Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2025 – 04:10 PM EST

PDB ID	:	9BZ4
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:

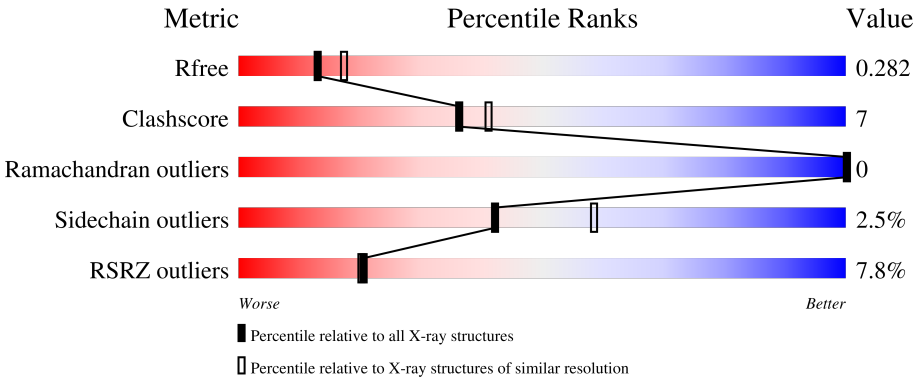
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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}	164625	1096 (2.46-2.46)
Clashscore	180529	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)
RSRZ outliers	164620	1096 (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 <=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	5% 77% 18% ·
1	B	468	7% 79% 16% 5%
1	C	468	10% 76% 17% · 6%
1	D	468	8% 74% 19% · 6%

2 Entry composition (i)

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.

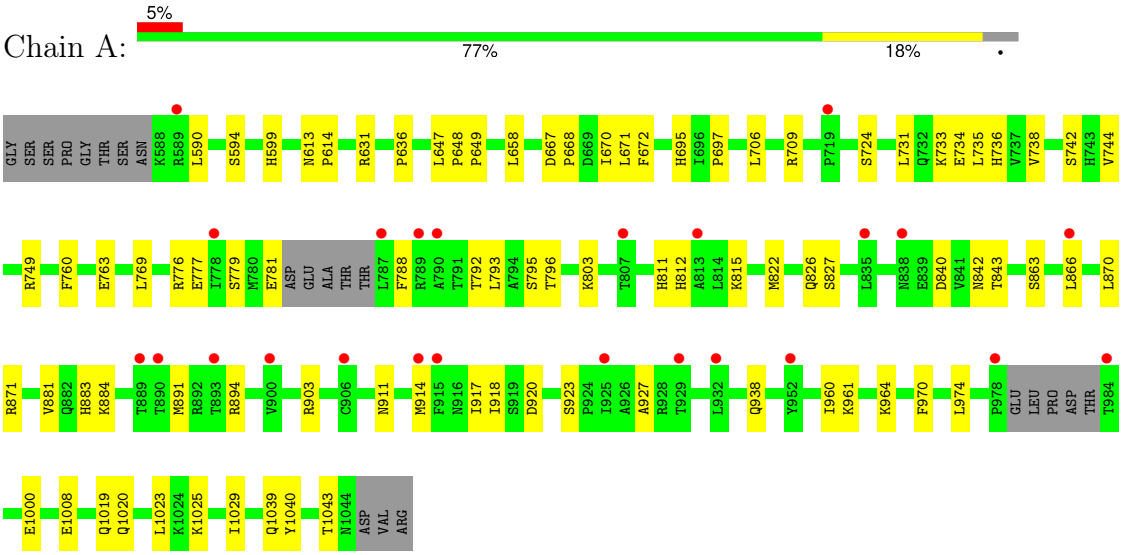
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	O	0	0
			6	6		
2	B	9	Total	O	0	0
			9	9		
2	C	4	Total	O	0	0
			4	4		
2	D	7	Total	O	0	0
			7	7		

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.

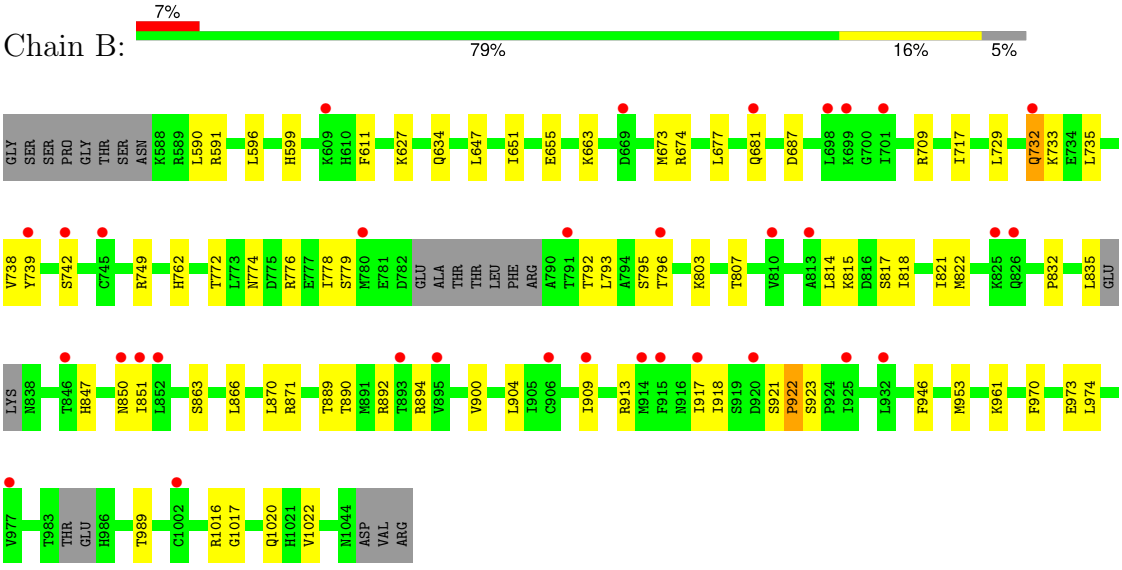
• Molecule 1: Ras GTPase-activating protein 1

Chain A:



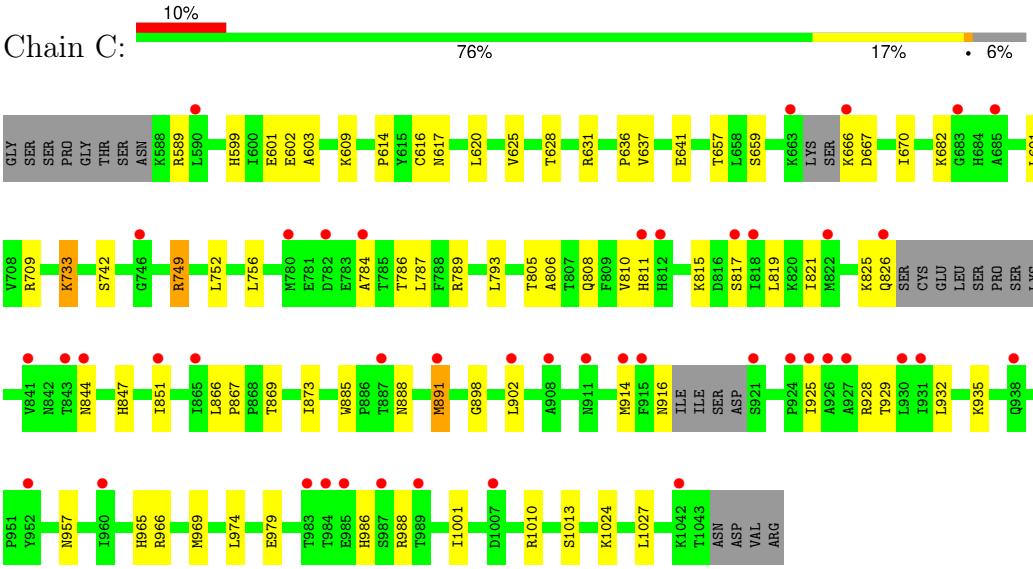
• Molecule 1: Ras GTPase-activating protein 1

Chain B:



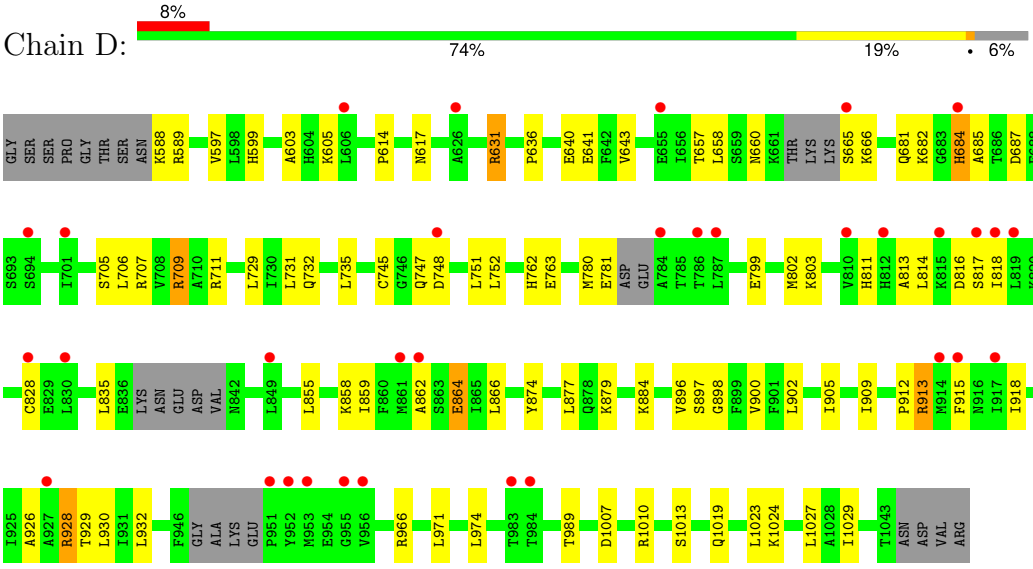
• Molecule 1: Ras GTPase-activating protein 1

Chain C:



• Molecule 1: Ras GTPase-activating protein 1

Chain D:



4 Data and refinement statistics (i)

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 87.52 – 2.45	Depositor EDS
% Data completeness (in resolution range)	95.7 (87.52-2.45) 96.1 (87.52-2.45)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	6959 reflections (5.12%)	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 , 59.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[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	0.25	0/3674	0.47	0/4963
1	B	0.28	1/3656 (0.0%)	0.48	1/4941 (0.0%)
1	C	0.25	0/3612	0.48	0/4883
1	D	0.25	0/3630	0.50	2/4906 (0.0%)
All	All	0.26	1/14572 (0.0%)	0.48	3/19693 (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	-5.31	1.33	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	691	LEU	CA-CB-CG	6.15	129.45	115.30
1	B	922	PRO	N-CD-CG	-5.49	94.96	103.20
1	D	780	MET	CG-SD-CE	5.21	108.53	100.20

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	3606	0	3693	50	1
1	B	3589	0	3666	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3545	0	3614	56	1
1	D	3563	0	3642	62	0
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	206	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 7.

All (206) 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:H	1:C:733:LYS:HD2	1.32	0.93
1:A:599:HIS:HB2	1:A:709:ARG:HB2	1.59	0.84
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: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:D:913:ARG:HD2	1:D:913:ARG:H	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: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:H	1:B:851:ILE:HD12	1.70	0.57
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:C:914:MET:SD	1:C:914:MET:N	2.82	0.52
1:C:945:GLU:H	1:C:945:GLU:CD	2.12	0.52
1:D:692:LEU:HD21	1:D:706:LEU:HB2	1.90	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:GLU:HB2	1:C:707:ARG:HG2	1.92	0.52
1:A:822:MET:HE2	1:A:918:ILE:HG21	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:665:SER:OG	1:D:666:LYS:N	2.43	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:D:909:ILE:O	1:D:930:LEU:HD23	2.12	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: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:D:781:GLU:O	1:D:884:LYS:NZ	2.42	0.49
1:C:617:ASN:HB2	1:C:657:THR:OG1	2.12	0.49
1:D:684:HIS:H	1:D:684:HIS:CD2	2.31	0.49
1:A:733:LYS:HG2	1:A:734:GLU:OE1	2.14	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:946:PHE:CZ	1:B:953:MET:HE2	2.51	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: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:862:ALA:C	1:D:864:GLU:N	2.71	0.44
1:D:825:LYS:HD3	1:D:825:LYS:HA	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
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:HE2	1:B:627:LYS:HB3	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:A:883:HIS:CD2	1:A:883:HIS:C	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:CZ	1:C:749:ARG:H	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: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:B:591:ARG:HB3	1:B:717:ILE:HB	2.01	0.43
1:D:605:LYS:HD3	1:D:605:LYS:HA	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:822:MET:HB3	1:B:822:MET:HE2	1.66	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

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 (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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1742/1872 (93%)	1705 (98%)	37 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	412/430 (96%)	404 (98%)	8 (2%)	52 67
1	B	411/430 (96%)	399 (97%)	12 (3%)	37 52
1	C	403/430 (94%)	393 (98%)	10 (2%)	42 58
1	D	408/430 (95%)	397 (97%)	11 (3%)	40 55
All	All	1634/1720 (95%)	1593 (98%)	41 (2%)	42 58

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	613	ASN
1	A	724	SER
1	A	776	ARG
1	A	779	SER
1	A	812	HIS
1	A	920	ASP
1	A	1000	GLU
1	A	1020	GLN
1	B	590	LEU
1	B	663	LYS
1	B	673	MET
1	B	681	GLN
1	B	687	ASP
1	B	732	GLN
1	B	749	ARG
1	B	795	SER
1	B	921	SER

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Mol	Chain	Res	Type
1	B	923	SER
1	B	961	LYS
1	B	1020	GLN
1	C	609	LYS
1	C	631	ARG
1	C	666	LYS
1	C	667	ASP
1	C	733	LYS
1	C	749	ARG
1	C	891	MET
1	C	966	ARG
1	C	979	GLU
1	C	988	ARG
1	D	631	ARG
1	D	684	HIS
1	D	709	ARG
1	D	816	ASP
1	D	835	LEU
1	D	864	GLU
1	D	879	LYS
1	D	913	ARG
1	D	928	ARG
1	D	966	ARG
1	D	1007	ASP

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	695	HIS
1	A	883	HIS
1	A	938	GLN
1	A	1038	ASN
1	C	811	HIS
1	C	826	GLN
1	D	599	HIS
1	D	624	GLN
1	D	684	HIS

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, 95^{th} 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%)	0.57	24 (5%)	32	32	47, 67, 111, 143	0
1	B	446/468 (95%)	0.66	33 (7%)	22	23	46, 70, 116, 159	0
1	C	439/468 (93%)	0.75	45 (10%)	13	14	45, 72, 131, 173	0
1	D	442/468 (94%)	0.78	37 (8%)	18	18	42, 76, 132, 167	0
All	All	1774/1872 (94%)	0.69	139 (7%)	20	20	42, 71, 126, 173	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	931	ILE	4.3
1	B	917	ILE	3.9
1	D	748	ASP	3.9
1	C	915	PHE	3.8
1	D	830	LEU	3.7
1	D	817	SER	3.7
1	B	810	VAL	3.5
1	B	1002	CYS	3.5
1	B	925	ILE	3.5
1	D	951	PRO	3.4
1	B	745	CYS	3.3
1	B	906	CYS	3.3
1	C	782	ASP	3.3
1	D	921	SER	3.3
1	C	812	HIS	3.2
1	D	915	PHE	3.1
1	C	927	ALA	3.0
1	D	922	PRO	3.0
1	D	819	LEU	3.0
1	D	701	ILE	3.0
1	A	925	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	890	THR	3.0
1	C	983	THR	2.9
1	C	685	ALA	2.9
1	C	843	THR	2.9
1	C	817	SER	2.9
1	D	821	ILE	2.8
1	D	955	GLY	2.8
1	B	909	ILE	2.8
1	A	838	ASN	2.8
1	D	828	CYS	2.8
1	C	865	ILE	2.7
1	D	914	MET	2.7
1	C	960	ILE	2.7
1	C	683	GLY	2.7
1	B	895	VAL	2.7
1	B	977	VAL	2.7
1	B	932	LEU	2.7
1	B	813	ALA	2.7
1	D	952	TYR	2.7
1	A	984	THR	2.7
1	C	818	ILE	2.7
1	B	825	LYS	2.6
1	A	790	ALA	2.6
1	D	927	ALA	2.6
1	A	893	THR	2.6
1	C	914	MET	2.6
1	D	786	THR	2.6
1	A	932	LEU	2.5
1	C	926	ALA	2.5
1	C	985	GLU	2.5
1	C	666	LYS	2.5
1	B	852	LEU	2.5
1	C	851	ILE	2.5
1	B	920	ASP	2.5
1	D	626	ALA	2.4
1	C	987	SER	2.4
1	B	850	ASN	2.4
1	A	787	LEU	2.4
1	A	952	TYR	2.4
1	A	813	ALA	2.4
1	D	655	GLU	2.4
1	B	699	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	861	MET	2.4
1	A	866	LEU	2.4
1	B	915	PHE	2.4
1	C	902	LEU	2.4
1	A	914	MET	2.4
1	D	953	MET	2.4
1	D	917	ILE	2.4
1	D	665	SER	2.4
1	A	929	THR	2.4
1	B	846	THR	2.4
1	B	893	THR	2.4
1	A	915	PHE	2.4
1	D	684	HIS	2.4
1	D	810	VAL	2.4
1	C	697	PRO	2.3
1	B	851	ILE	2.3
1	D	784	ALA	2.3
1	A	889	THR	2.3
1	C	989	THR	2.3
1	A	835	LEU	2.3
1	C	930	LEU	2.3
1	D	606	LEU	2.3
1	C	844	ASN	2.3
1	B	701	ILE	2.3
1	C	908	ALA	2.3
1	A	807	THR	2.3
1	D	849	LEU	2.3
1	D	818	ILE	2.3
1	D	812	HIS	2.3
1	B	826	GLN	2.3
1	D	787	LEU	2.2
1	B	739	TYR	2.2
1	B	609	LYS	2.2
1	D	983	THR	2.2
1	A	719	PRO	2.2
1	C	924	PRO	2.2
1	B	732	GLN	2.2
1	C	952	TYR	2.2
1	B	698	LEU	2.2
1	C	746	GLY	2.2
1	C	984	THR	2.2
1	C	925	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	891	MET	2.2
1	A	789	ARG	2.2
1	C	784	ALA	2.2
1	C	590	LEU	2.1
1	B	780	MET	2.1
1	A	978	PRO	2.1
1	C	780	MET	2.1
1	C	822	MET	2.1
1	B	796	THR	2.1
1	B	742	SER	2.1
1	A	906	CYS	2.1
1	B	669	ASP	2.1
1	C	663	LYS	2.1
1	C	1007	ASP	2.1
1	D	956	VAL	2.1
1	A	589	ARG	2.1
1	C	921	SER	2.1
1	C	911	ASN	2.1
1	C	811	HIS	2.1
1	A	900	VAL	2.1
1	B	791	THR	2.1
1	C	887	THR	2.1
1	D	924	PRO	2.1
1	B	681	GLN	2.1
1	C	826	GLN	2.1
1	C	1042	LYS	2.1
1	D	694	SER	2.1
1	C	841	VAL	2.0
1	D	815	LYS	2.0
1	D	984	THR	2.0
1	C	938	GLN	2.0
1	A	778	ILE	2.0
1	B	914	MET	2.0
1	D	862	ALA	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 monosaccharides 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.