



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:43 AM UTC

PDB ID : 9BZ4 / pdb_00009bz4
Title : Crystal structure of the C2 and GAP domains of human p120RasGAP
Authors : Paul, M.E.; Boggon, T.J.
Deposited on : 2024-05-24
Resolution : 2.45 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

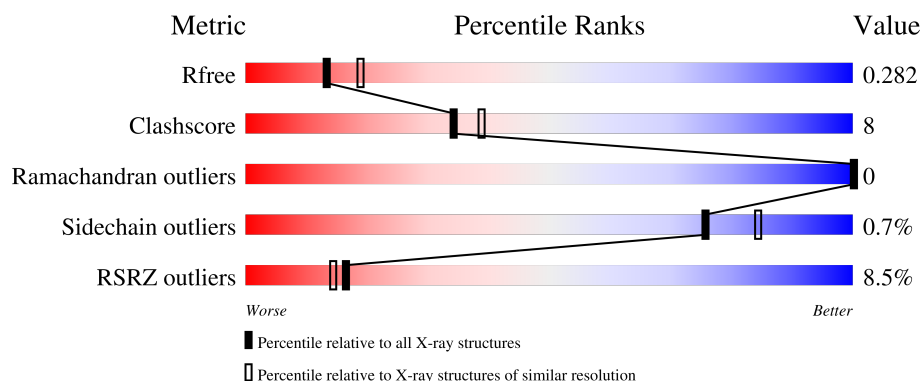
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	468	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>.</div> </div> </div>
1	B	468	<div> <div>7%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>5%</div> </div> </div>
1	C	468	<div> <div>10%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>6%</div> </div> </div>
1	D	468	<div> <div>9%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14329 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 Ras GTPase-activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3606	2294	630	661	21			
1	B	446	Total	C	N	O	S	0	0	0
			3589	2281	625	662	21			
1	C	439	Total	C	N	O	S	0	0	0
			3545	2255	618	652	20			
1	D	442	Total	C	N	O	S	0	0	0
			3563	2269	619	654	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	580	GLY	-	expression tag	UNP P20936
B	580	GLY	-	expression tag	UNP P20936
C	580	GLY	-	expression tag	UNP P20936
D	580	GLY	-	expression tag	UNP P20936

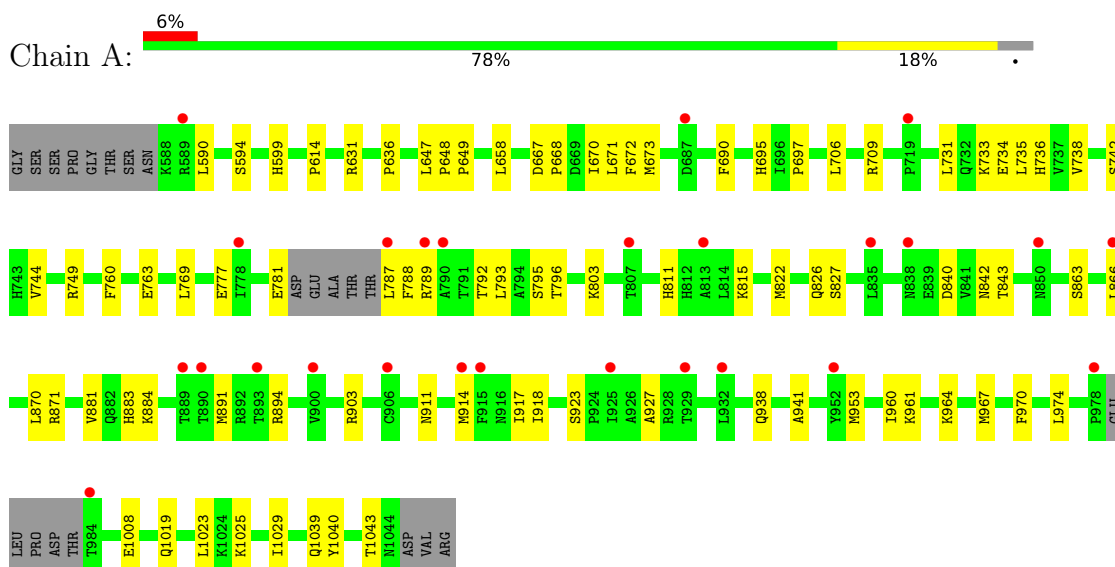
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	O	0	0
			6	6		
2	B	9	Total	O	0	0
			9	9		
2	C	4	Total	O	0	0
			4	4		
2	D	7	Total	O	0	0
			7	7		

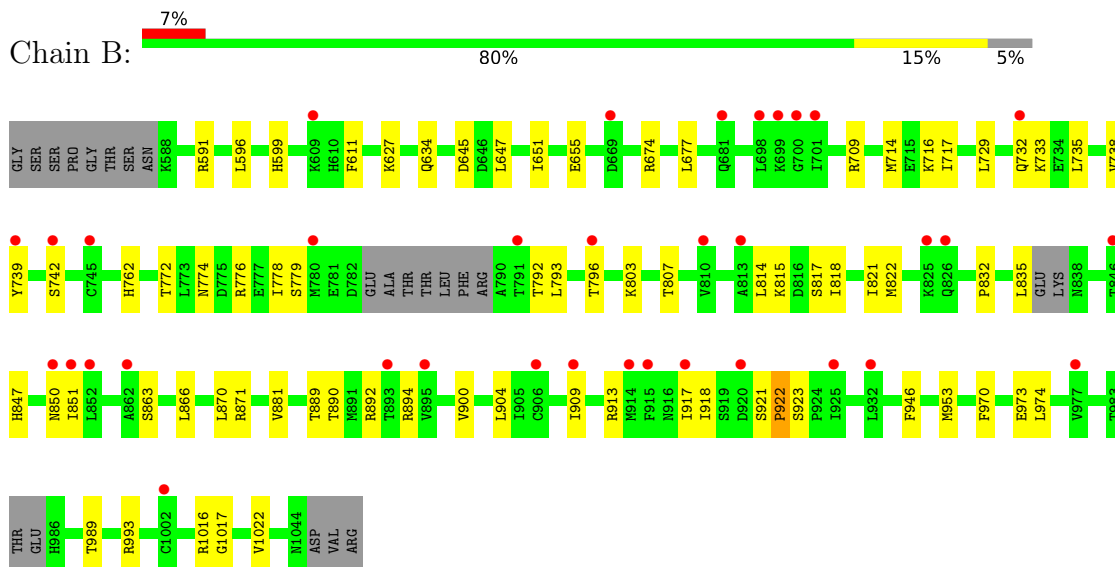
3 Residue-property plots [i](#)

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.

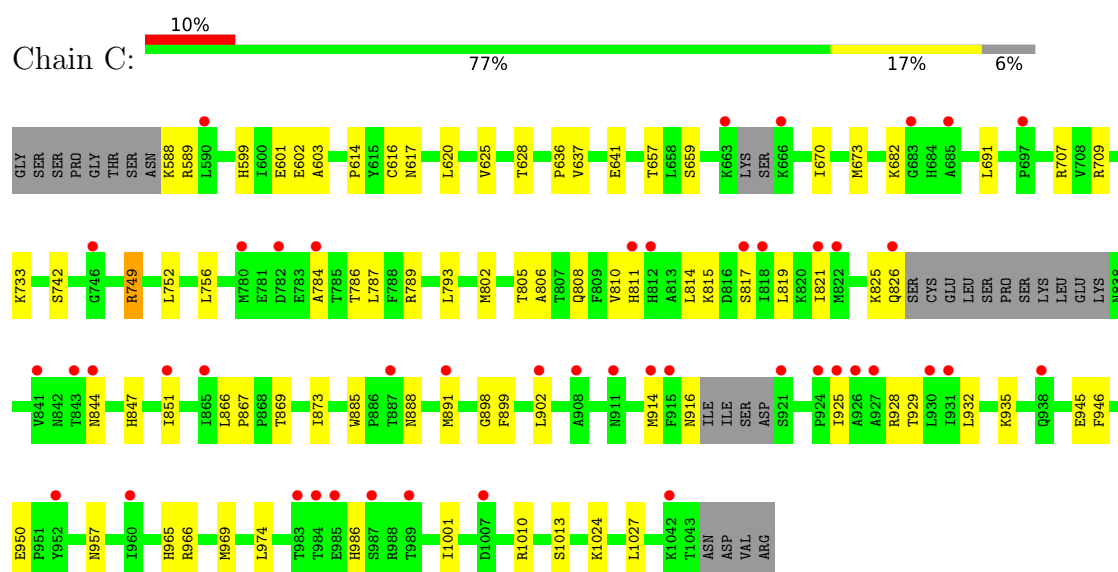
• Molecule 1: Ras GTPase-activating protein 1



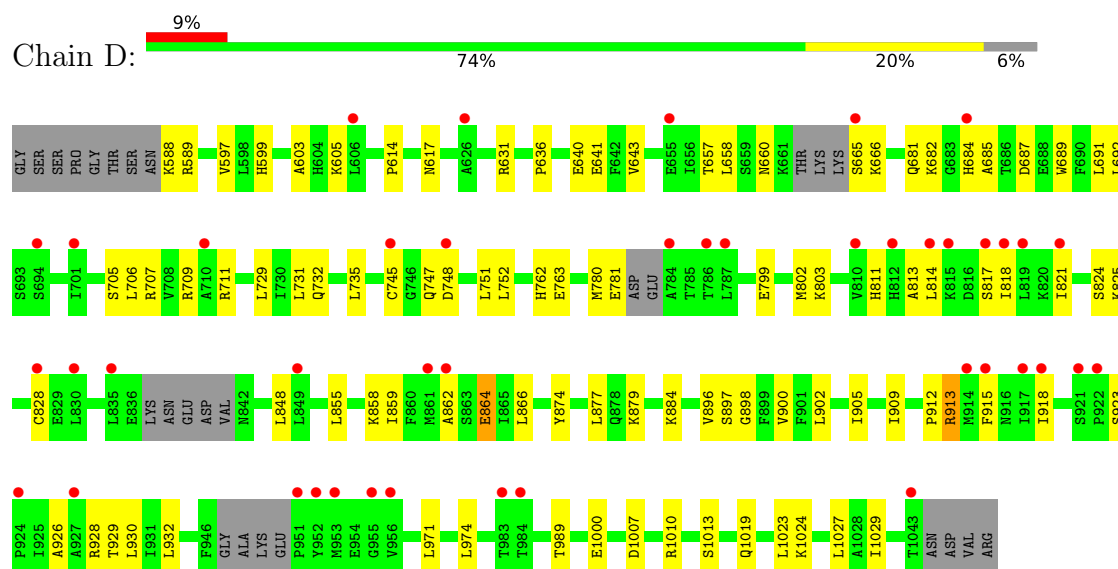
• Molecule 1: Ras GTPase-activating protein 1



• Molecule 1: Ras GTPase-activating protein 1



• Molecule 1: Ras GTPase-activating protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.89Å 94.04Å 96.71Å 95.81° 111.10° 108.51°	Depositor
Resolution (Å)	87.52 – 2.45 87.51 – 2.45	Depositor EDS
% Data completeness (in resolution range)	95.7 (87.52-2.45) 96.1 (87.51-2.45)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.228 , 0.284 0.228 , 0.282	Depositor DCC
R_{free} test set	3884 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14329	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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](#)

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	0.11	0/3674	0.28	0/4963
1	B	0.17	1/3656 (0.0%)	0.32	1/4941 (0.0%)
1	C	0.11	0/3612	0.29	0/4883
1	D	0.12	0/3630	0.32	0/4906
All	All	0.13	1/14572 (0.0%)	0.30	1/19693 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	922	PRO	CG-CD	-5.18	1.33	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	922	PRO	N-CD-CG	-5.49	94.96	103.20

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	3606	0	3693	55	1
1	B	3589	0	3666	45	0
1	C	3545	0	3614	59	1
1	D	3563	0	3642	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	6	0	0	1	0
2	B	9	0	0	0	0
2	C	4	0	0	0	0
2	D	7	0	0	0	0
All	All	14329	0	14615	220	1

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 8.

All (220) 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:733:LYS:HD2	1:C:733:LYS:H	1.32	0.93
1:A:599:HIS:HB2	1:A:709:ARG:HB2	1.59	0.84
1:B:822:MET:HE1	1:B:922:PRO:HA	1.65	0.78
1:D:814:LEU:HB3	1:D:818:ILE:HD11	1.63	0.78
1:D:631:ARG:NH1	1:D:640:GLU:OE2	2.15	0.78
1:C:866:LEU:HD12	1:C:974:LEU:HD11	1.65	0.78
1:C:826:GLN:NE2	1:C:844:ASN:OD1	2.16	0.78
1:D:599:HIS:HB2	1:D:709:ARG:HB2	1.66	0.78
1:B:821:ILE:HD11	1:B:851:ILE:HG21	1.65	0.77
1:B:714:MET:HE1	1:B:716:LYS:HD3	1.66	0.75
1:A:697:PRO:HG3	1:C:691:LEU:HD22	1.67	0.75
1:B:599:HIS:HB2	1:B:709:ARG:HB2	1.69	0.75
1:B:889:THR:O	1:B:892:ARG:NH1	2.20	0.74
1:C:599:HIS:HB2	1:C:709:ARG:HB2	1.71	0.72
1:A:742:SER:HB2	1:A:793:LEU:HD22	1.72	0.70
1:C:821:ILE:HD11	1:C:851:ILE:HG21	1.73	0.70
1:C:808:GLN:OE1	1:C:808:GLN:N	2.23	0.69
1:C:928:ARG:O	1:C:932:LEU:N	2.25	0.69
1:D:1010:ARG:HA	1:D:1027:LEU:HD11	1.74	0.69
1:B:742:SER:HB2	1:B:793:LEU:HD22	1.76	0.68
1:D:682:LYS:HD2	1:D:684:HIS:CE1	2.29	0.67
1:D:811:HIS:NE2	1:D:915:PHE:O	2.26	0.67
1:C:811:HIS:CE1	1:C:916:ASN:HD22	2.13	0.66
1:B:739:TYR:OH	1:B:776:ARG:HG3	1.96	0.66
1:A:788:PHE:O	1:A:903:ARG:NH2	2.30	0.65
1:C:742:SER:HB2	1:C:793:LEU:HD22	1.79	0.64
1:C:888:ASN:ND2	1:C:891:MET:HB2	2.13	0.64
1:B:863:SER:HB2	1:B:974:LEU:HD21	1.80	0.63
1:A:840:ASP:HB3	1:A:843:THR:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:691:LEU:HA	1:D:705:SER:HA	1.82	0.60
1:D:821:ILE:HA	1:D:824:SER:HB2	1.84	0.60
1:C:786:THR:HA	1:C:789:ARG:HD3	1.83	0.60
1:A:822:MET:HE2	1:A:918:ILE:HD13	1.83	0.60
1:D:913:ARG:H	1:D:913:ARG:HD2	1.68	0.59
1:A:594:SER:HB3	1:A:647:LEU:HB2	1.85	0.59
1:B:814:LEU:HD21	1:B:909:ILE:HG13	1.85	0.58
1:B:732:GLN:HA	1:B:733:LYS:HE2	1.84	0.58
1:B:818:ILE:O	1:B:822:MET:HG2	2.03	0.58
1:B:732:GLN:HE22	1:B:1022:VAL:HG21	1.69	0.58
1:B:832:PRO:HA	1:B:835:LEU:HD12	1.86	0.58
1:D:813:ALA:HB1	1:D:859:ILE:HA	1.84	0.58
1:D:874:TYR:HA	1:D:877:LEU:HD12	1.84	0.57
1:A:961:LYS:HA	1:A:964:LYS:HE2	1.85	0.57
1:C:945:GLU:H	1:C:945:GLU:CD	2.12	0.57
1:D:599:HIS:CE1	1:D:641:GLU:HB2	2.40	0.57
1:A:590:LEU:HD13	1:A:1040:TYR:HB3	1.86	0.57
1:B:851:ILE:HD12	1:B:851:ILE:H	1.70	0.57
1:B:822:MET:HE3	1:B:822:MET:HA	1.86	0.56
1:A:811:HIS:HA	1:A:917:ILE:HD11	1.88	0.56
1:B:611:PHE:O	1:B:634:GLN:NE2	2.37	0.56
1:A:911:ASN:HB3	1:A:914:MET:SD	2.46	0.56
1:D:599:HIS:HE1	1:D:641:GLU:HB2	1.70	0.56
1:C:805:THR:HB	1:C:867:PRO:HG2	1.86	0.56
1:C:815:LYS:O	1:C:819:LEU:HG	2.06	0.56
1:B:822:MET:SD	1:B:922:PRO:HB3	2.46	0.55
1:A:658:LEU:HD11	1:A:706:LEU:HD13	1.87	0.55
1:D:658:LEU:HD11	1:D:706:LEU:HD22	1.87	0.55
1:C:946:PHE:HD1	1:C:950:GLU:HG3	1.72	0.55
1:B:776:ARG:HA	1:B:779:SER:HB3	1.89	0.55
1:B:817:SER:O	1:B:821:ILE:HG12	2.06	0.54
1:C:821:ILE:HD12	1:C:929:THR:HG21	1.88	0.54
1:D:814:LEU:HD11	1:D:905:ILE:HD12	1.88	0.54
1:C:898:GLY:HA2	1:C:902:LEU:HB2	1.91	0.53
1:D:687:ASP:OD1	1:D:709:ARG:HG2	2.09	0.53
1:B:863:SER:HB3	1:B:970:PHE:HE1	1.73	0.53
1:C:811:HIS:HE1	1:C:916:ASN:HD22	1.57	0.53
1:D:681:GLN:HG3	1:D:682:LYS:H	1.73	0.53
1:B:822:MET:HE1	1:B:922:PRO:CA	2.39	0.52
1:C:914:MET:SD	1:C:914:MET:N	2.82	0.52
1:D:692:LEU:HD21	1:D:706:LEU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:PRO:HD3	1:C:589:ARG:HD2	1.90	0.52
1:D:1013:SER:HB2	1:D:1024:LYS:HD3	1.91	0.52
1:A:749:ARG:HD3	1:A:796:THR:HG21	1.92	0.52
1:C:601:GLU:HB2	1:C:707:ARG:HG2	1.92	0.52
1:C:929:THR:HA	1:C:932:LEU:HB2	1.91	0.52
1:C:806:ALA:O	1:C:810:VAL:HG23	2.09	0.52
1:B:655:GLU:HG2	1:B:674:ARG:HG3	1.93	0.51
1:C:602:GLU:HB3	1:C:637:VAL:HG22	1.93	0.51
1:A:614:PRO:HG2	1:A:636:PRO:HG3	1.93	0.51
1:D:780:MET:HE3	1:D:780:MET:HA	1.93	0.51
1:B:890:THR:O	1:B:894:ARG:HG3	2.11	0.51
1:D:813:ALA:HB2	1:D:862:ALA:HB3	1.93	0.50
1:B:774:ASN:O	1:B:778:ILE:HG13	2.11	0.50
1:B:847:HIS:O	1:B:851:ILE:HD12	2.11	0.50
1:B:847:HIS:O	1:B:850:ASN:N	2.43	0.50
1:D:817:SER:HB2	1:D:855:LEU:HD13	1.94	0.50
1:C:811:HIS:NE2	1:C:916:ASN:HB2	2.27	0.49
1:D:928:ARG:HH21	1:D:932:LEU:HD21	1.76	0.49
1:C:966:ARG:HA	1:C:969:MET:HE2	1.94	0.49
1:D:909:ILE:O	1:D:930:LEU:HD23	2.12	0.49
1:A:673:MET:HE2	1:A:690:PHE:CG	2.47	0.49
1:B:729:LEU:HD11	1:B:1022:VAL:HG13	1.95	0.49
1:B:762:HIS:HB2	1:B:989:THR:HG22	1.94	0.49
1:D:745:CYS:HB2	1:D:752:LEU:HD22	1.94	0.49
1:D:748:ASP:HB2	1:D:751:LEU:HB3	1.95	0.49
1:D:781:GLU:O	1:D:884:LYS:NZ	2.42	0.49
1:A:672:PHE:HB3	1:A:695:HIS:CE1	2.48	0.49
1:C:825:LYS:HG2	1:C:925:ILE:HG21	1.95	0.49
1:C:617:ASN:HB2	1:C:657:THR:OG1	2.12	0.49
1:D:684:HIS:CD2	1:D:684:HIS:H	2.31	0.49
1:A:733:LYS:HG2	1:A:734:GLU:OE1	2.14	0.48
1:A:883:HIS:C	1:A:883:HIS:CD2	2.91	0.48
1:C:869:THR:O	1:C:873:ILE:HG12	2.14	0.48
1:D:828:CYS:HB2	1:D:929:THR:HG23	1.95	0.48
1:D:913:ARG:H	1:D:913:ARG:CD	2.27	0.48
1:C:603:ALA:HB3	1:C:636:PRO:HD2	1.96	0.48
1:C:1013:SER:HB2	1:C:1024:LYS:HD3	1.96	0.48
1:C:965:HIS:O	1:C:969:MET:HG3	2.14	0.47
1:D:731:LEU:HD11	1:D:763:GLU:HG3	1.96	0.47
1:A:781:GLU:O	1:A:884:LYS:NZ	2.48	0.47
1:D:614:PRO:HG2	1:D:636:PRO:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:LEU:HD13	1:A:1040:TYR:CB	2.44	0.47
1:B:735:LEU:HB3	1:B:738:VAL:HB	1.96	0.47
1:A:744:VAL:HG12	1:A:1008:GLU:HG3	1.96	0.47
1:D:603:ALA:HB3	1:D:636:PRO:HD2	1.96	0.47
1:C:935:LYS:HG3	1:C:946:PHE:CE1	2.49	0.47
1:D:923:SER:H	1:D:926:ALA:HB3	1.80	0.47
1:B:815:LYS:HE3	1:B:917:ILE:O	2.15	0.47
1:D:685:ALA:N	1:D:711:ARG:HE	2.12	0.47
1:A:735:LEU:HB3	1:A:738:VAL:HB	1.97	0.46
1:D:912:PRO:HB2	1:D:918:ILE:HG12	1.96	0.46
1:B:871:ARG:NH2	1:B:973:GLU:O	2.49	0.46
1:D:665:SER:OG	1:D:666:LYS:N	2.43	0.46
1:A:938:GLN:NE2	2:A:1102:HOH:O	2.49	0.46
1:A:1025:LYS:O	1:A:1029:ILE:HG13	2.16	0.46
1:A:1039:GLN:O	1:A:1043:THR:HG23	2.16	0.46
1:A:734:GLU:HG3	1:A:736:HIS:CE1	2.50	0.46
1:D:597:VAL:HG22	1:D:643:VAL:HG22	1.98	0.46
1:C:784:ALA:HB2	1:C:885:TRP:CE2	2.51	0.45
1:C:811:HIS:HE1	1:C:916:ASN:ND2	2.14	0.45
1:D:813:ALA:HB2	1:D:862:ALA:CB	2.47	0.45
1:D:858:LYS:HB2	1:D:858:LYS:HE3	1.70	0.45
1:D:896:VAL:O	1:D:900:VAL:HG12	2.16	0.45
1:C:1010:ARG:HA	1:C:1027:LEU:HD11	1.98	0.45
1:C:817:SER:O	1:C:821:ILE:HG12	2.17	0.45
1:A:670:ILE:HG22	1:A:671:LEU:HG	1.98	0.45
1:C:733:LYS:HD2	1:C:733:LYS:N	2.15	0.45
1:D:588:LYS:HB3	1:D:589:ARG:H	1.61	0.45
1:D:802:MET:SD	1:D:874:TYR:OH	2.75	0.45
1:D:862:ALA:C	1:D:864:GLU:N	2.71	0.45
1:D:660:ASN:O	1:D:666:LYS:HB2	2.16	0.45
1:A:866:LEU:HD22	1:A:870:LEU:HD23	1.99	0.44
1:C:929:THR:HA	1:C:932:LEU:HD12	2.00	0.44
1:A:734:GLU:OE1	1:A:734:GLU:N	2.50	0.44
1:C:784:ALA:HB2	1:C:885:TRP:CD2	2.52	0.44
1:A:760:PHE:CD2	1:A:769:LEU:HB2	2.52	0.44
1:B:596:LEU:HB2	1:B:647:LEU:HD11	1.98	0.44
1:C:847:HIS:O	1:C:851:ILE:HD12	2.17	0.44
1:D:762:HIS:HD1	1:D:989:THR:HG1	1.65	0.44
1:D:825:LYS:HA	1:D:825:LYS:HD3	1.73	0.44
1:B:1016:ARG:HD2	1:B:1017:GLY:H	1.82	0.44
1:A:792:THR:O	1:A:796:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:732:GLN:O	1:D:735:LEU:HD12	2.18	0.44
1:A:815:LYS:NZ	1:A:917:ILE:O	2.32	0.43
1:B:627:LYS:HB3	1:B:627:LYS:HE2	1.68	0.43
1:B:866:LEU:HD22	1:B:870:LEU:HD23	1.99	0.43
1:A:631:ARG:HA	1:A:631:ARG:HD3	1.84	0.43
1:D:928:ARG:HD2	1:D:928:ARG:HA	1.75	0.43
1:A:803:LYS:HA	1:A:803:LYS:HD3	1.63	0.43
1:A:787:LEU:C	1:A:789:ARG:H	2.27	0.43
1:B:772:THR:O	1:B:776:ARG:HG2	2.19	0.43
1:B:900:VAL:O	1:B:904:LEU:HB3	2.18	0.43
1:C:749:ARG:H	1:C:749:ARG:CZ	2.30	0.43
1:B:729:LEU:O	1:B:732:GLN:HG2	2.18	0.43
1:D:866:LEU:HD12	1:D:974:LEU:HD21	2.00	0.43
1:A:787:LEU:HD21	1:A:891:MET:HE2	2.00	0.43
1:B:946:PHE:CZ	1:B:953:MET:HE2	2.54	0.43
1:D:813:ALA:HB3	1:D:814:LEU:HD12	2.00	0.43
1:A:863:SER:HB3	1:A:970:PHE:HE1	1.84	0.43
1:D:898:GLY:HA2	1:D:902:LEU:HB2	2.00	0.43
1:A:941:ALA:HA	1:A:967:MET:HE3	2.01	0.43
1:B:591:ARG:HB3	1:B:717:ILE:HB	2.01	0.43
1:C:673:MET:HE2	1:C:673:MET:HB2	1.86	0.43
1:D:605:LYS:HA	1:D:605:LYS:HD3	1.75	0.43
1:A:648:PRO:HA	1:C:589:ARG:HD3	2.01	0.42
1:A:777:GLU:O	1:A:781:GLU:HG2	2.19	0.42
1:A:960:ILE:O	1:A:964:LYS:HG3	2.19	0.42
1:C:620:LEU:HG	1:C:625:VAL:HG21	2.00	0.42
1:D:747:GLN:OE1	1:D:747:GLN:N	2.43	0.42
1:C:935:LYS:HG3	1:C:946:PHE:HE1	1.83	0.42
1:A:667:ASP:HA	1:A:668:PRO:HD3	1.91	0.42
1:B:803:LYS:NZ	1:B:807:THR:HG21	2.34	0.42
1:B:913:ARG:HB2	1:B:918:ILE:HD11	2.01	0.42
1:A:668:PRO:HB2	1:A:670:ILE:HD11	2.01	0.42
1:C:659:SER:HA	1:C:670:ILE:HD12	2.00	0.42
1:A:923:SER:O	1:A:927:ALA:N	2.37	0.42
1:C:752:LEU:HD23	1:C:1001:ILE:HD13	2.02	0.42
1:B:792:THR:O	1:B:796:THR:HG23	2.19	0.42
1:C:599:HIS:NE2	1:C:641:GLU:HG3	2.34	0.42
1:D:799:GLU:O	1:D:803:LYS:HG2	2.20	0.42
1:D:599:HIS:HB2	1:D:709:ARG:CB	2.43	0.42
1:D:729:LEU:HD22	1:D:1029:ILE:HD12	2.02	0.42
1:D:897:SER:HB2	1:D:971:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:617:ASN:HB2	1:D:657:THR:OG1	2.20	0.42
1:A:871:ARG:HB3	1:A:974:LEU:O	2.20	0.41
1:C:756:LEU:HD23	1:C:756:LEU:HA	1.94	0.41
1:D:818:ILE:HA	1:D:821:ILE:CD1	2.50	0.41
1:C:787:LEU:HD23	1:C:787:LEU:HA	1.83	0.41
1:C:946:PHE:N	1:C:957:ASN:OD1	2.54	0.41
1:D:762:HIS:ND1	1:D:989:THR:OG1	2.50	0.41
1:C:599:HIS:NE2	1:C:641:GLU:OE2	2.53	0.41
1:C:614:PRO:HG2	1:C:636:PRO:HG3	2.02	0.41
1:D:689:TRP:CE2	1:D:707:ARG:HB2	2.55	0.41
1:A:777:GLU:HG2	1:A:788:PHE:CE1	2.55	0.41
1:A:1019:GLN:O	1:A:1023:LEU:HG	2.20	0.41
1:D:974:LEU:HD23	1:D:974:LEU:HA	1.92	0.41
1:C:974:LEU:HD12	1:C:974:LEU:HA	1.81	0.41
1:A:731:LEU:HD11	1:A:763:GLU:HG3	2.03	0.41
1:A:974:LEU:HD23	1:A:974:LEU:HA	1.87	0.41
1:D:1019:GLN:HG2	1:D:1023:LEU:HD22	2.02	0.41
1:A:881:VAL:HG11	1:A:891:MET:HB3	2.02	0.40
1:A:894:ARG:HE	1:A:894:ARG:HB3	1.74	0.40
1:B:645:ASP:CG	1:B:993:ARG:HH22	2.29	0.40
1:A:826:GLN:OE1	1:A:827:SER:N	2.53	0.40
1:C:682:LYS:HD2	1:C:682:LYS:HA	1.84	0.40
1:A:953:MET:HE3	1:A:953:MET:HB3	1.83	0.40
1:C:616:CYS:HB2	1:C:628:THR:HG23	2.04	0.40
1:A:795:SER:HB2	1:A:903:ARG:HH12	1.85	0.40
1:B:651:ILE:HG22	1:B:677:LEU:HD11	2.03	0.40
1:C:802:MET:HE1	1:C:899:PHE:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:ASN:OD1	1:C:986:HIS:ND1[1_556]	2.17	0.03

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	441/468 (94%)	432 (98%)	9 (2%)	0	100	100
1	B	438/468 (94%)	431 (98%)	7 (2%)	0	100	100
1	C	431/468 (92%)	422 (98%)	9 (2%)	0	100	100
1	D	432/468 (92%)	420 (97%)	12 (3%)	0	100	100
All	All	1742/1872 (93%)	1705 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	412/430 (96%)	412 (100%)	0	100	100
1	B	411/430 (96%)	408 (99%)	3 (1%)	76	84
1	C	403/430 (94%)	400 (99%)	3 (1%)	76	84
1	D	408/430 (95%)	402 (98%)	6 (2%)	57	70
All	All	1634/1720 (95%)	1622 (99%)	12 (1%)	76	84

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	881	VAL
1	B	921	SER
1	B	923	SER
1	C	588	LYS
1	C	749	ARG
1	C	814	LEU
1	D	848	LEU
1	D	864	GLU

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Mol	Chain	Res	Type
1	D	879	LYS
1	D	913	ARG
1	D	1000	GLU
1	D	1007	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	634	GLN
1	A	695	HIS
1	A	812	HIS
1	A	883	HIS
1	A	938	GLN
1	A	1020	GLN
1	A	1038	ASN
1	B	599	HIS
1	B	652	ASN
1	B	888	ASN
1	B	939	ASN
1	B	965	HIS
1	B	1021	HIS
1	B	1035	GLN
1	C	604	HIS
1	C	610	HIS
1	C	613	ASN
1	C	695	HIS
1	C	732	GLN
1	C	811	HIS
1	C	916	ASN
1	D	624	GLN
1	D	684	HIS
1	D	847	HIS
1	D	963	ASN

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](#)

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	447/468 (95%)	0.66	26 (5%)	29	26	47, 67, 111, 143	0
1	B	446/468 (95%)	0.75	35 (7%)	19	16	46, 70, 116, 159	0
1	C	439/468 (93%)	0.84	46 (10%)	11	9	45, 72, 131, 173	0
1	D	442/468 (94%)	0.87	43 (9%)	13	11	42, 76, 132, 167	0
All	All	1774/1872 (94%)	0.78	150 (8%)	16	14	42, 71, 126, 173	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	931	ILE	4.3
1	B	917	ILE	4.0
1	C	915	PHE	3.9
1	D	748	ASP	3.9
1	D	830	LEU	3.8
1	D	817	SER	3.7
1	B	1002	CYS	3.7
1	B	810	VAL	3.6
1	B	925	ILE	3.6
1	B	906	CYS	3.5
1	B	745	CYS	3.5
1	D	951	PRO	3.4
1	D	921	SER	3.4
1	C	812	HIS	3.3
1	D	915	PHE	3.2
1	C	782	ASP	3.2
1	C	927	ALA	3.1
1	D	922	PRO	3.1
1	D	819	LEU	3.1
1	A	890	THR	3.0
1	C	983	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	828	CYS	3.0
1	D	701	ILE	3.0
1	D	821	ILE	3.0
1	A	925	ILE	2.9
1	C	685	ALA	2.9
1	C	817	SER	2.9
1	B	909	ILE	2.9
1	C	843	THR	2.9
1	D	955	GLY	2.9
1	C	865	ILE	2.8
1	A	838	ASN	2.8
1	C	818	ILE	2.8
1	C	960	ILE	2.8
1	D	914	MET	2.8
1	D	952	TYR	2.8
1	A	790	ALA	2.8
1	B	932	LEU	2.8
1	C	683	GLY	2.7
1	B	895	VAL	2.7
1	B	813	ALA	2.7
1	B	977	VAL	2.7
1	A	984	THR	2.7
1	D	927	ALA	2.6
1	B	825	LYS	2.6
1	C	914	MET	2.6
1	B	852	LEU	2.6
1	A	893	THR	2.6
1	C	926	ALA	2.6
1	A	932	LEU	2.6
1	D	786	THR	2.6
1	B	850	ASN	2.6
1	A	952	TYR	2.6
1	C	851	ILE	2.5
1	A	787	LEU	2.5
1	C	666	LYS	2.5
1	C	985	GLU	2.5
1	A	813	ALA	2.5
1	D	626	ALA	2.5
1	D	861	MET	2.5
1	D	917	ILE	2.5
1	A	866	LEU	2.5
1	B	915	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	893	THR	2.5
1	C	987	SER	2.5
1	A	914	MET	2.5
1	D	655	GLU	2.5
1	B	920	ASP	2.5
1	A	915	PHE	2.5
1	D	810	VAL	2.5
1	A	929	THR	2.5
1	B	846	THR	2.5
1	D	665	SER	2.5
1	C	697	PRO	2.4
1	B	851	ILE	2.4
1	D	606	LEU	2.4
1	D	784	ALA	2.4
1	D	953	MET	2.4
1	B	699	LYS	2.4
1	C	902	LEU	2.4
1	D	812	HIS	2.4
1	A	889	THR	2.4
1	C	989	THR	2.4
1	D	818	ILE	2.4
1	D	684	HIS	2.4
1	C	908	ALA	2.4
1	A	807	THR	2.4
1	B	701	ILE	2.4
1	C	930	LEU	2.4
1	C	844	ASN	2.4
1	D	849	LEU	2.3
1	C	952	TYR	2.3
1	B	826	GLN	2.3
1	A	835	LEU	2.3
1	B	739	TYR	2.3
1	C	924	PRO	2.3
1	C	984	THR	2.3
1	D	983	THR	2.3
1	B	698	LEU	2.3
1	C	925	ILE	2.3
1	A	906	CYS	2.3
1	D	787	LEU	2.3
1	B	609	LYS	2.3
1	C	746	GLY	2.2
1	B	732	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	780	MET	2.2
1	C	590	LEU	2.2
1	C	891	MET	2.2
1	A	719	PRO	2.2
1	A	978	PRO	2.2
1	D	956	VAL	2.2
1	B	796	THR	2.2
1	C	822	MET	2.2
1	A	778	ILE	2.2
1	B	742	SER	2.2
1	A	789	ARG	2.2
1	C	811	HIS	2.2
1	C	780	MET	2.2
1	C	921	SER	2.2
1	C	1007	ASP	2.2
1	D	924	PRO	2.2
1	C	841	VAL	2.1
1	C	911	ASN	2.1
1	B	791	THR	2.1
1	C	887	THR	2.1
1	D	694	SER	2.1
1	B	914	MET	2.1
1	C	826	GLN	2.1
1	C	784	ALA	2.1
1	D	814	LEU	2.1
1	D	984	THR	2.1
1	B	669	ASP	2.1
1	C	663	LYS	2.1
1	C	1042	LYS	2.1
1	A	900	VAL	2.1
1	B	681	GLN	2.1
1	D	710	ALA	2.1
1	D	862	ALA	2.1
1	D	1043	THR	2.1
1	C	938	GLN	2.1
1	A	589	ARG	2.1
1	D	918	ILE	2.1
1	D	815	LYS	2.1
1	B	862	ALA	2.0
1	A	850	ASN	2.0
1	D	835	LEU	2.0
1	A	687	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	745	CYS	2.0
1	B	700	GLY	2.0
1	C	821	ILE	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.