



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:23 AM UTC

PDB ID : 4IEG / pdb_00004ieg
Title : Structure and interactions of the RNA-dependent RNA polymerase from bacteriophage phi12 (P1 crystal form)
Authors : Ren, Z.; Franklin, M.C.; Ghose, R.
Deposited on : 2012-12-13
Resolution : 2.10 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

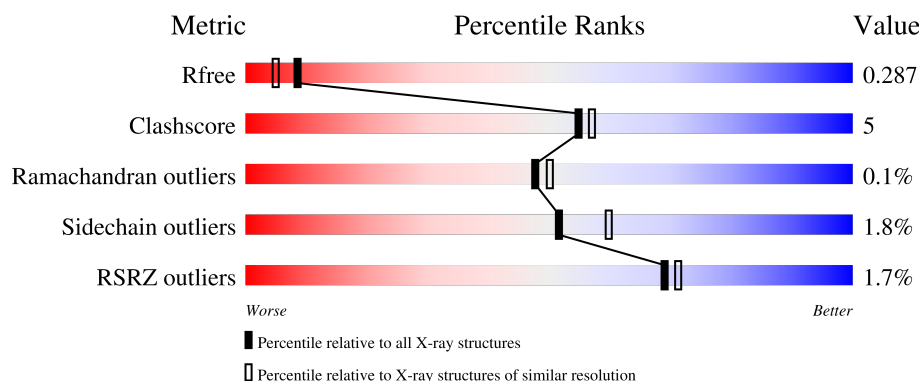
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	659	% 89% 9% ..
1	B	659	2% 86% 9% ..
1	C	659	2% 88% 10% ..
1	D	659	% 88% 9% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22601 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 RNA-dependent RNA polymerase P2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	3	0
			5260	3361	910	967	22			
1	B	634	Total	C	N	O	S	0	6	0
			5166	3305	889	950	22			
1	C	650	Total	C	N	O	S	0	5	0
			5281	3372	915	973	21			
1	D	643	Total	C	N	O	S	0	6	0
			5235	3348	903	962	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	MET	engineered mutation	UNP Q94M06
B	2	ALA	MET	engineered mutation	UNP Q94M06
C	2	ALA	MET	engineered mutation	UNP Q94M06
D	2	ALA	MET	engineered mutation	UNP Q94M06

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

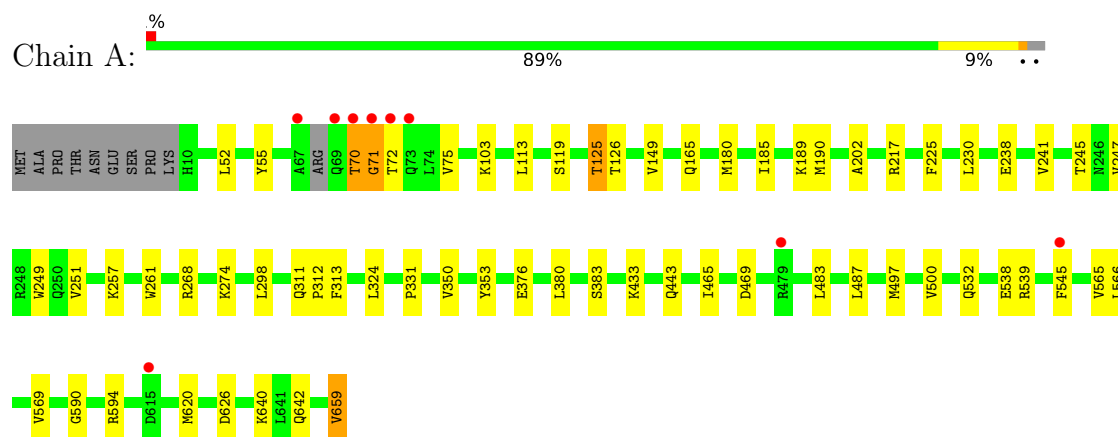
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	416	Total 416	O 416	0	0
3	B	422	Total 422	O 422	0	0
3	C	437	Total 437	O 437	0	0
3	D	380	Total 380	O 380	0	0

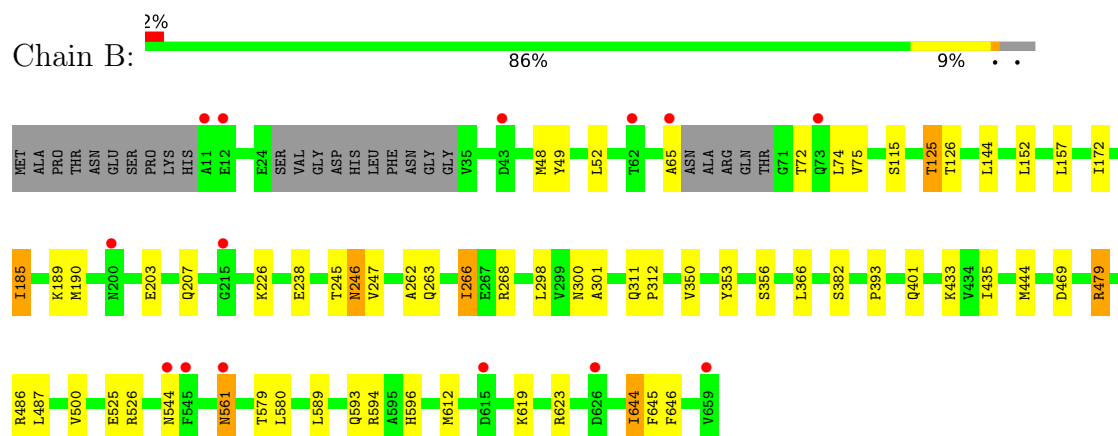
3 Residue-property plots [i](#)

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.

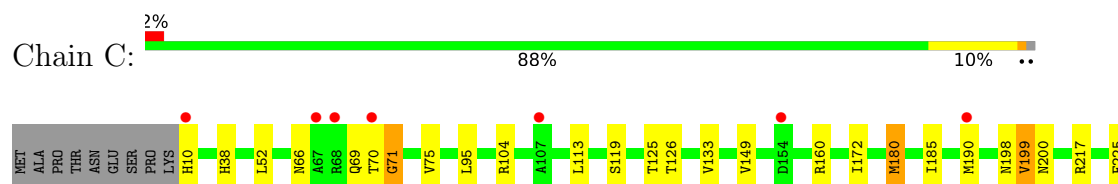
- Molecule 1: RNA-dependent RNA polymerase P2

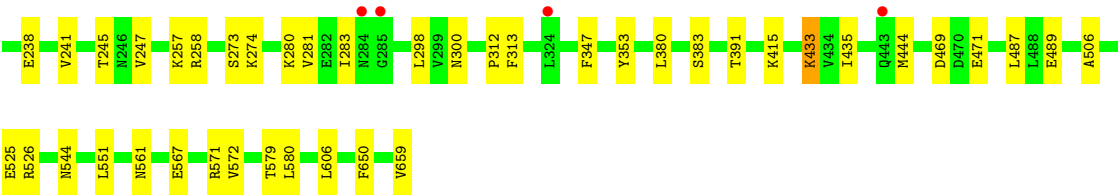


- Molecule 1: RNA-dependent RNA polymerase P2

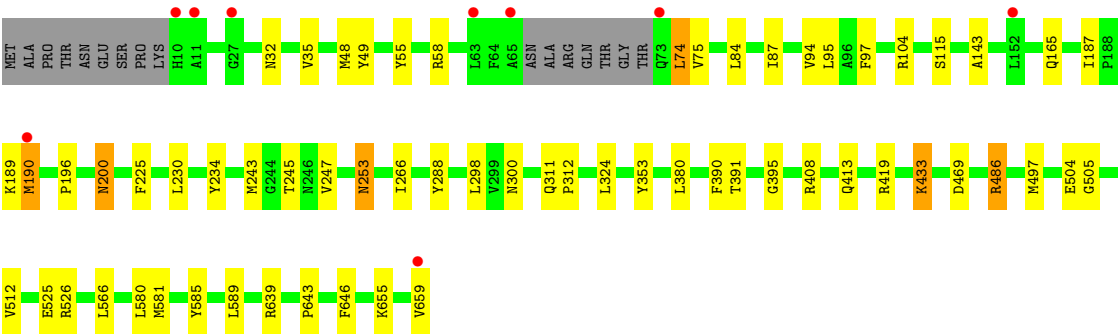
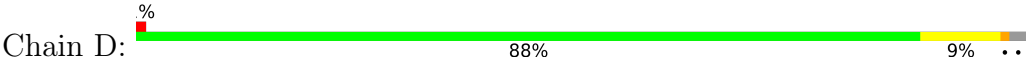


- Molecule 1: RNA-dependent RNA polymerase P2





● Molecule 1: RNA-dependent RNA polymerase P2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.87Å 94.47Å 96.48Å 75.16° 63.11° 83.79°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.3 (50.00-2.10) 92.6 (50.00-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.217 , 0.278 0.224 , 0.287	Depositor DCC
R_{free} test set	7276 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22601	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.56% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.53	0/5410	0.75	2/7327 (0.0%)
1	B	0.56	0/5321	0.75	0/7205
1	C	0.54	0/5438	0.73	0/7367
1	D	0.52	0/5394	0.73	0/7306
All	All	0.54	0/21563	0.74	2/29205 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	642	GLN	CA-C-N	6.93	127.22	119.32
1	A	642	GLN	C-N-CA	6.93	127.22	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	5260	0	5130	44	0
1	B	5166	0	5050	55	0
1	C	5281	0	5149	55	0
1	D	5235	0	5108	50	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	416	0	0	8	0
3	B	422	0	0	4	0
3	C	437	0	0	6	0
3	D	380	0	0	3	0
All	All	22601	0	20437	199	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 5.

All (199) 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:C:245[B]:THR:CG2	1:C:298[B]:LEU:HD11	1.17	1.57
1:C:245[B]:THR:CG2	1:C:298[B]:LEU:CD1	2.07	1.33
1:B:245[B]:THR:CG2	1:B:298[B]:LEU:HD11	1.75	1.16
1:C:75:VAL:HG12	1:C:247:VAL:HG23	1.28	1.13
1:C:245[B]:THR:HG23	1:C:298[B]:LEU:HD11	1.19	1.09
1:A:75:VAL:HG12	1:A:247:VAL:HG23	1.32	1.05
1:B:245[B]:THR:HG21	1:B:298[B]:LEU:HD11	1.08	1.04
1:C:75:VAL:CG1	1:C:247:VAL:HG23	1.86	1.04
1:C:245[B]:THR:HG21	1:C:298[B]:LEU:HD11	1.02	1.01
1:D:245[B]:THR:CG2	1:D:298[B]:LEU:HD11	1.94	0.98
1:B:245[B]:THR:CG2	1:B:298[B]:LEU:CD1	2.44	0.95
1:D:190[A]:MET:HA	1:D:190[A]:MET:CE	1.97	0.94
1:B:245[B]:THR:HG21	1:B:298[B]:LEU:CD1	1.96	0.94
1:D:190[A]:MET:HA	1:D:190[A]:MET:HE2	1.51	0.91
1:C:245[B]:THR:HG22	1:C:298[B]:LEU:HD11	1.53	0.90
1:C:75:VAL:HG12	1:C:247:VAL:CG2	2.04	0.87
1:D:245[B]:THR:HG21	1:D:298[B]:LEU:HD11	1.55	0.85
1:C:245[B]:THR:HG23	1:C:298[B]:LEU:CD1	1.91	0.85
1:B:612:MET:HE2	1:B:619:LYS:HZ3	1.45	0.82
1:A:75:VAL:HG12	1:A:247:VAL:CG2	2.09	0.81
1:B:612:MET:HE2	1:B:619:LYS:NZ	1.94	0.81
1:C:245[B]:THR:HG21	1:C:298[B]:LEU:CD1	1.90	0.79
1:A:75:VAL:CG1	1:A:247:VAL:HG23	2.10	0.79
1:A:324:LEU:HD11	1:A:659:VAL:HG21	1.63	0.78
1:D:245[B]:THR:HG23	1:D:298[B]:LEU:HD11	1.65	0.78
1:A:70:THR:HG22	3:A:1137:HOH:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245[B]:THR:HG22	1:C:298[B]:LEU:CD1	2.09	0.76
1:B:152:LEU:HD23	1:B:157:LEU:HD12	1.69	0.75
1:B:189:LYS:O	1:B:190[A]:MET:HE2	1.88	0.74
1:D:245[B]:THR:HG23	1:D:298[B]:LEU:CD1	2.17	0.74
1:A:125:THR:HG23	1:A:126:THR:O	1.89	0.72
1:B:65:ALA:O	3:B:1373:HOH:O	2.06	0.72
1:D:104:ARG:NH2	3:D:1285:HOH:O	2.22	0.72
1:B:52:LEU:HD11	1:B:238:GLU:HG2	1.72	0.72
1:A:245:THR:CG2	1:A:298[B]:LEU:HD11	2.19	0.71
1:A:245:THR:HG21	1:A:298[B]:LEU:HD11	1.71	0.71
1:D:190[A]:MET:CE	1:D:190[A]:MET:CA	2.69	0.71
1:D:200:ASN:C	1:D:200:ASN:HD22	2.00	0.70
1:B:125:THR:HG23	1:B:126:THR:O	1.93	0.69
1:C:353:TYR:CD2	1:C:469:ASP:HB3	2.29	0.67
1:B:185:ILE:HD11	1:B:312:PRO:HG3	1.77	0.66
1:D:190[A]:MET:HA	1:D:190[A]:MET:HE3	1.76	0.66
1:B:579:THR:HG22	1:B:580:LEU:HD12	1.78	0.66
1:B:185:ILE:HD11	1:B:312:PRO:CG	2.27	0.65
1:B:596:HIS:CE1	1:C:280:LYS:HE2	2.32	0.64
1:C:75:VAL:HG11	1:C:247:VAL:HG23	1.77	0.62
1:C:185:ILE:HD11	1:C:312:PRO:HG3	1.82	0.62
1:A:443:GLN:HB2	1:A:487:LEU:HD21	1.82	0.62
1:B:266:ILE:HD11	1:B:401:GLN:NE2	2.16	0.61
1:A:241:VAL:HG11	1:A:383:SER:HB3	1.82	0.61
1:A:149:VAL:HB	3:A:1484:HOH:O	2.01	0.60
1:D:353:TYR:CD2	1:D:469:ASP:HB3	2.36	0.60
1:C:579:THR:HB	1:C:580:LEU:HD12	1.81	0.60
1:B:612:MET:CE	1:B:619:LYS:HZ3	2.14	0.60
1:D:486:ARG:NH1	3:D:1354:HOH:O	2.35	0.60
1:C:571:ARG:NE	3:C:1165:HOH:O	2.34	0.60
1:B:561:ASN:HD22	1:B:561:ASN:N	1.98	0.59
1:D:324:LEU:HD21	1:D:659:VAL:HG21	1.84	0.59
1:C:52:LEU:HD11	1:C:238:GLU:HG2	1.84	0.58
1:C:149:VAL:HB	3:C:1187:HOH:O	2.03	0.58
1:B:75:VAL:HG12	1:B:247:VAL:HG23	1.85	0.58
1:A:566:LEU:HD22	3:A:1245:HOH:O	2.02	0.58
1:C:75:VAL:CG1	1:C:247:VAL:CG2	2.69	0.58
1:A:590:GLY:O	1:A:594:ARG:HG3	2.04	0.57
1:D:95:LEU:HD13	1:D:288:TYR:CZ	2.39	0.57
1:D:97:PHE:HA	1:D:580:LEU:HD23	1.86	0.57
1:A:52:LEU:HD11	1:A:238:GLU:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ILE:HD11	1:A:312:PRO:HG3	1.87	0.56
1:C:190:MET:O	1:C:200:ASN:ND2	2.38	0.56
1:A:165:GLN:CD	1:A:497:MET:HE2	2.31	0.56
1:C:274:LYS:NZ	3:C:1178:HOH:O	2.35	0.56
1:D:245[B]:THR:CG2	1:D:298[B]:LEU:CD1	2.72	0.56
1:B:74:LEU:HD22	1:B:393:PRO:HB2	1.88	0.56
1:B:353:TYR:CD2	1:B:469:ASP:HB3	2.41	0.55
1:D:200:ASN:C	1:D:200:ASN:ND2	2.64	0.55
1:D:75:VAL:HG12	1:D:247:VAL:HG23	1.88	0.55
1:B:593:GLN:HE22	1:C:258:ARG:H	1.54	0.55
1:A:539:ARG:HD3	1:A:545:PHE:HB2	1.88	0.55
1:C:104:ARG:HB2	1:C:572:VAL:CG1	2.38	0.54
1:B:152:LEU:HD21	1:B:356:SER:O	2.07	0.54
1:D:245[A]:THR:HG23	1:D:390:PHE:O	2.07	0.54
1:A:180:MET:HE1	1:A:313:PHE:HD1	1.73	0.53
1:D:245[A]:THR:HG21	1:D:391:THR:HB	1.90	0.53
1:B:266:ILE:HD11	1:B:401:GLN:CD	2.34	0.53
1:B:612:MET:CE	1:B:619:LYS:NZ	2.68	0.53
1:C:489:GLU:OE1	1:D:58:ARG:NH1	2.42	0.53
1:D:143:ALA:HB1	1:D:266:ILE:HD11	1.91	0.53
1:B:561:ASN:N	1:B:561:ASN:ND2	2.56	0.53
1:A:189:LYS:HA	1:A:202:ALA:HB2	1.91	0.52
1:B:172:ILE:HD12	1:B:435:ILE:HG12	1.91	0.52
1:C:66:ASN:OD1	1:C:198:ASN:ND2	2.40	0.51
1:D:525:GLU:O	1:D:526:ARG:C	2.53	0.51
1:B:350:VAL:HG22	1:B:500:VAL:HG22	1.93	0.51
1:D:408:ARG:O	1:D:413:GLN:NE2	2.43	0.51
1:B:75:VAL:CG1	1:B:247:VAL:HG23	2.41	0.51
1:C:172:ILE:HD12	1:C:435:ILE:HG12	1.92	0.51
1:A:443:GLN:CB	1:A:487:LEU:HD21	2.41	0.50
1:C:10:HIS:HE1	1:C:38:HIS:O	1.95	0.50
1:C:125:THR:HG23	1:C:126:THR:O	2.12	0.50
1:A:620:MET:HE3	3:A:1419:HOH:O	2.11	0.50
1:C:241:VAL:HG11	1:C:383:SER:OG	2.11	0.49
1:B:525:GLU:O	1:B:526:ARG:C	2.54	0.49
1:C:113:LEU:HD23	1:C:119:SER:HA	1.94	0.49
1:A:251:VAL:HG21	1:A:532:GLN:CD	2.38	0.49
1:C:580:LEU:HD12	1:C:580:LEU:N	2.28	0.49
1:C:95:LEU:HD11	1:C:283:ILE:HD12	1.94	0.49
1:D:75:VAL:CG1	1:D:247:VAL:HG23	2.43	0.49
1:B:185:ILE:HD11	1:B:312:PRO:CD	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:LEU:HB2	1:D:87:ILE:HD12	1.94	0.49
1:A:72:THR:HB	3:A:1493:HOH:O	2.12	0.48
1:D:243:MET:HE3	1:D:419:ARG:HG2	1.95	0.48
1:A:225:PHE:CZ	1:A:380:LEU:HA	2.48	0.48
1:B:185:ILE:HG23	1:B:311:GLN:NE2	2.27	0.48
1:C:561:ASN:ND2	1:C:567:GLU:OE2	2.46	0.48
1:B:185:ILE:CD1	1:B:312:PRO:HG3	2.41	0.48
1:B:486:ARG:HG2	3:B:1158:HOH:O	2.13	0.48
1:D:187:ILE:HB	1:D:639:ARG:HB2	1.94	0.48
1:C:104:ARG:HB2	1:C:572:VAL:HG11	1.95	0.48
1:A:70:THR:HG23	1:A:71:GLY:N	2.27	0.48
1:B:203:GLU:O	1:B:207:GLN:HG2	2.14	0.48
1:C:133:VAL:HG21	1:C:281:VAL:HG11	1.96	0.48
1:D:32:ASN:HD21	1:D:35:VAL:HG22	1.79	0.48
1:D:190[A]:MET:CA	1:D:190[A]:MET:HE3	2.41	0.48
1:A:350:VAL:HG22	1:A:500:VAL:HG22	1.96	0.47
1:C:180:MET:HE1	1:C:313:PHE:CD1	2.49	0.47
3:A:1328:HOH:O	1:C:160:ARG:NH1	2.46	0.47
1:B:246[A]:ASN:HD21	1:B:301:ALA:HB2	1.79	0.47
1:A:55:TYR:CE2	1:A:230:LEU:HD23	2.50	0.47
1:C:225:PHE:CZ	1:C:380:LEU:HA	2.49	0.47
1:B:245[B]:THR:HG23	1:B:298[B]:LEU:CD1	2.41	0.47
1:B:612:MET:HE1	1:B:623:ARG:NH1	2.30	0.47
1:B:185:ILE:HD12	1:B:646:PHE:CE2	2.49	0.47
1:D:245[B]:THR:HG23	1:D:298[B]:LEU:HD12	1.96	0.47
1:B:263:GLN:HA	1:B:266:ILE:HD13	1.97	0.46
1:B:612:MET:HE2	1:B:619:LYS:HZ2	1.76	0.46
1:D:311:GLN:N	1:D:312:PRO:HD2	2.30	0.46
1:D:433:LYS:HA	1:D:433:LYS:HE2	1.97	0.46
1:C:190:MET:HB3	1:C:544:ASN:ND2	2.31	0.46
1:A:483:LEU:HD12	1:A:483:LEU:O	2.16	0.46
1:B:245[A]:THR:HG22	1:B:300:ASN:ND2	2.30	0.46
1:C:70:THR:HG22	1:C:71:GLY:N	2.31	0.45
1:A:538:GLU:HG2	1:A:539:ARG:HG3	1.99	0.45
1:D:225:PHE:CZ	1:D:380:LEU:HA	2.52	0.45
1:D:74:LEU:HD11	1:D:395:GLY:C	2.42	0.45
1:C:245[A]:THR:HG21	1:C:391:THR:HB	1.98	0.45
1:B:444:MET:HG3	1:B:487:LEU:HD22	2.00	0.45
1:D:189:LYS:C	1:D:190[A]:MET:HE3	2.43	0.44
1:A:113:LEU:HD23	1:A:119:SER:HA	1.98	0.44
1:D:643:PRO:HA	1:D:646:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:GLU:O	1:C:526:ARG:C	2.60	0.44
1:A:149:VAL:HG13	3:A:1474:HOH:O	2.17	0.44
1:B:262:ALA:O	1:B:266:ILE:HG23	2.18	0.44
1:B:311:GLN:N	1:B:312:PRO:CD	2.81	0.43
1:B:579:THR:CG2	1:B:580:LEU:HD12	2.46	0.43
1:D:87:ILE:HG12	1:D:585:TYR:CG	2.53	0.43
1:D:48:MET:HG3	1:D:49:TYR:CD2	2.54	0.43
1:A:190[A]:MET:HE1	3:B:1515:HOH:O	2.19	0.43
1:B:48:MET:HG3	1:B:49:TYR:CD2	2.54	0.43
1:D:505:GLY:O	1:D:512:VAL:HG13	2.19	0.43
1:C:245[B]:THR:HG22	1:C:298[B]:LEU:HD12	1.99	0.43
1:A:165:GLN:CG	1:A:497:MET:HE2	2.48	0.43
1:B:152:LEU:CD2	1:B:157:LEU:HD12	2.45	0.43
1:B:644:ILE:HG22	1:B:645:PHE:CD2	2.54	0.43
1:D:94:VAL:HG22	1:D:581:MET:HE1	2.01	0.42
1:B:596:HIS:O	1:C:280:LYS:HE3	2.19	0.42
1:A:261:TRP:CD2	1:A:274:LYS:HD3	2.54	0.42
1:C:199:VAL:HG21	3:C:1489:HOH:O	2.19	0.42
1:D:165:GLN:CD	1:D:497:MET:HE2	2.44	0.42
1:B:245[B]:THR:CG2	1:B:298[B]:LEU:HD12	2.43	0.42
1:A:75:VAL:CG1	1:A:247:VAL:CG2	2.86	0.42
1:A:626:ASP:OD1	1:A:640:LYS:NZ	2.52	0.42
1:C:245[A]:THR:HG22	1:C:300:ASN:ND2	2.34	0.42
1:C:433:LYS:NZ	1:C:471:GLU:OE2	2.52	0.42
1:C:415:LYS:NZ	3:C:1487:HOH:O	2.39	0.42
1:A:311:GLN:N	1:A:312:PRO:CD	2.82	0.41
1:D:55:TYR:CE2	1:D:230:LEU:HD23	2.55	0.41
1:A:103:LYS:HD3	1:A:103:LYS:HA	1.84	0.41
1:B:479:ARG:HD3	3:B:1167:HOH:O	2.20	0.41
1:D:300:ASN:HD22	1:D:300:ASN:HA	1.74	0.41
1:C:347:PHE:CD1	1:C:506:ALA:HB1	2.55	0.41
1:A:565:VAL:O	1:A:569:VAL:HG23	2.20	0.41
1:C:180:MET:HE3	1:C:650:PHE:CE1	2.56	0.41
1:D:566:LEU:HD22	3:D:1210:HOH:O	2.21	0.41
1:B:190[B]:MET:HE3	1:B:190[B]:MET:HB2	1.91	0.41
1:B:561:ASN:ND2	1:C:273:SER:OG	2.54	0.41
1:C:571:ARG:CZ	3:C:1165:HOH:O	2.68	0.41
1:D:196:PRO:HB3	1:D:234:TYR:CE2	2.56	0.41
1:A:249:TRP:HB2	1:A:538:GLU:HG3	2.03	0.41
1:A:331:PRO:HG3	1:A:465:ILE:HG23	2.01	0.41
1:A:594:ARG:NH2	3:A:1158:HOH:O	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:GLU:H	1:A:376:GLU:CD	2.29	0.41
1:B:366:LEU:HD13	1:B:382:SER:HB2	2.03	0.41
1:D:243:MET:HE3	1:D:419:ARG:CG	2.51	0.41
1:C:444:MET:HG3	1:C:487:LEU:HD22	2.03	0.40
1:A:353:TYR:CD2	1:A:469:ASP:HB3	2.56	0.40
1:C:551:LEU:HD13	1:C:606:LEU:HD12	2.03	0.40
1:D:580:LEU:HD12	1:D:580:LEU:N	2.37	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	648/659 (98%)	634 (98%)	13 (2%)	1 (0%)	43	44
1	B	634/659 (96%)	618 (98%)	16 (2%)	0	100	100
1	C	653/659 (99%)	637 (98%)	15 (2%)	1 (0%)	43	44
1	D	645/659 (98%)	632 (98%)	13 (2%)	0	100	100
All	All	2580/2636 (98%)	2521 (98%)	57 (2%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	GLY
1	C	71	GLY

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	562/568 (99%)	555 (99%)	7 (1%)	63	72
1	B	554/568 (98%)	537 (97%)	17 (3%)	35	39
1	C	565/568 (100%)	558 (99%)	7 (1%)	63	72
1	D	561/568 (99%)	549 (98%)	12 (2%)	47	54
All	All	2242/2272 (99%)	2199 (98%)	43 (2%)	51	58

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	THR
1	A	125	THR
1	A	217	ARG
1	A	257	LYS
1	A	268	ARG
1	A	433	LYS
1	A	659	VAL
1	B	72	THR
1	B	115	SER
1	B	125	THR
1	B	144	LEU
1	B	185	ILE
1	B	226	LYS
1	B	246[A]	ASN
1	B	246[B]	ASN
1	B	266	ILE
1	B	268	ARG
1	B	433	LYS
1	B	479	ARG
1	B	544	ASN
1	B	561	ASN
1	B	589	LEU
1	B	594	ARG
1	B	644	ILE
1	C	69	GLN
1	C	180	MET
1	C	199	VAL
1	C	217	ARG
1	C	257	LYS
1	C	433	LYS

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Mol	Chain	Res	Type
1	C	659	VAL
1	D	74	LEU
1	D	115	SER
1	D	190[A]	MET
1	D	190[B]	MET
1	D	200	ASN
1	D	253[A]	ASN
1	D	253[B]	ASN
1	D	433	LYS
1	D	486	ARG
1	D	504	GLU
1	D	589	LEU
1	D	655	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	37	HIS
1	A	98	GLN
1	A	284	ASN
1	A	467	ASN
1	B	198	ASN
1	B	284	ASN
1	B	443	GLN
1	B	491	GLN
1	B	558	ASN
1	B	561	ASN
1	B	593	GLN
1	B	632	GLN
1	C	10	HIS
1	C	250	GLN
1	C	407	ASN
1	C	622	HIS
1	D	198	ASN
1	D	200	ASN
1	D	216	ASN
1	D	284	ASN
1	D	300	ASN
1	D	319	ASN
1	D	443	GLN
1	D	467	ASN

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Mol	Chain	Res	Type
1	D	491	GLN
1	D	522	GLN
1	D	593	GLN
1	D	622	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](#)

Of 4 ligands modelled in this entry, 4 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	649/659 (98%)	0.28	9 (1%) 73 75	13, 27, 39, 49	3 (0%)
1	B	634/659 (96%)	0.32	14 (2%) 62 65	14, 26, 41, 53	6 (0%)
1	C	650/659 (98%)	0.24	11 (1%) 69 71	13, 26, 37, 45	5 (0%)
1	D	643/659 (97%)	0.31	9 (1%) 73 75	12, 28, 42, 52	6 (0%)
All	All	2576/2636 (97%)	0.29	43 (1%) 69 71	12, 27, 40, 53	20 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	10	HIS	5.1
1	A	67	ALA	3.6
1	A	70	THR	3.2
1	A	479	ARG	3.0
1	D	73	GLN	2.9
1	B	11	ALA	2.8
1	D	659	VAL	2.8
1	A	69	GLN	2.7
1	B	65	ALA	2.6
1	B	43	ASP	2.6
1	B	545	PHE	2.6
1	B	561	ASN	2.6
1	A	73	GLN	2.5
1	D	11	ALA	2.5
1	B	626	ASP	2.5
1	C	443	GLN	2.5
1	B	73	GLN	2.4
1	A	72	THR	2.4
1	B	200	ASN	2.4
1	B	544	ASN	2.4
1	C	285	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	68	ARG	2.4
1	D	65	ALA	2.3
1	C	70	THR	2.3
1	A	615	ASP	2.3
1	A	545	PHE	2.2
1	C	190	MET	2.2
1	D	190[A]	MET	2.2
1	C	107	ALA	2.2
1	B	659	VAL	2.2
1	B	215	GLY	2.2
1	C	154[A]	ASP	2.2
1	C	67	ALA	2.1
1	B	62	THR	2.1
1	D	27	GLY	2.1
1	C	324	LEU	2.1
1	B	615	ASP	2.1
1	D	152	LEU	2.0
1	B	12	GLU	2.0
1	C	284	ASN	2.0
1	D	63	LEU	2.0
1	C	10	HIS	2.0
1	A	71	GLY	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(Å ²)	Q<0.9
2	MG	B	1001	1/1	0.84	0.19	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	1001	1/1	0.92	0.14	16,16,16,16	0
2	MG	C	1001	1/1	0.94	0.10	16,16,16,16	0
2	MG	D	1001	1/1	0.96	0.12	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.