Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 11:28 PM GMT

PDB ID	:	1XCG
Title	:	Crystal Structure of Human RhoA in complex with DH/PH fragment of PDZRHOGEF
Authors	:	Derewenda, U.; Oleksy, A.; Stevenson, A.S.; Korczynska, J.; Dauter, Z.; Somlyo, A.P.; Otlewski, J.; Somlyo, A.V.; Derewenda, Z.S.
Deposited on	:	2004-09-01
Resolution	:	2.50 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:

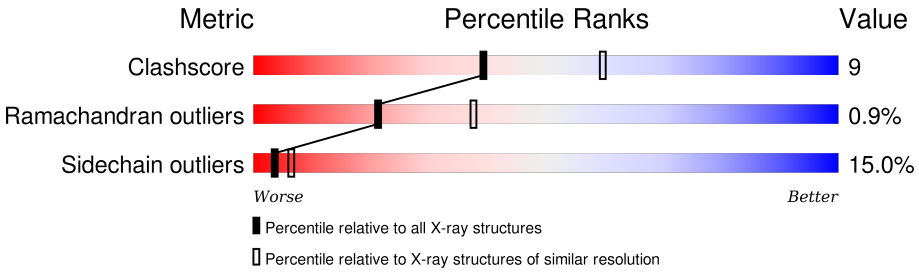
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	368	67% 25%
1	E	368	64% 31%
2	B	178	69% 29%
2	F	178	77% 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8750 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 Rho guanine nucleotide exchange factor 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2906	1837	519	535	15			
1	E	358	Total	C	N	O	S	0	0	0
			2931	1852	525	539	15			

- Molecule 2 is a protein called Transforming protein RhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	0	0
			1411	889	240	272	10			
2	F	178	Total	C	N	O	S	0	0	0
			1411	889	240	272	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	25	ASN	PHE	ENGINEERED	UNP P61586
F	25	ASN	PHE	ENGINEERED	UNP P61586

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	17	Total	O	0	0
			17	17		
3	E	30	Total	O	0	0
			30	30		
3	F	14	Total	O	0	0
			14	14		

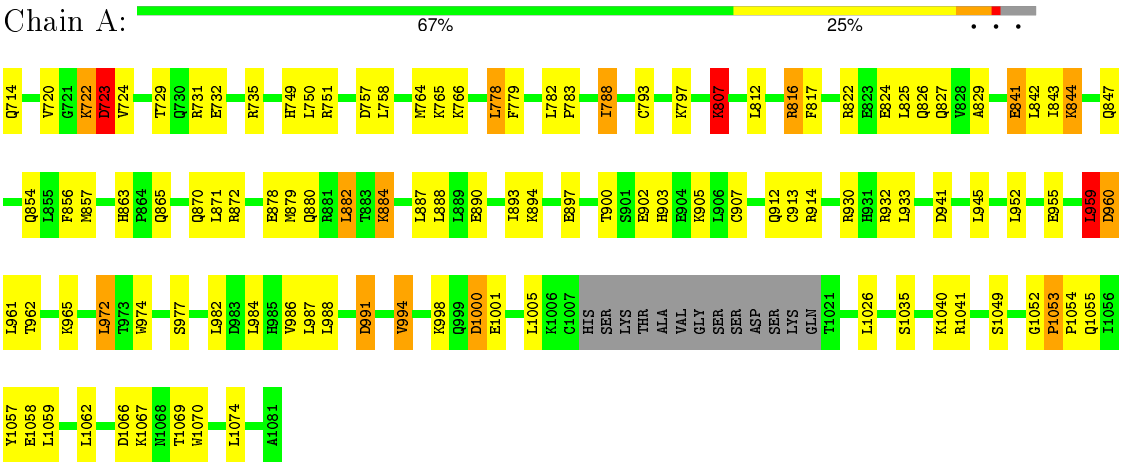
3 Residue-property plots (i)

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.

Note EDS was not executed.

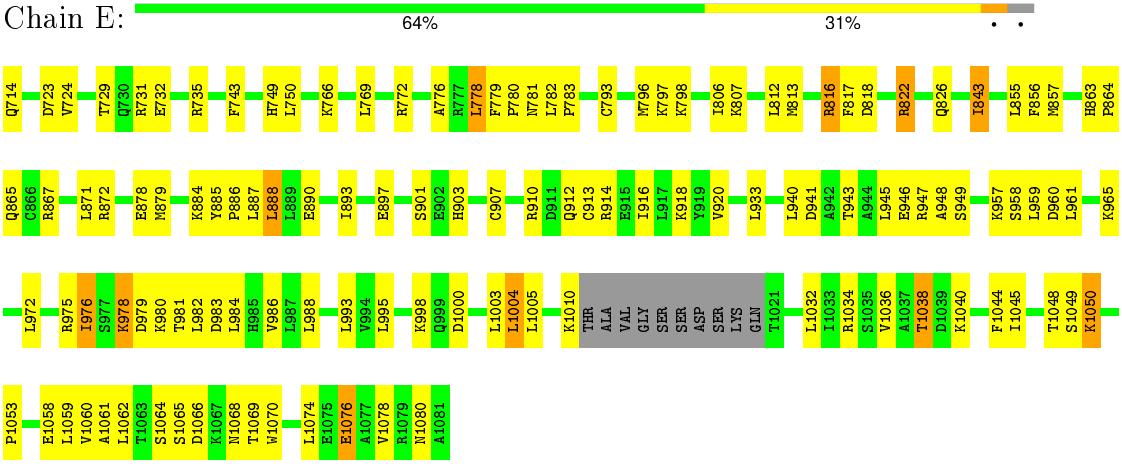
- Molecule 1: Rho guanine nucleotide exchange factor 11

Chain A:



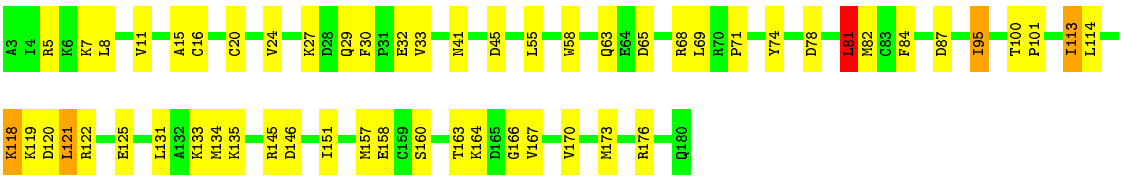
- Molecule 1: Rho guanine nucleotide exchange factor 11

Chain E:

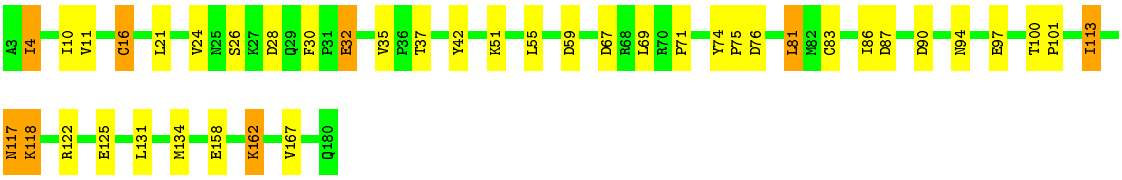


- Molecule 2: Transforming protein RhoA

Chain B:



• Molecule 2: Transforming protein RhoA



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.24Å 118.78Å 90.13Å 90.00° 114.34° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50	Depositor
% Data completeness (in resolution range)	96.8 (25.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.224 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8750	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

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	0.50	0/2950	0.74	7/3970 (0.2%)
1	E	0.51	0/2976	0.78	6/4004 (0.1%)
2	B	0.56	0/1438	0.82	6/1944 (0.3%)
2	F	0.56	0/1438	0.81	6/1944 (0.3%)
All	All	0.52	0/8802	0.78	25/11862 (0.2%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	65	ASP	CB-CG-OD2	7.30	124.87	118.30
1	E	723	ASP	CB-CG-OD2	7.13	124.72	118.30
2	F	90	ASP	CB-CG-OD2	6.61	124.25	118.30
2	B	81	LEU	CA-CB-CG	6.03	129.16	115.30
1	A	1000	ASP	CB-CG-OD2	6.02	123.72	118.30
1	E	1049	SER	O-C-N	5.82	132.01	122.70
2	F	87	ASP	CB-CG-OD2	5.81	123.53	118.30
2	B	78	ASP	CB-CG-OD2	5.75	123.47	118.30
2	F	76	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	723	ASP	CB-CG-OD2	5.61	123.35	118.30
2	B	45	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	991	ASP	CB-CG-OD2	5.43	123.19	118.30
1	E	818	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	757	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	941	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	960	ASP	CB-CG-OD2	5.24	123.02	118.30
2	F	59	ASP	CB-CG-OD2	5.20	122.98	118.30
1	E	1053	PRO	O-C-N	5.20	130.97	121.10
1	E	960	ASP	CB-CG-OD2	5.16	122.94	118.30
2	B	146	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	1066	ASP	CB-CG-OD2	5.13	122.92	118.30
2	F	81	LEU	CA-CB-CG	5.11	127.06	115.30
2	F	67	ASP	CB-CG-OD2	5.11	122.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	735	ARG	NE-CZ-NH2	-5.11	117.74	120.30
2	B	120	ASP	CB-CG-OD2	5.05	122.84	118.30

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	2906	0	2997	55	0
1	E	2931	0	3022	62	0
2	B	1411	0	1402	28	0
2	F	1411	0	1402	20	0
3	A	30	0	0	4	0
3	B	17	0	0	0	0
3	E	30	0	0	2	0
3	F	14	0	0	1	0
All	All	8750	0	8823	156	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 9.

All (156) 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:879:MET:HE3	2:B:69:LEU:HB3	1.48	0.94
1:E:822:ARG:HH11	1:E:826:GLN:HE22	1.05	0.93
1:A:879:MET:CE	2:B:69:LEU:HB3	2.03	0.88
1:E:1061:ALA:HB1	1:E:1066:ASP:HB3	1.56	0.86
1:A:822:ARG:HH11	1:A:912:GLN:HE22	1.22	0.86
1:A:959:LEU:HD12	1:A:1005:LEU:HD11	1.58	0.85
2:B:122:ARG:NH2	2:B:158:GLU:OE1	2.14	0.79
2:B:24:VAL:HG12	2:B:30:PHE:HA	1.67	0.77
1:E:863:HIS:HD2	1:E:865:GLN:H	1.32	0.76
1:A:778:LEU:HD13	1:A:779:PHE:CE2	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:PRO:O	1:A:1055:GLN:N	2.20	0.75
1:A:816:ARG:O	1:A:816:ARG:HD3	1.88	0.73
1:A:788:ILE:HD11	1:A:824:GLU:HG2	1.70	0.72
2:F:117:ASN:ND2	2:F:118:LYS:H	1.88	0.72
2:B:173:MET:HA	2:B:176:ARG:NH1	2.04	0.72
1:E:822:ARG:HE	1:E:912:GLN:NE2	1.87	0.71
2:B:163:THR:O	2:B:164:LYS:HB2	1.91	0.69
1:A:822:ARG:HH11	1:A:912:GLN:NE2	1.91	0.68
1:E:816:ARG:HD3	1:E:816:ARG:O	1.93	0.68
1:A:729:THR:HG23	1:A:732:GLU:H	1.60	0.67
2:B:157:MET:HG2	2:B:170:VAL:HG22	1.76	0.67
1:E:822:ARG:HH11	1:E:826:GLN:NE2	1.86	0.67
2:B:82:MET:SD	2:B:100:THR:HG22	2.34	0.66
1:E:872:ARG:HD3	3:E:37:HOH:O	1.95	0.66
1:E:863:HIS:CD2	1:E:865:GLN:HB2	2.30	0.66
1:E:1040:LYS:HD3	1:E:1064:SER:HB3	1.79	0.64
1:A:841:GLU:OE2	1:A:844:LYS:HE3	1.97	0.64
2:F:81:LEU:HD23	2:F:113:ILE:HG12	1.78	0.64
1:E:893:ILE:HG23	1:E:903:HIS:NE2	2.12	0.64
1:E:822:ARG:NH1	1:E:826:GLN:HE22	1.88	0.63
1:A:816:ARG:HD2	1:A:825:LEU:HD22	1.80	0.63
2:F:117:ASN:HD22	2:F:118:LYS:H	1.43	0.63
1:A:856:PHE:CD1	1:A:857:MET:HE2	2.34	0.63
1:E:856:PHE:CE2	1:E:857:MET:HE3	2.35	0.62
1:A:986:VAL:HG23	1:A:1070:TRP:CH2	2.35	0.62
1:A:749:HIS:HE1	1:A:878:GLU:OE1	1.84	0.61
1:A:972:LEU:HD22	1:A:986:VAL:HG21	1.82	0.61
1:E:879:MET:HE1	3:F:182:HOH:O	2.00	0.61
1:E:976:ILE:HD11	1:E:982:LEU:HG	1.81	0.61
2:B:84:PHE:HB3	2:B:95:ILE:CD1	2.31	0.60
2:F:81:LEU:CD2	2:F:113:ILE:HG12	2.32	0.60
1:E:822:ARG:HD2	1:E:826:GLN:NE2	2.17	0.60
2:B:122:ARG:HH22	2:B:158:GLU:CD	2.05	0.59
2:B:81:LEU:HD23	2:B:113:ILE:HG12	1.85	0.59
1:E:1045:ILE:HD12	1:E:1059:LEU:HD12	1.85	0.59
2:F:122:ARG:NH2	2:F:158:GLU:OE1	2.37	0.57
1:A:863:HIS:HD2	1:A:865:GLN:H	1.53	0.57
2:B:95:ILE:O	2:B:100:THR:HG23	2.05	0.57
1:A:893:ILE:HG23	1:A:903:HIS:NE2	2.21	0.56
1:A:879:MET:HE2	2:B:69:LEU:HB3	1.86	0.56
1:E:856:PHE:CE2	1:E:857:MET:CE	2.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1070:TRP:O	1:E:1074:LEU:HB2	2.04	0.56
1:E:856:PHE:HE2	1:E:857:MET:HE3	1.69	0.56
2:F:24:VAL:HG23	2:F:167:VAL:HG11	1.87	0.56
2:B:84:PHE:HB3	2:B:95:ILE:HD13	1.88	0.56
1:E:729:THR:HG23	1:E:732:GLU:H	1.71	0.55
1:E:856:PHE:HE2	1:E:857:MET:CE	2.19	0.55
1:A:1026:LEU:HD21	1:A:1057:TYR:CE1	2.42	0.55
1:E:863:HIS:CD2	1:E:865:GLN:H	2.19	0.55
2:F:10:ILE:HD11	2:F:83:CYS:SG	2.47	0.55
1:E:976:ILE:HD12	1:E:980:LYS:HG2	1.89	0.54
1:E:1045:ILE:HD11	1:E:1074:LEU:HD21	1.89	0.54
1:E:743:PHE:CE1	1:E:796:MET:HG2	2.43	0.54
2:B:81:LEU:CD2	2:B:113:ILE:HG12	2.37	0.53
2:B:71:PRO:HA	2:B:74:TYR:CD2	2.44	0.53
1:A:903:HIS:CE1	1:A:907:CYS:SG	3.02	0.53
1:A:749:HIS:CE1	1:A:878:GLU:OE1	2.62	0.53
1:A:822:ARG:HD3	1:A:912:GLN:NE2	2.25	0.52
2:B:100:THR:HG21	2:B:151:ILE:HG21	1.92	0.52
2:B:7:LYS:HE3	2:B:58:TRP:CE2	2.44	0.52
1:A:722:LYS:HG3	1:A:723:ASP:N	2.23	0.52
1:E:943:THR:HA	1:E:946:GLU:HG3	1.92	0.52
1:E:781:ASN:N	1:E:781:ASN:OD1	2.43	0.51
1:E:822:ARG:HD3	1:E:916:ILE:HG13	1.90	0.51
2:B:100:THR:N	2:B:101:PRO:HD2	2.26	0.50
1:A:856:PHE:HD1	1:A:857:MET:HE2	1.74	0.50
1:A:945:LEU:HD22	1:A:1005:LEU:HB3	1.92	0.50
1:E:984:LEU:HD13	1:E:995:LEU:HB3	1.94	0.50
1:A:986:VAL:HG23	1:A:1070:TRP:HH2	1.77	0.49
1:A:829:ALA:HB1	1:A:882:LEU:HD21	1.93	0.49
2:F:4:ILE:HG13	2:F:4:ILE:O	2.11	0.49
1:A:1058:GLU:OE1	1:E:1038:THR:HB	2.12	0.49
1:E:986:VAL:HG22	1:E:1070:TRP:CH2	2.47	0.49
1:A:879:MET:HE1	2:B:63:GLN:HG2	1.95	0.49
1:E:941:ASP:HB3	1:E:1004:LEU:HB3	1.95	0.49
1:A:933:LEU:HD22	1:A:961:LEU:HB3	1.95	0.48
1:A:822:ARG:HE	1:A:826:GLN:NE2	2.11	0.48
1:E:1034:ARG:HB2	1:E:1044:PHE:HB2	1.95	0.48
1:E:888:LEU:HD13	2:F:37:THR:HG21	1.96	0.48
1:A:991:ASP:N	1:A:991:ASP:OD1	2.47	0.48
1:E:945:LEU:HA	1:E:948:ALA:HB2	1.96	0.48
1:A:972:LEU:HD23	1:A:1059:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:MET:HE3	1:A:857:MET:HE1	1.96	0.48
2:B:157:MET:HG2	2:B:170:VAL:CG2	2.42	0.47
1:E:903:HIS:CE1	1:E:907:CYS:SG	3.07	0.47
1:A:863:HIS:CD2	1:A:865:GLN:H	2.32	0.47
2:F:16:CYS:O	2:F:16:CYS:SG	2.72	0.47
2:F:117:ASN:ND2	2:F:118:LYS:N	2.59	0.47
1:E:1074:LEU:O	1:E:1078:VAL:HG12	2.15	0.46
1:A:974:TRP:HB2	1:A:984:LEU:HD11	1.97	0.46
1:A:822:ARG:HD3	1:A:912:GLN:HE21	1.81	0.46
1:E:1040:LYS:O	1:E:1064:SER:HA	2.15	0.46
1:E:910:ARG:HD2	1:E:914:ARG:NH2	2.30	0.46
2:B:166:GLY:O	2:B:170:VAL:HG23	2.16	0.46
1:A:987:LEU:HB2	1:A:994:VAL:HG22	1.98	0.45
2:F:74:TYR:N	2:F:75:PRO:CD	2.79	0.45
1:A:817:PHE:O	1:A:912:GLN:HB3	2.16	0.45
1:A:880:GLN:NE2	3:A:77:HOH:O	2.50	0.45
1:A:735:ARG:NH2	1:A:807:LYS:O	2.37	0.45
1:E:778:LEU:HD13	1:E:779:PHE:CE2	2.51	0.45
1:E:749:HIS:HE1	1:E:878:GLU:OE1	1.98	0.45
1:E:933:LEU:HD22	1:E:961:LEU:HB3	1.98	0.45
1:E:822:ARG:HE	1:E:912:GLN:HE22	1.63	0.45
1:E:976:ILE:H	1:E:976:ILE:HG13	1.34	0.45
1:E:975:ARG:CZ	1:E:1060:VAL:HG21	2.47	0.45
1:A:974:TRP:HB2	1:A:984:LEU:CD1	2.47	0.44
1:A:827:GLN:HG3	3:A:67:HOH:O	2.17	0.44
1:E:978:LYS:O	1:E:979:ASP:HB2	2.17	0.44
1:A:932:ARG:HH12	2:B:68:ARG:NH2	2.15	0.44
2:B:8:LEU:HD11	2:B:81:LEU:HG	2.00	0.44
1:A:847:GLN:O	1:A:854:GLN:HB2	2.18	0.44
1:A:884:LYS:HA	1:A:884:LYS:HD2	1.73	0.44
1:E:772:ARG:HD3	1:E:772:ARG:HA	1.85	0.44
2:F:24:VAL:HG12	2:F:30:PHE:HA	1.99	0.44
2:F:71:PRO:HA	2:F:74:TYR:CD2	2.53	0.44
1:E:776:ALA:O	1:E:780:PRO:HA	2.18	0.43
1:A:900:THR:HG22	1:A:902:GLU:H	1.83	0.43
1:E:863:HIS:HD2	1:E:865:GLN:HB2	1.78	0.43
1:E:749:HIS:CE1	1:E:878:GLU:OE1	2.72	0.43
1:A:913:CYS:HB3	3:A:36:HOH:O	2.19	0.43
2:F:24:VAL:HG11	2:F:30:PHE:HD1	1.84	0.42
1:E:975:ARG:HB2	1:E:1058:GLU:HG2	2.00	0.42
1:E:817:PHE:CD2	1:E:913:CYS:SG	3.12	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:100:THR:N	2:F:101:PRO:HD2	2.34	0.42
1:E:812:LEU:HD23	1:E:813:MET:CE	2.49	0.42
1:A:890:GLU:OE1	1:A:914:ARG:NH2	2.53	0.42
1:E:843:ILE:HD12	1:E:843:ILE:HA	1.75	0.42
2:F:32:GLU:HG3	2:F:32:GLU:H	1.57	0.42
2:B:95:ILE:HG12	2:B:114:LEU:HD11	2.01	0.42
1:A:782:LEU:N	1:A:783:PRO:CD	2.82	0.42
2:B:118:LYS:HB3	2:B:121:LEU:HD22	2.02	0.42
1:E:1066:ASP:O	1:E:1069:THR:HB	2.20	0.41
1:E:1076:GLU:HG3	1:E:1080:ASN:HD21	1.85	0.41
1:E:782:LEU:N	1:E:783:PRO:CD	2.84	0.41
1:E:885:TYR:HB2	1:E:886:PRO:HD3	2.02	0.41
1:E:920:VAL:HG12	2:F:69:LEU:HD21	2.01	0.41
2:B:24:VAL:HG23	2:B:167:VAL:HG11	2.03	0.41
1:A:872:ARG:HD3	3:A:26:HOH:O	2.19	0.41
2:F:26:SER:HB3	2:F:42:TYR:CE2	2.54	0.41
1:A:870:GLN:HG3	2:B:5:ARG:NH1	2.36	0.41
1:A:986:VAL:CG2	1:A:1070:TRP:CH2	3.03	0.41
1:E:993:LEU:CD2	1:E:1045:ILE:HD13	2.50	0.41
1:A:856:PHE:CE1	1:A:857:MET:CE	3.04	0.40
1:E:867:ARG:NH1	3:E:84:HOH:O	2.41	0.40
2:F:94:ASN:HA	2:F:97:GLU:HB3	2.03	0.40
1:E:863:HIS:HD2	1:E:865:GLN:N	2.08	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	351/368 (95%)	333 (95%)	11 (3%)	7 (2%)	9 15
1	E	354/368 (96%)	335 (95%)	18 (5%)	1 (0%)	46 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	176/178 (99%)	165 (94%)	10 (6%)	1 (1%)	30 50
2	F	176/178 (99%)	169 (96%)	6 (3%)	1 (1%)	30 50
All	All	1057/1092 (97%)	1002 (95%)	45 (4%)	10 (1%)	21 37

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1054	PRO
1	A	1000	ASP
1	A	1052	GLY
1	A	807	LYS
1	A	959	LEU
1	A	1053	PRO
1	A	960	ASP
2	B	15	ALA
1	E	1050	LYS
2	F	162	LYS

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	323/334 (97%)	272 (84%)	51 (16%)	3 5
1	E	326/334 (98%)	273 (84%)	53 (16%)	3 5
2	B	156/156 (100%)	133 (85%)	23 (15%)	4 7
2	F	156/156 (100%)	139 (89%)	17 (11%)	8 15
All	All	961/980 (98%)	817 (85%)	144 (15%)	3 6

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	714	GLN
1	A	720	VAL

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Mol	Chain	Res	Type
1	A	722	LYS
1	A	723	ASP
1	A	724	VAL
1	A	731	ARG
1	A	750	LEU
1	A	751	ARG
1	A	758	LEU
1	A	765	LYS
1	A	766	LYS
1	A	778	LEU
1	A	788	ILE
1	A	793	CYS
1	A	797	LYS
1	A	807	LYS
1	A	812	LEU
1	A	816	ARG
1	A	841	GLU
1	A	842	LEU
1	A	843	ILE
1	A	844	LYS
1	A	871	LEU
1	A	882	LEU
1	A	884	LYS
1	A	887	LEU
1	A	888	LEU
1	A	894	LYS
1	A	897	GLU
1	A	905	LYS
1	A	930	ARG
1	A	952	LEU
1	A	955	GLU
1	A	959	LEU
1	A	962	THR
1	A	965	LYS
1	A	972	LEU
1	A	977	SER
1	A	982	LEU
1	A	988	LEU
1	A	994	VAL
1	A	998	LYS
1	A	1001	GLU
1	A	1035	SER

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Mol	Chain	Res	Type
1	A	1040	LYS
1	A	1041	ARG
1	A	1049	SER
1	A	1062	LEU
1	A	1067	LYS
1	A	1069	THR
1	A	1074	LEU
2	B	11	VAL
2	B	16	CYS
2	B	20	CYS
2	B	27	LYS
2	B	29	GLN
2	B	32	GLU
2	B	33	VAL
2	B	41	ASN
2	B	55	LEU
2	B	81	LEU
2	B	87	ASP
2	B	95	ILE
2	B	113	ILE
2	B	118	LYS
2	B	119	LYS
2	B	121	LEU
2	B	125	GLU
2	B	131	LEU
2	B	133	LYS
2	B	134	MET
2	B	135	LYS
2	B	145	ARG
2	B	160	SER
1	E	714	GLN
1	E	724	VAL
1	E	731	ARG
1	E	750	LEU
1	E	766	LYS
1	E	769	LEU
1	E	778	LEU
1	E	793	CYS
1	E	797	LYS
1	E	798	LYS
1	E	806	ILE
1	E	807	LYS

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Mol	Chain	Res	Type
1	E	816	ARG
1	E	822	ARG
1	E	843	ILE
1	E	855	LEU
1	E	864	PRO
1	E	871	LEU
1	E	884	LYS
1	E	887	LEU
1	E	888	LEU
1	E	890	GLU
1	E	897	GLU
1	E	901	SER
1	E	918	LYS
1	E	940	LEU
1	E	947	ARG
1	E	949	SER
1	E	957	LYS
1	E	958	SER
1	E	959	LEU
1	E	965	LYS
1	E	972	LEU
1	E	976	ILE
1	E	978	LYS
1	E	981	THR
1	E	983	ASP
1	E	988	LEU
1	E	998	LYS
1	E	1000	ASP
1	E	1003	LEU
1	E	1004	LEU
1	E	1005	LEU
1	E	1010	LYS
1	E	1032	LEU
1	E	1036	VAL
1	E	1038	THR
1	E	1048	THR
1	E	1050	LYS
1	E	1062	LEU
1	E	1065	SER
1	E	1068	ASN
1	E	1076	GLU
2	F	4	ILE

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Mol	Chain	Res	Type
2	F	11	VAL
2	F	16	CYS
2	F	21	LEU
2	F	28	ASP
2	F	32	GLU
2	F	35	VAL
2	F	51	LYS
2	F	55	LEU
2	F	86	ILE
2	F	113	ILE
2	F	117	ASN
2	F	118	LYS
2	F	125	GLU
2	F	131	LEU
2	F	134	MET
2	F	162	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	749	HIS
1	A	826	GLN
1	A	880	GLN
1	A	912	GLN
2	B	29	GLN
2	B	41	ASN
2	B	105	HIS
1	E	714	GLN
1	E	715	ASN
1	E	749	HIS
1	E	826	GLN
1	E	854	GLN
1	E	863	HIS
1	E	880	GLN
1	E	895	HIS
1	E	912	GLN
1	E	985	HIS
1	E	1080	ASN
2	F	41	ASN
2	F	117	ASN

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

There are no ligands in this entry.

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.