	D	332	4/4	0.91	0.32	12.51	60,61,61,63	0
3	EDO	C	334	4/4	0.91	0.28	10.14	44,48,52,56	0
6	PG5	B	330	12/12	0.86	0.37	7.74	73,75,76,76	0
3	EDO	B	329	4/4	0.93	0.26	6.62	37,43,46,48	0
3	EDO	A	331	4/4	0.83	0.36	5.80	60,60,60,61	0
3	EDO	D	330	4/4	0.90	0.30	5.50	37,40,41,41	0
3	EDO	C	333	4/4	0.83	0.21	5.45	46,46,46,49	0
4	PG4	A	333	13/13	0.77	0.37	4.43	67,73,75,76	0
2	K95	C	330	49/49	0.81	0.27	4.16	49,64,73,75	0
4	PG4	A	335	10/13	0.69	0.27	3.46	65,75,80,80	0
4	PG4	D	334	10/13	0.77	0.26	2.79	63,65,66,67	0
4	PG4	A	334	10/13	0.88	0.21	2.56	56,60,63,64	0
3	EDO	D	333	4/4	0.93	0.19	2.09	46,47,48,50	0
3	EDO	D	331	4/4	0.90	0.19	1.82	50,50,50,52	0
2	K95	C	329	49/49	0.87	0.21	1.28	38,56,65,66	0
2	K95	A	329	49/49	0.94	0.13	0.46	22,35,42,44	0
3	EDO	C	332	4/4	0.95	0.14	0.01	52,52,53,53	0
3	EDO	A	330	4/4	0.92	0.14	-0.06	46,46,47,50	0
5	ACT	A	336	4/4	0.81	0.31	-	75,75,75,75	0
7	NA	D	329	1/1	0.99	0.22	-	22,22,22,22	0
3	EDO	A	332	4/4	0.85	0.16	-	44,46,47,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.