WORLDWIDE PDB

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Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2023 – 07:16 AM EDT

PDB ID	:	4FGV
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)

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

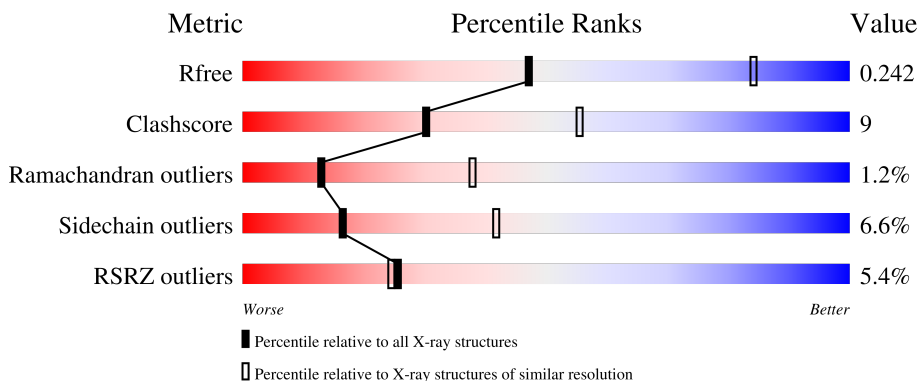|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
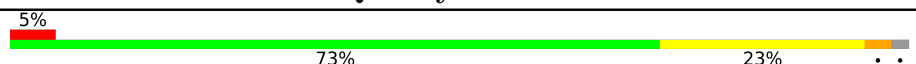*X-RAY DIFFRACTION*

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	Percentile Ranks	Value
Rfree		0.242
Clashscore		9
Ramachandran outliers		1.2%
Sidechain outliers		6.6%
RSRZ outliers		5.4%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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 <=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	5% ... 73% ... 23% ...

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 (i)

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)

Chain A:
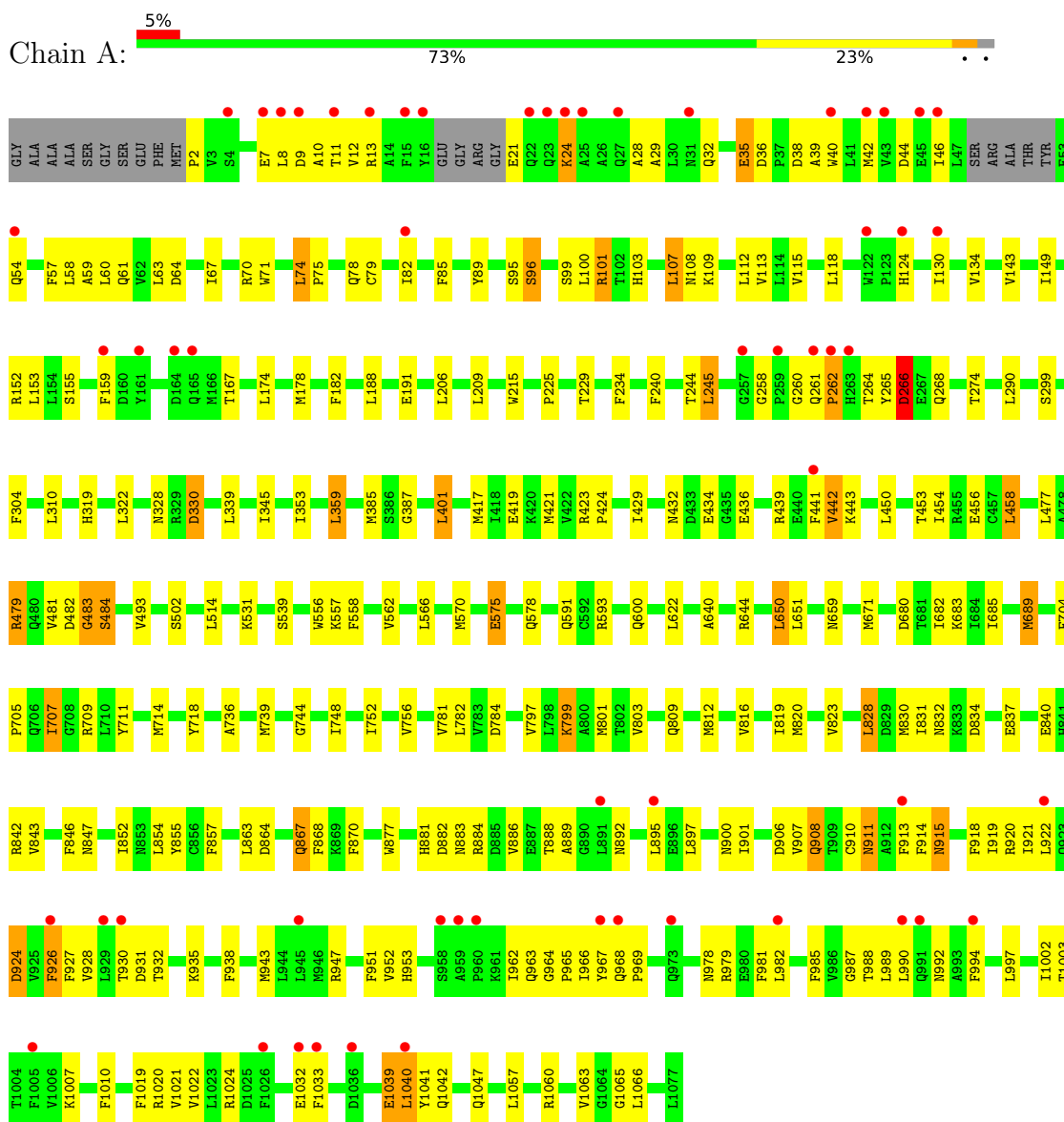
4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.11 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.220 , 0.243 0.215 , 0.242	Depositor DCC
R_{free} test set	2151 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	66.6	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 67.0	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	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: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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 ⓘ

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	0.26	0/8763	0.47	0/11858

There are no bond length outliers.

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	8595	0	8599	160	0
All	All	8595	0	8599	160	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 9.

All (160) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:689:MET:HE1	1:A:714:MET:HG2	1.86	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
1:A:482:ASP:C	1:A:484:SER:H	2.12	0.53
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:979:ARG:HH12	1:A:1007:LYS:HZ3	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:689:MET:HE3	1:A:752:ILE:HA	1.93	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
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:718:TYR:CZ	1:A:781:VAL:HG12	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:884:ARG:HH22	1:A:1042:GLN:CD	2.19	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: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: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
1:A:328:ASN:ND2	1:A:330:ASP:HB2	2.33	0.43
1:A:820:MET:HE1	1:A:852:ILE:HD13	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:915:ASN:HD22	1:A:915:ASN:C	2.23	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
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: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

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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%)	13	38

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%)	894 (93%)	63 (7%)	16	42

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	35	GLU
1	A	74	LEU
1	A	100	LEU

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Mol	Chain	Res	Type
1	A	101	ARG
1	A	107	LEU
1	A	152	ARG
1	A	191	GLU
1	A	206	LEU
1	A	209	LEU
1	A	245	LEU
1	A	266	ASP
1	A	274	THR
1	A	299	SER
1	A	330	ASP
1	A	359	LEU
1	A	385	MET
1	A	401	LEU
1	A	421	MET
1	A	434	GLU
1	A	442	VAL
1	A	458	LEU
1	A	479	ARG
1	A	514	LEU
1	A	531	LYS
1	A	557	LYS
1	A	566	LEU
1	A	575	GLU
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	680	ASP
1	A	689	MET
1	A	707	ILE
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	864	ASP

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Mol	Chain	Res	Type
1	A	867	GLN
1	A	868	PHE
1	A	897	LEU
1	A	908	GLN
1	A	911	ASN
1	A	915	ASN
1	A	919	ILE
1	A	920	ARG
1	A	924	ASP
1	A	926	PHE
1	A	981	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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	84	ASN
1	A	471	GLN
1	A	591	GLN
1	A	881	HIS
1	A	908	GLN
1	A	911	ASN
1	A	941	GLN
1	A	992	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides 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(Å²)	Q<0.9
1	A	1067/1086 (98%)	0.25	58 (5%)	25	24	31, 78, 179, 291	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	ARG	7.4
1	A	960	PRO	5.9
1	A	967	TYR	5.2
1	A	161	TYR	5.1
1	A	1033	PHE	4.9
1	A	11	THR	4.2
1	A	959	ALA	4.2
1	A	261	GLN	4.1
1	A	46	ILE	3.9
1	A	164	ASP	3.8
1	A	1040	LEU	3.8
1	A	990	LEU	3.7
1	A	929	LEU	3.6
1	A	22	GLN	3.6
1	A	16	TYR	3.5
1	A	15	PHE	3.5
1	A	23	GLN	3.4
1	A	7	GLU	3.2
1	A	9	ASP	3.1
1	A	122	TRP	3.1
1	A	1036	ASP	3.1
1	A	31	ASN	3.1
1	A	45	GLU	3.1
1	A	926	PHE	2.9
1	A	25	ALA	2.8
1	A	930	THR	2.8
1	A	945	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	124	HIS	2.7
1	A	895	LEU	2.7
1	A	1026	PHE	2.7
1	A	891	LEU	2.7
1	A	257	GLY	2.7
1	A	982	LEU	2.6
1	A	24	LYS	2.6
1	A	994	PHE	2.6
1	A	262	PRO	2.6
1	A	958	SER	2.5
1	A	968	GLN	2.5
1	A	159	PHE	2.5
1	A	441	PHE	2.5
1	A	54	GLN	2.5
1	A	4	SER	2.4
1	A	973	GLN	2.4
1	A	165	GLN	2.4
1	A	27	GLN	2.4
1	A	259	PRO	2.3
1	A	42	MET	2.3
1	A	43	VAL	2.3
1	A	991	GLN	2.3
1	A	263	HIS	2.3
1	A	82	ILE	2.3
1	A	8	LEU	2.2
1	A	1032	GLU	2.2
1	A	913	PHE	2.2
1	A	40	TRP	2.1
1	A	922	LEU	2.1
1	A	1005	PHE	2.1
1	A	130	ILE	2.1

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 monosaccharides 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.