



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:02 AM UTC

PDB ID : 3S5H / pdb_00003s5h
Title : Crystal structures of falcilysin, a M16 metalloprotease from the malaria parasite *Plasmodium falciparum*
Authors : Morgunova, E.; Ponpuak, M.; Istvan, E.; Popov, A.; Goldberg, D.; Eneqvist, T.
Deposited on : 2011-05-23
Resolution : 1.60 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

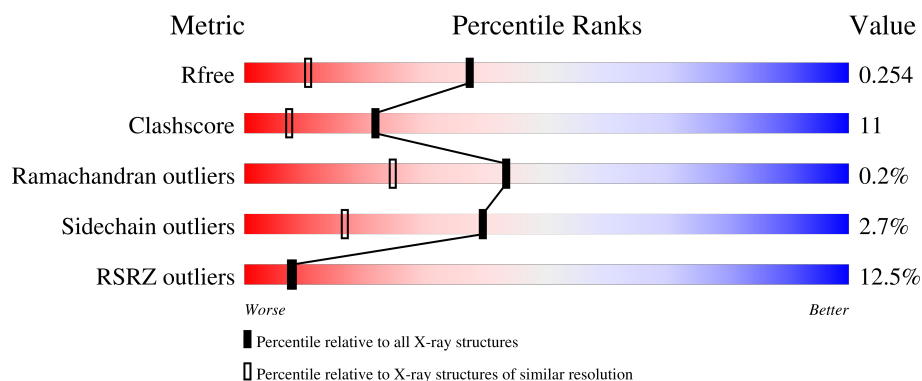
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	1193	11% 76% 13% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18600 atoms, of which 8924 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 Falcilysin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1078	Total	C	H	N	O	S	0	15	0
			17849	5747	8924	1454	1693	31			

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Co	0	0
			1	1		

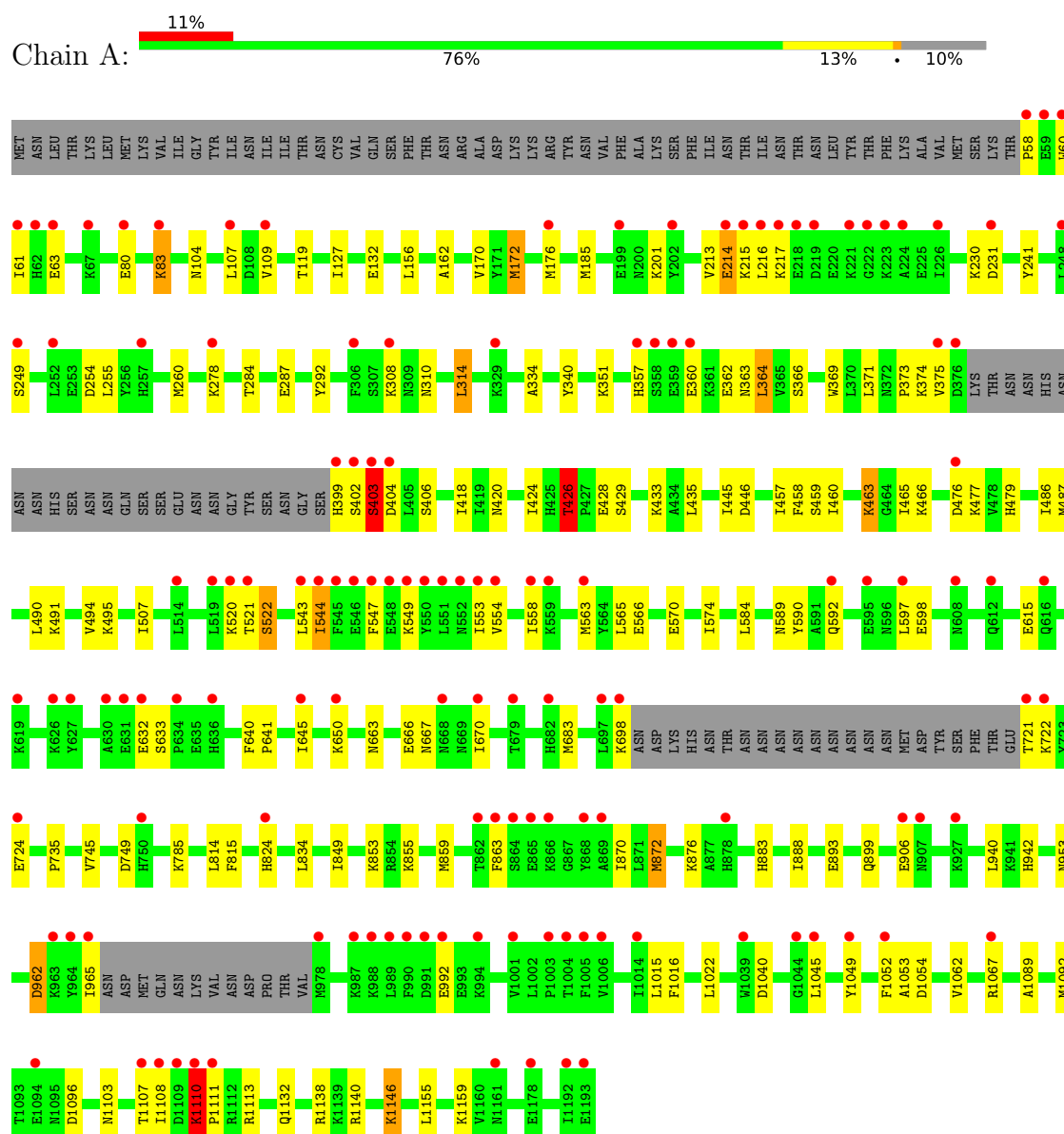
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	750	Total	O	0	0
			750	750		

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: Falcilysin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.54Å 107.16Å 128.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.47 – 1.60 49.47 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.6 (49.47-1.60) 94.4 (49.47-1.60)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.60Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.227 , 0.257 0.224 , 0.254	Depositor DCC
R_{free} test set	3235 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 35.5	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	0.92	EDS
Total number of atoms	18600	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: CO

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	0.92	5/9152 (0.1%)	0.97	7/12322 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	THR	CA-CB	6.48	1.59	1.53
1	A	162	ALA	CA-CB	-5.58	1.44	1.53
1	A	127	ILE	C-O	-5.45	1.20	1.24
1	A	1132	GLN	CD-OE1	5.24	1.33	1.23
1	A	334	ALA	CA-CB	-5.04	1.45	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	SER	N-CA-C	-7.14	95.59	110.80
1	A	58	PRO	N-CA-CB	6.74	110.41	103.00
1	A	1110	LYS	CA-C-N	6.51	126.27	119.76
1	A	1110	LYS	C-N-CA	6.51	126.27	119.76
1	A	310	ASN	N-CA-C	-6.42	101.67	109.57
1	A	590	TYR	N-CA-C	5.43	116.88	111.07
1	A	962	ASP	N-CA-C	-5.22	106.02	112.38

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	8925	8924	8927	193	0
2	A	1	0	0	0	0
3	A	750	0	0	68	0
All	All	9676	8924	8927	193	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 11.

All (193) 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:374:LYS:HA	1:A:402:SER:CA	1.91	1.00
1:A:374:LYS:HA	1:A:402:SER:HA	1.41	0.99
1:A:953:ASN:O	3:A:1916:HOH:O	1.82	0.96
1:A:374:LYS:HA	1:A:402:SER:N	1.97	0.78
1:A:870:ILE:HG13	3:A:1623:HOH:O	1.83	0.78
1:A:721:THR:HB	3:A:1863:HOH:O	1.82	0.77
1:A:547:PHE:CE1	3:A:1858:HOH:O	2.38	0.77
1:A:176[B]:MET:CE	3:A:1258:HOH:O	2.33	0.77
1:A:490:LEU:HB3	1:A:574[A]:ILE:HD11	1.66	0.75
1:A:176[B]:MET:CG	3:A:1258:HOH:O	2.35	0.75
1:A:683:MET:HE3	3:A:1675:HOH:O	1.87	0.74
1:A:418:ILE:CD1	1:A:507:ILE:HD11	2.19	0.73
1:A:176[B]:MET:HG2	3:A:1258:HOH:O	1.88	0.73
1:A:589:ASN:C	1:A:592:GLN:OE1	2.32	0.73
1:A:855:LYS:HE3	3:A:1455:HOH:O	1.87	0.72
1:A:899:GLN:NE2	3:A:1490:HOH:O	2.22	0.72
1:A:466:LYS:HD3	3:A:1907:HOH:O	1.90	0.71
1:A:899:GLN:HG3	3:A:1490:HOH:O	1.90	0.70
1:A:888:ILE:HD13	1:A:893:GLU:HG2	1.74	0.69
1:A:374:LYS:CA	1:A:402:SER:HA	2.21	0.68
1:A:814:LEU:HB3	3:A:1821:HOH:O	1.92	0.68
1:A:592:GLN:HB3	3:A:1577:HOH:O	1.92	0.67
1:A:170:VAL:HG12	1:A:172:MET:HG2	1.76	0.67
1:A:558:ILE:CD1	1:A:565:LEU:HG	2.25	0.66
1:A:663:ASN:ND2	1:A:666:GLU:HG3	2.11	0.66
1:A:834:LEU:HD22	3:A:1916:HOH:O	1.95	0.66
1:A:176[A]:MET:HG2	3:A:1258:HOH:O	1.94	0.65
1:A:589:ASN:HA	1:A:592:GLN:OE1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ILE:HG12	1:A:507:ILE:CD1	2.27	0.65
1:A:722:LYS:HE3	3:A:1777:HOH:O	1.97	0.64
1:A:362:GLU:HA	3:A:1907:HOH:O	1.98	0.64
1:A:373:PRO:O	1:A:402:SER:HA	1.98	0.64
1:A:870:ILE:CG1	3:A:1623:HOH:O	2.43	0.64
1:A:667:ASN:HB3	1:A:670:ILE:CD1	2.28	0.63
1:A:435:LEU:HD11	1:A:486[A]:ILE:HD11	1.79	0.63
1:A:815:PHE:O	3:A:1821:HOH:O	2.15	0.63
1:A:80:GLU:H	1:A:80:GLU:CD	2.06	0.63
1:A:215:LYS:CE	3:A:1717:HOH:O	2.47	0.63
1:A:824[A]:HIS:CD2	1:A:942:HIS:CE1	2.86	0.63
1:A:962:ASP:O	1:A:965:ILE:HG12	1.99	0.62
1:A:418:ILE:HD13	1:A:507:ILE:HD11	1.80	0.62
1:A:558:ILE:HD11	1:A:565:LEU:HD21	1.81	0.62
1:A:418:ILE:HG12	1:A:507:ILE:HD13	1.81	0.62
1:A:592:GLN:H	1:A:592:GLN:CD	2.07	0.62
1:A:357:HIS:NE2	1:A:592:GLN:NE2	2.49	0.61
1:A:520:LYS:HE2	3:A:1452:HOH:O	2.00	0.61
1:A:426:THR:HG23	1:A:428:GLU:H	1.64	0.61
1:A:215:LYS:HE3	3:A:1717:HOH:O	2.00	0.61
1:A:357:HIS:CE1	1:A:592:GLN:NE2	2.69	0.61
1:A:1040:ASP:O	1:A:1045[B]:LEU:HD13	1.99	0.61
1:A:424[B]:ILE:HD13	1:A:460:ILE:HD13	1.83	0.61
1:A:340:TYR:H	1:A:399:HIS:CB	2.14	0.60
1:A:888:ILE:CD1	1:A:893:GLU:HG2	2.31	0.60
1:A:255:LEU:HD21	1:A:366:SER:HB2	1.83	0.60
1:A:402:SER:CB	1:A:406:SER:N	2.64	0.60
1:A:374:LYS:NZ	1:A:399:HIS:HA	2.17	0.60
1:A:60:TRP:O	1:A:63:GLU:HG2	2.03	0.59
1:A:632:GLU:OE1	3:A:1845:HOH:O	2.17	0.59
1:A:109:VAL:HG23	1:A:176[A]:MET:HE1	1.84	0.58
1:A:667:ASN:HB3	1:A:670:ILE:HD11	1.84	0.58
1:A:899:GLN:CD	3:A:1490:HOH:O	2.47	0.57
1:A:1089:ALA:HA	1:A:1092:MET:HE3	1.86	0.57
1:A:1110:LYS:HB2	1:A:1111:PRO:HD2	1.87	0.57
1:A:254:ASP:HB3	3:A:1526:HOH:O	2.03	0.57
1:A:490:LEU:CB	1:A:574[A]:ILE:HD11	2.35	0.57
1:A:216:LEU:HD12	1:A:231:ASP:HA	1.87	0.56
1:A:834:LEU:CD2	3:A:1916:HOH:O	2.53	0.56
1:A:650:LYS:N	1:A:650:LYS:HD2	2.20	0.56
1:A:589:ASN:CA	1:A:592:GLN:OE1	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:O	3:A:1258:HOH:O	2.18	0.56
1:A:1022:LEU:C	1:A:1022:LEU:HD23	2.31	0.55
1:A:402:SER:CA	3:A:1725:HOH:O	2.55	0.55
1:A:418:ILE:CD1	1:A:507:ILE:CD1	2.85	0.55
1:A:645:ILE:HG22	3:A:1784:HOH:O	2.06	0.55
1:A:402:SER:CB	1:A:406:SER:CA	2.84	0.55
1:A:426:THR:HG21	3:A:1885:HOH:O	2.07	0.55
1:A:888:ILE:HD13	1:A:893:GLU:CG	2.37	0.54
1:A:374:LYS:HZ3	1:A:399:HIS:HA	1.72	0.54
1:A:1103:ASN:O	1:A:1107:THR:HG23	2.08	0.53
1:A:369:TRP:CZ2	1:A:487[A]:MET:HE1	2.43	0.53
1:A:953:ASN:C	3:A:1916:HOH:O	2.40	0.52
1:A:107:LEU:HD11	1:A:735:PRO:HG2	1.90	0.52
1:A:465:ILE:O	3:A:1907:HOH:O	2.19	0.52
1:A:872:MET:HA	1:A:872:MET:HE3	1.90	0.52
1:A:667:ASN:CG	1:A:670:ILE:HD13	2.35	0.52
1:A:721:THR:OG1	1:A:724:GLU:HG3	2.10	0.52
1:A:745:VAL:HG13	3:A:1821:HOH:O	2.09	0.51
1:A:176[B]:MET:HE3	3:A:1258:HOH:O	2.04	0.51
1:A:284:THR:OG1	1:A:287:GLU:HG3	2.11	0.51
1:A:1049:TYR:HB3	1:A:1067:ARG:HB2	1.93	0.50
1:A:213:VAL:C	1:A:214:GLU:HG3	2.36	0.50
1:A:402:SER:N	3:A:1305:HOH:O	2.45	0.50
1:A:375:VAL:CG1	1:A:403:SER:CB	2.89	0.50
1:A:683:MET:CE	3:A:1601:HOH:O	2.59	0.49
1:A:872:MET:SD	1:A:1052:PHE:CE2	3.05	0.49
1:A:369:TRP:CH2	1:A:487[A]:MET:HE1	2.48	0.49
1:A:558:ILE:HD11	1:A:565:LEU:CD2	2.43	0.49
1:A:544:ILE:C	1:A:544:ILE:HD12	2.38	0.49
1:A:278:LYS:HE3	3:A:1586:HOH:O	2.13	0.48
1:A:633:SER:HB2	3:A:1558:HOH:O	2.12	0.48
1:A:185:MET:HE1	1:A:314:LEU:HD11	1.95	0.48
1:A:745:VAL:CG1	3:A:1821:HOH:O	2.62	0.48
1:A:870:ILE:HD11	3:A:1469:HOH:O	2.12	0.48
1:A:176[B]:MET:CB	3:A:1258:HOH:O	2.62	0.48
1:A:563[B]:MET:HE3	1:A:566:GLU:CB	2.43	0.48
1:A:722:LYS:CE	3:A:1777:HOH:O	2.59	0.48
1:A:424[B]:ILE:CD1	1:A:460:ILE:HD13	2.44	0.47
1:A:375:VAL:HG13	1:A:403:SER:CB	2.44	0.47
1:A:520:LYS:HG2	1:A:521:THR:O	2.14	0.47
1:A:815:PHE:N	3:A:1821:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:PRO:O	1:A:402:SER:CB	2.62	0.47
1:A:1015:LEU:HD22	1:A:1159:LYS:CB	2.44	0.47
1:A:260:MET:HA	1:A:260:MET:HE2	1.96	0.47
1:A:426:THR:CG2	1:A:428:GLU:H	2.27	0.47
1:A:424[A]:ILE:C	1:A:424[A]:ILE:HD12	2.40	0.47
1:A:1052:PHE:CE2	1:A:1054:ASP:HB2	2.50	0.47
1:A:899:GLN:CG	3:A:1490:HOH:O	2.53	0.47
1:A:1108:ILE:O	1:A:1108:ILE:CG2	2.63	0.47
1:A:402:SER:CB	1:A:406:SER:HA	2.45	0.46
1:A:363:ASN:C	1:A:364:LEU:HD12	2.41	0.46
1:A:592:GLN:CB	3:A:1577:HOH:O	2.59	0.45
1:A:241:TYR:OH	1:A:598:GLU:OE2	2.24	0.45
1:A:418:ILE:CG1	1:A:507:ILE:CD1	2.95	0.45
1:A:863:PHE:HA	3:A:1623:HOH:O	2.15	0.45
1:A:992:GLU:H	1:A:992:GLU:CD	2.25	0.45
1:A:83:LYS:O	1:A:83:LYS:HG2	2.17	0.45
1:A:490:LEU:CB	1:A:574[A]:ILE:CD1	2.95	0.45
1:A:1140:ARG:HD2	1:A:1140:ARG:HA	1.83	0.45
1:A:402:SER:CB	3:A:1305:HOH:O	2.65	0.45
1:A:563[B]:MET:HE3	1:A:566:GLU:HB2	1.98	0.45
1:A:632:GLU:HB2	3:A:1845:HOH:O	2.17	0.45
1:A:176[A]:MET:CG	3:A:1258:HOH:O	2.59	0.45
1:A:420:ASN:O	1:A:424[A]:ILE:HG13	2.16	0.45
1:A:667:ASN:ND2	1:A:670:ILE:HD13	2.32	0.44
1:A:364:LEU:HG	1:A:463:LYS:HB3	2.00	0.44
1:A:424[B]:ILE:HG13	1:A:446:ASP:HB2	1.99	0.44
1:A:230:LYS:HE3	1:A:615:GLU:HG3	2.00	0.44
1:A:785:LYS:HD2	3:A:1487:HOH:O	2.16	0.44
1:A:872:MET:HB2	3:A:1722:HOH:O	2.17	0.44
1:A:433:LYS:HE3	3:A:1715:HOH:O	2.17	0.44
1:A:424[B]:ILE:HD13	1:A:460:ILE:CD1	2.46	0.44
1:A:491:LYS:NZ	3:A:1810:HOH:O	2.50	0.44
1:A:547:PHE:CD1	3:A:1858:HOH:O	2.69	0.44
1:A:632:GLU:HG2	3:A:1912:HOH:O	2.17	0.44
1:A:494:VAL:HG11	1:A:570:GLU:CG	2.48	0.43
1:A:558:ILE:CD1	1:A:565:LEU:CG	2.94	0.43
1:A:402:SER:C	3:A:1725:HOH:O	2.60	0.43
1:A:667:ASN:HB3	1:A:670:ILE:HD13	1.98	0.43
1:A:314:LEU:O	1:A:314:LEU:HG	2.16	0.43
1:A:351:LYS:NZ	1:A:476:ASP:OD1	2.50	0.43
1:A:490:LEU:HB3	1:A:574[A]:ILE:CD1	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1092:MET:HE3	1:A:1092:MET:HB2	1.68	0.43
1:A:230:LYS:O	1:A:231:ASP:HB3	2.19	0.43
1:A:1049:TYR:CB	1:A:1067:ARG:HB2	2.49	0.43
1:A:61:ILE:HG23	3:A:1260:HOH:O	2.19	0.43
1:A:495:LYS:HD3	3:A:1692:HOH:O	2.19	0.43
1:A:459:SER:HB3	3:A:1888:HOH:O	2.19	0.42
1:A:521:THR:O	1:A:522:SER:CB	2.66	0.42
1:A:1016:PHE:CZ	1:A:1155:LEU:HD21	2.55	0.42
1:A:1053:ALA:HA	1:A:1062:VAL:O	2.20	0.42
1:A:749:ASP:CG	3:A:1883:HOH:O	2.63	0.42
1:A:371:LEU:C	1:A:373:PRO:HD3	2.45	0.41
1:A:1092:MET:HG3	1:A:1096:ASP:HB2	2.01	0.41
1:A:254:ASP:CB	3:A:1526:HOH:O	2.65	0.41
1:A:375:VAL:HG11	1:A:403:SER:CB	2.49	0.41
1:A:1108:ILE:O	1:A:1108:ILE:HG22	2.18	0.41
1:A:83:LYS:NZ	1:A:104:ASN:H	2.18	0.41
1:A:477:LYS:HE2	3:A:1767:HOH:O	2.19	0.41
1:A:554:VAL:O	1:A:558:ILE:HG12	2.21	0.41
1:A:1089:ALA:O	1:A:1146:LYS:CE	2.68	0.41
1:A:418:ILE:CG1	1:A:507:ILE:HD11	2.51	0.41
1:A:445:ILE:O	1:A:460:ILE:HD12	2.21	0.41
1:A:463:LYS:HB2	1:A:463:LYS:HE2	1.83	0.41
1:A:278:LYS:CE	3:A:1586:HOH:O	2.69	0.41
1:A:824[A]:HIS:CD2	1:A:942:HIS:HE1	2.34	0.41
1:A:176[B]:MET:HE2	3:A:1258:HOH:O	2.11	0.41
1:A:476:ASP:HA	3:A:1664:HOH:O	2.21	0.41
1:A:849:ILE:CG2	1:A:853:LYS:HE3	2.51	0.41
1:A:1015:LEU:HD22	1:A:1159:LYS:HB3	2.03	0.41
1:A:457:ILE:HG22	1:A:458:PHE:N	2.35	0.40
1:A:876:LYS:HE2	1:A:883:HIS:CD2	2.57	0.40
1:A:549:LYS:O	1:A:553:ILE:HG12	2.21	0.40
1:A:597:LEU:HD23	1:A:597:LEU:HA	1.98	0.40
1:A:640:PHE:CG	1:A:641:PRO:HD2	2.57	0.40
1:A:640:PHE:CD2	1:A:641:PRO:HD2	2.57	0.40
1:A:872:MET:HE2	1:A:1062:VAL:HG11	2.03	0.40
1:A:1138:ARG:HA	3:A:1914:HOH:O	2.20	0.40
1:A:292:TYR:CD1	1:A:292:TYR:C	2.99	0.40
1:A:1052:PHE:CZ	1:A:1054:ASP:HB2	2.56	0.40
1:A:402:SER:CB	3:A:1725:HOH:O	2.69	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	1084/1193 (91%)	1055 (97%)	27 (2%)	2 (0%)	43 24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	403	SER
1	A	426	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	1004/1104 (91%)	977 (97%)	27 (3%)	39 16

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	LYS
1	A	132	GLU
1	A	172	MET
1	A	201	LYS
1	A	214	GLU
1	A	217	LYS
1	A	249	SER
1	A	308	LYS
1	A	314	LEU

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Mol	Chain	Res	Type
1	A	360	GLU
1	A	364	LEU
1	A	404	ASP
1	A	426	THR
1	A	463	LYS
1	A	479	HIS
1	A	522	SER
1	A	543	LEU
1	A	544	ILE
1	A	584	LEU
1	A	698	LYS
1	A	859	MET
1	A	872	MET
1	A	906	GLU
1	A	940	LEU
1	A	1110	LYS
1	A	1113	ARG
1	A	1146	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	141	ASN
1	A	161	ASN
1	A	271	ASN
1	A	443	ASN
1	A	474	ASN
1	A	538	ASN
1	A	726	ASN
1	A	760	ASN
1	A	804	ASN
1	A	857	ASN
1	A	901	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 1 ligands modelled in this entry, 1 is 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	399:HIS	C	402:SER	N	6.70

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	1078/1193 (90%)	0.76	135 (12%) 8 8	7, 22, 45, 77	14 (1%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	402	SER	15.1
1	A	399	HIS	10.8
1	A	403	SER	8.1
1	A	1108	ILE	6.0
1	A	224	ALA	6.0
1	A	965	ILE	5.5
1	A	550	TYR	4.8
1	A	1005	PHE	4.8
1	A	721	THR	4.5
1	A	358	SER	4.4
1	A	248	LEU	3.9
1	A	544	ILE	3.8
1	A	978	MET	3.8
1	A	226	ILE	3.7
1	A	863	PHE	3.7
1	A	58	PRO	3.7
1	A	1107	THR	3.7
1	A	1193	GLU	3.7
1	A	376	ASP	3.6
1	A	698	LYS	3.6
1	A	359	GLU	3.6
1	A	989	LEU	3.6
1	A	994	LYS	3.6
1	A	547	PHE	3.6
1	A	59	GLU	3.5
1	A	1049	TYR	3.5
1	A	219	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	223	LYS	3.4
1	A	595	GLU	3.4
1	A	109	VAL	3.4
1	A	218	GLU	3.4
1	A	558	ILE	3.4
1	A	543	LEU	3.3
1	A	357	HIS	3.3
1	A	404	ASP	3.2
1	A	221	LYS	3.2
1	A	551	LEU	3.2
1	A	1067	ARG	3.1
1	A	697	LEU	3.1
1	A	222	GLY	3.0
1	A	612[A]	GLN	3.0
1	A	553	ILE	3.0
1	A	1109	ASP	3.0
1	A	514	LEU	3.0
1	A	519	LEU	3.0
1	A	1003	PRO	3.0
1	A	992	GLU	3.0
1	A	682	HIS	2.9
1	A	61	ILE	2.9
1	A	824[A]	HIS	2.9
1	A	545	PHE	2.9
1	A	217	LYS	2.9
1	A	626	LYS	2.8
1	A	107	LEU	2.8
1	A	1006	VAL	2.8
1	A	724	GLU	2.8
1	A	865	GLU	2.8
1	A	1039	TRP	2.7
1	A	1052	PHE	2.7
1	A	634	PRO	2.7
1	A	1044	GLY	2.7
1	A	668	ASN	2.7
1	A	1110	LYS	2.7
1	A	552	ASN	2.7
1	A	83	LYS	2.7
1	A	375	VAL	2.7
1	A	521	THR	2.6
1	A	632	GLU	2.6
1	A	554	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	722	LYS	2.6
1	A	1161	ASN	2.6
1	A	67	LYS	2.5
1	A	645	ILE	2.5
1	A	963	LYS	2.5
1	A	176[A]	MET	2.5
1	A	63	GLU	2.5
1	A	360	GLU	2.5
1	A	631	GLU	2.5
1	A	630	ALA	2.5
1	A	559	LYS	2.5
1	A	563[A]	MET	2.5
1	A	548	GLU	2.5
1	A	60	TRP	2.5
1	A	215	LYS	2.5
1	A	987	LYS	2.4
1	A	750	HIS	2.4
1	A	869	ALA	2.4
1	A	1045[A]	LEU	2.4
1	A	592	GLN	2.4
1	A	214	GLU	2.4
1	A	868	TYR	2.4
1	A	308	LYS	2.4
1	A	80	GLU	2.3
1	A	1014	ILE	2.3
1	A	249	SER	2.3
1	A	991	ASP	2.3
1	A	329	LYS	2.3
1	A	619	LYS	2.3
1	A	670	ILE	2.3
1	A	549	LYS	2.3
1	A	650	LYS	2.3
1	A	597	LEU	2.3
1	A	1178	GLU	2.3
1	A	864	SER	2.3
1	A	278	LYS	2.3
1	A	1192	ILE	2.3
1	A	62	HIS	2.2
1	A	878	HIS	2.2
1	A	608	ASN	2.2
1	A	216	LEU	2.2
1	A	627	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	964	TYR	2.2
1	A	257	HIS	2.2
1	A	1094	GLU	2.2
1	A	1001	VAL	2.2
1	A	306	PHE	2.2
1	A	990	PHE	2.2
1	A	202	TYR	2.2
1	A	252	LEU	2.1
1	A	907	ASN	2.1
1	A	906	GLU	2.1
1	A	1111	PRO	2.1
1	A	476	ASP	2.1
1	A	636	HIS	2.1
1	A	231	ASP	2.1
1	A	616	GLN	2.1
1	A	862	THR	2.1
1	A	866	LYS	2.1
1	A	546	GLU	2.0
1	A	679	THR	2.0
1	A	1004	THR	2.0
1	A	199	GLU	2.0
1	A	520	LYS	2.0
1	A	927	LYS	2.0
1	A	988	LYS	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	CO	A	1195	1/1	0.80	0.12	40,40,40,40	1

6.5 Other polymers [i](#)

There are no such residues in this entry.