



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 02:23 PM EST

PDB ID : 1K8F
Title : CRYSTAL STRUCTURE OF THE HUMAN C-TERMINAL CAP1-ADENYLYL CYCLASE ASSOCIATED PROTEIN
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Deposited on : 2001-10-24
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

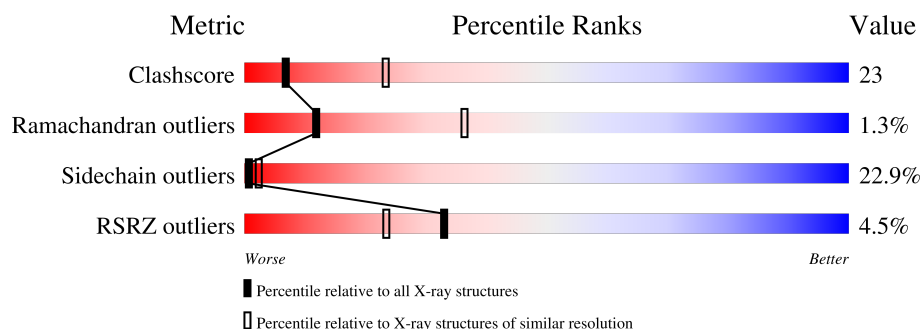
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	157	
1	B	157	
1	C	157	
1	D	157	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4864 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.

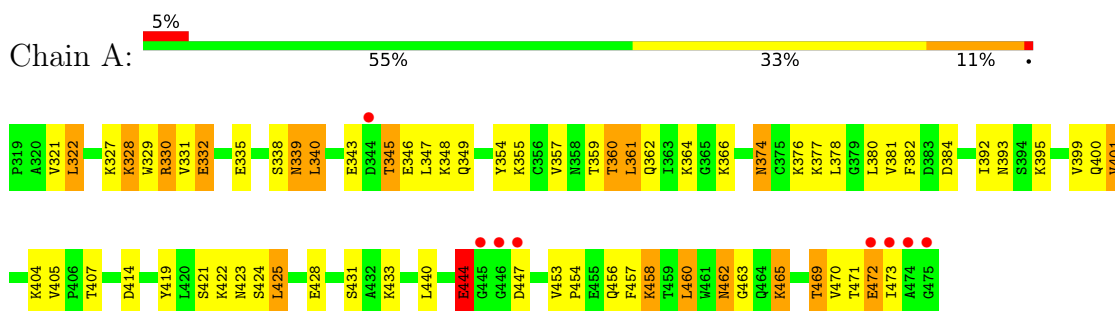
- Molecule 1 is a protein called ADENYLYL CYCLASE-ASSOCIATED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1216	771	198	241	6			
1	B	157	Total	C	N	O	S	0	0	0
			1216	771	198	241	6			
1	C	157	Total	C	N	O	S	0	0	0
			1216	771	198	241	6			
1	D	157	Total	C	N	O	S	0	0	0
			1216	771	198	241	6			

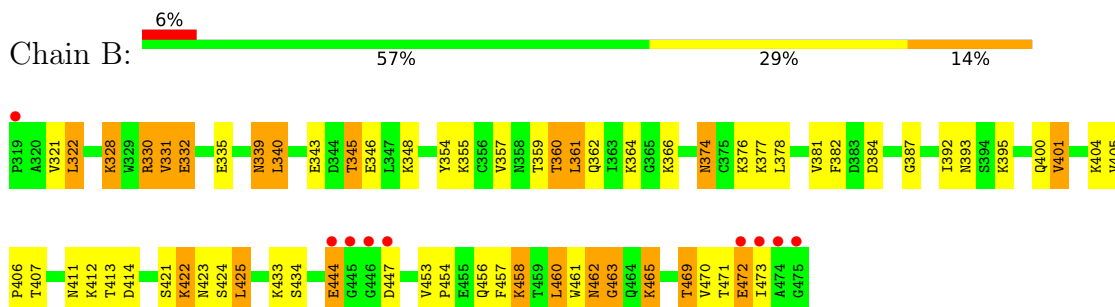
3 Residue-property plots

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.

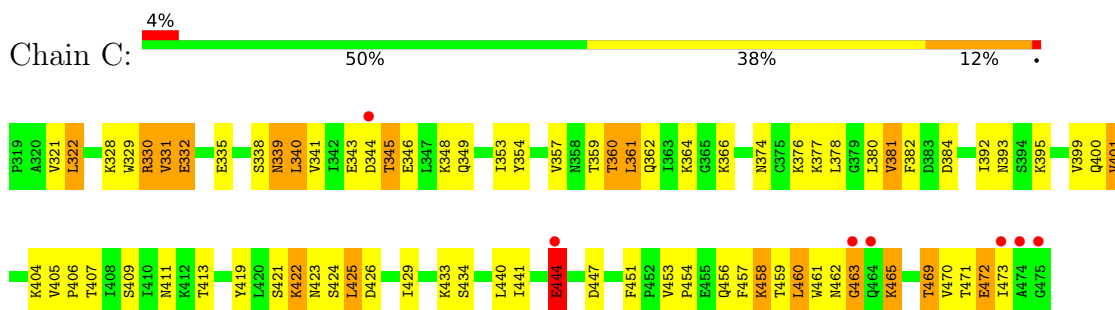
• Molecule 1: ADENYLYL CYCLASE-ASSOCIATED PROTEIN



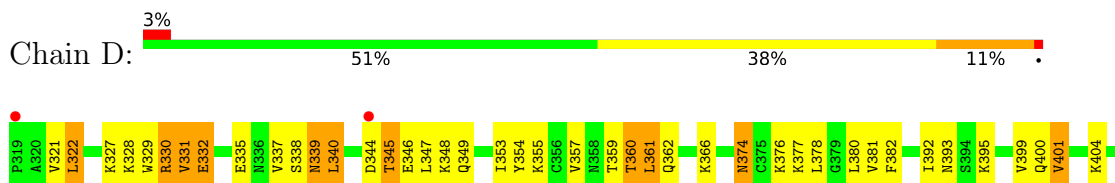
• Molecule 1: ADENYLYL CYCLASE-ASSOCIATED PROTEIN

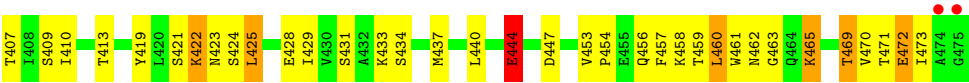


• Molecule 1: ADENYLYL CYCLASE-ASSOCIATED PROTEIN



• Molecule 1: ADENYLYL CYCLASE-ASSOCIATED PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.64Å 83.12Å 99.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 26.56 – 2.79	Depositor EDS
% Data completeness (in resolution range)	93.3 (10.00-2.80) 94.5 (26.56-2.79)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.11 (at 2.80Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.232 , 0.268 0.232 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4864	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	0/1232	0.65	1/1667 (0.1%)
1	B	0.32	0/1232	0.65	1/1667 (0.1%)
1	C	0.31	0/1232	0.64	1/1667 (0.1%)
1	D	0.32	0/1232	0.65	1/1667 (0.1%)
All	All	0.32	0/4928	0.65	4/6668 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	463	GLY	N-CA-C	-5.79	98.64	113.10
1	C	463	GLY	N-CA-C	-5.66	98.94	113.10
1	D	463	GLY	N-CA-C	-5.62	99.04	113.10
1	A	463	GLY	N-CA-C	-5.46	99.44	113.10

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	1216	0	1246	55	0
1	B	1216	0	1246	54	0
1	C	1216	0	1246	70	0
1	D	1216	0	1246	61	0
All	All	4864	0	4984	228	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 23.

All (228) 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:B:339:ASN:HD22	1:B:339:ASN:H	1.08	0.96
1:C:339:ASN:H	1:C:339:ASN:HD22	1.01	0.96
1:A:339:ASN:H	1:A:339:ASN:HD22	1.06	0.94
1:B:339:ASN:N	1:B:339:ASN:HD22	1.70	0.89
1:C:458:LYS:HE3	1:C:460:LEU:HD22	1.54	0.89
1:C:339:ASN:HD22	1:C:339:ASN:N	1.68	0.88
1:A:339:ASN:HD22	1:A:339:ASN:N	1.71	0.88
1:B:458:LYS:HE3	1:B:460:LEU:HD22	1.54	0.87
1:C:339:ASN:ND2	1:C:339:ASN:H	1.74	0.86
1:D:458:LYS:HE3	1:D:460:LEU:HD22	1.56	0.85
1:D:339:ASN:HD22	1:D:339:ASN:H	1.23	0.84
1:A:458:LYS:HE3	1:A:460:LEU:HD22	1.60	0.84
1:D:339:ASN:HD22	1:D:339:ASN:N	1.76	0.81
1:B:339:ASN:ND2	1:B:339:ASN:H	1.77	0.80
1:A:361:LEU:HD22	1:A:362:GLN:N	1.99	0.77
1:A:339:ASN:ND2	1:A:339:ASN:H	1.81	0.76
1:C:462:ASN:HB2	1:C:465:LYS:O	1.84	0.76
1:C:433:LYS:HA	1:D:433:LYS:HA	1.67	0.75
1:C:361:LEU:HD22	1:C:362:GLN:N	2.03	0.74
1:B:361:LEU:HD22	1:B:362:GLN:N	2.04	0.73
1:D:361:LEU:HD22	1:D:362:GLN:N	2.04	0.73
1:D:339:ASN:H	1:D:339:ASN:ND2	1.87	0.73
1:C:456:GLN:HE21	1:C:471:THR:HG21	1.56	0.71
1:A:457:PHE:CE2	1:A:470:VAL:HG22	2.27	0.70
1:B:456:GLN:HE21	1:B:471:THR:HG21	1.56	0.70
1:D:457:PHE:CE2	1:D:470:VAL:HG22	2.26	0.69
1:C:458:LYS:HD3	1:C:469:THR:HB	1.76	0.68
1:A:462:ASN:HB2	1:A:465:LYS:O	1.94	0.66
1:B:392:ILE:HG12	1:B:393:ASN:OD1	1.96	0.65
1:C:382:PHE:CZ	1:C:401:VAL:HG13	2.31	0.65
1:A:458:LYS:NZ	1:A:469:THR:HB	2.11	0.65
1:C:458:LYS:NZ	1:C:469:THR:HB	2.12	0.65
1:B:462:ASN:HB2	1:B:465:LYS:O	1.96	0.64
1:B:458:LYS:HD3	1:B:469:THR:HB	1.78	0.64
1:C:357:VAL:HA	1:C:376:LYS:O	1.96	0.64
1:C:382:PHE:CE1	1:C:401:VAL:HG13	2.32	0.64
1:D:392:ILE:HG12	1:D:393:ASN:OD1	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:462:ASN:HB2	1:D:465:LYS:O	1.97	0.63
1:C:392:ILE:HG12	1:C:393:ASN:OD1	1.98	0.63
1:D:357:VAL:HA	1:D:376:LYS:O	2.00	0.62
1:B:457:PHE:CE2	1:B:470:VAL:HG22	2.34	0.62
1:A:382:PHE:CE1	1:A:401:VAL:HG13	2.35	0.62
1:B:357:VAL:HA	1:B:376:LYS:O	1.99	0.62
1:A:382:PHE:CZ	1:A:401:VAL:HG13	2.35	0.61
1:A:321:VAL:HB	1:A:332:GLU:HG3	1.81	0.61
1:A:357:VAL:HA	1:A:376:LYS:O	2.01	0.61
1:A:361:LEU:HD22	1:A:362:GLN:H	1.63	0.61
1:A:457:PHE:CD2	1:A:470:VAL:HG22	2.36	0.61
1:A:454:PRO:HA	1:A:473:ILE:HG12	1.83	0.61
1:B:321:VAL:HB	1:B:332:GLU:HG3	1.83	0.61
1:B:454:PRO:HA	1:B:473:ILE:HG12	1.83	0.60
1:C:361:LEU:HD22	1:C:362:GLN:H	1.66	0.60
1:C:421:SER:O	1:C:425:LEU:HD13	2.02	0.60
1:A:456:GLN:HE21	1:A:471:THR:HG21	1.67	0.59
1:D:321:VAL:HB	1:D:332:GLU:HG3	1.84	0.59
1:A:458:LYS:HD3	1:A:469:THR:HB	1.83	0.59
1:C:321:VAL:HB	1:C:332:GLU:HG3	1.84	0.58
1:D:457:PHE:CD2	1:D:470:VAL:HG22	2.37	0.58
1:D:382:PHE:CE1	1:D:401:VAL:HG13	2.39	0.58
1:A:392:ILE:HG12	1:A:393:ASN:OD1	2.04	0.58
1:D:454:PRO:HA	1:D:473:ILE:HG12	1.84	0.58
1:D:458:LYS:NZ	1:D:469:THR:HB	2.19	0.58
1:A:472:GLU:CD	1:A:472:GLU:N	2.58	0.57
1:D:454:PRO:HA	1:D:473:ILE:CG1	2.34	0.57
1:B:472:GLU:H	1:B:472:GLU:CD	2.06	0.57
1:B:382:PHE:CE1	1:B:401:VAL:HG13	2.40	0.57
1:C:472:GLU:CD	1:C:472:GLU:H	2.08	0.56
1:B:458:LYS:NZ	1:B:469:THR:HB	2.20	0.56
1:C:461:TRP:NE1	1:C:463:GLY:HA2	2.19	0.56
1:B:454:PRO:HA	1:B:473:ILE:CG1	2.35	0.56
1:B:472:GLU:N	1:B:472:GLU:CD	2.58	0.56
1:C:451:PHE:CZ	1:D:461:TRP:CH2	2.94	0.56
1:A:454:PRO:HA	1:A:473:ILE:CG1	2.36	0.55
1:D:419:TYR:CE2	1:D:440:LEU:HG	2.41	0.55
1:D:458:LYS:HD3	1:D:469:THR:HB	1.89	0.55
1:A:472:GLU:H	1:A:472:GLU:CD	2.09	0.55
1:D:361:LEU:HD22	1:D:362:GLN:H	1.70	0.55
1:D:404:LYS:HE2	1:D:423:ASN:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:GLU:CD	1:C:472:GLU:N	2.59	0.55
1:C:457:PHE:CE2	1:C:470:VAL:HG22	2.42	0.55
1:A:458:LYS:CE	1:A:460:LEU:HD22	2.35	0.54
1:A:339:ASN:ND2	1:A:339:ASN:N	2.42	0.54
1:B:382:PHE:CZ	1:B:401:VAL:HG13	2.42	0.54
1:C:454:PRO:HA	1:C:473:ILE:CG1	2.38	0.54
1:B:361:LEU:HD22	1:B:362:GLN:H	1.71	0.54
1:A:404:LYS:HE2	1:A:423:ASN:O	2.08	0.53
1:C:454:PRO:HA	1:C:473:ILE:HG12	1.89	0.53
1:A:414:ASP:OD2	1:B:433:LYS:HE3	2.08	0.53
1:D:457:PHE:HE2	1:D:470:VAL:HG22	1.73	0.53
1:C:366:LYS:HG3	1:C:384:ASP:HB3	1.91	0.52
1:D:472:GLU:CD	1:D:472:GLU:N	2.63	0.52
1:C:404:LYS:HA	1:C:424:SER:HB3	1.91	0.52
1:D:456:GLN:HE21	1:D:471:THR:HG21	1.74	0.52
1:A:332:GLU:HB3	1:A:354:TYR:HB3	1.91	0.52
1:B:457:PHE:CD2	1:B:470:VAL:HG22	2.45	0.52
1:A:347:LEU:CD1	1:A:366:LYS:HD3	2.40	0.52
1:B:458:LYS:CE	1:B:460:LEU:HD22	2.35	0.52
1:C:459:THR:HB	1:D:429:ILE:HB	1.91	0.52
1:C:404:LYS:HE2	1:C:423:ASN:O	2.10	0.51
1:A:457:PHE:HE2	1:A:470:VAL:HG22	1.74	0.51
1:C:458:LYS:HG3	1:D:428:GLU:OE2	2.10	0.51
1:C:359:THR:HG22	1:C:360:THR:N	2.24	0.51
1:A:458:LYS:HZ2	1:A:469:THR:HB	1.75	0.51
1:D:332:GLU:HB3	1:D:354:TYR:HB3	1.92	0.50
1:C:380:LEU:HD23	1:C:399:VAL:HG13	1.93	0.50
1:B:421:SER:O	1:B:425:LEU:HD13	2.11	0.50
1:D:359:THR:HG22	1:D:360:THR:N	2.26	0.50
1:D:380:LEU:HD23	1:D:399:VAL:HG13	1.93	0.50
1:C:332:GLU:HB3	1:C:354:TYR:HB3	1.93	0.49
1:A:428:GLU:OE2	1:B:458:LYS:HG3	2.12	0.49
1:D:322:LEU:HA	1:D:330:ARG:O	2.12	0.49
1:A:359:THR:HG22	1:A:360:THR:N	2.25	0.49
1:C:451:PHE:CZ	1:D:461:TRP:HH2	2.29	0.49
1:D:472:GLU:CD	1:D:472:GLU:H	2.14	0.49
1:B:366:LYS:HG3	1:B:384:ASP:HB3	1.94	0.49
1:C:357:VAL:HB	1:C:376:LYS:HB3	1.95	0.49
1:B:404:LYS:HA	1:B:424:SER:HB3	1.93	0.49
1:C:331:VAL:HG22	1:C:331:VAL:O	2.12	0.48
1:D:382:PHE:CZ	1:D:401:VAL:HG13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:GLU:OE2	1:C:364:LYS:HD2	2.13	0.48
1:A:343:GLU:OE2	1:A:364:LYS:HD2	2.14	0.48
1:B:461:TRP:NE1	1:B:463:GLY:HA2	2.28	0.48
1:B:404:LYS:HE2	1:B:423:ASN:O	2.14	0.48
1:D:413:THR:O	1:D:434:SER:HB3	2.13	0.48
1:C:458:LYS:HZ2	1:C:469:THR:HB	1.79	0.48
1:D:329:TRP:NE1	1:D:349:GLN:OE1	2.45	0.48
1:A:472:GLU:OE1	1:A:472:GLU:N	2.48	0.47
1:A:340:LEU:HB3	1:A:361:LEU:HD23	1.95	0.47
1:B:332:GLU:HB3	1:B:354:TYR:HB3	1.97	0.47
1:B:343:GLU:OE2	1:B:364:LYS:HD2	2.14	0.47
1:D:340:LEU:HB3	1:D:361:LEU:HD23	1.97	0.47
1:A:322:LEU:HA	1:A:330:ARG:O	2.14	0.47
1:C:322:LEU:HA	1:C:330:ARG:O	2.15	0.47
1:D:458:LYS:CE	1:D:460:LEU:HD22	2.38	0.47
1:B:322:LEU:HA	1:B:330:ARG:O	2.15	0.47
1:D:329:TRP:HZ2	1:D:344:ASP:OD2	1.98	0.47
1:C:441:ILE:HG13	1:D:461:TRP:CE2	2.49	0.46
1:D:421:SER:O	1:D:425:LEU:HD13	2.15	0.46
1:A:322:LEU:CD2	1:A:340:LEU:HG	2.45	0.46
1:C:366:LYS:HG3	1:C:384:ASP:CB	2.44	0.46
1:C:405:VAL:O	1:C:405:VAL:HG13	2.15	0.46
1:B:359:THR:HG22	1:B:360:THR:N	2.31	0.46
1:C:339:ASN:ND2	1:C:339:ASN:N	2.39	0.46
1:C:340:LEU:HB3	1:C:361:LEU:HD23	1.98	0.46
1:A:329:TRP:NE1	1:A:349:GLN:OE1	2.45	0.46
1:B:405:VAL:HG13	1:B:405:VAL:O	2.15	0.46
1:C:461:TRP:HE1	1:C:463:GLY:HA2	1.80	0.46
1:C:422:LYS:HA	1:C:422:LYS:HD2	1.78	0.45
1:A:405:VAL:HG13	1:A:405:VAL:O	2.17	0.45
1:C:413:THR:O	1:C:434:SER:HB3	2.17	0.45
1:C:444:GLU:H	1:C:444:GLU:HG2	1.43	0.45
1:D:331:VAL:O	1:D:353:ILE:HA	2.16	0.45
1:D:355:LYS:HA	1:D:374:ASN:O	2.17	0.45
1:B:472:GLU:N	1:B:472:GLU:OE1	2.48	0.45
1:D:332:GLU:HA	1:D:354:TYR:O	2.16	0.45
1:D:338:SER:HA	1:D:360:THR:HB	1.97	0.45
1:B:355:LYS:HA	1:B:374:ASN:O	2.16	0.45
1:A:419:TYR:CE2	1:A:440:LEU:HG	2.52	0.45
1:A:457:PHE:CE1	1:B:457:PHE:CE1	3.05	0.45
1:B:331:VAL:O	1:B:331:VAL:HG22	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:TYR:CE2	1:C:440:LEU:HG	2.52	0.44
1:A:355:LYS:HA	1:A:374:ASN:O	2.17	0.44
1:C:339:ASN:O	1:C:341:VAL:HG23	2.18	0.44
1:C:457:PHE:CD2	1:C:470:VAL:HG22	2.52	0.44
1:D:404:LYS:HA	1:D:424:SER:HB3	1.99	0.44
1:A:433:LYS:HE3	1:B:414:ASP:OD2	2.18	0.44
1:B:457:PHE:HE2	1:B:470:VAL:HG22	1.79	0.44
1:B:456:GLN:NE2	1:B:471:THR:HG21	2.26	0.44
1:B:339:ASN:N	1:B:339:ASN:ND2	2.39	0.44
1:B:456:GLN:HE21	1:B:471:THR:CG2	2.29	0.44
1:D:444:GLU:HG2	1:D:444:GLU:H	1.37	0.44
1:D:354:TYR:CZ	1:D:355:LYS:HD2	2.52	0.44
1:C:329:TRP:NE1	1:C:349:GLN:OE1	2.48	0.44
1:B:422:LYS:HD2	1:B:422:LYS:HA	1.74	0.43
1:B:456:GLN:HB3	1:B:471:THR:OG1	2.18	0.43
1:C:329:TRP:HZ2	1:C:344:ASP:OD2	2.01	0.43
1:A:454:PRO:HG2	1:A:470:VAL:HG11	2.00	0.43
1:A:328:LYS:HD2	1:A:330:ARG:HG2	2.01	0.43
1:D:347:LEU:CD1	1:D:366:LYS:HD3	2.49	0.43
1:B:354:TYR:CE2	1:B:355:LYS:HD2	2.54	0.43
1:C:331:VAL:O	1:C:353:ILE:HA	2.18	0.43
1:D:454:PRO:HG2	1:D:470:VAL:HG11	2.00	0.43
1:D:456:GLN:HB3	1:D:471:THR:OG1	2.19	0.43
1:A:456:GLN:NE2	1:A:471:THR:HG21	2.33	0.43
1:A:359:THR:CG2	1:A:360:THR:N	2.81	0.42
1:B:328:LYS:HD2	1:B:330:ARG:HG2	2.01	0.42
1:C:458:LYS:CE	1:C:460:LEU:HD22	2.38	0.42
1:C:429:ILE:HB	1:D:459:THR:HB	2.01	0.42
1:C:461:TRP:CZ3	1:C:465:LYS:HA	2.54	0.42
1:D:331:VAL:O	1:D:331:VAL:HG22	2.20	0.42
1:A:332:GLU:HA	1:A:354:TYR:O	2.19	0.42
1:C:456:GLN:HG2	1:C:457:PHE:N	2.35	0.42
1:C:359:THR:CG2	1:C:360:THR:N	2.82	0.42
1:C:456:GLN:NE2	1:C:471:THR:HG21	2.30	0.42
1:B:413:THR:O	1:B:434:SER:HB3	2.20	0.42
1:C:322:LEU:C	1:C:322:LEU:HD12	2.40	0.42
1:D:329:TRP:CZ2	1:D:344:ASP:OD1	2.73	0.42
1:A:366:LYS:HG3	1:A:384:ASP:HB3	2.02	0.42
1:A:327:LYS:HB3	1:A:327:LYS:HE3	1.87	0.41
1:A:404:LYS:HA	1:A:424:SER:HB3	2.02	0.41
1:B:357:VAL:HB	1:B:376:LYS:HB3	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:ASN:ND2	1:D:339:ASN:N	2.43	0.41
1:A:421:SER:O	1:A:425:LEU:HD13	2.20	0.41
1:C:458:LYS:CD	1:C:469:THR:HB	2.48	0.41
1:B:387:GLY:O	1:B:406:PRO:HD2	2.21	0.41
1:C:338:SER:HA	1:C:360:THR:HB	2.02	0.41
1:D:327:LYS:HE3	1:D:327:LYS:HB3	1.90	0.41
1:A:338:SER:HA	1:A:360:THR:HB	2.02	0.41
1:A:380:LEU:HD23	1:A:399:VAL:HG13	2.01	0.41
1:B:393:ASN:ND2	1:B:412:LYS:HD2	2.35	0.41
1:C:426:ASP:OD1	1:C:426:ASP:N	2.53	0.41
1:C:457:PHE:HE2	1:C:470:VAL:HG22	1.86	0.41
1:D:359:THR:CG2	1:D:360:THR:N	2.83	0.41
1:C:322:LEU:CD2	1:C:340:LEU:HG	2.51	0.41
1:C:441:ILE:HG13	1:D:461:TRP:CD2	2.55	0.41
1:D:322:LEU:CD2	1:D:340:LEU:HG	2.51	0.41
1:B:392:ILE:HA	1:B:411:ASN:O	2.21	0.41
1:C:332:GLU:HA	1:C:354:TYR:O	2.21	0.41
1:C:405:VAL:HA	1:C:406:PRO:HD3	1.92	0.41
1:D:410:ILE:HD13	1:D:437:MET:HG2	2.02	0.41
1:A:444:GLU:H	1:A:444:GLU:HG2	1.35	0.41
1:B:332:GLU:HA	1:B:354:TYR:O	2.21	0.41
1:B:340:LEU:HB3	1:B:361:LEU:HD23	2.02	0.40
1:D:422:LYS:HD2	1:D:422:LYS:HA	1.77	0.40
1:C:362:GLN:HA	1:C:381:VAL:O	2.22	0.40
1:C:392:ILE:HA	1:C:411:ASN:O	2.21	0.40
1:A:322:LEU:HD12	1:A:322:LEU:C	2.42	0.40
1:D:354:TYR:CE2	1:D:355:LYS:HD2	2.57	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	155/157 (99%)	138 (89%)	15 (10%)	2 (1%)	12	36
1	B	155/157 (99%)	138 (89%)	15 (10%)	2 (1%)	12	36
1	C	155/157 (99%)	137 (88%)	16 (10%)	2 (1%)	12	36
1	D	155/157 (99%)	138 (89%)	15 (10%)	2 (1%)	12	36
All	All	620/628 (99%)	551 (89%)	61 (10%)	8 (1%)	12	36

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	444	GLU
1	B	444	GLU
1	C	444	GLU
1	D	444	GLU
1	B	345	THR
1	D	345	THR
1	A	345	THR
1	C	345	THR

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	142/142 (100%)	109 (77%)	33 (23%)	1	2
1	B	142/142 (100%)	110 (78%)	32 (22%)	1	2
1	C	142/142 (100%)	110 (78%)	32 (22%)	1	2
1	D	142/142 (100%)	109 (77%)	33 (23%)	1	2
All	All	568/568 (100%)	438 (77%)	130 (23%)	1	2

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	LEU
1	A	328	LYS
1	A	330	ARG

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Mol	Chain	Res	Type
1	A	331	VAL
1	A	332	GLU
1	A	335	GLU
1	A	339	ASN
1	A	340	LEU
1	A	345	THR
1	A	346	GLU
1	A	348	LYS
1	A	360	THR
1	A	361	LEU
1	A	374	ASN
1	A	377	LYS
1	A	378	LEU
1	A	381	VAL
1	A	395	LYS
1	A	400	GLN
1	A	401	VAL
1	A	407	THR
1	A	422	LYS
1	A	425	LEU
1	A	431	SER
1	A	444	GLU
1	A	447	ASP
1	A	453	VAL
1	A	458	LYS
1	A	460	LEU
1	A	462	ASN
1	A	465	LYS
1	A	469	THR
1	A	472	GLU
1	B	322	LEU
1	B	328	LYS
1	B	330	ARG
1	B	331	VAL
1	B	332	GLU
1	B	335	GLU
1	B	339	ASN
1	B	340	LEU
1	B	345	THR
1	B	346	GLU
1	B	348	LYS
1	B	360	THR

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Mol	Chain	Res	Type
1	B	361	LEU
1	B	374	ASN
1	B	377	LYS
1	B	378	LEU
1	B	381	VAL
1	B	395	LYS
1	B	400	GLN
1	B	401	VAL
1	B	407	THR
1	B	422	LYS
1	B	425	LEU
1	B	444	GLU
1	B	447	ASP
1	B	453	VAL
1	B	458	LYS
1	B	460	LEU
1	B	462	ASN
1	B	465	LYS
1	B	469	THR
1	B	472	GLU
1	C	322	LEU
1	C	328	LYS
1	C	330	ARG
1	C	331	VAL
1	C	332	GLU
1	C	335	GLU
1	C	339	ASN
1	C	340	LEU
1	C	345	THR
1	C	346	GLU
1	C	348	LYS
1	C	360	THR
1	C	361	LEU
1	C	374	ASN
1	C	377	LYS
1	C	378	LEU
1	C	381	VAL
1	C	395	LYS
1	C	400	GLN
1	C	401	VAL
1	C	407	THR
1	C	409	SER

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Mol	Chain	Res	Type
1	C	422	LYS
1	C	425	LEU
1	C	444	GLU
1	C	447	ASP
1	C	453	VAL
1	C	458	LYS
1	C	460	LEU
1	C	465	LYS
1	C	469	THR
1	C	472	GLU
1	D	322	LEU
1	D	328	LYS
1	D	330	ARG
1	D	331	VAL
1	D	332	GLU
1	D	335	GLU
1	D	337	VAL
1	D	339	ASN
1	D	340	LEU
1	D	345	THR
1	D	346	GLU
1	D	348	LYS
1	D	360	THR
1	D	361	LEU
1	D	374	ASN
1	D	377	LYS
1	D	378	LEU
1	D	381	VAL
1	D	395	LYS
1	D	400	GLN
1	D	401	VAL
1	D	407	THR
1	D	409	SER
1	D	422	LYS
1	D	425	LEU
1	D	431	SER
1	D	444	GLU
1	D	447	ASP
1	D	453	VAL
1	D	460	LEU
1	D	465	LYS
1	D	469	THR

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Mol	Chain	Res	Type
1	D	472	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	ASN
1	A	362	GLN
1	A	417	HIS
1	A	449	ASN
1	A	456	GLN
1	A	464	GLN
1	B	339	ASN
1	B	362	GLN
1	B	417	HIS
1	B	438	ASN
1	B	449	ASN
1	B	456	GLN
1	B	464	GLN
1	C	339	ASN
1	C	362	GLN
1	C	417	HIS
1	C	449	ASN
1	C	456	GLN
1	C	464	GLN
1	D	339	ASN
1	D	362	GLN
1	D	417	HIS
1	D	449	ASN
1	D	456	GLN
1	D	464	GLN

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	157/157 (100%)	-0.01	8 (5%) 28 19	4, 16, 44, 90	0
1	B	157/157 (100%)	-0.01	9 (5%) 23 15	2, 17, 46, 92	0
1	C	157/157 (100%)	0.04	7 (4%) 33 23	4, 19, 43, 89	0
1	D	157/157 (100%)	0.03	4 (2%) 57 47	4, 17, 41, 91	0
All	All	628/628 (100%)	0.01	28 (4%) 33 23	2, 18, 44, 92	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	475	GLY	13.6
1	B	475	GLY	11.5
1	B	474	ALA	10.1
1	D	475	GLY	10.0
1	C	475	GLY	9.1
1	D	474	ALA	8.8
1	A	446	GLY	4.1
1	B	473	ILE	4.1
1	C	474	ALA	4.0
1	A	474	ALA	3.8
1	B	319	PRO	3.5
1	C	344	ASP	3.3
1	B	444	GLU	3.1
1	D	344	ASP	3.1
1	C	464	GLN	2.8
1	C	463	GLY	2.8
1	B	447	ASP	2.7
1	A	447	ASP	2.6
1	C	444	GLU	2.5
1	D	319	PRO	2.4
1	A	344	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	445	GLY	2.3
1	A	473	ILE	2.3
1	B	446	GLY	2.3
1	A	472	GLU	2.3
1	B	445	GLY	2.2
1	C	473	ILE	2.1
1	B	472	GLU	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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.