



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:47 PM GMT

PDB ID : 4JHN
Title : The crystal structure of the RPGR RCC1-like domain
Authors : Waetzlich, D.; Vetter, I.; Wittinghofer, A.; Ismail, S.
Deposited on : 2013-03-05
Resolution : 1.70 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

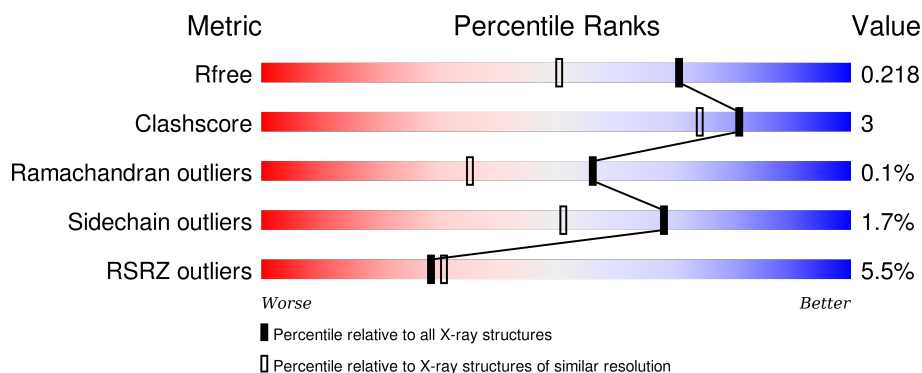
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	421	<div> <div>5%</div> <div>79% 6% 14%</div> </div>
1	B	421	<div> <div>4%</div> <div>82% • 14%</div> </div>
1	C	421	<div> <div>5%</div> <div>80% 5% • 14%</div> </div>
1	D	421	<div> <div>5%</div> <div>76% 9% • 14%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12042 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 X-linked retinitis pigmentosa GTPase regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	5	0
			2762	1753	473	520	16			
1	B	361	Total	C	N	O	S	0	6	0
			2756	1748	470	522	16			
1	C	361	Total	C	N	O	S	0	3	0
			2741	1739	465	520	17			
1	D	360	Total	C	N	O	S	0	5	0
			2744	1745	466	517	16			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	393	PRO	-	EXPRESSION TAG	UNP Q92834
A	394	ARG	-	EXPRESSION TAG	UNP Q92834
A	395	ARG	-	EXPRESSION TAG	UNP Q92834
A	396	PRO	-	EXPRESSION TAG	UNP Q92834
A	397	PRO	-	EXPRESSION TAG	UNP Q92834
A	398	ALA	-	EXPRESSION TAG	UNP Q92834
A	399	TYR	-	EXPRESSION TAG	UNP Q92834
A	400	VAL	-	EXPRESSION TAG	UNP Q92834
A	401	GLU	-	EXPRESSION TAG	UNP Q92834
A	402	GLN	-	EXPRESSION TAG	UNP Q92834
A	403	LYS	-	EXPRESSION TAG	UNP Q92834
A	404	LEU	-	EXPRESSION TAG	UNP Q92834
A	405	ILE	-	EXPRESSION TAG	UNP Q92834
A	406	SER	-	EXPRESSION TAG	UNP Q92834
A	407	GLU	-	EXPRESSION TAG	UNP Q92834
A	408	GLU	-	EXPRESSION TAG	UNP Q92834
A	409	ASP	-	EXPRESSION TAG	UNP Q92834
A	410	LEU	-	EXPRESSION TAG	UNP Q92834
A	411	ASN	-	EXPRESSION TAG	UNP Q92834
A	412	SER	-	EXPRESSION TAG	UNP Q92834
A	413	ALA	-	EXPRESSION TAG	UNP Q92834

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Chain	Residue	Modelled	Actual	Comment	Reference
A	414	VAL	-	EXPRESSION TAG	UNP Q92834
A	415	ASP	-	EXPRESSION TAG	UNP Q92834
A	416	HIS	-	EXPRESSION TAG	UNP Q92834
A	417	HIS	-	EXPRESSION TAG	UNP Q92834
A	418	HIS	-	EXPRESSION TAG	UNP Q92834
A	419	HIS	-	EXPRESSION TAG	UNP Q92834
A	420	HIS	-	EXPRESSION TAG	UNP Q92834
A	421	HIS	-	EXPRESSION TAG	UNP Q92834
B	393	PRO	-	EXPRESSION TAG	UNP Q92834
B	394	ARG	-	EXPRESSION TAG	UNP Q92834
B	395	ARG	-	EXPRESSION TAG	UNP Q92834
B	396	PRO	-	EXPRESSION TAG	UNP Q92834
B	397	PRO	-	EXPRESSION TAG	UNP Q92834
B	398	ALA	-	EXPRESSION TAG	UNP Q92834
B	399	TYR	-	EXPRESSION TAG	UNP Q92834
B	400	VAL	-	EXPRESSION TAG	UNP Q92834
B	401	GLU	-	EXPRESSION TAG	UNP Q92834
B	402	GLN	-	EXPRESSION TAG	UNP Q92834
B	403	LYS	-	EXPRESSION TAG	UNP Q92834
B	404	LEU	-	EXPRESSION TAG	UNP Q92834
B	405	ILE	-	EXPRESSION TAG	UNP Q92834
B	406	SER	-	EXPRESSION TAG	UNP Q92834
B	407	GLU	-	EXPRESSION TAG	UNP Q92834
B	408	GLU	-	EXPRESSION TAG	UNP Q92834
B	409	ASP	-	EXPRESSION TAG	UNP Q92834
B	410	LEU	-	EXPRESSION TAG	UNP Q92834
B	411	ASN	-	EXPRESSION TAG	UNP Q92834
B	412	SER	-	EXPRESSION TAG	UNP Q92834
B	413	ALA	-	EXPRESSION TAG	UNP Q92834
B	414	VAL	-	EXPRESSION TAG	UNP Q92834
B	415	ASP	-	EXPRESSION TAG	UNP Q92834
B	416	HIS	-	EXPRESSION TAG	UNP Q92834
B	417	HIS	-	EXPRESSION TAG	UNP Q92834
B	418	HIS	-	EXPRESSION TAG	UNP Q92834
B	419	HIS	-	EXPRESSION TAG	UNP Q92834
B	420	HIS	-	EXPRESSION TAG	UNP Q92834
B	421	HIS	-	EXPRESSION TAG	UNP Q92834
C	393	PRO	-	EXPRESSION TAG	UNP Q92834
C	394	ARG	-	EXPRESSION TAG	UNP Q92834
C	395	ARG	-	EXPRESSION TAG	UNP Q92834
C	396	PRO	-	EXPRESSION TAG	UNP Q92834
C	397	PRO	-	EXPRESSION TAG	UNP Q92834

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Chain	Residue	Modelled	Actual	Comment	Reference
C	398	ALA	-	EXPRESSION TAG	UNP Q92834
C	399	TYR	-	EXPRESSION TAG	UNP Q92834
C	400	VAL	-	EXPRESSION TAG	UNP Q92834
C	401	GLU	-	EXPRESSION TAG	UNP Q92834
C	402	GLN	-	EXPRESSION TAG	UNP Q92834
C	403	LYS	-	EXPRESSION TAG	UNP Q92834
C	404	LEU	-	EXPRESSION TAG	UNP Q92834
C	405	ILE	-	EXPRESSION TAG	UNP Q92834
C	406	SER	-	EXPRESSION TAG	UNP Q92834
C	407	GLU	-	EXPRESSION TAG	UNP Q92834
C	408	GLU	-	EXPRESSION TAG	UNP Q92834
C	409	ASP	-	EXPRESSION TAG	UNP Q92834
C	410	LEU	-	EXPRESSION TAG	UNP Q92834
C	411	ASN	-	EXPRESSION TAG	UNP Q92834
C	412	SER	-	EXPRESSION TAG	UNP Q92834
C	413	ALA	-	EXPRESSION TAG	UNP Q92834
C	414	VAL	-	EXPRESSION TAG	UNP Q92834
C	415	ASP	-	EXPRESSION TAG	UNP Q92834
C	416	HIS	-	EXPRESSION TAG	UNP Q92834
C	417	HIS	-	EXPRESSION TAG	UNP Q92834
C	418	HIS	-	EXPRESSION TAG	UNP Q92834
C	419	HIS	-	EXPRESSION TAG	UNP Q92834
C	420	HIS	-	EXPRESSION TAG	UNP Q92834
C	421	HIS	-	EXPRESSION TAG	UNP Q92834
D	393	PRO	-	EXPRESSION TAG	UNP Q92834
D	394	ARG	-	EXPRESSION TAG	UNP Q92834
D	395	ARG	-	EXPRESSION TAG	UNP Q92834
D	396	PRO	-	EXPRESSION TAG	UNP Q92834
D	397	PRO	-	EXPRESSION TAG	UNP Q92834
D	398	ALA	-	EXPRESSION TAG	UNP Q92834
D	399	TYR	-	EXPRESSION TAG	UNP Q92834
D	400	VAL	-	EXPRESSION TAG	UNP Q92834
D	401	GLU	-	EXPRESSION TAG	UNP Q92834
D	402	GLN	-	EXPRESSION TAG	UNP Q92834
D	403	LYS	-	EXPRESSION TAG	UNP Q92834
D	404	LEU	-	EXPRESSION TAG	UNP Q92834
D	405	ILE	-	EXPRESSION TAG	UNP Q92834
D	406	SER	-	EXPRESSION TAG	UNP Q92834
D	407	GLU	-	EXPRESSION TAG	UNP Q92834
D	408	GLU	-	EXPRESSION TAG	UNP Q92834
D	409	ASP	-	EXPRESSION TAG	UNP Q92834
D	410	LEU	-	EXPRESSION TAG	UNP Q92834

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Chain	Residue	Modelled	Actual	Comment	Reference
D	411	ASN	-	EXPRESSION TAG	UNP Q92834
D	412	SER	-	EXPRESSION TAG	UNP Q92834
D	413	ALA	-	EXPRESSION TAG	UNP Q92834
D	414	VAL	-	EXPRESSION TAG	UNP Q92834
D	415	ASP	-	EXPRESSION TAG	UNP Q92834
D	416	HIS	-	EXPRESSION TAG	UNP Q92834
D	417	HIS	-	EXPRESSION TAG	UNP Q92834
D	418	HIS	-	EXPRESSION TAG	UNP Q92834
D	419	HIS	-	EXPRESSION TAG	UNP Q92834
D	420	HIS	-	EXPRESSION TAG	UNP Q92834
D	421	HIS	-	EXPRESSION TAG	UNP Q92834

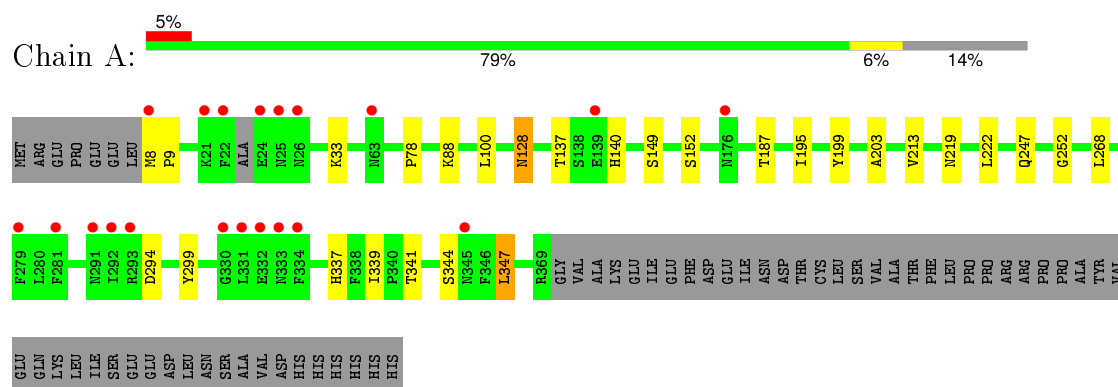
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	291	Total	O	0	0
			291	291		
2	B	260	Total	O	0	0
			260	260		
2	C	225	Total	O	0	0
			225	225		
2	D	263	Total	O	0	0
			263	263		

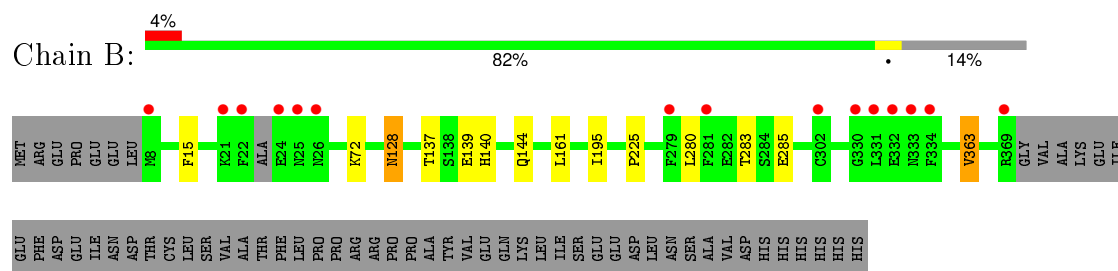
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

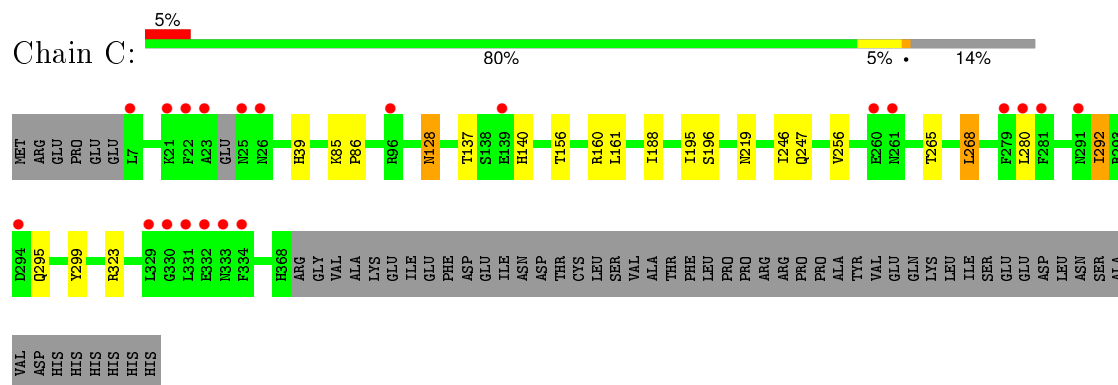
- Molecule 1: X-linked retinitis pigmentosa GTPase regulator



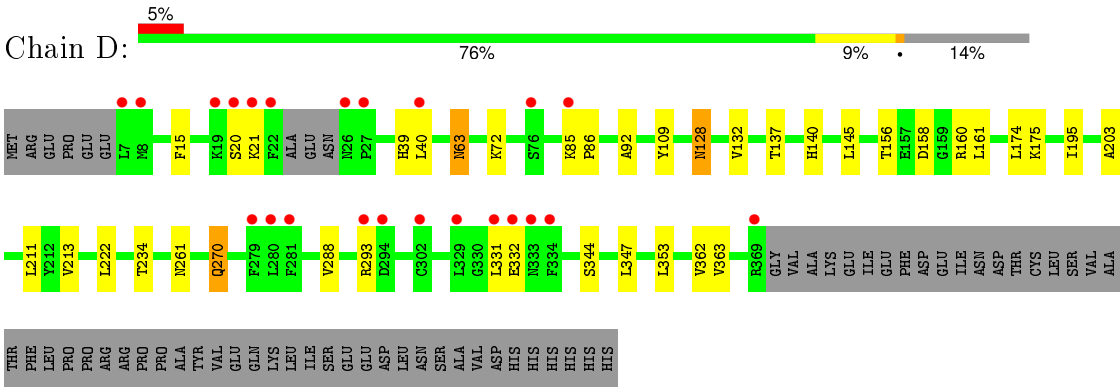
- Molecule 1: X-linked retinitis pigmentosa GTPase regulator



- Molecule 1: X-linked retinitis pigmentosa GTPase regulator



- Molecule 1: X-linked retinitis pigmentosa GTPase regulator



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.49Å 118.73Å 92.63Å 90.00° 101.54° 90.00°	Depositor
Resolution (Å)	29.83 – 1.70 29.83 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.83-1.70) 99.3 (29.83-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.57 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.6.0093	Depositor
R, R_{free}	0.185 , 0.218 0.185 , 0.218	Depositor DCC
R_{free} test set	6627 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 132539 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12042	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.67 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.6450e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.35	0/2840	0.50	0/3846
1	B	0.35	0/2834	0.49	0/3839
1	C	0.35	0/2809	0.50	0/3805
1	D	0.35	0/2822	0.51	0/3822
All	All	0.35	0/11305	0.50	0/15312

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 [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	2762	0	2706	18	0
1	B	2756	0	2686	10	0
1	C	2741	0	2671	13	0
1	D	2744	0	2686	30	0
2	A	291	0	0	7	0
2	B	260	0	0	1	0
2	C	225	0	0	1	0
2	D	263	0	0	5	0
All	All	12042	0	10749	71	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 3.

All (71) 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:187:THR:HG21	2:A:791:HOH:O	1.42	1.15
1:A:187:THR:CG2	2:A:791:HOH:O	1.93	1.15
1:D:145:LEU:HD13	2:D:932:HOH:O	1.55	1.06
1:D:145:LEU:CD1	2:D:932:HOH:O	2.11	0.96
1:C:161:LEU:HD11	1:C:195:ILE:HD13	1.58	0.85
1:A:199:TYR:HB2	2:A:732:HOH:O	1.76	0.85
1:B:137:THR:H	1:B:140:HIS:HD2	1.29	0.79
1:A:252:GLY:O	2:A:732:HOH:O	2.01	0.78
1:C:137:THR:H	1:C:140:HIS:HD2	1.32	0.78
1:D:92:ALA:HA	2:D:932:HOH:O	1.84	0.76
1:A:344:SER:HA	1:A:347:LEU:HD23	1.66	0.76
1:A:8:MET:HB3	1:A:9:PRO:HD3	1.71	0.72
1:D:288:VAL:HG11	1:D:293:ARG:HE	1.55	0.72
1:A:213[A]:VAL:HG21	1:A:222:LEU:O	1.89	0.71
1:B:161:LEU:HD11	1:B:195:ILE:HD13	1.72	0.71
1:D:137:THR:H	1:D:140:HIS:HD2	1.40	0.67
1:D:213[A]:VAL:HG21	1:D:222:LEU:O	1.95	0.67
1:A:149:SER:HB2	2:A:692:HOH:O	1.94	0.65
1:D:175:LYS:HG2	1:D:234:THR:HG22	1.80	0.63
1:D:270:GLN:H	1:D:270:GLN:HE21	1.45	0.63
1:B:280:LEU:HD21	1:B:283:THR:OG1	1.99	0.63
1:B:15:PHE:HB2	1:B:363:VAL:HG13	1.80	0.62
1:D:211[A]:LEU:CD2	1:D:213[A]:VAL:HG13	2.30	0.62
1:C:156:THR:HG22	1:C:160:ARG:H	1.65	0.61
1:D:15:PHE:HB2	1:D:363:VAL:HG13	1.82	0.61
1:A:137:THR:H	1:A:140:HIS:HD2	1.46	0.61
1:A:199:TYR:HD1	2:A:692:HOH:O	1.89	0.56
1:D:195:ILE:HD12	1:D:203:ALA:O	2.06	0.56
1:A:339:ILE:O	1:A:341:THR:HG23	2.06	0.56
1:B:161:LEU:HD11	1:B:195:ILE:CD1	2.38	0.54
1:A:195:ILE:HD12	1:A:203:ALA:O	2.07	0.53
1:D:145:LEU:HD12	2:D:932:HOH:O	1.95	0.53
1:D:109:TYR:CE2	1:D:132:VAL:HG22	2.44	0.52
1:D:270:GLN:N	1:D:270:GLN:HE21	2.07	0.52
1:A:247:GLN:HE22	1:A:299:TYR:HA	1.75	0.52
1:B:283:THR:HG22	1:B:285:GLU:H	1.76	0.51
1:A:128:ASN:C	1:A:128:ASN:HD22	2.13	0.50
1:C:195:ILE:HG13	1:C:196:SER:N	2.28	0.49
1:B:128:ASN:HD22	1:B:128:ASN:C	2.16	0.48
1:C:219:ASN:HB3	1:C:268:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:LEU:HD22	1:D:362:VAL:HG12	1.94	0.48
1:B:161:LEU:HD21	1:B:195:ILE:HD12	1.95	0.48
1:C:85:LYS:N	1:C:86:PRO:HD2	2.29	0.47
1:C:247:GLN:HE22	1:C:299:TYR:HA	1.79	0.47
1:D:331:LEU:CB	1:D:332:GLU:HB2	2.44	0.47
1:D:161:LEU:HD21	1:D:195:ILE:HD13	1.97	0.47
1:D:85:LYS:N	1:D:86:PRO:HD2	2.31	0.46
1:C:156:THR:CG2	1:C:160:ARG:H	2.28	0.45
1:A:337:HIS:ND1	1:A:341:THR:HG21	2.31	0.45
1:D:40:LEU:HD12	1:D:353:LEU:HD13	1.98	0.45
1:D:128:ASN:C	1:D:128:ASN:HD22	2.19	0.44
1:D:156:THR:HG22	1:D:160:ARG:H	1.81	0.44
1:D:156:THR:HG23	1:D:158:ASP:OD1	2.19	0.43
1:C:246:ILE:HG22	1:C:247:GLN:HG3	2.00	0.43
1:A:78:PRO:HB3	2:A:790:HOH:O	2.18	0.42
1:D:39:HIS:HD2	2:D:789:HOH:O	2.02	0.42
1:A:219:ASN:HB3	1:A:268:LEU:HG	2.01	0.42
1:D:344:SER:HA	1:D:347:LEU:HG	2.02	0.42
1:A:100:LEU:HD11	1:A:152:SER:HB3	2.00	0.42
1:D:331:LEU:CB	1:D:332:GLU:CA	2.98	0.42
1:C:292:ILE:HG12	1:C:292:ILE:O	2.20	0.42
1:D:331:LEU:CB	1:D:332:GLU:C	2.88	0.42
1:D:20:SER:O	1:D:21:LYS:HB2	2.19	0.42
1:D:211[A]:LEU:HD22	1:D:213[A]:VAL:HG13	2.01	0.41
1:D:156:THR:CG2	1:D:158:ASP:OD1	2.68	0.41
1:B:225:PRO:HB2	2:B:561:HOH:O	2.19	0.41
1:C:256:VAL:HG22	1:C:265:THR:HG22	2.02	0.41
1:C:39:HIS:HD2	2:C:569:HOH:O	2.04	0.41
1:D:63:ASN:H	1:D:63:ASN:HD22	1.68	0.41
1:B:144:GLN:NE2	1:B:195:ILE:H	2.19	0.41
1:C:128:ASN:HD22	1:C:128:ASN:C	2.24	0.41

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	362/421 (86%)	354 (98%)	8 (2%)	0	100	100
1	B	363/421 (86%)	355 (98%)	7 (2%)	1 (0%)	46	26
1	C	360/421 (86%)	356 (99%)	4 (1%)	0	100	100
1	D	361/421 (86%)	354 (98%)	6 (2%)	1 (0%)	46	26
All	All	1446/1684 (86%)	1419 (98%)	25 (2%)	2 (0%)	56	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	72	LYS
1	B	72	LYS

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	303/353 (86%)	298 (98%)	5 (2%)	68	51
1	B	302/353 (86%)	299 (99%)	3 (1%)	82	72
1	C	299/353 (85%)	292 (98%)	7 (2%)	58	37
1	D	300/353 (85%)	295 (98%)	5 (2%)	68	51
All	All	1204/1412 (85%)	1184 (98%)	20 (2%)	68	51

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	88	LYS
1	A	128	ASN
1	A	294	ASP
1	A	347	LEU
1	B	128	ASN

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Mol	Chain	Res	Type
1	B	139	GLU
1	B	363	VAL
1	C	128	ASN
1	C	188	ILE
1	C	268	LEU
1	C	280	LEU
1	C	292	ILE
1	C	295	GLN
1	C	323	ARG
1	D	63	ASN
1	D	128	ASN
1	D	174	LEU
1	D	261	ASN
1	D	270	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	128	ASN
1	A	140	HIS
1	A	184	GLN
1	A	226	ASN
1	A	232	HIS
1	A	236	GLN
1	A	247	GLN
1	B	128	ASN
1	B	140	HIS
1	B	144	GLN
1	B	226	ASN
1	B	236	GLN
1	B	247	GLN
1	C	25	ASN
1	C	128	ASN
1	C	140	HIS
1	C	184	GLN
1	C	226	ASN
1	C	227	GLN
1	C	236	GLN
1	C	247	GLN
1	D	34	ASN
1	D	39	HIS

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Mol	Chain	Res	Type
1	D	63	ASN
1	D	128	ASN
1	D	140	HIS
1	D	150	ASN
1	D	176	ASN
1	D	226	ASN
1	D	236	GLN
1	D	247	GLN
1	D	270	GLN
1	D	333	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 carbohydrates 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	361/421 (85%)	0.24	20 (5%) 29 31	12, 18, 33, 56	0
1	B	361/421 (85%)	0.24	15 (4%) 40 44	12, 19, 33, 49	0
1	C	361/421 (85%)	0.30	21 (5%) 26 28	12, 19, 37, 58	0
1	D	360/421 (85%)	0.26	23 (6%) 23 25	11, 18, 34, 60	0
All	All	1443/1684 (85%)	0.26	79 (5%) 29 31	11, 18, 35, 60	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	25	ASN	10.2
1	D	331	LEU	8.1
1	D	7	LEU	7.8
1	C	279	PHE	7.5
1	A	331	LEU	7.0
1	C	331	LEU	6.6
1	B	279	PHE	6.5
1	B	331	LEU	6.0
1	D	279	PHE	5.4
1	D	22	PHE	5.2
1	D	334	PHE	5.1
1	C	281	PHE	4.9
1	C	280	LEU	4.9
1	C	334	PHE	4.8
1	D	332	GLU	4.7
1	A	22	PHE	4.6
1	A	279	PHE	4.6
1	A	293	ARG	4.5
1	C	7	LEU	4.5
1	A	330	GLY	4.3
1	A	281	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	333	ASN	4.2
1	D	76	SER	4.0
1	B	8	MET	3.9
1	D	20	SER	3.9
1	B	25	ASN	3.9
1	A	334	PHE	3.8
1	C	21	LYS	3.7
1	C	333	ASN	3.7
1	A	21	LYS	3.7
1	B	334	PHE	3.6
1	A	25	ASN	3.5
1	A	26	ASN	3.5
1	C	332	GLU	3.5
1	A	333	ASN	3.5
1	B	281	PHE	3.4
1	D	281	PHE	3.4
1	A	8	MET	3.3
1	C	330	GLY	3.3
1	B	332	GLU	3.3
1	C	22	PHE	3.2
1	C	260	GLU	3.1
1	B	22	PHE	3.1
1	C	294	ASP	3.1
1	A	139	GLU	3.1
1	C	261	ASN	3.1
1	D	26	ASN	3.0
1	B	302	CYS	3.0
1	C	26	ASN	2.9
1	B	333	ASN	2.9
1	B	21	LYS	2.9
1	B	369	ARG	2.9
1	A	332	GLU	2.9
1	D	21	LYS	2.8
1	C	23	ALA	2.8
1	B	330	GLY	2.8
1	B	26	ASN	2.6
1	D	369	ARG	2.5
1	D	302	CYS	2.4
1	A	291	ASN	2.4
1	B	24	GLU	2.3
1	D	19	LYS	2.3
1	D	27	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	329	LEU	2.3
1	A	24	GLU	2.2
1	D	85	LYS	2.2
1	A	292	ILE	2.2
1	A	63	ASN	2.2
1	C	291	ASN	2.2
1	C	139	GLU	2.1
1	C	96	ARG	2.1
1	A	345	ASN	2.1
1	D	40	LEU	2.1
1	D	293	ARG	2.1
1	D	294	ASP	2.1
1	A	176	ASN	2.0
1	D	280	LEU	2.0
1	D	329	LEU	2.0
1	D	8	MET	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 carbohydrates 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.