



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:59 PM EDT

PDB ID : 5CIO / pdb_00005cio
Title : Crystal structure of PqqF
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Deposited on : 2015-07-13
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
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

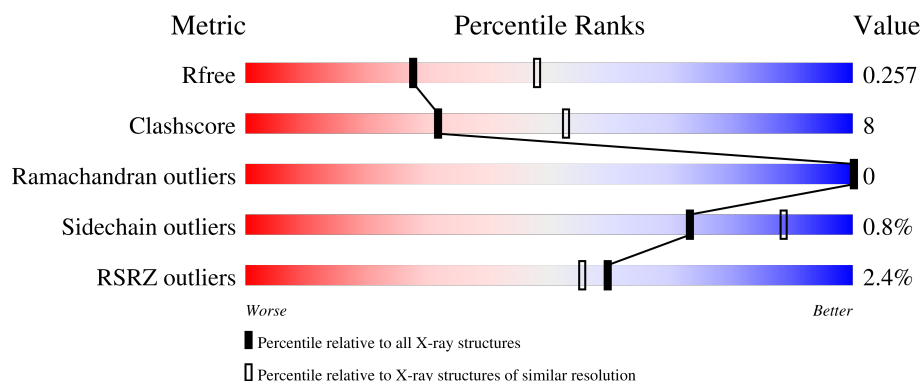
1 Overall quality at a glance

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	793	
1	B	793	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12021 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 pyrroloquinoline quinone biosynthesis protein PqqF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	770	Total	C	N	O	S	0	0	0
			5950	3755	1113	1065	17			
1	B	766	Total	C	N	O	S	0	0	0
			5922	3741	1105	1059	17			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

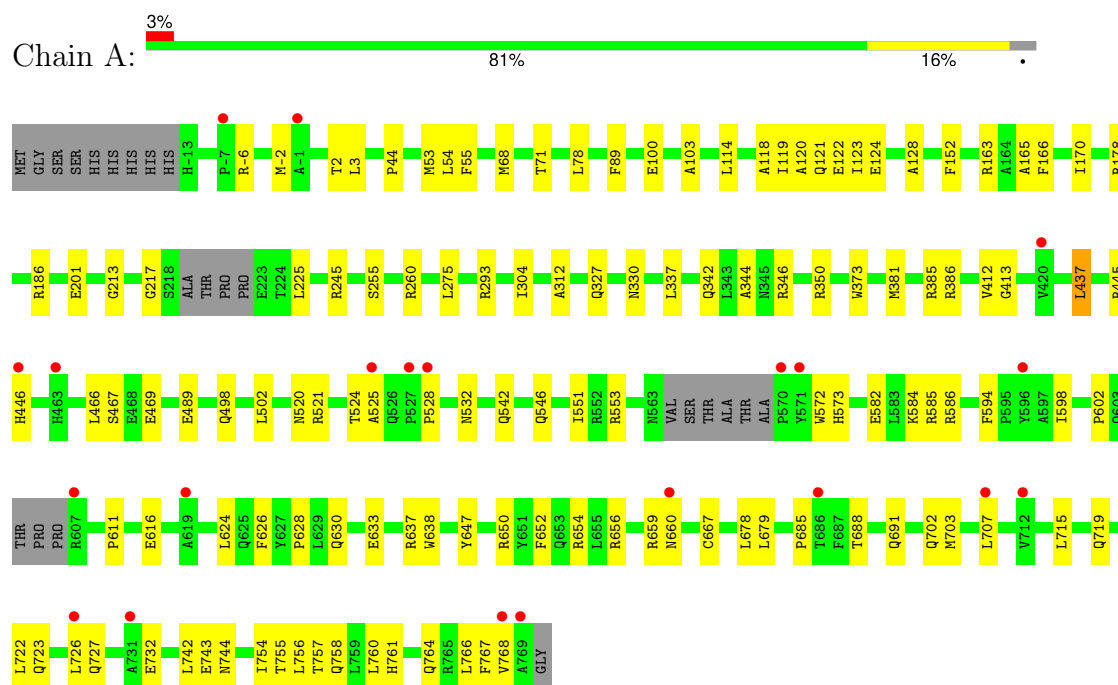
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	75	Total	O	0	0
			75	75		
3	B	72	Total	O	0	0
			72	72		

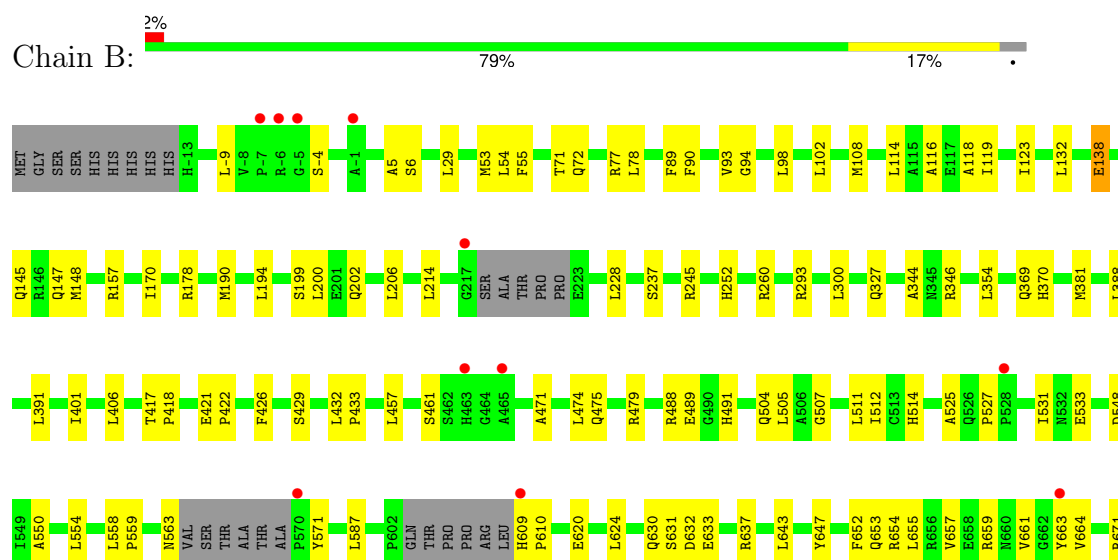
3 Residue-property plots

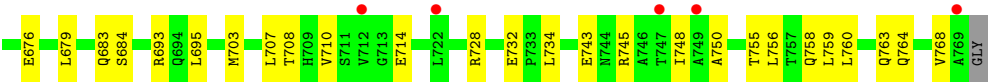
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: pyrroloquinoline quinone biosynthesis protein PqqF



- Molecule 1: pyrroloquinoline quinone biosynthesis protein PqqF





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.09Å 133.37Å 92.11Å 90.00° 119.40° 90.00°	Depositor
Resolution (Å)	47.51 – 2.50 47.51 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.51-2.50) 99.4 (47.51-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.199 , 0.255 0.204 , 0.257	Depositor DCC
R_{free} test set	3200 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.064 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12021	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: ZN

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	0.49	6/6094 (0.1%)	0.63	0/8293
1	B	0.42	0/6066	0.60	0/8256
All	All	0.46	6/12160 (0.0%)	0.62	0/16549

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	445	ARG	NE-CZ	-11.57	1.20	1.33
1	A	445	ARG	CZ-NH2	-10.20	1.20	1.33
1	A	521	ARG	NE-CZ	-7.97	1.24	1.33
1	A	445	ARG	CD-NE	-7.10	1.36	1.46
1	A	445	ARG	CZ-NH1	-6.62	1.23	1.32
1	A	521	ARG	CZ-NH1	-6.33	1.23	1.32

There are no bond angle outliers.

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	5950	0	5881	95	1
1	B	5922	0	5862	102	1
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	75	0	0	5	0
3	B	72	0	0	2	0
All	All	12021	0	11743	190	1

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 8.

All (190) 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:756:LEU:HG	1:B:760:LEU:CD1	2.05	0.86
1:B:764:GLN:OE1	1:B:768:VAL:HG21	1.76	0.85
1:B:764:GLN:OE1	1:B:768:VAL:HG11	1.77	0.83
1:A:520:ASN:O	1:A:524:THR:HG23	1.79	0.82
1:B:755:THR:HG23	1:B:758:GLN:H	1.47	0.79
1:B:671:ARG:NH1	1:B:743:GLU:OE2	2.18	0.77
1:A:-2:MET:HE2	1:B:732:GLU:HB3	1.67	0.77
1:A:659:ARG:NH1	3:A:901:HOH:O	2.17	0.76
1:B:671:ARG:NH2	1:B:676:GLU:OE1	2.19	0.75
1:A:633:GLU:O	1:A:637:ARG:HG3	1.90	0.71
1:A:650:ARG:O	1:A:654:ARG:HG3	1.90	0.70
1:A:346:ARG:HH22	1:A:489:GLU:CD	1.99	0.70
1:A:437:LEU:HD11	1:A:586:ARG:HD2	1.74	0.69
1:B:655:LEU:HD23	1:B:661:VAL:HG21	1.73	0.69
1:A:582:GLU:CD	1:A:585:ARG:HH12	2.01	0.69
1:A:659:ARG:O	3:A:901:HOH:O	2.10	0.68
1:A:255:SER:HB3	1:B:370:HIS:CG	2.27	0.68
1:B:293:ARG:NH2	3:B:901:HOH:O	2.26	0.68
1:B:346:ARG:HH22	1:B:489:GLU:CD	2.01	0.68
1:A:667:CYS:SG	1:A:678:LEU:HD21	2.34	0.68
1:A:123:ILE:HG23	1:A:166:PHE:HD2	1.59	0.68
1:A:342:GLN:OE1	1:B:6:SER:OG	2.08	0.67
1:A:121:GLN:HG2	1:A:660:ASN:HD21	1.58	0.66
1:A:756:LEU:HD23	1:A:760:LEU:HG	1.75	0.66
1:A:756:LEU:CD2	1:A:760:LEU:HG	2.25	0.66
1:A:293:ARG:NH2	3:A:902:HOH:O	2.29	0.65
1:A:186:ARG:HD3	1:A:217:GLY:O	1.97	0.65
1:B:708:THR:HG22	1:B:760:LEU:HD21	1.77	0.64
1:B:138:GLU:OE1	1:B:245:ARG:NH2	2.30	0.64
1:A:758:GLN:HA	1:A:761:HIS:HB3	1.80	0.63
1:B:432:LEU:HD21	1:B:511:LEU:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:LEU:HD23	1:A:760:LEU:HD23	1.81	0.61
1:B:116:ALA:O	1:B:170:ILE:HD11	2.00	0.61
1:A:413:GLY:HA2	3:A:930:HOH:O	2.02	0.60
1:B:55:PHE:CE1	1:B:78:LEU:HD21	2.36	0.60
1:B:620:GLU:OE2	1:B:683:GLN:NE2	2.35	0.60
1:B:756:LEU:HG	1:B:760:LEU:HD12	1.80	0.60
1:A:437:LEU:HD11	1:A:586:ARG:CD	2.32	0.60
1:B:260:ARG:HG2	1:B:344:ALA:HB1	1.84	0.59
1:A:528:PRO:O	1:A:532:ASN:ND2	2.34	0.59
1:B:633:GLU:O	1:B:637:ARG:HG3	2.03	0.59
1:B:102:LEU:HD11	1:B:194:LEU:HD21	1.85	0.58
1:B:346:ARG:NH2	1:B:489:GLU:OE2	2.30	0.57
1:B:432:LEU:HD11	1:B:514:HIS:ND1	2.19	0.57
1:B:54:LEU:HB3	1:B:108:MET:HE3	1.87	0.57
1:A:124:GLU:OE1	1:A:163:ARG:NH2	2.38	0.57
1:A:553:ARG:NH1	1:A:616:GLU:OE2	2.38	0.57
1:A:120:ALA:HB2	1:A:170:ILE:HD12	1.88	0.56
1:B:764:GLN:OE1	1:B:768:VAL:CG2	2.52	0.56
1:A:659:ARG:O	1:A:659:ARG:HG3	2.06	0.56
1:B:756:LEU:O	1:B:760:LEU:HD12	2.05	0.55
1:B:98:LEU:HD23	1:B:206:LEU:HD13	1.88	0.55
1:B:707:LEU:O	1:B:710:VAL:HG12	2.07	0.55
1:A:121:GLN:CG	1:A:660:ASN:HD21	2.19	0.55
1:A:346:ARG:NH1	1:A:489:GLU:OE1	2.39	0.55
1:A:524:THR:OG1	1:A:525:ALA:N	2.39	0.55
1:B:119:ILE:O	1:B:123:ILE:HG13	2.06	0.55
1:A:53:MET:HE1	1:A:118:ALA:HB3	1.89	0.54
1:B:421:GLU:HG2	1:B:422:PRO:HD2	1.89	0.54
1:A:-6:ARG:HH21	1:B:77:ARG:HD3	1.72	0.54
1:A:678:LEU:HD23	1:A:679:LEU:N	2.23	0.54
1:B:764:GLN:OE1	1:B:768:VAL:CG1	2.53	0.54
1:A:54:LEU:HD12	1:A:89:PHE:CZ	2.43	0.53
1:B:190:MET:HE1	1:B:214:LEU:HD22	1.91	0.53
1:A:201:GLU:HG3	1:B:507:GLY:HA2	1.91	0.53
1:A:626:PHE:O	1:A:628:PRO:HD3	2.09	0.53
1:B:114:LEU:HD12	1:B:178:ARG:HG3	1.90	0.53
1:B:654:ARG:O	1:B:659:ARG:HG3	2.09	0.53
1:A:754:ILE:HG23	1:A:758:GLN:HG2	1.90	0.52
1:A:678:LEU:HD23	1:A:679:LEU:H	1.74	0.52
1:B:426:PHE:HZ	1:B:429:SER:HB3	1.75	0.52
1:A:385:ARG:O	1:A:386:ARG:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:LEU:HD13	1:A:572:TRP:HZ2	1.74	0.52
1:A:446:HIS:CE1	1:A:584:LYS:HB2	2.44	0.51
1:B:54:LEU:HD12	1:B:89:PHE:CZ	2.45	0.51
1:A:754:ILE:CG2	1:A:758:GLN:HG2	2.39	0.51
1:B:78:LEU:C	1:B:78:LEU:HD23	2.36	0.51
1:B:53:MET:HE1	1:B:118:ALA:HB3	1.93	0.51
1:B:157:ARG:NH1	3:B:903:HOH:O	2.27	0.50
1:A:755:THR:OG1	1:A:758:GLN:OE1	2.24	0.50
1:A:764:GLN:O	1:A:768:VAL:HG22	2.11	0.50
1:A:55:PHE:CE1	1:A:78:LEU:HD21	2.47	0.50
1:B:252:HIS:CD2	1:B:293:ARG:HD2	2.47	0.50
1:A:722:LEU:O	1:A:726:LEU:HG	2.12	0.49
1:A:756:LEU:CD2	1:A:760:LEU:CD1	2.91	0.49
1:A:594:PHE:CD2	1:A:598:ILE:HD11	2.47	0.49
1:A:466:LEU:HD13	1:A:572:TRP:CZ2	2.48	0.49
1:B:624:LEU:HD11	1:B:679:LEU:HD11	1.94	0.49
1:A:44:PRO:HB2	1:A:165:ALA:HB1	1.95	0.48
1:A:756:LEU:CD2	1:A:760:LEU:CG	2.90	0.48
1:A:260:ARG:HG2	1:A:344:ALA:HB1	1.95	0.48
1:B:748:ILE:C	1:B:750:ALA:N	2.70	0.48
1:A:766:LEU:HD23	1:A:767:PHE:CZ	2.48	0.48
1:B:252:HIS:NE2	1:B:293:ARG:HD2	2.29	0.48
1:A:624:LEU:HD11	1:A:679:LEU:HD11	1.96	0.48
1:A:128:ALA:HB1	1:A:685:PRO:HG3	1.96	0.47
1:A:756:LEU:HD22	1:A:760:LEU:CD1	2.44	0.47
1:B:432:LEU:CD2	1:B:511:LEU:HA	2.43	0.47
1:B:637:ARG:HH21	1:B:748:ILE:CG1	2.27	0.47
1:A:703:MET:O	1:A:707:LEU:HB2	2.14	0.47
1:A:756:LEU:HD23	1:A:756:LEU:O	2.14	0.47
1:A:764:GLN:HG3	1:A:768:VAL:HG21	1.97	0.47
1:B:432:LEU:HD12	1:B:433:PRO:HD2	1.96	0.47
1:B:609:HIS:O	1:B:630:GLN:NE2	2.47	0.47
1:B:631:SER:OG	1:B:632:ASP:N	2.48	0.47
1:B:479:ARG:NH2	1:B:533:GLU:OE2	2.38	0.47
1:A:68:MET:HA	1:A:78:LEU:HD13	1.97	0.47
1:A:327:GLN:O	1:A:330:ASN:HB2	2.16	0.46
1:B:471:ALA:HA	1:B:474:LEU:HD12	1.98	0.46
1:B:703:MET:HA	1:B:703:MET:HE3	1.96	0.46
1:B:72:GLN:NE2	1:B:652:PHE:CD1	2.83	0.46
1:A:551:ILE:HG13	1:B:-9:LEU:HD13	1.98	0.46
1:A:611:PRO:HA	1:A:628:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:THR:HG21	1:B:78:LEU:HB2	1.98	0.46
1:B:327:GLN:OE1	1:B:381:MET:HE1	2.16	0.46
1:A:638:TRP:CH2	1:A:722:LEU:HB3	2.51	0.46
1:A:647:TYR:HA	1:A:703:MET:HE2	1.98	0.45
1:B:199:SER:OG	1:B:202:GLN:HG3	2.17	0.45
1:B:728:ARG:O	1:B:745:ARG:NH2	2.47	0.45
1:A:245:ARG:HG2	1:A:304:ILE:HG23	1.98	0.45
1:A:573:HIS:NE2	1:A:602:PRO:HD2	2.32	0.45
1:A:756:LEU:HD22	1:A:760:LEU:HD11	1.99	0.45
1:B:5:ALA:HB2	1:B:200:LEU:HD13	1.96	0.45
1:B:710:VAL:HG23	1:B:714:GLU:OE1	2.16	0.45
1:A:346:ARG:O	1:A:350:ARG:HG3	2.16	0.45
1:B:461:SER:OG	1:B:571:TYR:O	2.26	0.45
1:B:559:PRO:O	1:B:563:ASN:ND2	2.49	0.45
1:A:312:ALA:HB2	1:A:412:VAL:HG12	1.98	0.45
1:A:346:ARG:NH2	1:A:489:GLU:OE2	2.49	0.45
1:B:228:LEU:HD12	1:B:300:LEU:HD21	1.98	0.45
1:B:527:PRO:O	1:B:531:ILE:HD12	2.16	0.45
1:A:152:PHE:CD2	1:A:225:LEU:HD22	2.52	0.45
1:B:653:GLN:O	1:B:657:VAL:HG22	2.17	0.45
1:A:467:SER:C	1:A:469:GLU:H	2.25	0.45
1:B:728:ARG:HE	1:B:728:ARG:HB3	1.64	0.44
1:B:756:LEU:HG	1:B:760:LEU:HD11	1.97	0.44
1:A:652:PHE:CZ	1:A:656:ARG:HG2	2.52	0.44
1:B:237:SER:HA	1:B:391:LEU:O	2.17	0.44
1:A:71:THR:HG21	1:A:78:LEU:HB2	2.00	0.44
1:B:512:ILE:HG22	1:B:587:LEU:HD21	2.00	0.44
1:B:29:LEU:C	1:B:29:LEU:HD23	2.43	0.44
1:B:90:PHE:HD2	1:B:354:LEU:HD11	1.82	0.44
1:A:498:GLN:HB2	3:A:915:HOH:O	2.18	0.44
1:B:346:ARG:NH1	1:B:489:GLU:OE1	2.39	0.44
1:B:432:LEU:HD13	1:B:488:ARG:HD3	2.00	0.43
1:B:631:SER:HG	1:B:633:GLU:H	1.62	0.43
1:A:2:THR:O	1:A:3:LEU:HD23	2.18	0.43
1:B:72:GLN:NE2	1:B:652:PHE:CG	2.86	0.43
1:B:138:GLU:CD	1:B:245:ARG:HH22	2.26	0.43
1:B:748:ILE:C	1:B:750:ALA:H	2.27	0.43
1:A:275:LEU:HA	1:A:275:LEU:HD23	1.80	0.43
1:B:145:GLN:OE1	1:B:245:ARG:HD3	2.18	0.43
1:A:337:LEU:HD21	1:A:373:TRP:CD1	2.54	0.43
1:B:475:GLN:O	1:B:479:ARG:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:LEU:HD21	1:B:695:LEU:HB3	2.01	0.43
1:A:502:LEU:HD11	1:A:742:LEU:HD11	2.00	0.43
1:B:647:TYR:OH	1:B:763:GLN:NE2	2.47	0.42
1:A:723:GLN:O	1:A:727:GLN:HG2	2.18	0.42
1:A:756:LEU:CD2	1:A:760:LEU:HD11	2.49	0.42
1:B:93:VAL:HG23	1:B:94:GLY:O	2.19	0.42
1:A:327:GLN:HG3	1:A:381:MET:HE1	2.01	0.42
1:A:114:LEU:HD12	1:A:178:ARG:HG2	2.01	0.42
1:A:654:ARG:NH1	1:A:702:GLN:OE1	2.51	0.42
1:B:401:ILE:HB	1:B:406:LEU:HD12	2.02	0.42
1:B:457:LEU:CD2	1:B:504:GLN:HG2	2.50	0.42
1:B:756:LEU:O	1:B:760:LEU:CD1	2.67	0.42
1:A:688:THR:OG1	1:A:691:GLN:HG3	2.20	0.42
1:B:525:ALA:O	1:B:527:PRO:HD3	2.19	0.42
1:B:637:ARG:NH2	1:B:748:ILE:HD11	2.35	0.42
1:A:764:GLN:NE2	1:A:768:VAL:HG11	2.35	0.42
1:A:715:LEU:HD21	1:A:719:GLN:HE21	1.84	0.41
1:B:643:LEU:HG	1:B:759:LEU:HD11	2.00	0.41
1:A:-6:ARG:HH21	1:B:77:ARG:CD	2.33	0.41
1:B:550:ALA:O	1:B:554:LEU:HG	2.20	0.41
1:B:488:ARG:O	1:B:489:GLU:HB2	2.19	0.41
1:B:417:THR:O	1:B:418:PRO:C	2.64	0.41
1:A:78:LEU:HD23	1:A:78:LEU:C	2.46	0.41
1:B:132:LEU:HD22	1:B:663:TYR:CE1	2.55	0.41
1:B:663:TYR:HD1	1:B:664:VAL:HG23	1.85	0.41
1:A:100:GLU:O	1:A:103:ALA:HB3	2.20	0.41
1:A:467:SER:C	1:A:469:GLU:N	2.79	0.41
1:A:542:GLN:O	1:A:546:GLN:HG2	2.20	0.41
1:A:743:GLU:O	1:A:744:ASN:HB2	2.20	0.41
1:B:148:MET:CE	1:B:388:LEU:HB2	2.51	0.41
1:B:381:MET:HE2	1:B:381:MET:HB3	1.93	0.40
1:B:491:HIS:CG	1:B:734:LEU:HD11	2.57	0.40
1:B:558:LEU:HB3	1:B:559:PRO:HD3	2.03	0.40
1:B:609:HIS:HA	1:B:610:PRO:HD3	1.95	0.40
1:A:119:ILE:O	1:A:122:GLU:N	2.55	0.40
1:B:661:VAL:O	1:B:684:SER:OG	2.32	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLY:CA	1:B:693:ARG:NH2[4_748]	2.15	0.05

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	762/793 (96%)	719 (94%)	43 (6%)	0	100	100
1	B	758/793 (96%)	732 (97%)	26 (3%)	0	100	100
All	All	1520/1586 (96%)	1451 (96%)	69 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	595/616 (97%)	591 (99%)	4 (1%)	76	89
1	B	593/616 (96%)	587 (99%)	6 (1%)	68	86
All	All	1188/1232 (96%)	1178 (99%)	10 (1%)	73	88

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	437	LEU
1	A	630	GLN
1	A	732	GLU

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Mol	Chain	Res	Type
1	A	757	THR
1	B	-4	SER
1	B	138	GLU
1	B	147	GLN
1	B	369	GLN
1	B	505	LEU
1	B	548	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	147	GLN
1	A	174	GLN
1	A	179	GLN
1	A	195	GLN
1	A	356	GLN
1	A	376	GLN
1	A	497	HIS
1	A	514	HIS
1	A	537	ASN
1	A	542	GLN
1	A	563	ASN
1	A	653	GLN
1	A	660	ASN
1	A	735	GLN
1	B	86	GLN
1	B	309	HIS
1	B	376	GLN
1	B	497	HIS
1	B	526	GLN
1	B	621	HIS
1	B	727	GLN

5.3.3 RNA ⓘ

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	770/793 (97%)	0.14	21 (2%) 56 51	29, 53, 93, 105	0
1	B	766/793 (96%)	-0.03	16 (2%) 63 59	28, 48, 86, 102	0
All	All	1536/1586 (96%)	0.06	37 (2%) 59 55	28, 51, 91, 105	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	769	ALA	4.4
1	A	726	LEU	3.0
1	B	-1	ALA	2.9
1	A	463	HIS	2.8
1	B	-7	PRO	2.8
1	B	663	TYR	2.8
1	A	528	PRO	2.6
1	B	217	GLY	2.6
1	A	570	PRO	2.5
1	A	712	VAL	2.5
1	A	-1	ALA	2.5
1	B	609	HIS	2.5
1	B	463	HIS	2.4
1	A	-7	PRO	2.4
1	A	596	TYR	2.4
1	A	686	THR	2.4
1	B	747	THR	2.4
1	B	-5	GLY	2.4
1	A	768	VAL	2.4
1	B	769	ALA	2.3
1	A	420	VAL	2.3
1	B	570	PRO	2.2
1	A	527	PRO	2.2
1	A	619	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	731	ALA	2.2
1	B	528	PRO	2.1
1	A	607	ARG	2.1
1	A	446	HIS	2.1
1	A	525	ALA	2.1
1	B	465	ALA	2.1
1	A	707	LEU	2.1
1	B	722	LEU	2.0
1	B	-6	ARG	2.0
1	B	712	VAL	2.0
1	B	749	ALA	2.0
1	A	660	ASN	2.0
1	A	571	TYR	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
2	ZN	A	801	1/1	0.99	0.03	53,53,53,53	0
2	ZN	A	802	1/1	0.99	0.03	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.