



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:02 PM UTC

PDB ID : 4FGV / pdb_00004fgv
Title : Crystal structure of free CRM1 (crystal form 1)
Authors : Monecke, T.; Neumann, P.; Dickmanns, A.; Ficner, R.
Deposited on : 2012-06-05
Resolution : 2.94 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

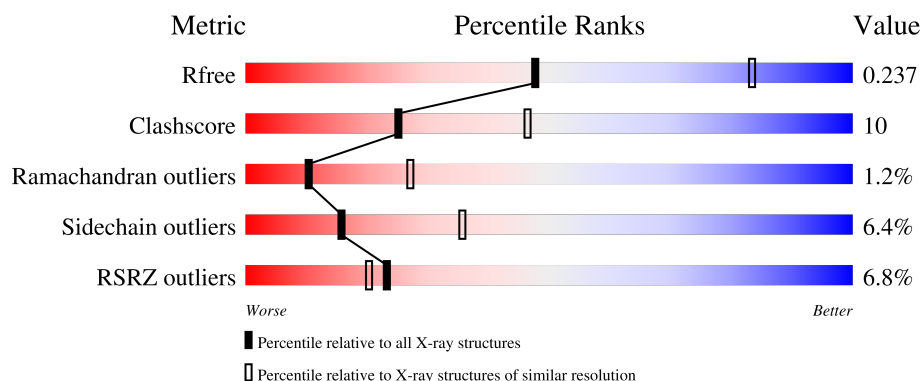
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	1086	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8595 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.

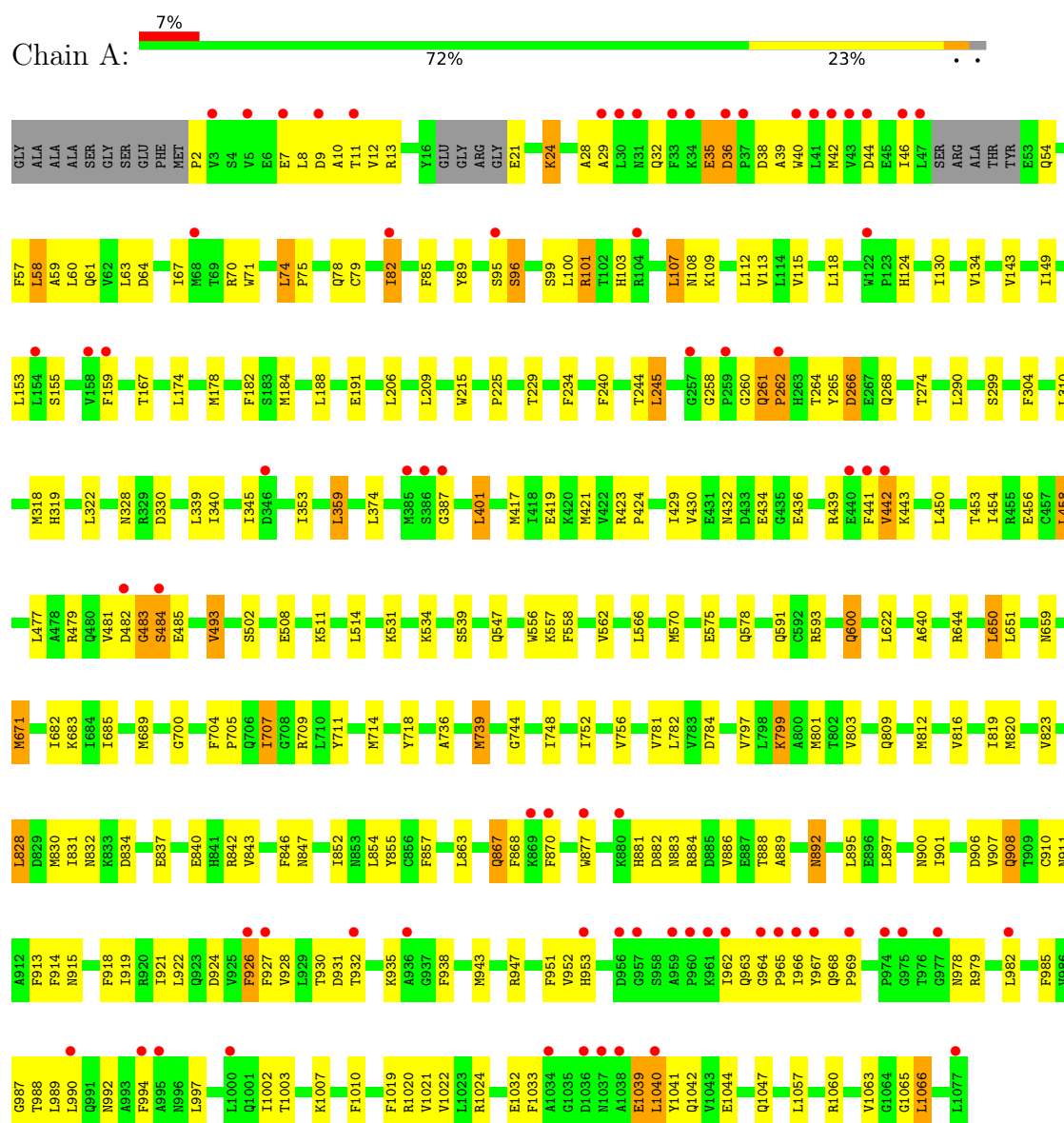
- Molecule 1 is a protein called Chromosome region maintenance 1 (CRM1) or Exportin 1 (Xpo1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1067	8595	5484	1448	1600	63	0	0	0

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: Chromosome region maintenance 1 (CRM1) or Exportin 1 (Xpo1)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.12Å 139.07Å 174.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.85 – 2.94 45.85 – 2.94	Depositor EDS
% Data completeness (in resolution range)	95.8 (45.85-2.94) 95.6 (45.85-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.220 , 0.243 0.212 , 0.237	Depositor DCC
R_{free} test set	2151 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.0	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8595	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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	0.36	0/8763	0.81	9/11858 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	GLU	N-CA-C	-8.33	103.22	112.72
1	A	700	GLY	CA-C-N	5.43	125.77	119.47
1	A	700	GLY	C-N-CA	5.43	125.77	119.47
1	A	261	GLN	CA-C-N	-5.31	113.20	119.84
1	A	261	GLN	C-N-CA	-5.31	113.20	119.84
1	A	36	ASP	CA-C-N	-5.26	113.11	118.85
1	A	36	ASP	C-N-CA	-5.26	113.11	118.85
1	A	600	GLN	CA-C-N	5.12	125.15	119.32
1	A	600	GLN	C-N-CA	5.12	125.15	119.32

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	8595	0	8599	167	0
All	All	8595	0	8599	167	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 10.

All (167) 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:911:ASN:HD21	1:A:966:ILE:HG12	1.41	0.85
1:A:258:GLY:HA3	1:A:262:PRO:HD2	1.63	0.80
1:A:134:VAL:HG22	1:A:188:LEU:HD12	1.64	0.80
1:A:932:THR:O	1:A:935:LYS:NZ	2.18	0.77
1:A:13:ARG:HD2	1:A:24:LYS:HG2	1.65	0.76
1:A:908:GLN:HE21	1:A:908:GLN:H	1.34	0.75
1:A:359:LEU:HD12	1:A:453:THR:HG23	1.69	0.74
1:A:834:ASP:HB3	1:A:837:GLU:HB2	1.68	0.74
1:A:479:ARG:HH21	1:A:483:GLY:HA3	1.56	0.70
1:A:261:GLN:HB2	1:A:262:PRO:HD3	1.73	0.69
1:A:820:MET:HE1	1:A:852:ILE:HD13	1.72	0.69
1:A:134:VAL:HG21	1:A:184:MET:HE2	1.78	0.66
1:A:883:ASN:HB3	1:A:886:VAL:HG12	1.79	0.64
1:A:895:LEU:HD21	1:A:943:MET:HG3	1.78	0.64
1:A:38:ASP:O	1:A:42:MET:HB2	1.99	0.62
1:A:1024:ARG:HG3	1:A:1040:LEU:HD12	1.81	0.61
1:A:689:MET:HE1	1:A:714:MET:HG2	1.83	0.60
1:A:264:THR:OG1	1:A:266:ASP:OD1	2.19	0.60
1:A:994:PHE:HE2	1:A:1032:GLU:H	1.48	0.60
1:A:429:ILE:HD11	1:A:539:SER:HB2	1.85	0.58
1:A:63:LEU:HD23	1:A:113:VAL:HG11	1.85	0.58
1:A:482:ASP:C	1:A:484:SER:H	2.12	0.58
1:A:979:ARG:HH12	1:A:1007:LYS:NZ	2.00	0.58
1:A:60:LEU:HD22	1:A:113:VAL:HG21	1.85	0.58
1:A:64:ASP:HA	1:A:67:ILE:HD12	1.86	0.57
1:A:914:PHE:O	1:A:918:PHE:HB2	2.03	0.57
1:A:907:VAL:O	1:A:911:ASN:HB2	2.03	0.57
1:A:482:ASP:O	1:A:484:SER:N	2.37	0.56
1:A:908:GLN:H	1:A:908:GLN:NE2	2.03	0.56
1:A:888:THR:O	1:A:892:ASN:HB2	2.05	0.56
1:A:439:ARG:HH11	1:A:575:GLU:HG2	1.70	0.55
1:A:54:GLN:HA	1:A:57:PHE:HD2	1.70	0.55
1:A:989:LEU:HA	1:A:992:ASN:HD22	1.72	0.55
1:A:938:PHE:HE1	1:A:1020:ARG:HG3	1.72	0.55
1:A:268:GLN:N	1:A:268:GLN:OE1	2.40	0.54
1:A:837:GLU:O	1:A:842:ARG:NH2	2.40	0.54
1:A:997:LEU:HD23	1:A:1002:ILE:HG12	1.89	0.54
1:A:35:GLU:HG2	1:A:70:ARG:NH2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:968:GLN:HB3	1:A:969:PRO:HD2	1.90	0.53
1:A:1021:VAL:HG22	1:A:1024:ARG:NH2	2.23	0.53
1:A:953:HIS:HB3	1:A:1010:PHE:CD1	2.44	0.53
1:A:828:LEU:HD11	1:A:870:PHE:CG	2.43	0.53
1:A:74:LEU:HG	1:A:75:PRO:HD2	1.91	0.53
1:A:682:ILE:HD13	1:A:744:GLY:HA3	1.90	0.53
1:A:685:ILE:HG21	1:A:748:ILE:HG23	1.91	0.52
1:A:967:TYR:CD2	1:A:968:GLN:HG2	2.45	0.52
1:A:310:LEU:HG	1:A:353:ILE:HD13	1.90	0.52
1:A:593:ARG:HG3	1:A:640:ALA:HB2	1.91	0.52
1:A:843:VAL:O	1:A:847:ASN:ND2	2.42	0.52
1:A:927:PHE:O	1:A:931:ASP:HB2	2.10	0.52
1:A:906:ASP:HB3	1:A:908:GLN:NE2	2.25	0.52
1:A:924:ASP:O	1:A:928:VAL:HG23	2.10	0.52
1:A:935:LYS:HB3	1:A:1039:GLU:HB2	1.91	0.52
1:A:987:GLY:HA2	1:A:990:LEU:HD12	1.92	0.52
1:A:319:HIS:HB3	1:A:322:LEU:HD13	1.91	0.51
1:A:419:GLU:HA	1:A:493:VAL:HG11	1.91	0.51
1:A:556:TRP:CE2	1:A:600:GLN:HG3	2.44	0.51
1:A:40:TRP:HA	1:A:85:PHE:CE2	2.45	0.51
1:A:9:ASP:HA	1:A:12:VAL:HB	1.92	0.51
1:A:75:PRO:HG2	1:A:78:GLN:HB2	1.93	0.51
1:A:450:LEU:O	1:A:454:ILE:HG13	2.10	0.50
1:A:881:HIS:HD2	1:A:882:ASP:N	2.09	0.50
1:A:831:ILE:HG23	1:A:842:ARG:HG3	1.93	0.50
1:A:290:LEU:HB3	1:A:345:ILE:HD11	1.93	0.50
1:A:884:ARG:HH22	1:A:1042:GLN:CD	2.19	0.50
1:A:155:SER:O	1:A:159:PHE:HB3	2.11	0.50
1:A:96:SER:HB3	1:A:99:SER:HB2	1.93	0.49
1:A:130:ILE:O	1:A:134:VAL:HG23	2.11	0.49
1:A:432:ASN:ND2	1:A:436:GLU:HB3	2.26	0.49
1:A:962:ILE:HG22	1:A:964:GLY:H	1.77	0.49
1:A:432:ASN:HD21	1:A:436:GLU:HB3	1.78	0.49
1:A:423:ARG:HH22	1:A:443:LYS:HE3	1.79	0.48
1:A:1060:ARG:HA	1:A:1066:LEU:HD23	1.96	0.48
1:A:842:ARG:HD2	1:A:877:TRP:CZ2	2.49	0.48
1:A:234:PHE:HB2	1:A:244:THR:HG21	1.95	0.48
1:A:44:ASP:HB2	1:A:89:TYR:OH	2.13	0.48
1:A:953:HIS:HB3	1:A:1010:PHE:HD1	1.79	0.48
1:A:95:SER:HA	1:A:143:VAL:HG23	1.96	0.47
1:A:103:HIS:O	1:A:107:LEU:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:MET:HE3	1:A:752:ILE:HA	1.95	0.47
1:A:952:VAL:HG13	1:A:978:ASN:HB3	1.96	0.47
1:A:42:MET:HG2	1:A:59:ALA:HB2	1.96	0.47
1:A:911:ASN:ND2	1:A:966:ILE:HG12	2.21	0.47
1:A:245:LEU:HD12	1:A:304:PHE:CE1	2.50	0.46
1:A:799:LYS:O	1:A:803:VAL:HG23	2.16	0.46
1:A:830:MET:O	1:A:834:ASP:HB2	2.16	0.46
1:A:834:ASP:CB	1:A:837:GLU:HB2	2.42	0.46
1:A:901:ILE:HG21	1:A:913:PHE:CD2	2.51	0.46
1:A:318:MET:HA	1:A:318:MET:HE3	1.98	0.46
1:A:718:TYR:CZ	1:A:781:VAL:HG12	2.51	0.46
1:A:240:PHE:O	1:A:244:THR:HG23	2.16	0.45
1:A:570:MET:O	1:A:578:GLN:NE2	2.39	0.45
1:A:831:ILE:O	1:A:842:ARG:NH1	2.45	0.45
1:A:2:PRO:HG2	1:A:7:GLU:HB2	1.99	0.45
1:A:883:ASN:HB3	1:A:886:VAL:CG1	2.45	0.45
1:A:915:ASN:HD22	1:A:915:ASN:C	2.23	0.45
1:A:9:ASP:C	1:A:11:THR:H	2.25	0.45
1:A:820:MET:HG2	1:A:863:LEU:HD13	1.99	0.45
1:A:683:LYS:HE3	1:A:683:LYS:HB2	1.82	0.45
1:A:863:LEU:HG	1:A:867:GLN:HB2	1.98	0.45
1:A:29:ALA:O	1:A:32:GLN:NE2	2.48	0.44
1:A:108:ASN:O	1:A:112:LEU:HG	2.17	0.44
1:A:149:ILE:O	1:A:153:LEU:HG	2.17	0.44
1:A:479:ARG:HD3	1:A:479:ARG:HA	1.74	0.44
1:A:508:GLU:H	1:A:508:GLU:CD	2.25	0.44
1:A:881:HIS:CD2	1:A:883:ASN:H	2.34	0.44
1:A:67:ILE:O	1:A:71:TRP:HB2	2.18	0.44
1:A:910:CYS:SG	1:A:911:ASN:N	2.90	0.44
1:A:417:MET:HB3	1:A:458:LEU:HD13	1.99	0.44
1:A:951:PHE:HA	1:A:963:GLN:HB2	2.00	0.44
1:A:797:VAL:O	1:A:801:MET:HG2	2.18	0.44
1:A:8:LEU:HA	1:A:46:ILE:HD11	1.99	0.44
1:A:174:LEU:HD23	1:A:178:MET:HG3	1.99	0.44
1:A:477:LEU:O	1:A:481:VAL:HG23	2.18	0.44
1:A:115:VAL:HA	1:A:118:LEU:HD12	2.01	0.43
1:A:442:VAL:HG22	1:A:443:LYS:H	1.83	0.43
1:A:985:PHE:O	1:A:988:THR:OG1	2.30	0.43
1:A:101:ARG:H	1:A:101:ARG:HG2	1.60	0.43
1:A:182:PHE:CE1	1:A:215:TRP:HB3	2.54	0.43
1:A:812:MET:O	1:A:816:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASN:ND2	1:A:330:ASP:HB2	2.33	0.43
1:A:58:LEU:O	1:A:61:GLN:HB3	2.18	0.43
1:A:819:ILE:O	1:A:823:VAL:HB	2.18	0.43
1:A:482:ASP:C	1:A:484:SER:N	2.77	0.43
1:A:671:MET:HE3	1:A:671:MET:HA	2.01	0.43
1:A:39:ALA:O	1:A:42:MET:HB3	2.18	0.43
1:A:558:PHE:O	1:A:562:VAL:HG13	2.19	0.43
1:A:707:ILE:O	1:A:711:TYR:HB2	2.19	0.43
1:A:943:MET:O	1:A:947:ARG:HG2	2.18	0.43
1:A:857:PHE:HZ	1:A:901:ILE:HD13	1.84	0.42
1:A:930:THR:HA	1:A:1033:PHE:HZ	1.83	0.42
1:A:82:ILE:HA	1:A:85:PHE:HB3	1.99	0.42
1:A:650:LEU:HD12	1:A:650:LEU:HA	1.89	0.42
1:A:659:ASN:HB3	1:A:709:ARG:NH2	2.33	0.42
1:A:857:PHE:CE1	1:A:900:ASN:HB3	2.54	0.42
1:A:846:PHE:CE2	1:A:889:ALA:HB1	2.54	0.42
1:A:10:ALA:O	1:A:28:ALA:HB2	2.19	0.42
1:A:265:TYR:O	1:A:268:GLN:N	2.51	0.42
1:A:401:LEU:HD12	1:A:401:LEU:HA	1.85	0.42
1:A:901:ILE:HG21	1:A:913:PHE:HD2	1.84	0.42
1:A:968:GLN:HE21	1:A:969:PRO:HD2	1.85	0.42
1:A:502:SER:O	1:A:1065:GLY:HA2	2.20	0.42
1:A:109:LYS:O	1:A:113:VAL:HG23	2.20	0.42
1:A:1019:PHE:O	1:A:1022:VAL:HG12	2.19	0.42
1:A:328:ASN:HD21	1:A:330:ASP:HB2	1.85	0.41
1:A:809:GLN:HG2	1:A:855:TYR:HB3	2.01	0.41
1:A:947:ARG:HA	1:A:947:ARG:HD2	1.86	0.41
1:A:1024:ARG:HH12	1:A:1044:GLU:CD	2.28	0.41
1:A:556:TRP:CD2	1:A:600:GLN:HG3	2.55	0.41
1:A:11:THR:HG21	1:A:58:LEU:HD22	2.03	0.41
1:A:423:ARG:HH22	1:A:443:LYS:NZ	2.18	0.41
1:A:423:ARG:HA	1:A:424:PRO:HD3	1.91	0.41
1:A:967:TYR:HB2	1:A:978:ASN:OD1	2.21	0.41
1:A:225:PRO:O	1:A:229:THR:HG23	2.21	0.41
1:A:828:LEU:HD11	1:A:870:PHE:CB	2.51	0.41
1:A:1024:ARG:HD2	1:A:1041:TYR:CE1	2.56	0.41
1:A:79:CYS:HA	1:A:82:ILE:HG22	2.03	0.41
1:A:1003:THR:O	1:A:1007:LYS:HG2	2.20	0.40
1:A:967:TYR:CE2	1:A:968:GLN:HG2	2.57	0.40
1:A:13:ARG:O	1:A:21:GLU:N	2.55	0.40
1:A:339:LEU:HD23	1:A:339:LEU:HA	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LEU:HD21	1:A:456:GLU:HG2	2.03	0.40
1:A:704:PHE:CG	1:A:705:PRO:HD3	2.57	0.40
1:A:736:ALA:HA	1:A:739:MET:HG3	2.04	0.40
1:A:922:LEU:O	1:A:926:PHE:HB2	2.21	0.40
1:A:9:ASP:C	1:A:11:THR:N	2.80	0.40
1:A:423:ARG:HH22	1:A:443:LYS:CE	2.34	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	1061/1086 (98%)	987 (93%)	61 (6%)	13 (1%)	10	27

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	921	ILE
1	A	483	GLY
1	A	124	HIS
1	A	262	PRO
1	A	266	ASP
1	A	387	GLY
1	A	260	GLY
1	A	441	PHE
1	A	484	SER
1	A	167	THR
1	A	36	ASP
1	A	96	SER
1	A	965	PRO

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	957/971 (99%)	896 (94%)	61 (6%)	16	36

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	35	GLU
1	A	58	LEU
1	A	74	LEU
1	A	82	ILE
1	A	100	LEU
1	A	101	ARG
1	A	107	LEU
1	A	191	GLU
1	A	206	LEU
1	A	209	LEU
1	A	245	LEU
1	A	274	THR
1	A	299	SER
1	A	340	ILE
1	A	359	LEU
1	A	374	LEU
1	A	401	LEU
1	A	421	MET
1	A	430	VAL
1	A	434	GLU
1	A	442	VAL
1	A	458	LEU
1	A	493	VAL
1	A	511	LYS
1	A	514	LEU
1	A	531	LYS
1	A	534	LYS
1	A	547	GLN
1	A	557	LYS

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Mol	Chain	Res	Type
1	A	566	LEU
1	A	591	GLN
1	A	622	LEU
1	A	644	ARG
1	A	650	LEU
1	A	651	LEU
1	A	671	MET
1	A	707	ILE
1	A	739	MET
1	A	756	VAL
1	A	782	LEU
1	A	784	ASP
1	A	799	LYS
1	A	828	LEU
1	A	832	ASN
1	A	840	GLU
1	A	854	LEU
1	A	867	GLN
1	A	868	PHE
1	A	892	ASN
1	A	897	LEU
1	A	908	GLN
1	A	919	ILE
1	A	926	PHE
1	A	982	LEU
1	A	1039	GLU
1	A	1040	LEU
1	A	1047	GLN
1	A	1057	LEU
1	A	1063	VAL
1	A	1066	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	65	ASN
1	A	78	GLN
1	A	84	ASN
1	A	92	GLN
1	A	344	GLN
1	A	471	GLN

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Mol	Chain	Res	Type
1	A	591	GLN
1	A	767	GLN
1	A	822	ASN
1	A	832	ASN
1	A	881	HIS
1	A	908	GLN
1	A	911	ASN
1	A	941	GLN
1	A	992	ASN

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 [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	1067/1086 (98%)	0.28	73 (6%) 23 20	31, 78, 179, 291	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	158	VAL	5.7
1	A	441	PHE	4.5
1	A	967	TYR	4.5
1	A	41	LEU	4.2
1	A	47	LEU	4.0
1	A	442	VAL	3.9
1	A	969	PRO	3.9
1	A	36	ASP	3.8
1	A	40	TRP	3.8
1	A	385	MET	3.8
1	A	1040	LEU	3.6
1	A	927	PHE	3.4
1	A	1036	ASP	3.3
1	A	159	PHE	3.2
1	A	994	PHE	3.1
1	A	259	PRO	3.0
1	A	68	MET	2.9
1	A	962	ILE	2.9
1	A	956	ASP	2.9
1	A	482	ASP	2.9
1	A	1077	LEU	2.9
1	A	33	PHE	2.8
1	A	880	LYS	2.8
1	A	1038	ALA	2.8
1	A	387	GLY	2.8
1	A	42	MET	2.6
1	A	964	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	932	THR	2.6
1	A	262	PRO	2.6
1	A	82	ILE	2.6
1	A	5	VAL	2.6
1	A	870	PHE	2.6
1	A	31	ASN	2.6
1	A	975	GLY	2.5
1	A	104	ARG	2.5
1	A	95	SER	2.4
1	A	484	SER	2.4
1	A	34	LYS	2.4
1	A	386	SER	2.4
1	A	960	PRO	2.4
1	A	974	PRO	2.4
1	A	3	VAL	2.4
1	A	440	GLU	2.4
1	A	936	ALA	2.4
1	A	257	GLY	2.3
1	A	926	PHE	2.3
1	A	965	PRO	2.3
1	A	29	ALA	2.3
1	A	46	ILE	2.3
1	A	961	LYS	2.3
1	A	37	PRO	2.3
1	A	957	GLY	2.3
1	A	953	HIS	2.3
1	A	122	TRP	2.3
1	A	995	ALA	2.2
1	A	1034	ALA	2.2
1	A	959	ALA	2.2
1	A	982	LEU	2.2
1	A	44	ASP	2.1
1	A	7	GLU	2.1
1	A	9	ASP	2.1
1	A	1037	ASN	2.1
1	A	30	LEU	2.1
1	A	1000	LEU	2.1
1	A	877	TRP	2.1
1	A	869	LYS	2.0
1	A	43	VAL	2.0
1	A	977	GLY	2.0
1	A	154	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	990	LEU	2.0
1	A	966	ILE	2.0
1	A	11	THR	2.0
1	A	346	ASP	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.