



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:38 AM GMT

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 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/ValidationPDFNotes.html>

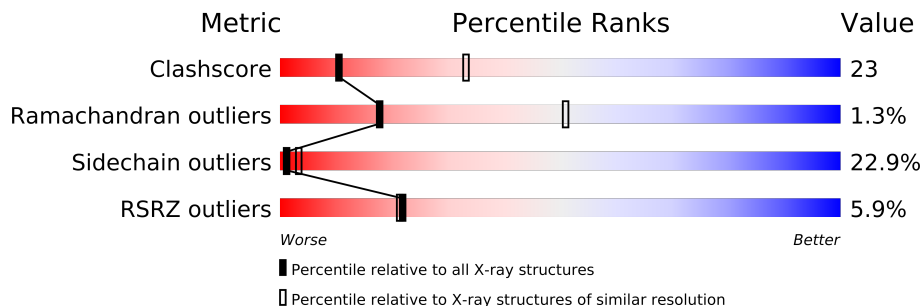
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance





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	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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.

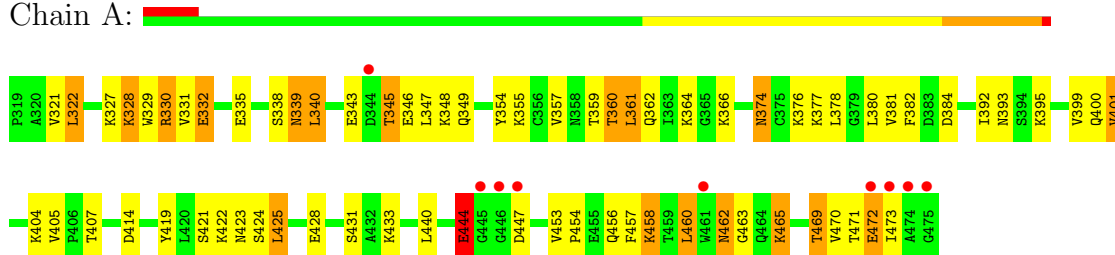
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1216	771	198	241	6			
1	B	157	Total	C	N	O	S	0	0	0
			1216	771	198	241	6			
1	C	157	Total	C	N	O	S	0	0	0
			1216	771	198	241	6			
1	D	157	Total	C	N	O	S	0	0	0
			1216	771	198	241	6			

3 Residue-property plots

These plots are drawn for all protein, RNA 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: ADENYLYL CYCLASE-ASSOCIATED PROTEIN

Chain A:



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.	DCC
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 13.7	EDS
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 16711 reflections	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1216	0	1246	61	0
All	All	4864	0	4984	228	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

All (228) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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:361:LEU:HD22	1:A:362:GLN:H	1.63	0.61
1:A:454:PRO:HA	1:A:473:ILE:HG12	1.83	0.61
1:A:457:PHE:CD2	1:A:470:VAL:HG22	2.36	0.61
1:B:321:VAL:HB	1:B:332:GLU:HG3	1.83	0.61
1:A:357:VAL:HA	1:A:376:LYS:O	2.01	0.61
1:C:361:LEU:HD22	1:C:362:GLN:H	1.66	0.60
1:B:454:PRO:HA	1:B:473:ILE:HG12	1.83	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:458:LYS:NZ	1:D:469:THR:HB	2.19	0.58
1:D:454:PRO:HA	1:D:473:ILE:HG12	1.84	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:D:458:LYS:HD3	1:D:469:THR:HB	1.89	0.55
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:361:LEU:HD22	1:D:362:GLN:H	1.70	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:472:GLU:H	1:A:472:GLU:CD	2.09	0.55
1:D:404:LYS:HE2	1:D:423:ASN:O	2.06	0.55
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:C:454:PRO:HA	1:C:473:ILE:HG12	1.89	0.53
1:A:404:LYS:HE2	1:A:423:ASN:O	2.08	0.53
1:D:457:PHE:HE2	1:D:470:VAL:HG22	1.73	0.53
1:A:414:ASP:OD2	1:B:433:LYS:HE3	2.08	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:B:457:PHE:CD2	1:B:470:VAL:HG22	2.45	0.52
1:A:332:GLU:HB3	1:A:354:TYR:HB3	1.91	0.52
1:B:458:LYS:CE	1:B:460:LEU:HD22	2.35	0.52
1:A:347:LEU:CD1	1:A:366:LYS:HD3	2.40	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:D:380:LEU:HD23	1:D: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: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: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:A:359:THR:HG22	1:A:360:THR:N	2.25	0.49
1:C:357:VAL:HB	1:C:376:LYS:HB3	1.95	0.49
1:B:366:LYS:HG3	1:B:384:ASP:HB3	1.94	0.49
1:B:404:LYS:HA	1:B:424:SER:HB3	1.93	0.49
1:D:382:PHE:CZ	1:D:401:VAL:HG13	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:331:VAL:HG22	1:C:331:VAL:O	2.12	0.48
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:D:340:LEU:HB3	1:D:361:LEU:HD23	1.97	0.47
1:B:343:GLU:OE2	1:B:364:LYS:HD2	2.14	0.47
1:A:322:LEU:HA	1:A:330:ARG:O	2.14	0.47
1:D:458:LYS:CE	1:D:460:LEU:HD22	2.38	0.47
1:C:322:LEU:HA	1:C:330:ARG:O	2.15	0.47
1:D:329:TRP:HZ2	1:D:344:ASP:OD2	1.98	0.47
1:B:322:LEU:HA	1:B:330:ARG:O	2.15	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: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:B:359:THR:HG22	1:B:360:THR:N	2.31	0.46
1:A:329:TRP:NE1	1:A:349:GLN:OE1	2.45	0.46
1:C:461:TRP:HE1	1:C:463:GLY:HA2	1.80	0.46
1:B:405:VAL:HG13	1:B:405:VAL:O	2.15	0.46
1:C:422:LYS:HA	1:C:422:LYS:HD2	1.78	0.45
1:C:413:THR:O	1:C:434:SER:HB3	2.17	0.45
1:A:405:VAL:HG13	1:A:405:VAL:O	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:D:332:GLU:HA	1:D:354:TYR:O	2.16	0.45
1:B:472:GLU:N	1:B:472:GLU:OE1	2.48	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:C:419:TYR:CE2	1:C:440:LEU:HG	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:331:VAL:O	1:B:331:VAL:HG22	2.16	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:355:LYS:HA	1:A:374:ASN:O	2.17	0.44
1:B:457:PHE:HE2	1:B:470:VAL:HG22	1.79	0.44
1:A:433:LYS:HE3	1:B:414:ASP:OD2	2.18	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: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:B:422:LYS:HD2	1:B:422:LYS:HA	1.74	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:D:454:PRO:HG2	1:D:470:VAL:HG11	2.00	0.43
1:B:354:TYR:CE2	1:B:355:LYS:HD2	2.54	0.43
1:D:456:GLN:HB3	1:D:471:THR:OG1	2.19	0.43
1:C:331:VAL:O	1:C:353:ILE:HA	2.18	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:C:458:LYS:CE	1:C:460:LEU:HD22	2.38	0.42
1:B:328:LYS:HD2	1:B:330:ARG:HG2	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:C:429:ILE:HB	1:D:459:THR:HB	2.01	0.42
1:C:456:GLN:HG2	1:C:457:PHE:N	2.35	0.42
1:A:332:GLU:HA	1:A:354:TYR:O	2.19	0.42
1:C:456:GLN:NE2	1:C:471:THR:HG21	2.30	0.42
1:C:359:THR:CG2	1:C:360:THR:N	2.82	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:B:413:THR:O	1:B:434:SER:HB3	2.20	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:D:339:ASN:ND2	1:D:339:ASN:N	2.43	0.41
1:B:357:VAL:HB	1:B:376:LYS:HB3	2.00	0.41
1:A:404:LYS:HA	1:A:424:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:458:LYS:CD	1:C:469:THR:HB	2.48	0.41
1:A:421:SER:O	1:A:425:LEU:HD13	2.20	0.41
1:C:338:SER:HA	1:C:360:THR:HB	2.02	0.41
1:B:387:GLY:O	1:B:406:PRO:HD2	2.21	0.41
1:D:327:LYS:HE3	1:D:327:LYS:HB3	1.90	0.41
1:C:457:PHE:HE2	1:C:470:VAL:HG22	1.86	0.41
1:B:393:ASN:ND2	1:B:412:LYS:HD2	2.35	0.41
1:D:359:THR:CG2	1:D:360:THR:N	2.83	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:C:426:ASP:OD1	1:C:426:ASP:N	2.53	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%)	18	51
1	B	155/157 (99%)	138 (89%)	15 (10%)	2 (1%)	18	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	155/157 (99%)	137 (88%)	16 (10%)	2 (1%)	18	51
1	D	155/157 (99%)	138 (89%)	15 (10%)	2 (1%)	18	51
All	All	620/628 (99%)	551 (89%)	61 (10%)	8 (1%)	18	51

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	3
1	B	142/142 (100%)	110 (78%)	32 (22%)	1	3
1	C	142/142 (100%)	110 (78%)	32 (22%)	1	3
1	D	142/142 (100%)	109 (77%)	33 (23%)	1	3
All	All	568/568 (100%)	438 (77%)	130 (23%)	1	3

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
1	A	331	VAL
1	A	332	GLU
1	A	335	GLU

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Mol	Chain	Res	Type
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
1	B	361	LEU
1	B	374	ASN
1	B	377	LYS

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Mol	Chain	Res	Type
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
1	C	422	LYS
1	C	425	LEU
1	C	444	GLU

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Mol	Chain	Res	Type
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
1	D	472	GLU

Some 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 chains 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 ⓘ

There are no ligands in this entry.

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	157/157 (100%)	0.12	9 (5%) 23 23	4, 16, 44, 90	0
1	B	157/157 (100%)	0.14	11 (7%) 16 14	2, 17, 46, 92	0
1	C	157/157 (100%)	0.20	10 (6%) 19 17	4, 19, 43, 89	0
1	D	157/157 (100%)	0.16	7 (4%) 32 33	4, 17, 41, 91	0
All	All	628/628 (100%)	0.16	37 (5%) 22 21	2, 18, 44, 92	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	475	GLY	14.2
1	B	474	ALA	13.6
1	B	475	GLY	13.3
1	D	474	ALA	10.5
1	D	475	GLY	10.0
1	C	475	GLY	9.9
1	A	474	ALA	5.3
1	B	473	ILE	5.1
1	C	474	ALA	4.7
1	A	446	GLY	4.4
1	B	319	PRO	4.2
1	C	344	ASP	3.8
1	D	344	ASP	3.7
1	C	464	GLN	3.6
1	C	463	GLY	3.5
1	A	447	ASP	3.4
1	A	472	GLU	3.4
1	B	444	GLU	3.3
1	B	447	ASP	3.3
1	B	472	GLU	3.1
1	D	319	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	444	GLU	2.8
1	A	473	ILE	2.8
1	A	445	GLY	2.7
1	C	445	GLY	2.6
1	C	339	ASN	2.5
1	D	445	GLY	2.5
1	B	446	GLY	2.5
1	C	358	ASN	2.4
1	B	445	GLY	2.4
1	A	344	ASP	2.4
1	A	461	TRP	2.2
1	C	473	ILE	2.2
1	D	443	THR	2.1
1	B	344	ASP	2.1
1	D	472	GLU	2.1
1	B	471	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.