



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:12 AM UTC

PDB ID : 1RQX / pdb_00001rqx
Title : Crystal structure of ACC Deaminase complexed with Inhibitor
Authors : Karthikeyan, S.; Zhao, Z.; Kao, C.L.; Zhou, Q.; Tao, Z.; Zhang, H.; Liu, H.W.
Deposited on : 2003-12-07
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

<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

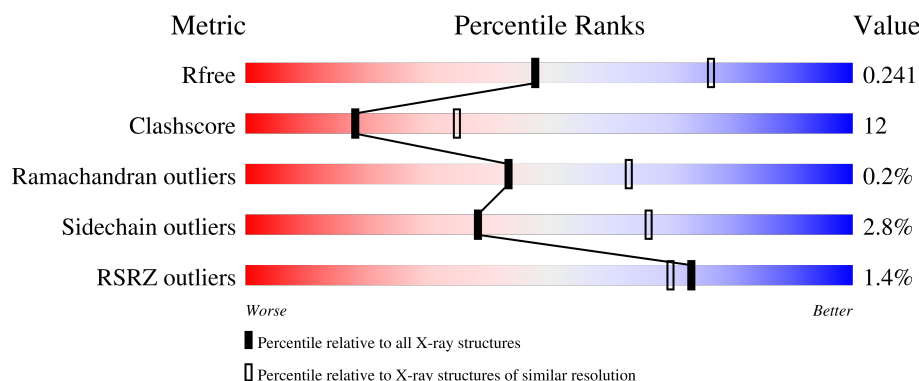
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	338	0% 75% 20% ..
1	B	338	0% 74% 22% ..
1	C	338	2% 67% 31% .
1	D	338	2% 67% 29% ..

2 Entry composition [i](#)

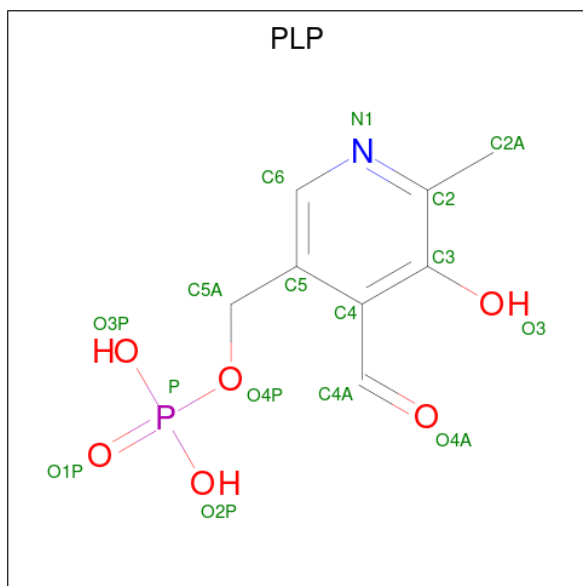
There are 4 unique types of molecules in this entry. The entry contains 10525 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1-aminocyclopropane-1-carboxylate deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2514	1576	451	472	15			
1	B	328	Total	C	N	O	S	0	0	0
			2488	1561	445	467	15			
1	C	338	Total	C	N	O	S	0	0	0
			2571	1614	461	481	15			
1	D	329	Total	C	N	O	S	0	0	0
			2499	1567	449	468	15			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



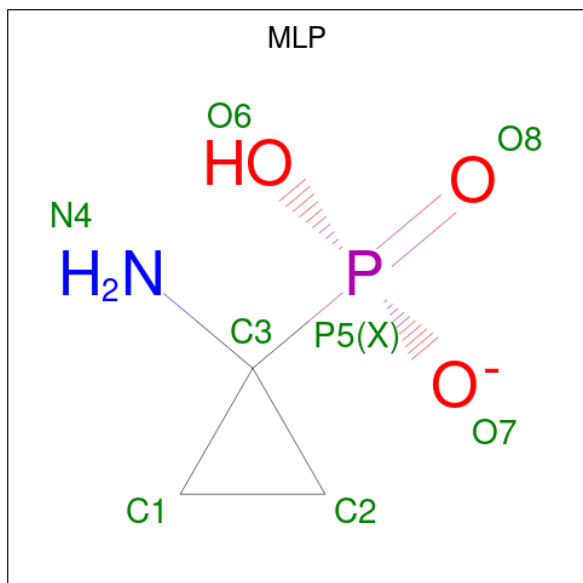
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is 1-AMINOCYCLOPROPYLPHOSPHONATE (CCD ID: MLP) (formula: $C_3H_7NO_3P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			8	3	1	3	1		
3	B	1	Total	C	N	O	P	0	0
			8	3	1	3	1		
3	C	1	Total	C	N	O	P	0	0
			8	3	1	3	1		
3	D	1	Total	C	N	O	P	0	0
			8	3	1	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total	O	0	0
			94	94		
4	B	99	Total	O	0	0
			99	99		
4	C	86	Total	O	0	0
			86	86		

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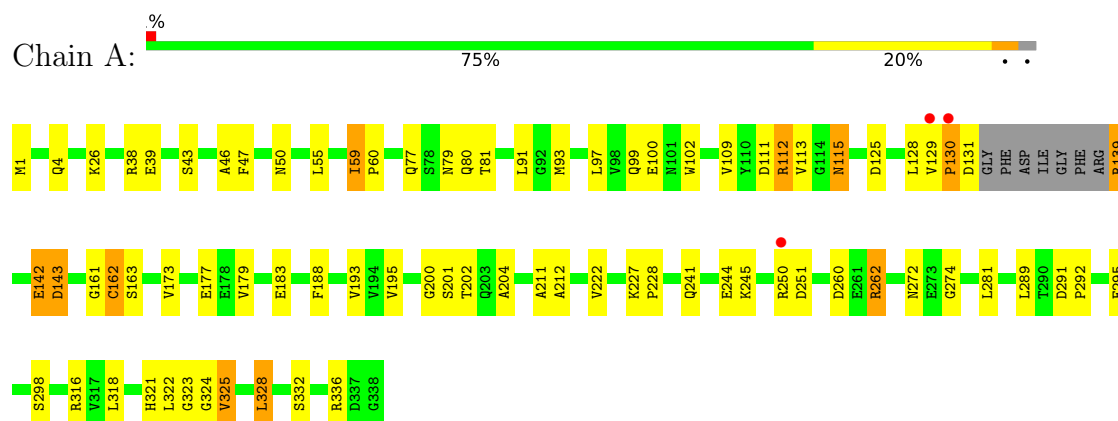
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	82	Total	O	0	0
			82	82		

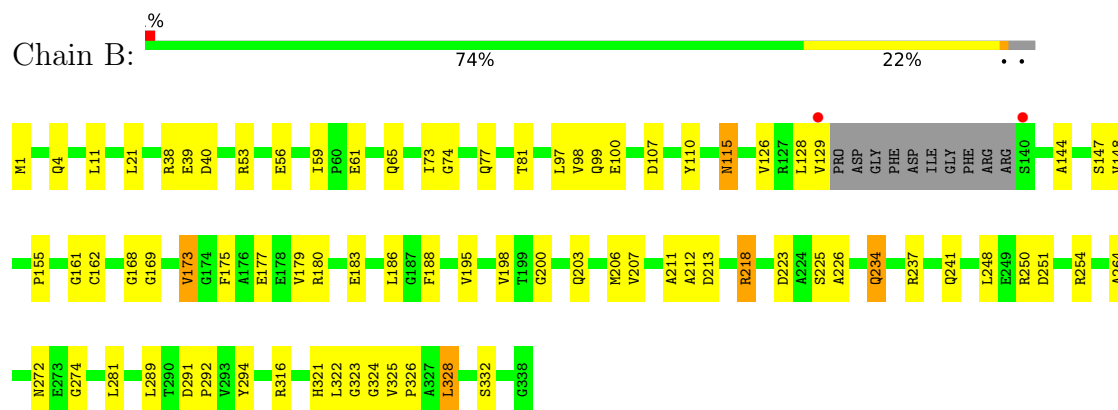
3 Residue-property plots [i](#)

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.

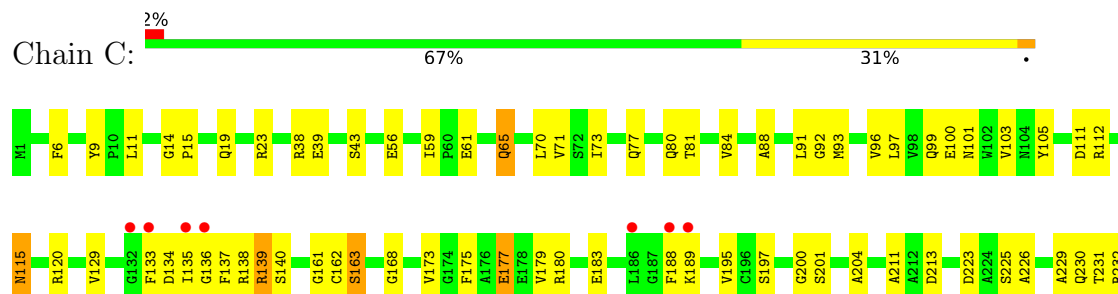
- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

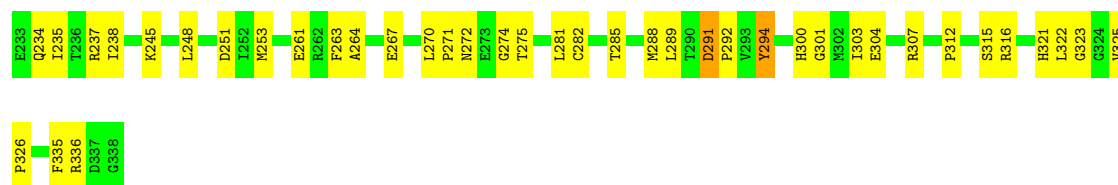


- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

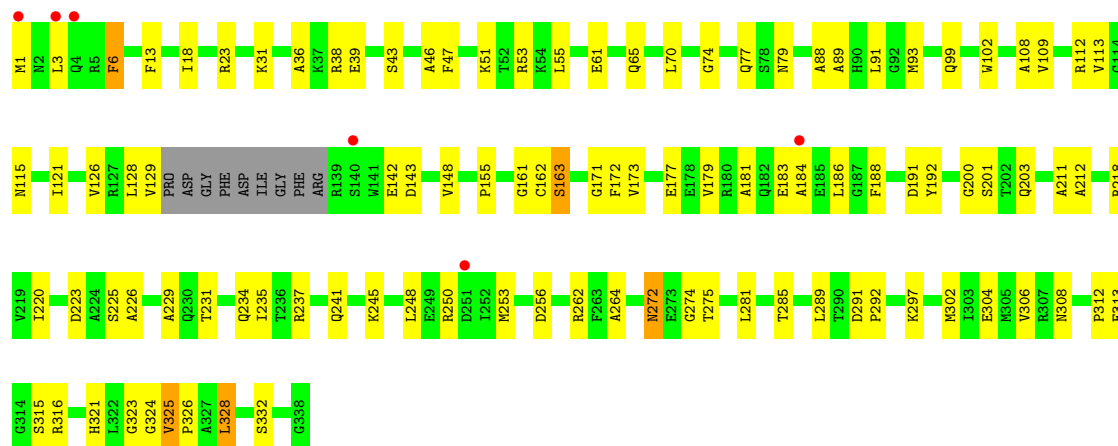


- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase





- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.76Å 68.59Å 350.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 2.50 48.75 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.5 (48.75-2.50) 91.6 (48.75-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.43 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.248 0.194 , 0.241	Depositor DCC
R_{free} test set	2689 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.045 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10525	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLP, PLP

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	0.58	1/2561 (0.0%)	1.08	16/3461 (0.5%)
1	B	0.56	1/2534 (0.0%)	1.08	12/3424 (0.4%)
1	C	0.56	0/2621	1.05	16/3542 (0.5%)
1	D	0.54	1/2545 (0.0%)	1.07	11/3438 (0.3%)
All	All	0.56	3/10261 (0.0%)	1.07	55/13865 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	59	ILE	CA-CB	8.68	1.58	1.54
1	A	325	VAL	CA-CB	6.43	1.58	1.53
1	D	325	VAL	CA-CB	5.07	1.57	1.53

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	200	GLY	N-CA-C	14.95	131.28	113.79
1	A	200	GLY	N-CA-C	14.33	134.87	114.67
1	B	200	GLY	N-CA-C	12.38	130.35	114.25
1	D	173	VAL	N-CA-C	-11.85	98.75	110.72
1	B	173	VAL	N-CA-C	-11.24	98.74	111.00
1	C	173	VAL	N-CA-C	-10.54	99.52	111.00
1	A	173	VAL	N-CA-C	-10.41	99.65	111.00
1	D	163	SER	N-CA-C	9.64	122.79	111.02
1	A	163	SER	N-CA-C	8.57	120.31	110.97
1	C	200	GLY	N-CA-C	7.74	131.52	113.18
1	C	163	SER	N-CA-C	7.51	120.18	111.02
1	D	211	ALA	N-CA-C	-7.50	103.12	111.82
1	B	211	ALA	N-CA-C	-7.45	103.18	111.82
1	B	115	ASN	N-CA-C	7.30	118.88	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	262	ARG	N-CA-C	7.11	121.06	112.38
1	C	38	ARG	N-CA-C	6.52	119.87	108.52
1	A	211	ALA	N-CA-C	-6.50	104.61	112.54
1	C	43	SER	N-CA-C	6.43	118.62	108.79
1	A	38	ARG	N-CA-C	6.41	119.67	108.52
1	A	262	ARG	N-CA-C	6.41	120.36	112.54
1	B	291	ASP	CA-C-N	6.35	125.97	119.56
1	B	291	ASP	C-N-CA	6.35	125.97	119.56
1	D	38	ARG	N-CA-C	6.32	119.43	109.39
1	C	39	GLU	N-CA-C	-6.26	104.90	112.54
1	D	332	SER	N-CA-C	6.02	117.84	111.28
1	C	168	GLY	N-CA-C	6.02	121.27	113.27
1	B	38	ARG	N-CA-C	5.93	118.82	109.39
1	A	115	ASN	N-CA-C	5.92	117.40	111.07
1	A	162	CYS	N-CA-C	-5.81	104.89	113.72
1	A	332	SER	N-CA-C	5.80	117.60	111.28
1	C	115	ASN	N-CA-C	5.74	117.21	111.07
1	C	211	ALA	N-CA-C	-5.68	105.23	111.82
1	B	53	ARG	N-CA-C	-5.66	105.19	111.36
1	B	168	GLY	N-CA-C	5.53	121.07	113.99
1	C	291	ASP	CA-C-N	5.51	125.13	119.56
1	C	291	ASP	C-N-CA	5.51	125.13	119.56
1	A	125	ASP	N-CA-C	-5.50	99.55	108.41
1	C	197	SER	N-CA-C	5.48	118.03	108.76
1	D	108	ALA	N-CA-C	5.46	118.00	111.71
1	B	21	LEU	N-CA-C	-5.43	101.40	109.11
1	A	227	LYS	CA-C-N	5.41	126.60	119.84
1	A	227	LYS	C-N-CA	5.41	126.60	119.84
1	B	324	GLY	N-CA-C	5.40	122.54	115.36
1	B	332	SER	N-CA-C	5.33	117.08	111.28
1	C	59	ILE	CB-CA-C	-5.32	108.65	113.70
1	D	43	SER	N-CA-C	5.26	117.25	108.99
1	C	294	TYR	N-CA-C	5.25	117.14	108.48
1	A	50	ASN	N-CA-C	5.14	116.88	111.28
1	D	6	PHE	CA-C-N	5.13	124.89	119.76
1	D	6	PHE	C-N-CA	5.13	124.89	119.76
1	A	43	SER	N-CA-C	5.12	117.02	108.99
1	A	59	ILE	CB-CA-C	-5.11	108.85	113.70
1	A	202	THR	N-CA-C	-5.06	105.67	111.14
1	C	300	HIS	N-CA-C	-5.05	105.66	111.07
1	C	65	GLN	N-CA-C	-5.02	106.93	113.16

There are no chirality outliers.

There are no planarity outliers.

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	2514	0	2485	50	0
1	B	2488	0	2461	55	0
1	C	2571	0	2538	71	0
1	D	2499	0	2474	75	0
2	A	15	0	7	1	0
2	B	15	0	7	0	0
2	C	15	0	7	0	0
2	D	15	0	7	0	0
3	A	8	0	5	1	0
3	B	8	0	5	0	0
3	C	8	0	5	1	0
3	D	8	0	5	0	0
4	A	94	0	0	5	0
4	B	99	0	0	2	0
4	C	86	0	0	2	0
4	D	82	0	0	4	0
All	All	10525	0	10006	245	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 12.

All (245) 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:1:MET:HE3	1:D:212:ALA:HB2	1.34	1.06
1:B:1:MET:HE3	1:B:212:ALA:HB2	1.38	1.04
1:B:272:ASN:HD22	1:B:274:GLY:H	1.12	0.95
1:A:81:THR:HB	1:A:97:LEU:HD13	1.49	0.94
1:A:272:ASN:HD22	1:A:274:GLY:H	1.22	0.86
1:C:100:GLU:OE1	1:C:135:ILE:HG12	1.80	0.80
1:C:251:ASP:O	1:C:253:MET:HE2	1.83	0.79
1:C:272:ASN:HD22	1:C:274:GLY:H	1.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:GLN:HE22	1:C:115:ASN:H	1.32	0.76
1:B:250:ARG:HG2	1:B:251:ASP:H	1.52	0.74
1:B:272:ASN:ND2	1:B:274:GLY:H	1.82	0.74
1:B:321:HIS:HD2	1:B:323:GLY:H	1.33	0.74
1:C:180:ARG:HD3	1:C:213:ASP:OD2	1.89	0.72
1:B:237:ARG:O	1:B:241:GLN:HG3	1.89	0.72
1:C:134:ASP:HB3	1:C:137:PHE:HB3	1.71	0.72
1:A:272:ASN:HD22	1:A:274:GLY:N	1.87	0.71
1:C:100:GLU:HB2	1:C:135:ILE:HD13	1.74	0.70
1:D:142:GLU:HB2	4:D:552:HOH:O	1.91	0.70
1:A:77:GLN:HE22	1:A:115:ASN:H	1.39	0.69
4:B:578:HOH:O	1:D:112:ARG:HD2	1.91	0.68
1:D:1:MET:CE	1:D:212:ALA:HB2	2.19	0.68
1:D:234:GLN:HG2	1:D:237:ARG:HH21	1.59	0.66
1:B:61:GLU:HG2	1:B:65:GLN:NE2	2.10	0.66
1:A:289:LEU:O	1:A:321:HIS:HE1	1.77	0.66
1:B:250:ARG:HG2	1:B:251:ASP:N	2.10	0.65
1:C:73:ILE:HD11	1:C:135:ILE:HD12	1.78	0.65
1:D:223:ASP:O	1:D:264:ALA:HB2	1.96	0.64
1:B:292:PRO:HD3	1:B:328:LEU:HD13	1.80	0.64
1:B:77:GLN:HE22	1:B:115:ASN:H	1.44	0.64
1:A:1:MET:HE3	1:A:212:ALA:HB2	1.79	0.64
1:D:292:PRO:HD3	1:D:328:LEU:CD1	2.28	0.63
1:B:272:ASN:HD22	1:B:274:GLY:N	1.89	0.63
1:A:109:VAL:O	1:A:113:VAL:HG22	1.99	0.62
1:D:179:VAL:O	1:D:183:GLU:HG3	2.00	0.62
1:D:191:ASP:O	1:D:218:ARG:HD3	1.99	0.62
1:D:218:ARG:HG2	1:D:218:ARG:HH11	1.64	0.62
1:D:272:ASN:HD22	1:D:274:GLY:N	1.97	0.62
1:C:188:PHE:CE1	1:C:316:ARG:HD2	2.35	0.61
1:D:272:ASN:HD22	1:D:274:GLY:H	1.48	0.61
1:C:321:HIS:HD2	1:C:323:GLY:H	1.48	0.61
1:D:77:GLN:HE22	1:D:115:ASN:H	1.48	0.61
1:C:272:ASN:HD22	1:C:274:GLY:N	1.99	0.61
1:C:234:GLN:O	1:C:238:ILE:HG13	2.00	0.60
1:D:61:GLU:HG2	1:D:65:GLN:NE2	2.16	0.60
1:D:220:ILE:N	1:D:220:ILE:HD12	2.16	0.60
1:A:250:ARG:HG2	1:A:251:ASP:N	2.17	0.60
1:D:321:HIS:HD2	1:D:323:GLY:H	1.50	0.60
1:C:100:GLU:HG2	1:C:101:ASN:H	1.67	0.59
1:B:99:GLN:HB2	1:B:128:LEU:HD23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:VAL:HG11	1:D:155:PRO:HB3	1.83	0.58
1:A:250:ARG:HG2	1:A:251:ASP:H	1.68	0.58
1:B:186:LEU:HB3	1:B:188:PHE:CE2	2.38	0.58
1:B:289:LEU:O	1:B:321:HIS:HE1	1.85	0.58
1:C:223:ASP:O	1:C:264:ALA:HB2	2.03	0.58
1:D:272:ASN:ND2	1:D:275:THR:H	2.01	0.58
1:A:161:GLY:O	1:A:162:CYS:HB2	2.04	0.58
1:B:321:HIS:CD2	1:B:323:GLY:H	2.19	0.58
1:C:232:ARG:NH2	1:C:261:GLU:OE2	2.37	0.58
1:C:23:ARG:NH1	1:D:89:ALA:O	2.37	0.58
1:B:169:GLY:O	1:B:173:VAL:HG23	2.04	0.57
1:C:81:THR:HB	1:C:97:LEU:HD13	1.85	0.57
1:C:133:PHE:CZ	1:C:138:ARG:HD2	2.38	0.57
1:B:1:MET:CE	1:B:212:ALA:HB2	2.25	0.57
1:C:19:GLN:NE2	1:D:13:PHE:HE1	2.02	0.56
1:D:161:GLY:O	1:D:162:CYS:HB2	2.04	0.56
1:B:272:ASN:ND2	1:B:274:GLY:N	2.50	0.56
1:D:220:ILE:HD12	1:D:220:ILE:H	1.71	0.56
1:D:302:MET:O	1:D:306:VAL:HG23	2.06	0.56
1:A:321:HIS:HD2	1:A:323:GLY:H	1.54	0.56
1:D:225:SER:O	1:D:226:ALA:HB3	2.05	0.55
1:D:218:ARG:O	1:D:220:ILE:HD12	2.06	0.55
1:C:100:GLU:HG3	1:C:129:VAL:CG2	2.36	0.55
1:A:325:VAL:O	1:A:328:LEU:HB2	2.07	0.55
1:D:51:LYS:HE3	1:D:161:GLY:HA2	1.88	0.55
1:D:39:GLU:HB2	1:D:321:HIS:O	2.07	0.55
1:A:142:GLU:HG3	4:A:565:HOH:O	2.08	0.54
1:C:138:ARG:O	1:C:139:ARG:HB2	2.08	0.54
1:A:241:GLN:HB3	4:A:577:HOH:O	2.08	0.54
1:B:180:ARG:HD3	1:B:213:ASP:OD2	2.07	0.54
1:D:192:TYR:HB3	1:D:220:ILE:CD1	2.37	0.54
1:D:312:PRO:HG2	1:D:315:SER:OG	2.07	0.54
1:D:183:GLU:HB3	1:D:188:PHE:O	2.08	0.54
1:D:297:LYS:HG2	4:D:565:HOH:O	2.07	0.54
1:B:99:GLN:HG3	1:B:126:VAL:HG13	1.91	0.53
1:B:179:VAL:O	1:B:183:GLU:HG3	2.09	0.53
1:B:11:LEU:N	1:B:56:GLU:OE2	2.27	0.53
1:C:133:PHE:CE1	1:C:138:ARG:HD2	2.44	0.53
1:B:61:GLU:HG2	1:B:65:GLN:HE21	1.74	0.52
1:B:81:THR:HB	1:B:97:LEU:HD13	1.91	0.52
1:C:100:GLU:OE2	1:C:134:ASP:HA	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ARG:O	1:A:143:ASP:HB2	2.10	0.52
1:B:73:ILE:HG13	1:B:98:VAL:HB	1.91	0.52
1:C:138:ARG:O	1:C:139:ARG:CB	2.58	0.52
1:C:231:THR:O	1:C:235:ILE:HG13	2.10	0.51
1:D:61:GLU:CG	1:D:65:GLN:NE2	2.73	0.51
1:D:234:GLN:HG2	1:D:237:ARG:NH2	2.25	0.51
1:B:161:GLY:O	1:B:162:CYS:HB2	2.10	0.51
1:A:4:GLN:OE1	1:A:4:GLN:N	2.41	0.51
1:D:325:VAL:O	1:D:328:LEU:HB2	2.11	0.51
1:A:188:PHE:CD1	1:A:188:PHE:C	2.89	0.51
1:C:103:VAL:HG12	1:C:105:TYR:HB2	1.93	0.51
1:D:218:ARG:HG2	1:D:218:ARG:NH1	2.26	0.51
1:C:312:PRO:O	1:C:315:SER:OG	2.27	0.50
1:A:272:ASN:ND2	1:A:274:GLY:N	2.58	0.50
1:B:39:GLU:HB2	1:B:321:HIS:O	2.12	0.50
1:A:111:ASP:OD1	1:A:112:ARG:HG2	2.12	0.50
1:B:100:GLU:HG2	1:B:129:VAL:HG21	1.93	0.50
1:C:91:LEU:HD13	1:C:93:MET:HE2	1.93	0.50
1:D:250:ARG:NH1	1:D:256:ASP:OD2	2.42	0.50
1:B:198:VAL:HG21	1:B:294:TYR:CE1	2.47	0.50
1:A:79:ASN:OD1	1:A:324:GLY:HA2	2.11	0.50
1:C:188:PHE:HB3	4:C:585:HOH:O	2.12	0.50
1:B:1:MET:HE2	1:B:248:LEU:HD13	1.94	0.49
1:C:120:ARG:HD2	4:D:547:HOH:O	2.12	0.49
1:B:254:ARG:HG3	4:B:548:HOH:O	2.12	0.49
1:C:183:GLU:CD	1:C:189:LYS:HD3	2.36	0.49
1:C:6:PHE:CZ	1:C:245:LYS:HD2	2.47	0.49
1:D:203:GLN:OE1	1:D:235:ILE:HD13	2.13	0.49
1:A:195:VAL:HG23	1:A:322:LEU:HD11	1.94	0.49
1:C:111:ASP:C	1:C:112:ARG:HG2	2.37	0.49
1:A:26:LYS:NZ	4:A:573:HOH:O	2.45	0.49
1:B:198:VAL:HG21	1:B:294:TYR:HE1	1.77	0.49
1:D:231:THR:O	1:D:235:ILE:HG13	2.13	0.49
1:C:195:VAL:HG23	1:C:322:LEU:HD11	1.94	0.48
1:C:100:GLU:HG2	1:C:101:ASN:N	2.28	0.48
1:D:292:PRO:HD3	1:D:328:LEU:HD12	1.95	0.48
1:C:201:SER:HA	1:C:204:ALA:HB3	1.94	0.48
1:C:234:GLN:HG3	1:C:237:ARG:NH2	2.28	0.48
1:A:111:ASP:C	1:A:112:ARG:HG2	2.39	0.48
1:C:161:GLY:O	1:C:162:CYS:HB2	2.14	0.48
1:C:80:GLN:O	1:C:84:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:TYR:OH	3:C:501:MLP:O6	2.27	0.47
1:D:46:ALA:O	1:D:47:PHE:HB2	2.13	0.47
1:D:163:SER:HA	1:D:201:SER:HB3	1.97	0.47
1:D:188:PHE:CG	1:D:316:ARG:NH1	2.83	0.47
1:B:292:PRO:HD3	1:B:328:LEU:CD1	2.45	0.47
1:D:99:GLN:HB2	1:D:128:LEU:HD23	1.97	0.47
1:A:59:ILE:HB	1:A:60:PRO:HD3	1.97	0.46
1:A:272:ASN:ND2	1:A:274:GLY:H	2.02	0.46
1:C:100:GLU:CD	1:C:135:ILE:H	2.23	0.46
1:D:181:ALA:O	1:D:184:ALA:HB3	2.15	0.46
1:C:289:LEU:O	1:C:321:HIS:HE1	1.99	0.46
1:C:335:PHE:CG	1:D:121:ILE:HD11	2.50	0.46
1:B:99:GLN:HG3	1:B:126:VAL:CG1	2.46	0.46
1:C:229:ALA:HB3	4:C:519:HOH:O	2.15	0.46
1:A:91:LEU:HD13	1:A:93:MET:HE2	1.97	0.46
1:C:61:GLU:O	1:C:65:GLN:HG3	2.15	0.46
1:C:263:PHE:HE1	1:C:304:GLU:HG2	1.81	0.46
1:B:40:ASP:CB	1:B:323:GLY:HA2	2.45	0.46
1:B:148:VAL:HG11	1:B:155:PRO:HB3	1.97	0.46
1:D:109:VAL:O	1:D:113:VAL:HG22	2.16	0.46
1:A:80:GLN:N	3:A:501:MLP:O8	2.41	0.46
1:A:228:PRO:HG3	4:A:516:HOH:O	2.14	0.46
1:D:325:VAL:N	1:D:326:PRO:CD	2.79	0.46
1:D:61:GLU:CG	1:D:65:GLN:HE21	2.29	0.45
1:C:11:LEU:N	1:C:56:GLU:OE2	2.43	0.45
1:D:192:TYR:HD2	1:D:220:ILE:HD11	1.81	0.45
1:B:175:PHE:CE1	1:B:206:MET:HE2	2.51	0.45
1:B:325:VAL:O	1:B:328:LEU:HB2	2.16	0.45
1:C:175:PHE:O	1:C:179:VAL:HG23	2.16	0.45
1:D:186:LEU:HB3	1:D:188:PHE:CE2	2.52	0.45
1:A:55:LEU:O	1:A:59:ILE:HG12	2.17	0.45
1:B:203:GLN:O	1:B:207:VAL:HG23	2.17	0.45
1:B:218:ARG:HH11	1:B:218:ARG:CG	2.30	0.45
1:D:291:ASP:HB2	1:D:292:PRO:HD2	1.97	0.45
1:D:253:MET:O	1:D:256:ASP:HB2	2.17	0.45
1:D:74:GLY:HA2	1:D:102:TRP:CH2	2.51	0.45
1:A:193:VAL:HA	1:A:318:LEU:O	2.17	0.44
1:D:53:ARG:HD3	1:D:171:GLY:O	2.16	0.44
1:D:191:ASP:OD2	1:D:315:SER:HA	2.17	0.44
1:A:241:GLN:NE2	1:A:245:LYS:HD3	2.31	0.44
1:B:234:GLN:HE21	1:B:234:GLN:HB2	1.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLN:N	1:A:4:GLN:CD	2.75	0.44
1:C:129:VAL:HB	1:C:133:PHE:CG	2.52	0.44
1:C:23:ARG:HD3	1:C:285:THR:O	2.18	0.44
1:C:225:SER:O	1:C:226:ALA:HB3	2.18	0.44
1:A:129:VAL:O	1:A:129:VAL:HG23	2.18	0.44
1:B:144:ALA:O	1:B:147:SER:HB3	2.18	0.44
1:B:223:ASP:O	1:B:264:ALA:HB2	2.18	0.44
1:B:148:VAL:HG12	1:B:155:PRO:HD3	2.00	0.43
1:D:237:ARG:O	1:D:241:GLN:HG3	2.18	0.43
1:A:39:GLU:HB2	1:A:321:HIS:O	2.18	0.43
1:A:291:ASP:HB2	1:A:292:PRO:HD2	1.99	0.43
1:B:325:VAL:HG13	1:B:328:LEU:HD22	1.99	0.43
1:C:325:VAL:N	1:C:326:PRO:CD	2.80	0.43
1:D:91:LEU:HD12	1:D:93:MET:HE3	2.00	0.43
1:A:139:ARG:N	4:A:566:HOH:O	2.51	0.43
1:B:99:GLN:CG	1:B:126:VAL:HG13	2.49	0.43
1:D:289:LEU:O	1:D:321:HIS:HE1	2.02	0.43
1:C:177:GLU:OE1	1:C:180:ARG:NH2	2.51	0.43
1:A:336:ARG:HH11	1:A:336:ARG:HG2	1.83	0.43
1:D:99:GLN:HG3	1:D:126:VAL:HG13	2.00	0.43
1:C:135:ILE:HG22	1:C:140:SER:OG	2.17	0.43
1:C:9:TYR:CE1	1:C:91:LEU:HD21	2.54	0.43
1:D:23:ARG:HD3	1:D:285:THR:O	2.19	0.43
1:C:263:PHE:CE2	1:C:301:GLY:HA2	2.54	0.43
1:A:295:GLU:OE2	2:A:401:PLP:N1	2.52	0.43
1:C:19:GLN:NE2	1:D:13:PHE:CE1	2.86	0.43
1:D:39:GLU:CD	1:D:53:ARG:HH21	2.26	0.43
1:D:192:TYR:HB3	1:D:220:ILE:HD13	2.01	0.43
1:C:291:ASP:HB2	1:C:292:PRO:CD	2.49	0.42
1:D:304:GLU:HG3	1:D:308:ASN:ND2	2.34	0.42
1:A:241:GLN:HE22	1:A:245:LYS:HD3	1.83	0.42
1:B:225:SER:O	1:B:226:ALA:HB3	2.19	0.42
1:C:161:GLY:C	1:C:163:SER:H	2.27	0.42
1:C:282:CYS:SG	1:C:288:MET:HE2	2.59	0.42
1:D:31:LYS:HB3	1:D:313:GLU:HG3	2.01	0.42
1:B:218:ARG:NH1	1:B:218:ARG:HG3	2.33	0.42
1:C:70:LEU:HD12	1:C:88:ALA:HB2	1.99	0.42
1:C:135:ILE:HG13	1:C:136:GLY:N	2.34	0.42
1:A:139:ARG:HA	1:A:139:ARG:HD3	1.84	0.42
1:C:336:ARG:HG2	1:C:336:ARG:HH11	1.84	0.42
1:A:179:VAL:O	1:A:183:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:GLY:HA2	1:D:23:ARG:CZ	2.49	0.42
1:D:6:PHE:CZ	1:D:245:LYS:HG2	2.54	0.42
1:C:14:GLY:O	1:C:15:PRO:C	2.61	0.42
1:C:71:VAL:HG22	1:C:96:VAL:HB	2.02	0.42
1:D:70:LEU:HD12	1:D:88:ALA:HB2	2.02	0.42
1:A:112:ARG:HH22	1:C:111:ASP:CG	2.28	0.42
1:B:107:ASP:HB3	1:B:110:TYR:HB2	2.02	0.42
1:D:188:PHE:CD2	1:D:316:ARG:NH1	2.88	0.42
1:C:267:GLU:HB2	1:C:270:LEU:HD12	2.02	0.41
1:D:192:TYR:CD2	1:D:220:ILE:HD11	2.55	0.41
1:B:218:ARG:HA	1:B:218:ARG:HD2	1.88	0.41
1:B:325:VAL:N	1:B:326:PRO:CD	2.83	0.41
1:A:289:LEU:O	1:A:321:HIS:CE1	2.66	0.41
1:D:18:ILE:HA	1:D:36:ALA:O	2.21	0.41
1:A:99:GLN:HB2	1:A:128:LEU:HD23	2.02	0.41
1:A:201:SER:HA	1:A:204:ALA:HB3	2.02	0.41
1:B:195:VAL:HG23	1:B:322:LEU:HD11	2.01	0.41
1:D:79:ASN:OD1	1:D:324:GLY:HA2	2.21	0.41
1:A:260:ASP:OD2	1:A:262:ARG:NH2	2.39	0.41
1:B:188:PHE:CG	1:B:316:ARG:NH1	2.89	0.41
1:C:272:ASN:ND2	1:C:275:THR:H	2.19	0.41
1:D:53:ARG:HD2	1:D:172:PHE:CE1	2.56	0.41
1:D:229:ALA:HA	4:D:574:HOH:O	2.20	0.41
1:A:100:GLU:HB2	1:A:102:TRP:CD1	2.56	0.41
1:A:222:VAL:HG11	1:A:298:SER:HA	2.03	0.41
1:C:230:GLN:HE21	1:C:230:GLN:HB3	1.65	0.40
1:D:51:LYS:O	1:D:55:LEU:HG	2.21	0.40
1:B:73:ILE:HG12	1:B:74:GLY:N	2.37	0.40
1:B:186:LEU:HD13	1:B:188:PHE:CZ	2.57	0.40
1:C:303:ILE:HG22	1:C:307:ARG:HH12	1.85	0.40
1:A:46:ALA:O	1:A:47:PHE:HB2	2.22	0.40
1:A:188:PHE:CE1	1:A:316:ARG:CD	3.05	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	327/338 (97%)	317 (97%)	9 (3%)	1 (0%)	36	55
1	B	324/338 (96%)	317 (98%)	7 (2%)	0	100	100
1	C	336/338 (99%)	319 (95%)	16 (5%)	1 (0%)	36	55
1	D	325/338 (96%)	311 (96%)	14 (4%)	0	100	100
All	All	1312/1352 (97%)	1264 (96%)	46 (4%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	PRO
1	C	139	ARG

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	258/264 (98%)	248 (96%)	10 (4%)	28	55
1	B	255/264 (97%)	249 (98%)	6 (2%)	43	70
1	C	263/264 (100%)	258 (98%)	5 (2%)	50	76
1	D	256/264 (97%)	248 (97%)	8 (3%)	35	62
All	All	1032/1056 (98%)	1003 (97%)	29 (3%)	38	66

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	ARG
1	A	130	PRO
1	A	131	ASP
1	A	139	ARG

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Mol	Chain	Res	Type
1	A	142	GLU
1	A	143	ASP
1	A	177	GLU
1	A	244	GLU
1	A	281	LEU
1	A	328	LEU
1	B	4	GLN
1	B	177	GLU
1	B	218	ARG
1	B	234	GLN
1	B	281	LEU
1	B	328	LEU
1	C	99	GLN
1	C	177	GLU
1	C	248	LEU
1	C	271	PRO
1	C	281	LEU
1	D	3	LEU
1	D	129	VAL
1	D	143	ASP
1	D	177	GLU
1	D	248	LEU
1	D	272	ASN
1	D	281	LEU
1	D	328	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	77	GLN
1	A	90	HIS
1	A	99	GLN
1	A	117	GLN
1	A	230	GLN
1	A	234	GLN
1	A	241	GLN
1	A	272	ASN
1	A	321	HIS
1	B	65	GLN
1	B	77	GLN
1	B	99	GLN

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Mol	Chain	Res	Type
1	B	230	GLN
1	B	234	GLN
1	B	272	ASN
1	B	300	HIS
1	B	321	HIS
1	C	2	ASN
1	C	19	GLN
1	C	77	GLN
1	C	99	GLN
1	C	182	GLN
1	C	230	GLN
1	C	234	GLN
1	C	272	ASN
1	C	321	HIS
1	D	2	ASN
1	D	65	GLN
1	D	77	GLN
1	D	83	GLN
1	D	90	HIS
1	D	241	GLN
1	D	272	ASN
1	D	321	HIS

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 [i](#)

8 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	MLP	C	501	2	5,8,8	4.47	3 (60%)	5,14,14	2.15	2 (40%)
3	MLP	B	501	2	5,8,8	4.69	3 (60%)	5,14,14	2.15	2 (40%)
2	PLP	A	401	1,3	15,15,16	1.65	3 (20%)	21,22,23	1.03	0
2	PLP	B	401	1,3	15,15,16	1.69	2 (13%)	21,22,23	1.09	0
3	MLP	D	501	2	5,8,8	4.76	3 (60%)	5,14,14	2.08	2 (40%)
2	PLP	C	401	1,3	15,15,16	1.54	3 (20%)	21,22,23	1.06	0
3	MLP	A	501	2	5,8,8	4.73	4 (80%)	5,14,14	2.39	2 (40%)
2	PLP	D	401	1,3	15,15,16	1.70	3 (20%)	21,22,23	1.11	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	MLP	C	501	2	-	0/0/13/13	0/1/1/1
3	MLP	B	501	2	-	0/0/13/13	0/1/1/1
2	PLP	A	401	1,3	-	0/6/6/8	0/1/1/1
2	PLP	B	401	1,3	-	0/6/6/8	0/1/1/1
3	MLP	D	501	2	-	0/0/13/13	0/1/1/1
2	PLP	C	401	1,3	-	0/6/6/8	0/1/1/1
3	MLP	A	501	2	-	0/0/13/13	0/1/1/1
2	PLP	D	401	1,3	-	0/6/6/8	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	MLP	C2-C1	-9.34	1.27	1.50
3	A	501	MLP	C2-C1	-9.30	1.27	1.50
3	C	501	MLP	C2-C1	-9.09	1.28	1.50
3	B	501	MLP	C2-C1	-9.03	1.28	1.50
2	B	401	PLP	C5-C4	4.20	1.45	1.40
2	C	401	PLP	C5-C4	4.19	1.45	1.40
2	A	401	PLP	C5-C4	4.03	1.45	1.40
2	D	401	PLP	C3-C2	4.03	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	MLP	P5-O8	4.01	1.57	1.50
3	B	501	MLP	P5-O8	3.78	1.56	1.50
2	D	401	PLP	C5-C4	3.65	1.44	1.40
3	A	501	MLP	P5-O8	3.59	1.56	1.50
2	B	401	PLP	C3-C2	3.38	1.44	1.41
3	C	501	MLP	P5-O8	3.21	1.55	1.50
3	B	501	MLP	P5-O7	-3.13	1.46	1.54
2	A	401	PLP	C3-C2	3.10	1.44	1.41
2	A	401	PLP	C6-C5	2.54	1.42	1.37
2	C	401	PLP	C6-C5	2.47	1.42	1.37
2	D	401	PLP	C6-C5	2.45	1.42	1.37
3	A	501	MLP	P5-O7	-2.36	1.48	1.54
3	D	501	MLP	P5-O7	-2.32	1.48	1.54
3	C	501	MLP	P5-O7	-2.29	1.48	1.54
3	A	501	MLP	P5-C3	-2.20	1.79	1.83
2	C	401	PLP	C3-C2	2.18	1.43	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	MLP	O7-P5-O6	4.29	120.34	108.24
3	B	501	MLP	O7-P5-O6	3.71	118.70	108.24
3	D	501	MLP	O7-P5-O6	3.50	118.11	108.24
3	C	501	MLP	O7-P5-O6	3.49	118.09	108.24
3	C	501	MLP	O6-P5-C3	-2.36	100.58	106.62
3	B	501	MLP	O6-P5-C3	-2.32	100.68	106.62
3	D	501	MLP	O6-P5-C3	-2.28	100.78	106.62
3	A	501	MLP	O6-P5-C3	-2.03	101.41	106.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	MLP	1	0
2	A	401	PLP	1	0
3	A	501	MLP	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	331/338 (97%)	-0.16	3 (0%) 81 78	18, 34, 55, 75	0
1	B	328/338 (97%)	-0.18	2 (0%) 85 83	17, 35, 59, 74	0
1	C	338/338 (100%)	0.04	7 (2%) 63 59	21, 37, 60, 74	0
1	D	329/338 (97%)	0.07	6 (1%) 67 64	22, 39, 63, 78	0
All	All	1326/1352 (98%)	-0.06	18 (1%) 73 70	17, 36, 60, 78	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	135	ILE	4.0
1	A	130	PRO	3.3
1	C	186	LEU	3.0
1	D	140	SER	3.0
1	C	136	GLY	2.9
1	C	188	PHE	2.9
1	B	129	VAL	2.8
1	A	129	VAL	2.6
1	B	140	SER	2.4
1	D	184	ALA	2.2
1	D	251	ASP	2.2
1	D	3	LEU	2.2
1	A	250	ARG	2.2
1	C	133	PHE	2.1
1	C	132	GLY	2.1
1	C	189	LYS	2.1
1	D	1	MET	2.1
1	D	4	GLN	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
3	MLP	D	501	8/8	0.95	0.11	37,38,39,39	0
2	PLP	D	401	15/16	0.96	0.07	27,31,35,35	0
3	MLP	B	501	8/8	0.96	0.08	33,35,36,36	0
3	MLP	C	501	8/8	0.96	0.09	31,34,35,36	0
2	PLP	C	401	15/16	0.96	0.07	29,34,37,38	0
2	PLP	A	401	15/16	0.97	0.07	26,30,33,35	0
2	PLP	B	401	15/16	0.98	0.06	24,28,30,31	0
3	MLP	A	501	8/8	0.99	0.05	28,30,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.