



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:58 AM UTC

PDB ID : 2NVP / pdb_00002nvp
Title : X-Ray Crystal Structure of Protein CPF_0428 from Clostridium perfringens.
Northeast Structural Genomics Consortium Target CpR63.
Authors : Forouhar, F.; Chen, Y.; Seetharaman, J.; Cunningham, K.; Ma, L.-C.; Fang,
Y.; Baran, M.C.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong,
L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2006-11-13
Resolution : 2.20 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

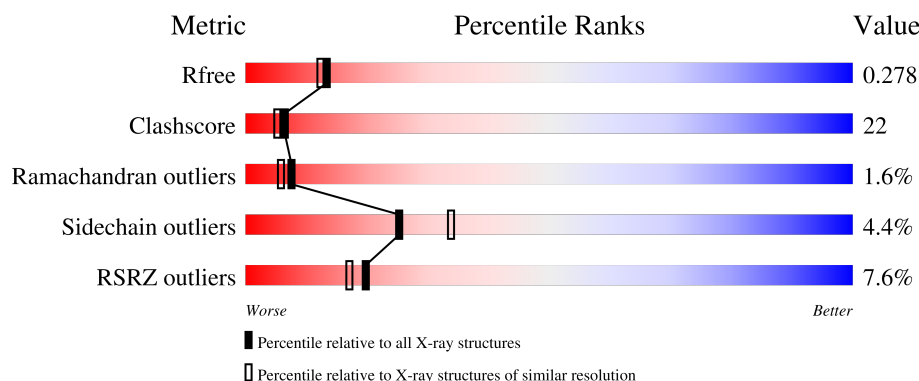
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	435	7% 59% 36% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3809 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 Hypothetical protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	Se	0	0	0
			3540	2271	576	679	5	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q0TU05
A	40	MSE	MET	modified residue	UNP Q0TU05
A	61	MSE	MET	modified residue	UNP Q0TU05
A	167	MSE	MET	modified residue	UNP Q0TU05
A	211	MSE	MET	modified residue	UNP Q0TU05
A	233	MSE	MET	modified residue	UNP Q0TU05
A	292	MSE	MET	modified residue	UNP Q0TU05
A	298	MSE	MET	modified residue	UNP Q0TU05
A	363	MSE	MET	modified residue	UNP Q0TU05
A	391	MSE	MET	modified residue	UNP Q0TU05
A	428	LEU	-	cloning artifact	UNP Q0TU05
A	429	GLU	-	cloning artifact	UNP Q0TU05
A	430	HIS	-	expression tag	UNP Q0TU05
A	431	HIS	-	expression tag	UNP Q0TU05
A	432	HIS	-	expression tag	UNP Q0TU05
A	433	HIS	-	expression tag	UNP Q0TU05
A	434	HIS	-	expression tag	UNP Q0TU05
A	435	HIS	-	expression tag	UNP Q0TU05

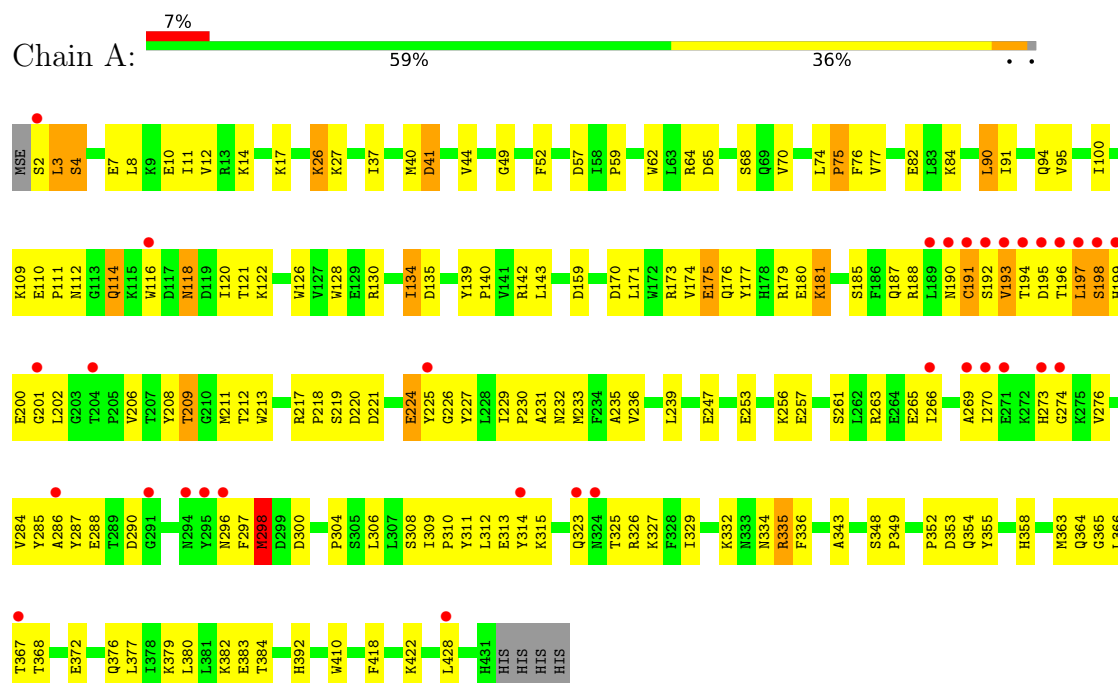
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	269	Total	O	0	0
			269	269		

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: Hypothetical protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.86Å 47.74Å 84.38Å 90.00° 96.03° 90.00°	Depositor
Resolution (Å)	19.92 – 2.20 19.92 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.8 (19.92-2.20) 96.5 (19.92-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.29	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.245 0.247 , 0.278	Depositor DCC
R_{free} test set	5324 reflections (7.64%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3809	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.43	0/3625	0.83	3/4889 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SER	N-CA-C	-6.23	105.46	114.12
1	A	348	SER	CA-C-N	5.19	124.99	119.28
1	A	348	SER	C-N-CA	5.19	124.99	119.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3540	0	3392	152	0
2	A	269	0	0	17	0
All	All	3809	0	3392	152	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 22.

All (152) 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:A:121:THR:HG22	1:A:130:ARG:HH11	1.21	1.05
1:A:175:GLU:HG3	1:A:213:TRP:HB3	1.55	0.85
1:A:326:ARG:HH11	1:A:367:THR:HG23	1.46	0.81
1:A:253:GLU:HB3	2:A:617:HOH:O	1.80	0.80
1:A:358:HIS:HD2	1:A:392:HIS:H	1.25	0.79
1:A:297:PHE:HA	2:A:564:HOH:O	1.84	0.76
1:A:208:TYR:HB2	2:A:694:HOH:O	1.88	0.73
1:A:332:LYS:HG2	2:A:631:HOH:O	1.89	0.70
1:A:121:THR:HG22	1:A:130:ARG:NH1	2.04	0.69
1:A:121:THR:CG2	1:A:130:ARG:HH11	2.03	0.69
1:A:134:ILE:CG1	1:A:231:ALA:HB1	2.23	0.69
1:A:358:HIS:CD2	1:A:392:HIS:H	2.10	0.69
1:A:343:ALA:HB2	1:A:380:LEU:HD22	1.76	0.68
1:A:12:VAL:HG21	1:A:40:MSE:HG2	1.75	0.68
1:A:74:LEU:O	1:A:77:VAL:HG22	1.94	0.67
1:A:134:ILE:HG12	1:A:231:ALA:HB1	1.77	0.67
1:A:121:THR:HG22	1:A:122:LYS:H	1.61	0.66
1:A:217:ARG:HB3	1:A:218:PRO:HD2	1.76	0.66
1:A:229:ILE:O	1:A:233:MSE:HG3	1.96	0.65
1:A:199:HIS:O	1:A:200:GLU:HB2	1.95	0.65
1:A:177:TYR:HB3	1:A:180:GLU:HB2	1.79	0.65
1:A:94:GLN:HE22	1:A:140:PRO:HA	1.62	0.64
1:A:197:LEU:HA	1:A:201:GLY:H	1.62	0.64
1:A:309:ILE:HB	1:A:310:PRO:HD3	1.81	0.63
1:A:40:MSE:HA	1:A:40:MSE:HE2	1.81	0.62
1:A:192:SER:C	1:A:194:THR:H	2.08	0.62
1:A:358:HIS:HE1	1:A:384:THR:OG1	1.82	0.62
1:A:276:VAL:HB	1:A:297:PHE:HZ	1.65	0.61
1:A:312:LEU:O	1:A:313:GLU:HB2	2.00	0.61
1:A:173:ARG:HA	1:A:176:GLN:HE21	1.66	0.60
1:A:366:LEU:HD21	1:A:418:PHE:HA	1.83	0.60
1:A:195:ASP:OD2	1:A:197:LEU:HB3	2.02	0.60
1:A:233:MSE:HE2	1:A:314:TYR:CE2	2.37	0.60
1:A:197:LEU:HA	1:A:201:GLY:N	2.18	0.58
1:A:311:TYR:HB2	1:A:363:MSE:HE1	1.83	0.58
1:A:219:SER:O	1:A:220:ASP:HB2	2.03	0.58
1:A:14:LYS:HE3	2:A:572:HOH:O	2.03	0.58
1:A:74:LEU:HB2	1:A:75:PRO:HD3	1.86	0.58
1:A:364:GLN:HG2	1:A:377:LEU:HD11	1.85	0.58
1:A:121:THR:CG2	1:A:130:ARG:HD3	2.35	0.56
1:A:326:ARG:NH1	1:A:368:THR:HB	2.21	0.56
1:A:121:THR:HG23	1:A:185:SER:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LYS:H	1:A:26:LYS:CD	2.19	0.55
1:A:232:ASN:O	1:A:236:VAL:HG23	2.07	0.55
1:A:188:ARG:H	1:A:195:ASP:HB2	1.72	0.55
1:A:379:LYS:O	1:A:383:GLU:HG3	2.06	0.55
1:A:263:ARG:HG2	1:A:263:ARG:HH11	1.73	0.54
1:A:26:LYS:H	1:A:26:LYS:HD3	1.73	0.54
1:A:196:THR:O	1:A:198:SER:N	2.41	0.54
1:A:298:MSE:HE2	1:A:335:ARG:NH1	2.22	0.54
1:A:94:GLN:NE2	1:A:140:PRO:HA	2.23	0.54
1:A:121:THR:HG21	1:A:130:ARG:HD3	1.91	0.53
1:A:57:ASP:O	1:A:59:PRO:HD3	2.08	0.53
1:A:225:TYR:HB2	1:A:288:GLU:HB3	1.90	0.53
1:A:206:VAL:HB	1:A:227:TYR:CE1	2.44	0.52
1:A:230:PRO:HB3	1:A:306:LEU:HD12	1.90	0.52
1:A:311:TYR:HB2	1:A:363:MSE:CE	2.39	0.52
1:A:177:TYR:HB2	1:A:181:LYS:HD3	1.90	0.52
1:A:364:GLN:HA	1:A:367:THR:HG22	1.92	0.52
1:A:193:VAL:HA	2:A:548:HOH:O	2.10	0.52
1:A:363:MSE:O	1:A:363:MSE:HE3	2.10	0.51
1:A:177:TYR:HB3	1:A:180:GLU:HG3	1.92	0.51
1:A:247:GLU:HB2	1:A:256:LYS:HD2	1.93	0.51
1:A:177:TYR:HB3	1:A:180:GLU:CG	2.40	0.51
1:A:188:ARG:HB3	1:A:195:ASP:HB3	1.93	0.51
1:A:372:GLU:O	1:A:376:GLN:HG3	2.11	0.51
1:A:100:ILE:HD13	1:A:126:TRP:HB3	1.93	0.50
1:A:11:ILE:CD1	1:A:82:GLU:HG3	2.41	0.50
1:A:177:TYR:HB3	1:A:180:GLU:CB	2.41	0.50
1:A:12:VAL:CG2	1:A:40:MSE:HG2	2.42	0.50
1:A:206:VAL:HB	1:A:227:TYR:HE1	1.75	0.50
1:A:3:LEU:HA	2:A:491:HOH:O	2.11	0.50
1:A:336:PHE:CZ	1:A:349:PRO:HG3	2.47	0.50
1:A:120:ILE:HB	1:A:187:GLN:HB2	1.93	0.49
1:A:284:VAL:HG13	1:A:325:THR:HA	1.94	0.49
1:A:134:ILE:HD11	1:A:231:ALA:O	2.12	0.49
1:A:197:LEU:HD12	1:A:200:GLU:HA	1.94	0.49
1:A:352:PRO:O	1:A:355:TYR:HB2	2.12	0.49
1:A:221:ASP:HB2	2:A:563:HOH:O	2.12	0.49
1:A:290:ASP:HB3	2:A:574:HOH:O	2.11	0.49
1:A:27:LYS:HB3	1:A:382:LYS:HD2	1.94	0.49
1:A:190:ASN:O	1:A:191:CYS:HB3	2.12	0.49
1:A:10:GLU:HG3	2:A:570:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HA	2:A:685:HOH:O	2.12	0.48
1:A:233:MSE:HE2	1:A:314:TYR:CD2	2.49	0.48
1:A:261:SER:O	1:A:265:GLU:HG3	2.14	0.48
1:A:335:ARG:HD3	1:A:336:PHE:CD1	2.48	0.48
1:A:74:LEU:C	1:A:76:PHE:H	2.22	0.48
1:A:276:VAL:HB	1:A:297:PHE:CZ	2.48	0.47
1:A:4:SER:HB3	1:A:7:GLU:OE1	2.14	0.47
1:A:110:GLU:HB2	1:A:111:PRO:HD2	1.96	0.47
1:A:323:GLN:O	1:A:327:LYS:HG3	2.14	0.47
1:A:365:GLY:HA3	1:A:418:PHE:CE1	2.48	0.47
1:A:142:ARG:HD2	2:A:468:HOH:O	2.15	0.47
1:A:62:TRP:HB2	1:A:65:ASP:HB3	1.97	0.47
1:A:353:ASP:O	1:A:354:GLN:HB2	2.15	0.46
1:A:84:LYS:HB2	2:A:665:HOH:O	2.15	0.46
1:A:112:ASN:OD1	1:A:114:GLN:HB2	2.16	0.46
1:A:229:ILE:HD12	1:A:286:ALA:C	2.41	0.46
1:A:336:PHE:CE1	1:A:349:PRO:HG3	2.51	0.46
1:A:91:ILE:O	1:A:95:VAL:HG23	2.15	0.46
1:A:230:PRO:HG3	1:A:287:TYR:CE1	2.51	0.46
1:A:52:PHE:CE2	1:A:109:LYS:HA	2.51	0.45
1:A:218:PRO:HB3	1:A:304:PRO:HD2	1.98	0.45
1:A:229:ILE:N	1:A:230:PRO:HD2	2.31	0.45
1:A:382:LYS:HE3	2:A:642:HOH:O	2.15	0.45
1:A:192:SER:C	1:A:194:THR:N	2.74	0.45
1:A:134:ILE:HD13	1:A:235:ALA:HB2	1.98	0.45
1:A:134:ILE:HG13	1:A:231:ALA:HB1	1.97	0.45
1:A:121:THR:HG22	1:A:122:LYS:N	2.29	0.44
1:A:175:GLU:HB3	1:A:212:THR:OG1	2.17	0.44
1:A:116:TRP:HB2	1:A:128:TRP:NE1	2.32	0.44
1:A:266:ILE:O	1:A:270:ILE:HG13	2.17	0.44
1:A:263:ARG:HG2	1:A:263:ARG:NH1	2.33	0.44
1:A:287:TYR:CD2	1:A:288:GLU:HG3	2.53	0.44
1:A:269:ALA:O	1:A:273:HIS:HB2	2.18	0.43
1:A:170:ASP:O	1:A:174:VAL:HG23	2.18	0.43
1:A:171:LEU:C	1:A:171:LEU:HD23	2.44	0.43
1:A:335:ARG:HD3	1:A:336:PHE:HD1	1.83	0.43
1:A:120:ILE:HA	2:A:683:HOH:O	2.17	0.43
1:A:300:ASP:HB3	2:A:558:HOH:O	2.18	0.43
1:A:308:SER:O	1:A:309:ILE:C	2.59	0.43
1:A:64:ARG:HG3	1:A:139:TYR:CE2	2.54	0.43
1:A:40:MSE:HE2	1:A:44:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLU:OE2	1:A:298:MSE:HE3	2.18	0.43
1:A:70:VAL:HG21	1:A:90:LEU:HD12	2.00	0.43
1:A:314:TYR:CD2	1:A:315:LYS:HG2	2.54	0.43
1:A:329:ILE:HA	1:A:334:ASN:HB2	2.01	0.43
1:A:90:LEU:HD13	1:A:143:LEU:CD2	2.49	0.42
1:A:74:LEU:O	1:A:76:PHE:N	2.52	0.42
1:A:211:MSE:HB2	1:A:227:TYR:CD2	2.53	0.42
1:A:2:SER:O	1:A:8:LEU:HG	2.20	0.42
1:A:49:GLY:HA2	2:A:508:HOH:O	2.19	0.42
1:A:4:SER:HB3	1:A:7:GLU:CD	2.45	0.42
1:A:209:THR:HG23	1:A:211:MSE:H	1.85	0.42
1:A:68:SER:HB3	1:A:410:TRP:CZ3	2.55	0.42
1:A:134:ILE:HG13	1:A:135:ASP:N	2.33	0.42
1:A:325:THR:O	1:A:329:ILE:HG12	2.20	0.42
1:A:179:ARG:NH2	1:A:202:LEU:HD12	2.35	0.42
1:A:118:ASN:HD22	1:A:118:ASN:HA	1.60	0.41
1:A:233:MSE:HB3	1:A:314:TYR:CG	2.55	0.41
1:A:40:MSE:CE	1:A:44:VAL:HG21	2.51	0.41
1:A:253:GLU:O	1:A:257:GLU:HG3	2.19	0.41
1:A:332:LYS:HA	1:A:332:LYS:HD3	1.86	0.41
1:A:68:SER:HB3	1:A:410:TRP:CE3	2.56	0.41
1:A:364:GLN:HA	1:A:367:THR:CG2	2.50	0.41
1:A:37:ILE:O	1:A:41:ASP:HB2	2.20	0.40
1:A:288:GLU:HB2	1:A:296:ASN:HB2	2.03	0.40
1:A:422:LYS:HA	1:A:422:LYS:HD3	1.96	0.40
1:A:274:GLY:O	1:A:285:TYR:HA	2.21	0.40
1:A:343:ALA:HB1	1:A:380:LEU:HD13	2.04	0.40
1:A:192:SER:O	1:A:193:VAL:HB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	428/435 (98%)	390 (91%)	31 (7%)	7 (2%)	7 6

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	VAL
1	A	197	LEU
1	A	298	MSE
1	A	191	CYS
1	A	209	THR
1	A	75	PRO
1	A	226	GLY

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	385/380 (101%)	368 (96%)	17 (4%)	25 34

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	4	SER
1	A	17	LYS
1	A	26	LYS
1	A	41	ASP
1	A	90	LEU
1	A	114	GLN
1	A	118	ASN
1	A	134	ILE
1	A	159	ASP
1	A	175	GLU
1	A	181	LYS
1	A	224	GLU
1	A	239	LEU

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Mol	Chain	Res	Type
1	A	298	MSE
1	A	335	ARG
1	A	428	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	94	GLN
1	A	118	ASN
1	A	176	GLN
1	A	190	ASN
1	A	268	ASN
1	A	296	ASN
1	A	358	HIS
1	A	364	GLN
1	A	431	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](#)

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 ⓘ

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	421/435 (96%)	0.48	32 (7%) 20 17	12, 31, 53, 62	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	SER	5.2
1	A	197	LEU	4.0
1	A	195	ASP	3.8
1	A	270	ILE	3.8
1	A	199	HIS	3.3
1	A	196	THR	3.2
1	A	194	THR	3.1
1	A	269	ALA	2.9
1	A	198	SER	2.9
1	A	116	TRP	2.7
1	A	428	LEU	2.6
1	A	191	CYS	2.6
1	A	324	ASN	2.5
1	A	314	TYR	2.5
1	A	193	VAL	2.4
1	A	271	GLU	2.4
1	A	204	THR	2.4
1	A	367	THR	2.4
1	A	190	ASN	2.4
1	A	189	LEU	2.3
1	A	296	ASN	2.3
1	A	225	TYR	2.3
1	A	201	GLY	2.2
1	A	286	ALA	2.2
1	A	192	SER	2.2
1	A	266	ILE	2.2
1	A	274	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	273	HIS	2.1
1	A	323	GLN	2.1
1	A	295	TYR	2.1
1	A	291	GLY	2.1
1	A	294	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.