Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:57 AM GMT

PDB ID	:	2JIT
Title	:	CRYSTAL STRUCTURE OF EGFR KINASE DOMAIN T790M MUTATION
Authors	:	Yun, C.-H.; Mengwasser, K.E.; Toms, A.V.; Woo, M.S.; Greulich, H.; Wong, K.-K.; Meyerson, M.; Eck, M.J.
Deposited on	:	2007-07-01
Resolution	:	3.10 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:

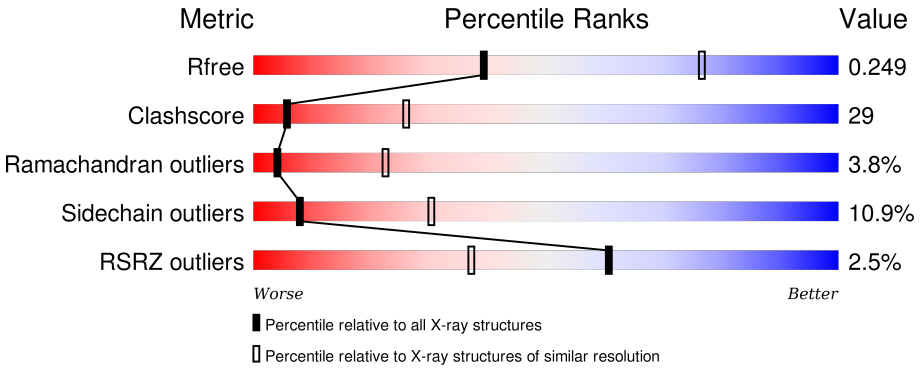
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	327	2% 49% 34% 7% • 9%
1	B	327	3% 46% 41% 7% • 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4886 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 EPIDERMAL GROWTH FACTOR RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2363	1519	400	428	16			
1	B	312	Total	C	N	O	S	0	0	0
			2450	1578	416	439	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	790	MET	THR	ENGINEERED MUTATION	UNP P00533
B	790	MET	THR	ENGINEERED MUTATION	UNP P00533

- Molecule 2 is water.

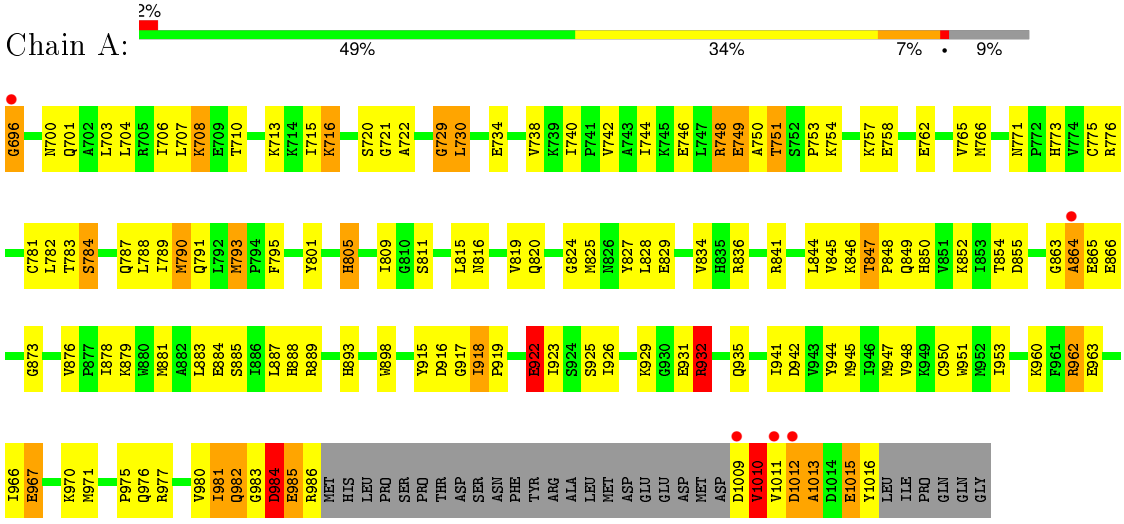
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	25	Total	O	0	0
			25	25		
2	B	48	Total	O	0	0
			48	48		

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.

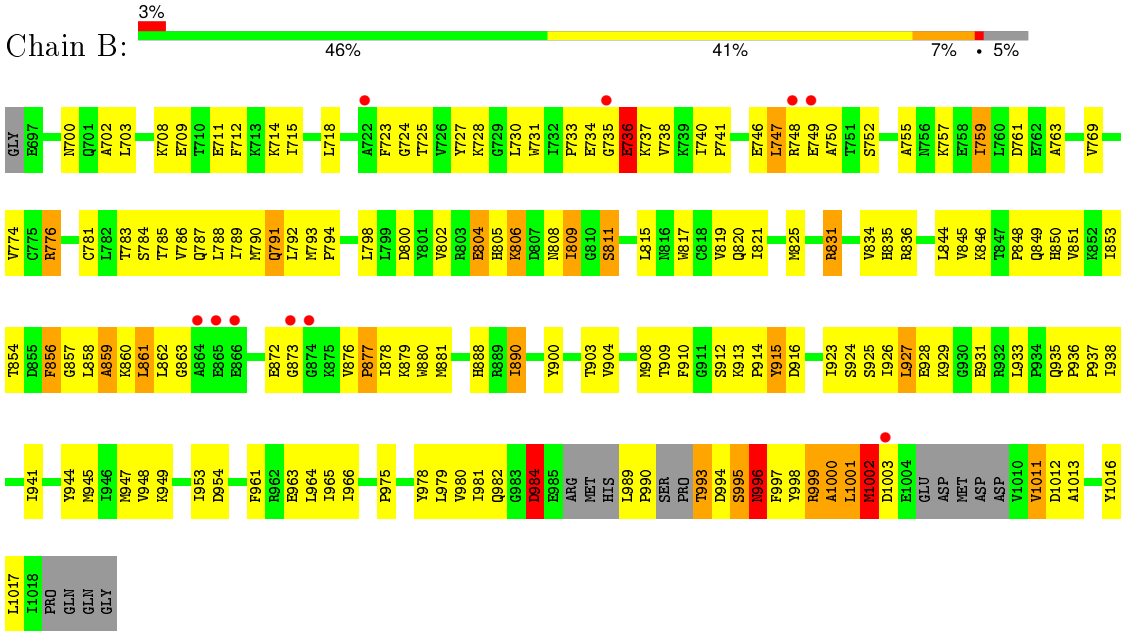
- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR

Chain A:



- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.89Å 90.30Å 164.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.42 – 3.10 24.42 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (24.42-3.10) 99.2 (24.42-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.73 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.3.0026	Depositor
R, R_{free}	0.207 , 0.249 0.205 , 0.249	Depositor DCC
R_{free} test set	759 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	58.4	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 15027 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4886	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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

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	0.74	4/2413 (0.2%)	0.68	1/3266 (0.0%)
1	B	0.83	8/2502 (0.3%)	0.73	3/3388 (0.1%)
All	All	0.78	12/4915 (0.2%)	0.71	4/6654 (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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	696	GLY	N-CA	7.36	1.57	1.46
1	B	873	GLY	C-O	7.09	1.34	1.23
1	B	733	PRO	C-O	6.27	1.35	1.23
1	B	877	PRO	N-CD	6.22	1.56	1.47
1	B	748	ARG	CZ-NH1	5.69	1.40	1.33
1	B	804	GLU	CB-CG	5.61	1.62	1.52
1	A	781	CYS	CB-SG	-5.60	1.72	1.81
1	A	762	GLU	CB-CG	5.50	1.62	1.52
1	B	733	PRO	N-CD	5.35	1.55	1.47
1	B	736	GLU	CB-CG	5.34	1.62	1.52
1	A	970	LYS	CE-NZ	5.26	1.62	1.49
1	B	736	GLU	CD-OE1	5.24	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	748	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	B	748	ARG	NE-CZ-NH1	5.58	123.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	733	PRO	N-CD-CG	-5.43	95.05	103.20
1	A	932	ARG	NE-CZ-NH2	-5.17	117.72	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	932	ARG	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	2363	0	2392	140	0
1	B	2450	0	2450	152	0
2	A	25	0	0	2	0
2	B	48	0	0	3	0
All	All	4886	0	4842	281	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 29.

All (281) 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:715:ILE:HG12	1:A:729:GLY:HA2	1.21	1.16
1:B:736:GLU:HG3	1:B:1016:TYR:OH	1.44	1.14
1:A:1015:GLU:O	1:A:1015:GLU:HG2	1.45	1.14
1:B:989:LEU:CB	1:B:990:PRO:CD	2.30	1.10
1:B:834:VAL:H	1:B:860:LYS:CB	1.66	1.08
1:B:1001:LEU:O	1:B:1002:MET:HB2	1.54	1.03
1:A:775:CYS:SG	1:A:854:THR:HG22	1.99	1.02
1:A:1011:VAL:HG13	1:A:1012:ASP:H	1.24	1.01
1:A:1011:VAL:HG13	1:A:1012:ASP:N	1.71	1.01
1:A:722:ALA:HA	1:A:748:ARG:HH22	1.24	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:ASP:O	1:A:1010:VAL:HG22	1.60	1.00
1:A:1009:ASP:O	1:A:1010:VAL:HG13	1.60	0.99
1:A:775:CYS:SG	1:A:854:THR:CG2	2.51	0.99
1:A:1009:ASP:C	1:A:1010:VAL:HG22	1.85	0.95
1:B:989:LEU:CB	1:B:990:PRO:HD2	1.96	0.94
1:A:1011:VAL:CG1	1:A:1012:ASP:N	2.30	0.91
1:A:783:THR:HG21	1:A:787:GLN:HE21	1.38	0.88
1:B:835:HIS:O	1:B:836:ARG:HB2	1.80	0.81
1:A:775:CYS:CB	1:A:854:THR:HG22	2.11	0.80
1:A:1015:GLU:CG	1:A:1015:GLU:O	2.30	0.80
1:A:748:ARG:HG2	1:A:748:ARG:HH11	1.47	0.80
1:A:1009:ASP:O	1:A:1010:VAL:CG2	2.30	0.80
1:B:994:ASP:O	1:B:995:SER:CB	2.30	0.79
1:A:1009:ASP:O	1:A:1010:VAL:CG1	2.30	0.79
1:A:746:GLU:HG3	1:A:787:GLN:HG2	1.64	0.79
1:B:820:GLN:HE22	1:B:851:VAL:H	1.31	0.79
1:B:738:VAL:CG2	1:B:1011:VAL:HG11	2.12	0.78
1:B:738:VAL:CG2	1:B:1011:VAL:CG1	2.61	0.78
1:A:782:LEU:HD21	1:B:948:VAL:HG13	1.64	0.78
1:B:738:VAL:HG21	1:B:1011:VAL:HG11	1.64	0.77
1:B:989:LEU:CB	1:B:990:PRO:HD3	2.15	0.76
1:B:776:ARG:HH22	1:B:1017:LEU:HD12	1.50	0.76
1:A:793:MET:HG3	1:A:846:LYS:HA	1.65	0.76
1:B:834:VAL:N	1:B:860:LYS:CB	2.47	0.76
1:B:945:MET:HG3	1:B:949:LYS:HE3	1.68	0.76
1:B:759:ILE:HG21	1:B:786:VAL:HB	1.68	0.76
1:B:825:MET:HE3	1:B:853:ILE:HD13	1.69	0.75
1:A:771:ASN:ND2	1:A:773:HIS:H	1.84	0.74
1:B:1001:LEU:O	1:B:1002:MET:CB	2.32	0.74
1:B:845:VAL:HA	1:B:851:VAL:HG12	1.69	0.74
1:B:811:SER:HB2	1:B:975:PRO:CB	2.17	0.73
1:A:775:CYS:HB2	1:A:854:THR:HG22	1.71	0.73
1:B:718:LEU:HG	1:B:728:LYS:HB2	1.71	0.71
1:B:999:ARG:O	1:B:1000:ALA:C	2.29	0.71
1:A:1009:ASP:C	1:A:1010:VAL:CG2	2.59	0.70
1:A:722:ALA:CA	1:A:748:ARG:HH22	2.04	0.70
1:A:1012:ASP:C	1:A:1012:ASP:OD1	2.30	0.69
1:B:781:CYS:HB3	1:B:787:GLN:HG3	1.73	0.69
1:A:829:GLU:HG3	1:A:893:HIS:CD2	2.28	0.69
1:A:715:ILE:HG12	1:A:729:GLY:CA	2.13	0.68
1:B:984:ASP:O	1:B:984:ASP:CG	2.30	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:811:SER:HB2	1:B:975:PRO:HB3	1.74	0.68
1:A:776:ARG:H	1:A:791:GLN:HE21	1.41	0.67
1:A:700:ASN:ND2	1:B:941:ILE:HG21	2.11	0.66
1:B:915:TYR:H	1:B:933:LEU:HD21	1.61	0.66
1:B:808:ASN:HB3	1:B:989:LEU:HA	1.77	0.66
1:B:995:SER:O	1:B:998:TYR:N	2.29	0.65
1:B:848:PRO:HD3	1:B:993:THR:HG21	1.78	0.65
1:B:820:GLN:NE2	1:B:851:VAL:H	1.94	0.65
1:A:980:VAL:O	1:A:980:VAL:HG12	1.97	0.65
1:A:984:ASP:O	1:A:986:ARG:N	2.30	0.65
1:B:1000:ALA:O	1:B:1002:MET:N	2.30	0.65
1:A:1012:ASP:OD1	1:A:1013:ALA:N	2.30	0.65
1:B:781:CYS:SG	1:B:783:THR:HG23	2.37	0.64
1:B:995:SER:O	1:B:997:PHE:N	2.30	0.64
1:A:696:GLY:N	2:A:2001:HOH:O	2.30	0.64
1:A:1012:ASP:O	1:A:1013:ALA:HB2	1.98	0.63
1:A:1015:GLU:O	1:A:1016:TYR:C	2.37	0.63
1:A:795:PHE:HB2	1:A:845:VAL:HB	1.80	0.63
1:A:1009:ASP:O	1:A:1010:VAL:CB	2.46	0.62
1:A:811:SER:HB3	1:A:981:ILE:HD12	1.81	0.62
1:A:863:GLY:O	1:A:865:GLU:N	2.33	0.62
1:A:887:LEU:C	1:A:888:HIS:ND1	2.53	0.62
1:B:738:VAL:CG2	1:B:1011:VAL:HG13	2.29	0.62
1:B:746:GLU:HB3	1:B:787:GLN:HB3	1.82	0.62
1:B:735:GLY:O	1:B:737:LYS:N	2.34	0.61
1:A:751:THR:O	1:A:753:PRO:HD3	1.99	0.61
1:B:995:SER:C	1:B:997:PHE:N	2.53	0.60
1:B:961:PHE:O	1:B:965:ILE:HG13	2.02	0.60
1:B:1000:ALA:O	1:B:1001:LEU:C	2.40	0.60
1:A:703:LEU:HA	1:B:935:GLN:HE22	1.67	0.60
1:B:996:ASN:N	1:B:996:ASN:OD1	2.30	0.60
1:A:793:MET:HG3	1:A:846:LYS:CA	2.31	0.60
1:B:700:ASN:OD1	1:B:702:ALA:HB2	2.01	0.60
1:A:721:GLY:O	1:A:748:ARG:NH2	2.34	0.59
1:B:805:HIS:O	1:B:809:ILE:CG1	2.50	0.59
1:B:1000:ALA:O	1:B:1003:ASP:N	2.36	0.58
1:A:829:GLU:HG3	1:A:893:HIS:CG	2.37	0.58
1:A:784:SER:HA	1:B:953:ILE:HG13	1.84	0.58
1:B:854:THR:CG2	2:B:2026:HOH:O	2.51	0.58
1:B:860:LYS:O	1:B:862:LEU:HG	2.03	0.58
1:B:877:PRO:O	1:B:881:MET:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:ILE:HG22	1:A:716:LYS:HE3	1.85	0.58
1:B:736:GLU:CG	1:B:1016:TYR:OH	2.37	0.57
1:B:835:HIS:O	1:B:836:ARG:CB	2.51	0.57
1:B:878:ILE:HD12	1:B:878:ILE:H	1.70	0.57
1:B:792:LEU:HD23	1:B:844:LEU:HD11	1.87	0.57
1:B:858:LEU:O	1:B:860:LYS:N	2.38	0.56
1:B:888:HIS:HB2	1:B:890:ILE:HG22	1.87	0.56
1:A:825:MET:HA	1:A:828:LEU:HD12	1.85	0.56
1:B:858:LEU:O	1:B:859:ALA:C	2.43	0.56
1:A:847:THR:OG1	1:A:849:GLN:OE1	2.23	0.56
1:B:878:ILE:HD12	1:B:878:ILE:N	2.19	0.56
1:A:985:GLU:O	1:A:986:ARG:C	2.44	0.56
1:A:963:GLU:O	1:A:966:ILE:HG12	2.07	0.55
1:A:811:SER:OG	1:A:975:PRO:HB2	2.06	0.55
1:A:793:MET:HB2	1:A:844:LEU:HB3	1.89	0.55
1:B:999:ARG:O	1:B:1002:MET:HB2	2.06	0.55
1:A:885:SER:O	1:A:889:ARG:HA	2.06	0.55
1:A:748:ARG:HG2	1:A:748:ARG:NH1	2.21	0.55
1:A:704:LEU:H	1:B:935:GLN:HE22	1.55	0.55
1:B:805:HIS:O	1:B:809:ILE:HG12	2.06	0.54
1:B:811:SER:HB2	1:B:975:PRO:HB2	1.87	0.54
1:B:793:MET:HB3	1:B:794:PRO:HD2	1.89	0.54
1:A:844:LEU:HG	1:A:854:THR:HG21	1.90	0.54
1:A:944:TYR:HD1	1:A:947:MET:HE3	1.73	0.54
1:A:771:ASN:HD22	1:A:773:HIS:H	1.55	0.54
1:B:820:GLN:NE2	1:B:851:VAL:HG22	2.23	0.54
1:B:995:SER:C	1:B:997:PHE:H	2.09	0.54
1:A:887:LEU:O	1:A:888:HIS:ND1	2.41	0.54
1:B:763:ALA:HB2	1:B:788:LEU:HD22	1.90	0.54
1:A:805:HIS:ND1	1:A:805:HIS:N	2.54	0.53
1:B:815:LEU:O	1:B:819:VAL:HG23	2.09	0.53
1:A:801:TYR:OH	1:A:848:PRO:HG3	2.09	0.53
1:B:740:ILE:HG21	1:B:1013:ALA:HB2	1.90	0.53
1:A:811:SER:HB3	1:A:981:ILE:CD1	2.39	0.53
1:A:847:THR:HG23	1:A:850:HIS:HB3	1.89	0.53
1:A:700:ASN:HB3	1:B:941:ILE:HG22	1.92	0.52
1:B:909:THR:HB	1:B:912:SER:OG	2.09	0.52
1:A:947:MET:O	1:A:950:CYS:HB2	2.10	0.52
1:B:978:TYR:O	1:B:979:LEU:HD12	2.10	0.52
1:B:900:TYR:CE2	1:B:964:LEU:HD13	2.44	0.52
1:A:700:ASN:O	1:A:701:GLN:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:GLY:O	1:A:866:GLU:N	2.42	0.52
1:B:736:GLU:HG3	1:B:1016:TYR:CZ	2.40	0.52
1:A:708:LYS:HG2	1:B:931:GLU:HB2	1.92	0.52
1:A:983:GLY:O	1:A:984:ASP:C	2.48	0.51
1:A:844:LEU:HG	1:A:854:THR:CG2	2.40	0.51
1:B:860:LYS:O	1:B:861:LEU:C	2.49	0.51
1:A:750:ALA:O	1:B:954:ASP:HB2	2.10	0.51
1:A:847:THR:CG2	1:A:850:HIS:HB3	2.41	0.51
1:B:806:LYS:HG3	1:B:910:PHE:HB3	1.93	0.51
1:A:715:ILE:HG22	1:A:716:LYS:HG2	1.92	0.51
1:B:757:LYS:HE3	1:B:761:ASP:OD2	2.11	0.51
1:B:825:MET:CE	1:B:853:ILE:HD13	2.40	0.51
1:A:883:LEU:HG	1:A:887:LEU:HD13	1.93	0.51
1:B:769:VAL:HG11	1:B:774:VAL:HG11	1.92	0.50
1:B:913:LYS:HB2	1:B:916:ASP:HB2	1.93	0.50
1:B:700:ASN:OD1	1:B:702:ALA:CB	2.59	0.50
1:A:715:ILE:C	1:A:716:LYS:HG2	2.31	0.50
1:A:863:GLY:O	1:A:864:ALA:C	2.50	0.50
1:B:998:TYR:O	1:B:999:ARG:O	2.30	0.50
1:B:820:GLN:HE22	1:B:851:VAL:N	2.06	0.50
1:B:879:LYS:HE2	1:B:915:TYR:O	2.12	0.50
1:A:878:ILE:H	1:A:878:ILE:HD12	1.77	0.50
1:A:944:TYR:O	1:A:948:VAL:HG23	2.11	0.50
1:A:834:VAL:HG12	1:A:836:ARG:HG3	1.93	0.50
1:B:999:ARG:O	1:B:1000:ALA:O	2.30	0.49
1:A:932:ARG:NH2	1:A:951:TRP:O	2.45	0.49
1:A:713:LYS:O	1:A:729:GLY:HA3	2.12	0.49
1:B:989:LEU:O	1:B:990:PRO:O	2.30	0.49
1:B:915:TYR:H	1:B:933:LEU:CD2	2.25	0.49
1:A:898:TRP:CH2	1:A:932:ARG:NH2	2.80	0.49
1:B:984:ASP:O	1:B:984:ASP:OD1	2.30	0.49
1:B:935:GLN:HB2	1:B:944:TYR:CE1	2.48	0.49
1:B:715:ILE:HD11	1:B:730:LEU:HG	1.94	0.49
1:A:931:GLU:O	1:A:932:ARG:NE	2.46	0.49
1:A:754:LYS:O	1:A:758:GLU:HG3	2.13	0.49
1:B:738:VAL:HG21	1:B:1011:VAL:CG1	2.36	0.48
1:B:811:SER:H	1:B:981:ILE:HD12	1.77	0.48
1:A:944:TYR:HA	1:A:947:MET:HE2	1.95	0.48
1:A:935:GLN:HB2	1:A:944:TYR:CE2	2.49	0.48
1:B:776:ARG:HG2	1:B:791:GLN:OE1	2.14	0.48
1:A:715:ILE:HG22	1:A:716:LYS:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1016:TYR:HD1	1:B:1017:LEU:HD23	1.79	0.47
1:B:854:THR:HG22	2:B:2026:HOH:O	2.12	0.47
1:B:802:VAL:HG22	1:B:910:PHE:HA	1.96	0.47
1:A:982:GLN:H	1:A:982:GLN:HG3	1.40	0.47
1:B:817:TRP:O	1:B:821:ILE:HG12	2.14	0.47
1:A:782:LEU:CD2	1:B:948:VAL:HG13	2.37	0.47
1:B:749:GLU:O	1:B:750:ALA:HB3	2.13	0.47
1:A:849:GLN:OE1	1:A:849:GLN:N	2.48	0.47
1:B:738:VAL:HG23	1:B:1011:VAL:CG1	2.44	0.47
1:A:879:LYS:HD3	1:A:915:TYR:HB2	1.96	0.47
1:A:815:LEU:O	1:A:819:VAL:HG23	2.15	0.47
1:A:919:PRO:HD2	1:A:922:GLU:OE2	2.15	0.47
1:A:1012:ASP:O	1:A:1013:ALA:CB	2.63	0.47
1:A:700:ASN:ND2	1:B:941:ILE:CG2	2.77	0.47
1:B:789:ILE:HD12	1:B:789:ILE:N	2.30	0.47
1:A:941:ILE:O	1:A:945:MET:HB2	2.15	0.47
1:A:776:ARG:O	1:A:791:GLN:HG3	2.15	0.46
1:A:983:GLY:O	1:A:986:ARG:CB	2.63	0.46
1:B:938:ILE:HD12	1:B:979:LEU:HG	1.97	0.46
1:B:963:GLU:O	1:B:966:ILE:HG12	2.16	0.46
1:B:747:LEU:HD12	1:B:785:THR:HG22	1.97	0.46
1:A:980:VAL:O	1:A:980:VAL:CG1	2.62	0.46
1:A:740:ILE:O	1:A:742:VAL:HG13	2.15	0.46
1:A:776:ARG:NH1	2:A:2009:HOH:O	2.49	0.46
1:B:924:SER:O	1:B:928:GLU:HG3	2.16	0.46
1:B:811:SER:N	1:B:981:ILE:HD12	2.31	0.46
1:A:863:GLY:H	1:A:866:GLU:HB2	1.80	0.46
1:B:750:ALA:HB1	1:B:784:SER:O	2.16	0.46
1:B:846:LYS:HE3	1:B:1012:ASP:OD1	2.16	0.45
1:B:999:ARG:O	1:B:1001:LEU:O	2.34	0.45
1:A:748:ARG:CG	1:A:748:ARG:NH1	2.78	0.45
1:A:960:LYS:O	1:A:963:GLU:HG3	2.16	0.45
1:B:709:GLU:HA	1:B:712:PHE:CZ	2.52	0.45
1:B:805:HIS:O	1:B:809:ILE:HG13	2.16	0.45
1:B:878:ILE:HA	1:B:881:MET:HE2	1.98	0.45
1:B:980:VAL:O	1:B:980:VAL:HG12	2.17	0.45
1:A:704:LEU:H	1:B:935:GLN:NE2	2.14	0.45
1:B:926:ILE:HG13	1:B:927:LEU:N	2.31	0.45
1:B:763:ALA:HB2	1:B:788:LEU:CD2	2.47	0.45
1:B:995:SER:O	1:B:996:ASN:C	2.55	0.45
1:B:923:ILE:HA	1:B:926:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:SER:O	1:A:929:LYS:HD3	2.17	0.44
1:A:748:ARG:HB3	1:A:749:GLU:OE1	2.17	0.44
1:A:748:ARG:HG3	1:A:749:GLU:HG3	2.00	0.44
1:A:708:LYS:C	1:A:710:THR:H	2.21	0.44
1:B:1016:TYR:CD1	1:B:1017:LEU:HD23	2.53	0.43
1:B:925:SER:O	1:B:929:LYS:HG2	2.18	0.43
1:B:860:LYS:O	1:B:862:LEU:N	2.51	0.43
1:B:854:THR:HG21	2:B:2026:HOH:O	2.14	0.43
1:B:714:LYS:HD3	1:B:727:TYR:CG	2.54	0.43
1:A:824:GLY:O	1:A:827:TYR:HB3	2.17	0.43
1:B:854:THR:HG22	1:B:856:PHE:H	1.83	0.43
1:B:880:TRP:CZ2	1:B:914:PRO:HG2	2.53	0.43
1:B:998:TYR:O	1:B:999:ARG:C	2.56	0.43
1:B:904:VAL:O	1:B:908:MET:HG2	2.18	0.43
1:B:831:ARG:HH11	1:B:831:ARG:HG2	1.83	0.43
1:A:765:VAL:HG23	1:A:766:MET:N	2.34	0.43
1:A:984:ASP:O	1:A:985:GLU:C	2.56	0.43
1:B:790:MET:SD	1:B:854:THR:HG23	2.59	0.43
1:B:800:ASP:O	1:B:804:GLU:HG3	2.18	0.43
1:B:752:SER:O	1:B:755:ALA:N	2.51	0.42
1:B:825:MET:CE	1:B:853:ILE:HG21	2.50	0.42
1:A:805:HIS:O	1:A:809:ILE:HG13	2.19	0.42
1:A:878:ILE:HA	1:A:881:MET:SD	2.59	0.42
1:A:931:GLU:O	1:A:932:ARG:HD3	2.20	0.42
1:B:723:PHE:CD2	1:B:724:GLY:N	2.88	0.42
1:B:915:TYR:CZ	1:B:933:LEU:HG	2.54	0.42
1:A:935:GLN:HB2	1:A:944:TYR:CD2	2.54	0.42
1:A:931:GLU:O	1:A:932:ARG:CD	2.67	0.42
1:A:773:HIS:HA	1:A:852:LYS:HG2	2.01	0.42
1:B:731:TRP:CE3	1:B:740:ILE:HD12	2.54	0.42
1:B:708:LYS:O	1:B:711:GLU:HB2	2.20	0.42
1:A:706:ILE:C	1:A:707:LEU:HD23	2.40	0.42
1:A:744:ILE:HA	1:A:788:LEU:O	2.20	0.42
1:A:962:ARG:HG3	1:A:962:ARG:H	1.67	0.42
1:A:962:ARG:HE	1:A:962:ARG:HB2	1.65	0.42
1:B:857:GLY:C	1:B:859:ALA:N	2.74	0.41
1:A:708:LYS:C	1:A:710:THR:N	2.74	0.41
1:B:927:LEU:HD12	1:B:927:LEU:HA	1.87	0.41
1:A:730:LEU:N	1:A:730:LEU:HD23	2.35	0.41
1:A:790:MET:H	1:A:790:MET:HG2	1.76	0.41
1:B:878:ILE:CD1	1:B:878:ILE:H	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:846:LYS:HD3	1:B:850:HIS:ND1	2.35	0.41
1:B:944:TYR:HA	1:B:947:MET:CE	2.50	0.41
1:B:759:ILE:HA	1:B:759:ILE:HD13	1.93	0.41
1:B:944:TYR:HA	1:B:947:MET:HE3	2.02	0.41
1:A:932:ARG:HD3	1:A:932:ARG:HA	1.59	0.41
1:B:936:PRO:HA	1:B:937:PRO:HD3	1.95	0.41
1:A:984:ASP:C	1:A:986:ARG:N	2.73	0.41
1:A:750:ALA:CB	1:A:784:SER:O	2.68	0.41
1:A:722:ALA:HA	1:A:748:ARG:NH2	2.09	0.41
1:B:876:VAL:HG23	1:B:878:ILE:HD11	2.01	0.41
1:B:741:PRO:O	1:B:792:LEU:HB2	2.21	0.41
1:A:967:GLU:O	1:A:971:MET:HG3	2.21	0.41
1:A:917:GLY:O	1:A:918:ILE:C	2.58	0.41
1:A:966:ILE:HG13	1:A:967:GLU:N	2.34	0.41
1:A:783:THR:CG2	1:A:787:GLN:HG3	2.51	0.41
1:A:750:ALA:HB2	1:A:784:SER:O	2.21	0.41
1:B:821:ILE:HG12	1:B:821:ILE:H	1.70	0.41
1:A:922:GLU:HG3	1:A:926:ILE:HD11	2.02	0.41
1:A:916:ASP:O	1:A:918:ILE:N	2.53	0.41
1:A:816:ASN:O	1:A:820:GLN:HG3	2.20	0.41
1:B:998:TYR:O	1:B:1001:LEU:O	2.38	0.40
1:A:1012:ASP:OD1	1:A:1013:ALA:HB3	2.21	0.40
1:B:913:LYS:HG2	1:B:913:LYS:H	1.76	0.40
1:B:876:VAL:HA	1:B:877:PRO:HD3	1.87	0.40
1:A:829:GLU:HA	1:A:893:HIS:NE2	2.35	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	295/327 (90%)	242 (82%)	42 (14%)	11 (4%)	4 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	304/327 (93%)	261 (86%)	31 (10%)	12 (4%)	4 22
All	All	599/654 (92%)	503 (84%)	73 (12%)	23 (4%)	4 22

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	864	ALA
1	A	984	ASP
1	A	985	GLU
1	A	1010	VAL
1	A	1013	ALA
1	B	736	GLU
1	B	859	ALA
1	B	995	SER
1	B	999	ARG
1	B	1000	ALA
1	A	922	GLU
1	B	863	GLY
1	B	915	TYR
1	B	984	ASP
1	B	996	ASN
1	B	1002	MET
1	A	855	ASP
1	B	872	GLU
1	A	729	GLY
1	B	1001	LEU
1	A	873	GLY
1	A	923	ILE
1	A	918	ILE

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	255/287 (89%)	223 (88%)	32 (12%)	6 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	259/287 (90%)	235 (91%)	24 (9%)	11 39
All	All	514/574 (90%)	458 (89%)	56 (11%)	8 30

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	708	LYS
1	A	716	LYS
1	A	720	SER
1	A	730	LEU
1	A	734	GLU
1	A	738	VAL
1	A	748	ARG
1	A	749	GLU
1	A	751	THR
1	A	757	LYS
1	A	784	SER
1	A	789	ILE
1	A	790	MET
1	A	793	MET
1	A	805	HIS
1	A	841	ARG
1	A	847	THR
1	A	876	VAL
1	A	884	GLU
1	A	922	GLU
1	A	942	ASP
1	A	953	ILE
1	A	962	ARG
1	A	967	GLU
1	A	976	GLN
1	A	977	ARG
1	A	981	ILE
1	A	982	GLN
1	A	984	ASP
1	A	1010	VAL
1	A	1012	ASP
1	A	1015	GLU
1	B	703	LEU
1	B	725	THR
1	B	734	GLU
1	B	747	LEU

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Mol	Chain	Res	Type
1	B	759	ILE
1	B	776	ARG
1	B	791	GLN
1	B	798	LEU
1	B	806	LYS
1	B	809	ILE
1	B	811	SER
1	B	831	ARG
1	B	849	GLN
1	B	856	PHE
1	B	861	LEU
1	B	890	ILE
1	B	903	THR
1	B	927	LEU
1	B	982	GLN
1	B	984	ASP
1	B	993	THR
1	B	996	ASN
1	B	1002	MET
1	B	1011	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	756	ASN
1	A	771	ASN
1	A	787	GLN
1	A	791	GLN
1	A	816	ASN
1	A	842	ASN
1	A	894	GLN
1	A	935	GLN
1	B	805	HIS
1	B	820	GLN
1	B	849	GLN
1	B	935	GLN

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

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	299/327 (91%)	-0.33	5 (1%) 73 52	31, 49, 72, 110	0
1	B	312/327 (95%)	-0.27	10 (3%) 51 27	22, 45, 95, 109	0
All	All	611/654 (93%)	-0.30	15 (2%) 61 37	22, 47, 87, 110	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	865	GLU	4.7
1	B	735	GLY	3.8
1	A	1012	ASP	3.7
1	B	864	ALA	3.5
1	A	1011	VAL	3.2
1	B	873	GLY	2.8
1	B	866	GLU	2.6
1	B	749	GLU	2.6
1	B	874	GLY	2.6
1	A	696	GLY	2.5
1	B	722	ALA	2.5
1	B	748	ARG	2.3
1	B	1003	ASP	2.1
1	A	864	ALA	2.1
1	A	1009	ASP	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.