Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:27 AM GMT

PDB ID	:	2D5G
Title	:	Structure of ubiquitin fold protein R767E mutant
Authors	:	Shibata, N.; Higuchi, Y.
Deposited on	:	2005-11-01
Resolution	:	3.20 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

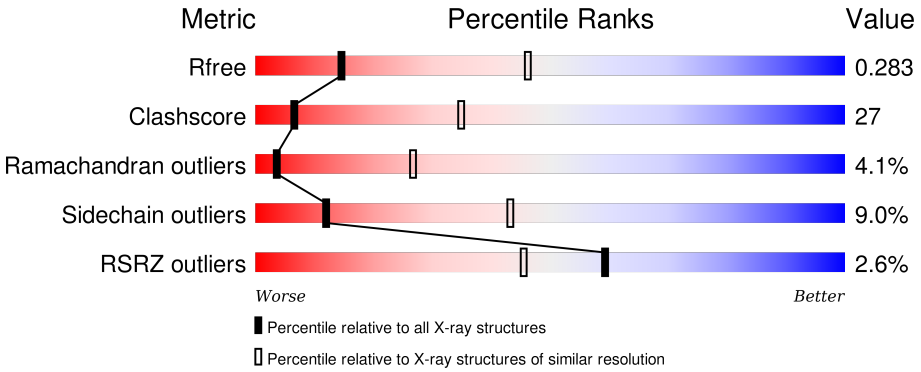
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 <=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	85	55% 36% 6%
1	B	85	40% 48% 11%
1	C	85	44% 48% 6%
1	D	85	6% 53% 39%
1	E	85	5% 39% 51% 6%

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Mol	Chain	Length	Quality of chain
1	F	85	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4066 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 Axin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	83	Total	C	N	O	S	0	0	0
			677	441	104	129	3			
1	B	85	Total	C	N	O	S	0	0	0
			691	451	106	131	3			
1	C	83	Total	C	N	O	S	0	0	0
			677	441	104	129	3			
1	D	83	Total	C	N	O	S	0	0	0
			677	441	104	129	3			
1	E	80	Total	C	N	O	S	0	0	0
			657	431	101	123	2			
1	F	83	Total	C	N	O	S	0	0	0
			677	441	104	129	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	767	GLU	ARG	ENGINEERED	UNP O70239
B	767	GLU	ARG	ENGINEERED	UNP O70239
C	767	GLU	ARG	ENGINEERED	UNP O70239
D	767	GLU	ARG	ENGINEERED	UNP O70239
E	767	GLU	ARG	ENGINEERED	UNP O70239
F	767	GLU	ARG	ENGINEERED	UNP O70239

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Hg	0	0
			1	1		
2	E	1	Total	Hg	0	0
			1	1		
2	B	2	Total	Hg	0	0
			2	2		

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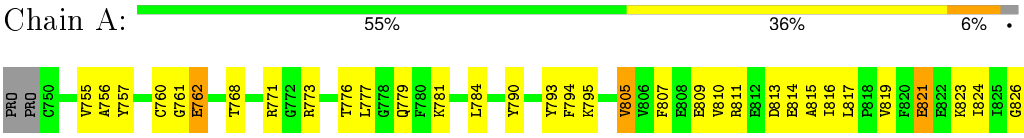
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	2	Total Hg 2 2	0	0
2	A	2	Total Hg 2 2	0	0
2	F	2	Total Hg 2 2	0	0

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.

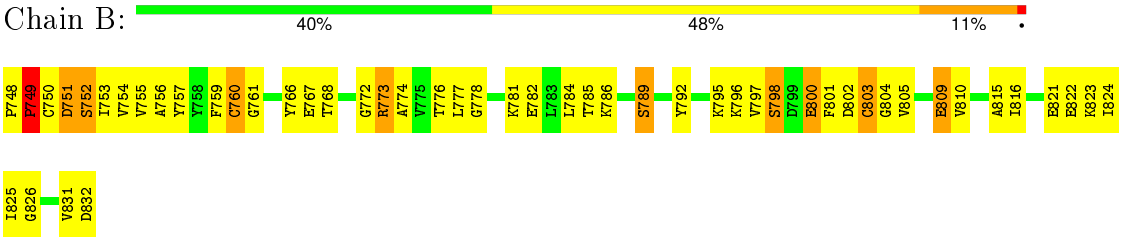
- Molecule 1: Axin-1

Chain A:



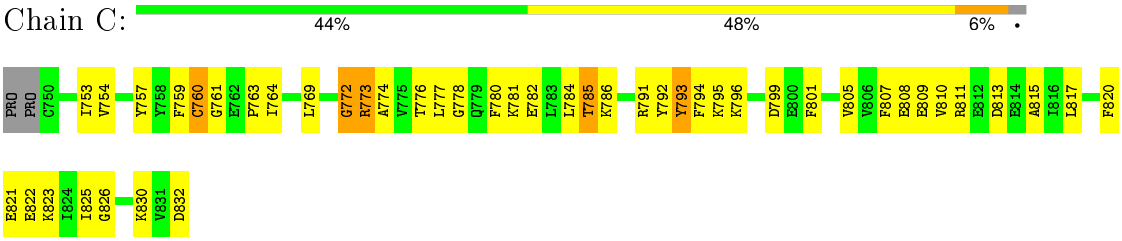
- Molecule 1: Axin-1

Chain B:



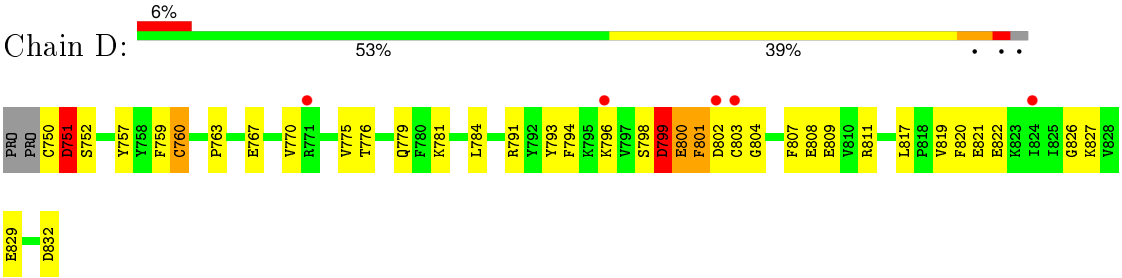
- Molecule 1: Axin-1

Chain C:



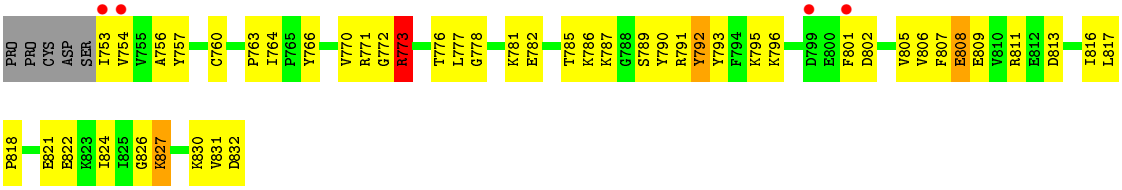
- Molecule 1: Axin-1

Chain D:



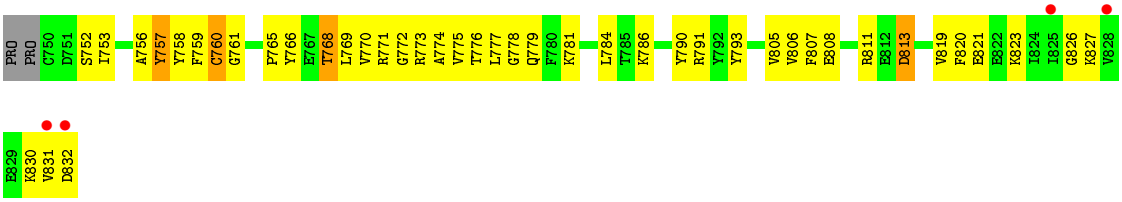
- Molecule 1: Axin-1

Chain E:



- Molecule 1: Axin-1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	125.55Å 125.55Å 115.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.18 – 3.20 49.18 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.18-3.20) 99.4 (49.18-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.29 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.314 0.223 , 0.283	Depositor DCC
R_{free} test set	1059 reflections (9.53%)	DCC
Wilson B-factor (Å^2)	93.5	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 71.2	EDS
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 22416 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4066	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.68	0/691	0.69	0/929
1	B	0.63	0/707	0.70	0/952
1	C	0.64	0/691	0.66	0/929
1	D	0.61	0/691	0.76	3/929 (0.3%)
1	E	0.53	0/671	0.59	0/902
1	F	0.58	0/691	0.60	0/929
All	All	0.61	0/4142	0.67	3/5570 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	800	GLU	CA-C-N	7.85	134.47	117.20
1	D	800	GLU	O-C-N	-5.74	113.52	122.70
1	D	800	GLU	N-CA-C	5.46	125.74	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	771	ARG	Peptide
1	C	793	TYR	Sidechain

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	677	0	671	31	0
1	B	691	0	684	44	0
1	C	677	0	671	41	0
1	D	677	0	670	33	0
1	E	657	0	657	43	0
1	F	677	0	670	36	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	1	0
2	D	1	0	0	0	0
2	E	1	0	0	1	0
2	F	2	0	0	1	0
All	All	4066	0	4023	221	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 27.

All (221) 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:777:LEU:HD22	1:A:810:VAL:HG12	1.38	1.04
1:D:798:SER:HB3	1:D:804:GLY:HA2	1.42	1.01
1:D:800:GLU:O	1:D:800:GLU:OE1	1.79	1.00
1:F:757:TYR:CE1	1:F:766:TYR:HB2	2.00	0.97
1:C:763:PRO:HG2	1:C:764:ILE:HD12	1.46	0.96
1:D:803:CYS:N	1:D:804:GLY:HA3	1.78	0.95
1:B:781:LYS:HA	1:B:784:LEU:HD23	1.54	0.88
1:B:753:ILE:HD11	1:B:773:ARG:O	1.76	0.85
1:D:798:SER:HB3	1:D:804:GLY:CA	2.08	0.83
1:F:760:CYS:SG	2:F:609:HG:HG	1.97	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:748:PRO:N	1:B:749:PRO:CD	2.46	0.78
1:F:757:TYR:HD1	1:F:757:TYR:H	1.32	0.78
1:C:795:LYS:HD2	1:C:825:ILE:HG21	1.65	0.77
1:E:763:PRO:HG2	1:E:764:ILE:HD12	1.66	0.75
1:A:781:LYS:HA	1:A:784:LEU:HD23	1.70	0.74
1:B:781:LYS:HA	1:B:784:LEU:CD2	2.18	0.72
1:B:798:SER:HB3	1:B:801:PHE:HB2	1.70	0.72
1:C:760:CYS:SG	2:C:606:HG:HG	2.07	0.71
1:F:757:TYR:HE1	1:F:766:TYR:HB2	1.55	0.70
1:F:777:LEU:HG	1:F:781:LYS:HE3	1.73	0.70
1:F:830:LYS:HE3	1:F:831:VAL:O	1.92	0.70
1:C:785:THR:HB	1:C:786:LYS:HD2	1.74	0.69
1:C:777:LEU:HD22	1:C:810:VAL:HG12	1.74	0.69
1:F:820:PHE:CE2	1:F:821:GLU:HG3	2.29	0.68
1:C:753:ILE:HD11	1:C:773:ARG:O	1.94	0.68
1:A:781:LYS:HA	1:A:784:LEU:CD2	2.24	0.67
1:F:760:CYS:SG	1:F:790:TYR:HE1	2.18	0.67
1:E:778:GLY:O	1:E:782:GLU:HG3	1.96	0.65
1:E:796:LYS:HD2	1:E:818:PRO:HG3	1.77	0.65
1:B:773:ARG:HD3	1:B:773:ARG:O	1.96	0.64
1:B:759:PHE:O	1:B:761:GLY:N	2.30	0.64
1:D:794:PHE:CE1	1:D:817:LEU:HD13	2.33	0.64
1:E:790:TYR:HD1	1:E:830:LYS:HA	1.63	0.63
1:A:776:THR:HG22	1:A:816:ILE:HD13	1.78	0.63
1:E:764:ILE:HD12	1:E:764:ILE:H	1.64	0.62
1:D:802:ASP:C	1:D:804:GLY:HA3	2.19	0.62
1:C:764:ILE:H	1:C:764:ILE:HD12	1.63	0.62
1:F:757:TYR:N	1:F:757:TYR:HD1	1.98	0.62
1:E:760:CYS:SG	2:E:608:HG:HG	2.18	0.62
1:D:776:THR:OG1	1:D:779:GLN:HG3	2.00	0.61
1:A:807:PHE:CE1	1:A:827:LYS:HD2	2.35	0.61
1:D:798:SER:HB3	1:D:804:GLY:C	2.20	0.61
1:B:748:PRO:N	1:B:749:PRO:HD2	2.16	0.61
1:F:757:TYR:N	1:F:757:TYR:CD1	2.69	0.60
1:F:807:PHE:CZ	1:F:827:LYS:HE2	2.36	0.60
1:B:759:PHE:C	1:B:761:GLY:H	2.04	0.60
1:B:781:LYS:CA	1:B:784:LEU:HD23	2.30	0.60
1:D:798:SER:CB	1:D:804:GLY:C	2.70	0.60
1:B:778:GLY:O	1:B:782:GLU:HG3	2.01	0.59
1:C:830:LYS:HD3	1:C:832:ASP:OD1	2.02	0.59
1:C:772:GLY:C	1:C:774:ALA:H	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:800:GLU:O	1:D:800:GLU:CD	2.40	0.59
1:E:771:ARG:HG3	1:E:772:GLY:N	2.18	0.58
1:D:832:ASP:OD2	1:E:786:LYS:HA	2.02	0.58
1:E:753:ILE:HD13	1:E:824:ILE:HG13	1.86	0.58
1:D:750:CYS:SG	1:D:751:ASP:N	2.75	0.58
1:F:777:LEU:CG	1:F:781:LYS:HE3	2.33	0.57
1:F:776:THR:HG23	1:F:779:GLN:OE1	2.04	0.57
1:A:790:TYR:CD1	1:A:830:LYS:HA	2.39	0.57
1:B:751:ASP:O	1:B:752:SER:HB3	2.05	0.57
1:B:756:ALA:HB2	1:B:767:GLU:HG3	1.85	0.57
1:A:793:TYR:HB3	1:A:807:PHE:HB3	1.87	0.57
1:D:798:SER:O	1:D:799:ASP:C	2.44	0.57
1:D:752:SER:HB2	1:D:770:VAL:O	2.04	0.57
1:A:823:LYS:HB2	1:A:823:LYS:HZ3	1.69	0.57
1:E:753:ILE:CD1	1:E:824:ILE:HG13	2.35	0.56
1:F:753:ILE:HG13	1:F:773:ARG:HA	1.86	0.56
1:F:753:ILE:HD11	1:F:773:ARG:HD3	1.86	0.56
1:C:757:TYR:HA	1:C:826:GLY:O	2.05	0.56
1:A:755:VAL:HG22	1:A:824:ILE:HD12	1.86	0.56
1:E:816:ILE:HD13	1:E:816:ILE:N	2.21	0.56
1:C:820:PHE:CD2	1:C:821:GLU:HG3	2.42	0.55
1:C:786:LYS:HD2	1:C:786:LYS:N	2.21	0.55
1:B:757:TYR:CE2	1:B:759:PHE:HB2	2.41	0.55
1:E:792:TYR:CD1	1:E:792:TYR:N	2.73	0.55
1:B:796:LYS:HG2	1:B:797:VAL:N	2.22	0.55
1:D:796:LYS:HD2	1:D:808:GLU:HB2	1.88	0.55
1:A:777:LEU:HG	1:A:781:LYS:HD2	1.88	0.55
1:B:754:VAL:HB	1:B:823:LYS:HG2	1.88	0.55
1:B:772:GLY:O	1:B:774:ALA:N	2.40	0.55
1:B:795:LYS:HG2	1:B:805:VAL:HG11	1.88	0.55
1:D:803:CYS:N	1:D:804:GLY:CA	2.62	0.54
1:B:757:TYR:HE2	1:B:759:PHE:HB2	1.73	0.54
1:A:823:LYS:HD3	1:B:800:GLU:OE2	2.08	0.54
1:A:776:THR:HA	1:A:815:ALA:O	2.08	0.54
1:E:776:THR:HG22	1:E:816:ILE:HD12	1.91	0.53
1:C:781:LYS:HA	1:C:784:LEU:HD13	1.91	0.53
1:E:796:LYS:HD3	1:E:808:GLU:HB3	1.90	0.52
1:B:777:LEU:HD22	1:B:810:VAL:HG12	1.92	0.52
1:F:793:TYR:HB3	1:F:807:PHE:HB3	1.91	0.52
1:A:830:LYS:HE3	1:A:832:ASP:CG	2.29	0.52
1:B:748:PRO:N	1:B:749:PRO:HD3	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:759:PHE:O	1:C:760:CYS:C	2.48	0.52
1:F:807:PHE:CE2	1:F:827:LYS:HG3	2.45	0.52
1:A:795:LYS:HG2	1:A:805:VAL:HG11	1.91	0.51
1:F:769:LEU:N	1:F:769:LEU:HD12	2.26	0.51
1:E:793:TYR:HB3	1:E:807:PHE:HB3	1.93	0.51
1:B:802:ASP:O	1:B:804:GLY:N	2.44	0.51
1:E:805:VAL:HG12	1:E:806:VAL:N	2.25	0.51
1:F:805:VAL:HG12	1:F:806:VAL:N	2.25	0.51
1:C:784:LEU:N	1:C:784:LEU:HD12	2.25	0.51
1:A:809:GLU:CD	1:A:811:ARG:HH11	2.14	0.51
1:C:769:LEU:HD12	1:C:769:LEU:H	1.76	0.51
1:E:790:TYR:CD1	1:E:830:LYS:HA	2.45	0.50
1:D:791:ARG:HB3	1:D:809:GLU:OE2	2.11	0.50
1:B:757:TYR:HA	1:B:826:GLY:O	2.12	0.50
1:A:794:PHE:CE2	1:A:817:LEU:HD22	2.47	0.50
1:B:759:PHE:C	1:B:761:GLY:N	2.65	0.50
1:C:772:GLY:O	1:C:773:ARG:HG2	2.12	0.50
1:B:753:ILE:HG22	1:B:754:VAL:H	1.77	0.50
1:B:766:TYR:CD1	1:B:766:TYR:N	2.80	0.50
1:C:793:TYR:HA	1:C:808:GLU:O	2.11	0.50
1:D:775:VAL:HG13	1:D:779:GLN:HB2	1.94	0.49
1:D:791:ARG:HD3	1:E:785:THR:HG22	1.93	0.49
1:F:752:SER:HA	1:F:771:ARG:HA	1.93	0.49
1:E:796:LYS:HD3	1:E:808:GLU:CB	2.42	0.49
1:E:809:GLU:HB3	1:F:768:THR:HB	1.95	0.49
1:D:791:ARG:CD	1:E:785:THR:HG22	2.42	0.49
1:A:757:TYR:HA	1:A:826:GLY:O	2.13	0.48
1:E:821:GLU:O	1:E:822:GLU:HB2	2.12	0.48
1:B:772:GLY:C	1:B:774:ALA:H	2.16	0.48
1:C:795:LYS:HD2	1:C:825:ILE:CG2	2.37	0.48
1:C:794:PHE:CE2	1:C:817:LEU:HD22	2.47	0.48
1:B:789:SER:O	1:B:831:VAL:HG23	2.13	0.48
1:D:798:SER:HB2	1:D:804:GLY:C	2.34	0.48
1:E:791:ARG:HD3	1:E:809:GLU:OE2	2.14	0.48
1:E:778:GLY:HA2	1:E:813:ASP:OD1	2.14	0.48
1:E:796:LYS:HZ2	1:E:808:GLU:HG2	1.79	0.48
1:B:776:THR:HG22	1:B:816:ILE:HD13	1.95	0.47
1:C:764:ILE:N	1:C:764:ILE:HD12	2.28	0.47
1:D:757:TYR:HA	1:D:826:GLY:O	2.14	0.47
1:E:796:LYS:NZ	1:E:808:GLU:HG2	2.30	0.47
1:E:764:ILE:HD12	1:E:764:ILE:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:821:GLU:O	1:D:822:GLU:HB2	2.15	0.47
1:A:821:GLU:HB3	1:A:823:LYS:NZ	2.30	0.47
1:A:773:ARG:HG3	1:A:773:ARG:HH11	1.80	0.47
1:F:752:SER:HB2	1:F:770:VAL:O	2.15	0.46
1:C:754:VAL:HB	1:C:823:LYS:HG2	1.97	0.46
1:F:759:PHE:O	1:F:761:GLY:N	2.48	0.46
1:B:831:VAL:O	1:B:832:ASP:HB2	2.14	0.46
1:D:800:GLU:O	1:D:800:GLU:CG	2.63	0.46
1:C:781:LYS:HE3	1:C:813:ASP:OD1	2.15	0.46
1:B:755:VAL:HG22	1:B:824:ILE:HB	1.96	0.46
1:B:759:PHE:CD1	1:B:760:CYS:HB3	2.51	0.46
1:F:757:TYR:HA	1:F:826:GLY:O	2.17	0.45
1:A:794:PHE:CD2	1:A:817:LEU:HD22	2.51	0.45
1:E:796:LYS:HD2	1:E:818:PRO:CG	2.46	0.45
1:E:831:VAL:O	1:E:832:ASP:CB	2.65	0.45
1:E:778:GLY:HA3	1:E:813:ASP:HB3	1.98	0.45
1:D:793:TYR:HB3	1:D:807:PHE:HB3	1.98	0.44
1:A:814:GLU:OE1	1:A:814:GLU:HA	2.17	0.44
1:E:781:LYS:HD2	1:E:813:ASP:OD1	2.16	0.44
1:D:760:CYS:HB3	1:D:829:GLU:HA	1.98	0.44
1:C:792:TYR:N	1:C:792:TYR:CD1	2.84	0.44
1:C:792:TYR:O	1:C:809:GLU:HA	2.18	0.44
1:B:753:ILE:HG22	1:B:754:VAL:N	2.33	0.44
1:B:750:CYS:O	1:B:751:ASP:HB3	2.18	0.44
1:D:781:LYS:HA	1:D:784:LEU:HD23	1.99	0.44
1:F:786:LYS:N	1:F:786:LYS:HD2	2.32	0.44
1:C:772:GLY:O	1:C:774:ALA:N	2.46	0.44
1:C:821:GLU:O	1:C:822:GLU:HB2	2.18	0.44
1:C:769:LEU:HD12	1:C:769:LEU:N	2.32	0.44
1:E:756:ALA:HA	1:E:766:TYR:O	2.17	0.44
1:F:778:GLY:HA2	1:F:813:ASP:OD1	2.17	0.44
1:A:756:ALA:CB	1:B:801:PHE:HZ	2.30	0.44
1:A:807:PHE:CZ	1:A:827:LYS:HD2	2.53	0.44
1:E:777:LEU:CA	1:E:817:LEU:HD21	2.48	0.43
1:A:821:GLU:HB3	1:A:823:LYS:HZ1	1.83	0.43
1:E:773:ARG:HA	1:E:773:ARG:HE	1.83	0.43
1:D:796:LYS:HZ3	1:D:808:GLU:CD	2.22	0.43
1:C:793:TYR:HB3	1:C:807:PHE:HB3	2.00	0.43
1:E:757:TYR:HA	1:E:826:GLY:O	2.18	0.43
1:F:760:CYS:HG	1:F:790:TYR:HE1	1.66	0.43
1:E:753:ILE:HG12	1:E:754:VAL:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:VAL:HG13	1:A:823:LYS:O	2.19	0.43
1:E:807:PHE:CE2	1:E:827:LYS:HG3	2.54	0.43
1:E:801:PHE:CD2	1:E:806:VAL:HG11	2.54	0.43
1:B:798:SER:CB	1:B:801:PHE:HB2	2.44	0.43
1:D:799:ASP:O	1:D:800:GLU:HB3	2.19	0.43
1:B:776:THR:HA	1:B:815:ALA:O	2.19	0.43
1:C:753:ILE:HG22	1:C:754:VAL:N	2.34	0.42
1:B:821:GLU:O	1:B:822:GLU:HB2	2.19	0.42
1:C:776:THR:HA	1:C:815:ALA:O	2.19	0.42
1:F:781:LYS:HA	1:F:784:LEU:HD13	2.00	0.42
1:E:801:PHE:CE2	1:E:806:VAL:HG11	2.54	0.42
1:C:778:GLY:O	1:C:782:GLU:HG3	2.19	0.42
1:F:819:VAL:HG13	1:F:823:LYS:O	2.18	0.42
1:C:796:LYS:NZ	1:C:808:GLU:OE1	2.52	0.42
1:A:761:GLY:O	1:A:762:GLU:C	2.57	0.42
1:F:756:ALA:HA	1:F:766:TYR:O	2.20	0.42
1:E:777:LEU:CG	1:E:781:LYS:HE3	2.49	0.42
1:B:792:TYR:O	1:B:809:GLU:HG2	2.18	0.42
1:E:781:LYS:HG2	1:E:792:TYR:CE2	2.54	0.42
1:F:793:TYR:HA	1:F:808:GLU:O	2.19	0.42
1:D:759:PHE:O	1:D:760:CYS:C	2.57	0.42
1:A:777:LEU:O	1:A:781:LYS:HG3	2.20	0.42
1:C:772:GLY:C	1:C:774:ALA:N	2.72	0.42
1:F:775:VAL:HG13	1:F:779:GLN:HB2	2.02	0.42
1:C:757:TYR:HB3	1:C:780:PHE:HZ	1.85	0.42
1:C:763:PRO:HG2	1:C:764:ILE:CD1	2.34	0.42
1:A:823:LYS:NZ	1:A:823:LYS:HB2	2.35	0.42
1:F:757:TYR:HE1	1:F:766:TYR:CB	2.30	0.42
1:A:790:TYR:HD1	1:A:830:LYS:HA	1.81	0.42
1:B:756:ALA:O	1:B:825:ILE:HA	2.20	0.42
1:E:792:TYR:HD1	1:E:792:TYR:N	2.17	0.42
1:E:776:THR:HG22	1:E:816:ILE:CD1	2.49	0.42
1:F:777:LEU:CD2	1:F:781:LYS:HE3	2.50	0.41
1:F:805:VAL:CG1	1:F:806:VAL:N	2.82	0.41
1:C:759:PHE:O	1:C:761:GLY:N	2.52	0.41
1:D:796:LYS:NZ	1:D:808:GLU:CD	2.73	0.41
1:C:801:PHE:HE2	1:D:767:GLU:OE1	2.03	0.41
1:B:784:LEU:N	1:B:784:LEU:HD22	2.36	0.41
1:A:776:THR:N	1:A:779:GLN:OE1	2.47	0.41
1:C:777:LEU:CD2	1:C:810:VAL:HG12	2.47	0.41
1:D:819:VAL:CG1	1:D:820:PHE:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:LYS:O	1:A:830:LYS:HG3	2.20	0.40
1:C:805:VAL:HG13	1:C:820:PHE:CE1	2.56	0.40
1:C:785:THR:HB	1:C:786:LYS:CD	2.48	0.40
1:B:756:ALA:HA	1:B:766:TYR:O	2.22	0.40
1:B:792:TYR:O	1:B:809:GLU:HA	2.22	0.40
1:F:758:TYR:CD2	1:F:765:PRO:HB3	2.56	0.40

There are no symmetry-related clashes.

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	81/85 (95%)	73 (90%)	6 (7%)	2 (2%)	7 41
1	B	83/85 (98%)	70 (84%)	8 (10%)	5 (6%)	2 16
1	C	81/85 (95%)	75 (93%)	3 (4%)	3 (4%)	4 29
1	D	81/85 (95%)	67 (83%)	9 (11%)	5 (6%)	2 14
1	E	78/85 (92%)	70 (90%)	6 (8%)	2 (3%)	7 40
1	F	81/85 (95%)	74 (91%)	4 (5%)	3 (4%)	4 29
All	All	485/510 (95%)	429 (88%)	36 (7%)	20 (4%)	3 27

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	760	CYS
1	B	749	PRO
1	B	752	SER
1	B	803	CYS
1	C	773	ARG
1	D	799	ASP

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Mol	Chain	Res	Type
1	E	773	ARG
1	F	760	CYS
1	B	760	CYS
1	C	760	CYS
1	D	751	ASP
1	D	760	CYS
1	D	763	PRO
1	A	762	GLU
1	B	751	ASP
1	D	801	PHE
1	E	802	ASP
1	F	772	GLY
1	F	774	ALA
1	C	772	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	74/76 (97%)	68 (92%)	6 (8%)	15 51
1	B	76/76 (100%)	66 (87%)	10 (13%)	5 23
1	C	74/76 (97%)	70 (95%)	4 (5%)	27 68
1	D	74/76 (97%)	69 (93%)	5 (7%)	20 59
1	E	71/76 (93%)	62 (87%)	9 (13%)	5 25
1	F	74/76 (97%)	68 (92%)	6 (8%)	15 51
All	All	443/456 (97%)	403 (91%)	40 (9%)	12 43

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	768	THR
1	A	805	VAL
1	A	813	ASP
1	A	821	GLU

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Mol	Chain	Res	Type
1	A	827	LYS
1	A	832	ASP
1	B	749	PRO
1	B	768	THR
1	B	773	ARG
1	B	785	THR
1	B	786	LYS
1	B	789	SER
1	B	798	SER
1	B	800	GLU
1	B	803	CYS
1	B	809	GLU
1	C	785	THR
1	C	791	ARG
1	C	799	ASP
1	C	811	ARG
1	D	751	ASP
1	D	799	ASP
1	D	801	PHE
1	D	811	ARG
1	D	827	LYS
1	E	770	VAL
1	E	773	ARG
1	E	787	LYS
1	E	789	SER
1	E	792	TYR
1	E	795	LYS
1	E	808	GLU
1	E	811	ARG
1	E	827	LYS
1	F	757	TYR
1	F	768	THR
1	F	791	ARG
1	F	811	ARG
1	F	813	ASP
1	F	832	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	83/85 (97%)	-0.07	0 100 100	28, 50, 105, 133	0
1	B	85/85 (100%)	-0.16	0 100 100	33, 58, 118, 157	0
1	C	83/85 (97%)	-0.28	0 100 100	23, 55, 104, 148	0
1	D	83/85 (97%)	0.32	5 (6%) 25 14	37, 74, 137, 170	0
1	E	80/85 (94%)	0.04	4 (5%) 32 19	47, 92, 140, 158	0
1	F	83/85 (97%)	0.29	4 (4%) 34 21	44, 81, 136, 147	0
All	All	497/510 (97%)	0.02	13 (2%) 59 45	23, 69, 133, 170	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	825	ILE	4.3
1	F	832	ASP	3.2
1	D	802	ASP	3.1
1	D	803	CYS	3.0
1	D	796	LYS	2.9
1	D	771	ARG	2.9
1	E	799	ASP	2.7
1	E	753	ILE	2.7
1	F	828	VAL	2.5
1	E	801	PHE	2.5
1	D	824	ILE	2.4
1	E	754	VAL	2.2
1	F	831	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	HG	B	603	1/1	0.99	0.17	-0.68	76,76,76,76	0
2	HG	A	601	1/1	0.98	0.17	-	114,114,114,114	1
2	HG	B	604	1/1	0.97	0.15	-	81,81,81,81	0
2	HG	D	607	1/1	0.99	0.17	-	96,96,96,96	0
2	HG	F	610	1/1	0.96	0.11	-	100,100,100,100	1
2	HG	E	608	1/1	0.98	0.16	-	95,95,95,95	0
2	HG	C	605	1/1	0.95	0.17	-	113,113,113,113	1
2	HG	A	602	1/1	0.98	0.16	-	81,81,81,81	0
2	HG	F	609	1/1	0.97	0.13	-	88,88,88,88	0
2	HG	C	606	1/1	0.97	0.17	-	97,97,97,97	0

6.5 Other polymers (i)

There are no such residues in this entry.