Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 10:38 AM EDT

PDB ID	:	2RF9
Title	:	Crystal structure of the complex between the EGFR kinase domain and a Mig6 peptide
Authors	:	Zhang, X.; Pickin, K.A.; Bose, R.; Jura, N.; Cole, P.A.; Kuriyan, J.
Deposited on	:	2007-09-28
Resolution	:	3.50 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

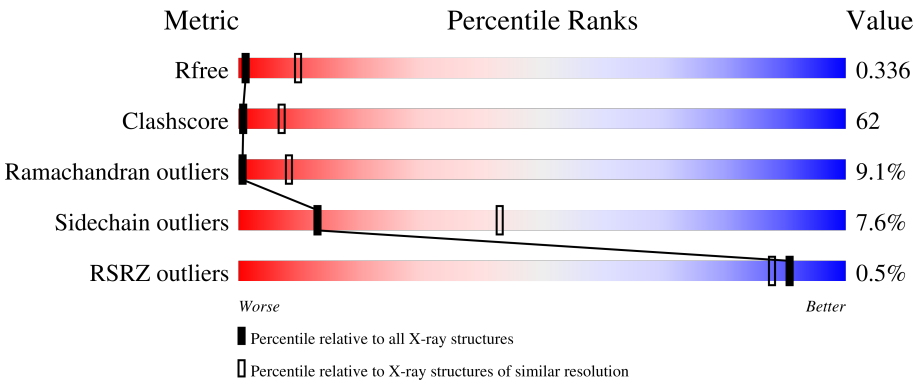
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.50 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))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	330	25% 48% 11% 15%
1	B	330	% 24% 49% 8% 18%
2	C	65	25% 15% • 58%
2	D	65	25% 11% 5% 60%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4435 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
			Total	C	N	O	S			
1	A	280	2068	1336	345	372	15	0	0	0
1	B	269	2010	1298	334	363	15	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	669	GLY	-	expression tag	UNP P00533
A	670	ALA	-	expression tag	UNP P00533
A	671	MET	-	expression tag	UNP P00533
B	669	GLY	-	expression tag	UNP P00533
B	670	ALA	-	expression tag	UNP P00533
B	671	MET	-	expression tag	UNP P00533

- Molecule 2 is a protein called ERBB receptor feedback inhibitor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	27	183	119	27	36	1	0	0	0
2	D	26	174	113	26	34	1	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	310	GLY	-	expression tag	UNP Q9UJM3
C	311	PRO	-	expression tag	UNP Q9UJM3
C	312	LEU	-	expression tag	UNP Q9UJM3
C	313	GLY	-	expression tag	UNP Q9UJM3
C	314	SER	-	expression tag	UNP Q9UJM3
D	310	GLY	-	expression tag	UNP Q9UJM3

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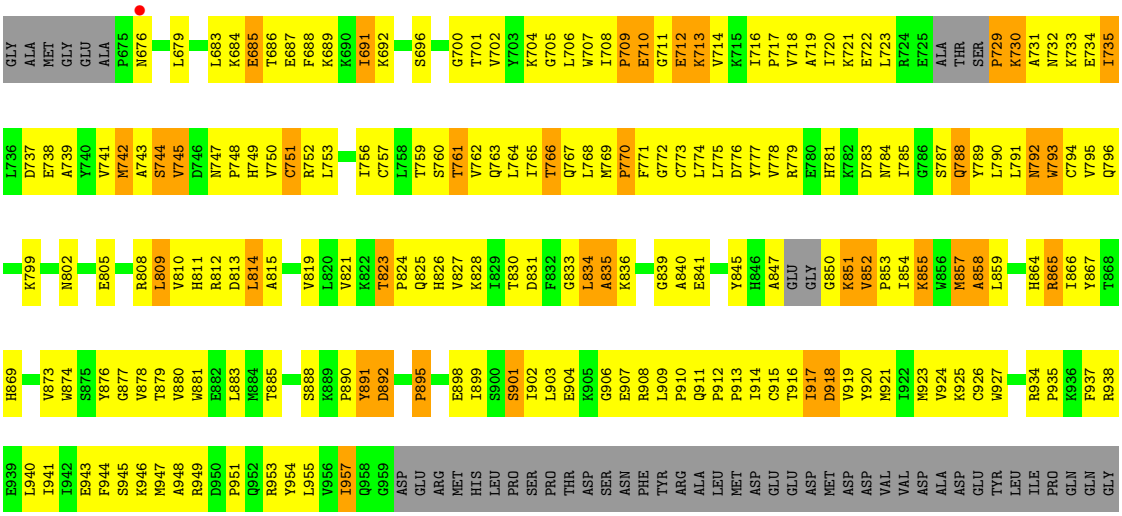
Chain	Residue	Modelled	Actual	Comment	Reference
D	311	PRO	-	expression tag	UNP Q9UJM3
D	312	LEU	-	expression tag	UNP Q9UJM3
D	313	GLY	-	expression tag	UNP Q9UJM3
D	314	SER	-	expression tag	UNP Q9UJM3

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.

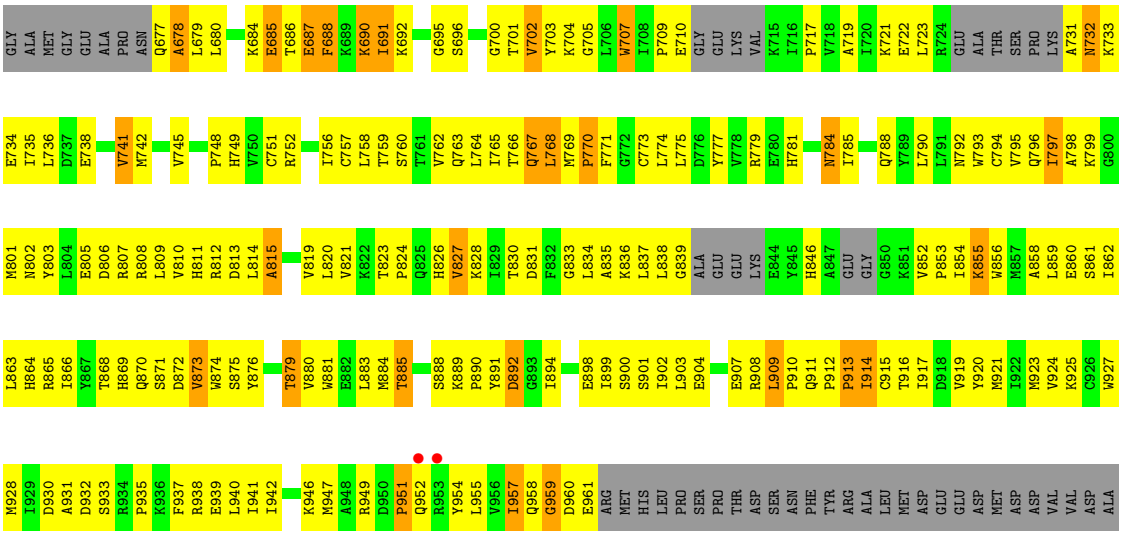
• Molecule 1: Epidermal growth factor receptor

Chain A: 25% 48% 11% 15%



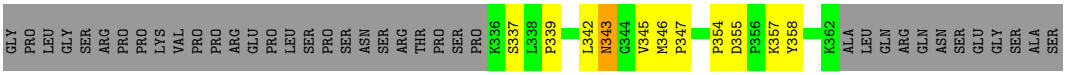
• Molecule 1: Epidermal growth factor receptor

Chain B: % 24% 49% 8% 18%



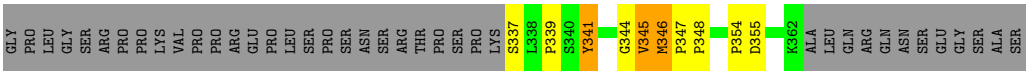
• Molecule 2: ERBB receptor feedback inhibitor 1

Chain C:



• Molecule 2: ERBB receptor feedback inhibitor 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	188.76Å 42.65Å 99.73Å 90.00° 109.12° 90.00°	Depositor
Resolution (Å)	47.11 – 3.50 47.11 – 3.49	Depositor EDS
% Data completeness (in resolution range)	84.5 (47.11-3.50) 84.1 (47.11-3.49)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 3.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.272 , 0.329 0.275 , 0.336	Depositor DCC
R_{free} test set	495 reflections (5.45%)	wwPDB-VP
Wilson B-factor (Å^2)	70.1	Xtriage
Anisotropy	0.699	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 106.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	4435	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.45% 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 (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.48	0/2114	0.74	1/2887 (0.0%)
1	B	0.46	0/2054	0.74	0/2800
2	C	0.65	0/190	0.77	0/264
2	D	0.57	0/181	0.83	0/251
All	All	0.48	0/4539	0.74	1/6202 (0.0%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	729	PRO	N-CA-CB	5.40	109.78	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	891	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	2068	0	1961	258	0
1	B	2010	0	1902	249	0
2	C	183	0	152	18	0
2	D	174	0	138	27	0
All	All	4435	0	4153	532	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 62.

All (532) 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)
2:D:341:TYR:CE2	2:D:347:PRO:HD2	1.80	1.17
2:D:341:TYR:HE2	2:D:347:PRO:HD2	0.95	1.09
2:D:339:PRO:CB	2:D:341:TYR:HE1	1.71	1.03
1:A:907:GLU:O	1:A:908:ARG:HD3	1.57	1.03
1:B:808:ARG:HH11	1:B:839:GLY:HA2	1.23	1.03
2:D:339:PRO:HB3	2:D:341:TYR:HE1	1.27	0.98
2:D:341:TYR:HE2	2:D:347:PRO:CD	1.78	0.96
1:A:859:LEU:HD13	1:A:903:LEU:HD23	1.47	0.95
1:B:696:SER:HB2	1:B:701:THR:HG22	1.49	0.93
1:A:739:ALA:HA	1:A:742:MET:HB3	1.50	0.93
2:D:339:PRO:HB2	2:D:341:TYR:CE1	2.04	0.93
1:A:864:HIS:O	1:A:866:ILE:HG13	1.68	0.92
2:D:341:TYR:CE2	2:D:347:PRO:CD	2.52	0.91
2:D:339:PRO:CB	2:D:341:TYR:CE1	2.54	0.91
1:A:775:LEU:HG	1:A:779:ARG:HE	1.36	0.89
1:A:812:ARG:HG3	1:A:867:TYR:CD2	2.08	0.89
1:B:781:HIS:O	1:B:785:ILE:HG13	1.75	0.86
1:B:696:SER:HA	1:B:701:THR:HA	1.58	0.86
1:B:902:ILE:HB	1:B:907:GLU:HG3	1.56	0.86
1:B:707:TRP:CE2	1:B:709:PRO:HG3	2.11	0.86
1:A:795:VAL:HG22	1:A:944:PHE:HB3	1.59	0.85
1:B:880:VAL:O	1:B:884:MET:HG2	1.75	0.85
1:B:696:SER:CB	1:B:701:THR:HG22	2.06	0.84
1:A:873:VAL:HG12	1:A:926:CYS:HB3	1.59	0.84
1:B:876:TYR:O	1:B:880:VAL:HG23	1.77	0.83
1:A:757:CYS:HB3	1:A:763:GLN:HB2	1.59	0.83
1:A:688:PHE:HA	1:A:706:LEU:O	1.79	0.83
1:B:815:ALA:O	1:B:819:VAL:HG23	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:GLU:O	1:A:707:TRP:HD1	1.63	0.82
1:B:777:TYR:OH	1:B:824:PRO:HG3	1.80	0.81
1:A:880:VAL:HB	1:A:923:MET:CE	2.11	0.80
1:B:881:TRP:N	1:B:923:MET:HE3	1.96	0.80
1:A:721:LYS:HZ1	1:A:830:THR:HG21	1.46	0.80
1:B:758:LEU:HD23	1:B:762:VAL:HG23	1.61	0.80
1:A:947:MET:HA	1:A:954:TYR:CE1	2.16	0.80
1:A:948:ALA:O	1:A:951:PRO:HD3	1.82	0.80
1:A:702:VAL:HG22	1:A:721:LYS:HA	1.61	0.80
1:A:830:THR:HG22	1:A:831:ASP:H	1.46	0.80
1:A:899:ILE:O	1:A:903:LEU:HB2	1.81	0.80
1:B:808:ARG:NH1	1:B:839:GLY:HA2	1.97	0.80
1:A:729:PRO:C	1:A:731:ALA:H	1.85	0.80
1:A:839:GLY:O	1:A:841:GLU:N	2.15	0.80
1:B:707:TRP:NE1	1:B:709:PRO:HG3	1.98	0.79
1:B:757:CYS:HB3	1:B:763:GLN:HB2	1.64	0.79
1:B:954:TYR:O	1:B:955:LEU:HD23	1.82	0.79
1:A:733:LYS:HE3	1:A:737:ASP:OD2	1.83	0.79
1:A:909:LEU:HD13	1:A:927:TRP:CH2	2.18	0.78
1:B:939:GLU:HA	1:B:942:ILE:HD12	1.65	0.78
1:B:769:MET:HG3	1:B:820:LEU:HD13	1.66	0.78
1:B:919:VAL:HG21	1:B:955:LEU:HD21	1.66	0.77
1:A:772:GLY:O	1:A:821:VAL:HG23	1.84	0.77
1:B:794:CYS:HA	1:B:797:ILE:HD12	1.65	0.76
1:A:721:LYS:NZ	1:A:830:THR:HG21	2.01	0.76
1:A:812:ARG:CZ	1:A:834:LEU:O	2.33	0.76
1:B:691:ILE:HB	1:B:704:LYS:O	1.86	0.75
1:A:911:GLN:NE2	2:C:339:PRO:HG3	2.02	0.75
1:B:702:VAL:CG2	1:B:721:LYS:HG2	2.16	0.75
1:A:753:LEU:HD11	1:A:764:LEU:HD22	1.68	0.75
1:A:702:VAL:HG13	1:A:720:ILE:O	1.87	0.74
1:B:775:LEU:HD11	1:B:779:ARG:HE	1.52	0.74
1:B:773:CYS:SG	1:B:775:LEU:HB3	2.28	0.74
1:B:793:TRP:O	1:B:797:ILE:HG13	1.85	0.74
1:A:760:SER:O	1:A:761:THR:HG23	1.87	0.74
1:B:930:ASP:O	1:B:933:SER:HB3	1.87	0.73
1:A:909:LEU:N	1:A:909:LEU:HD12	2.04	0.73
1:A:880:VAL:HB	1:A:923:MET:HE1	1.69	0.72
1:B:881:TRP:HB2	1:B:923:MET:HE1	1.71	0.72
1:B:795:VAL:HG12	1:B:799:LYS:HE3	1.71	0.72
1:A:753:LEU:HD12	1:A:766:THR:HG23	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:688:PHE:HA	1:B:707:TRP:HA	1.70	0.72
1:B:947:MET:HA	1:B:954:TYR:CE1	2.25	0.72
1:A:696:SER:HB3	1:A:701:THR:HG23	1.70	0.72
1:A:830:THR:HG22	1:A:831:ASP:N	2.05	0.71
1:B:814:LEU:HD12	1:B:815:ALA:H	1.56	0.71
1:B:738:GLU:O	1:B:741:VAL:HG23	1.90	0.71
1:A:859:LEU:HD13	1:A:903:LEU:CD2	2.21	0.70
1:B:885:THR:HB	1:B:888:SER:HB2	1.71	0.70
1:B:899:ILE:O	1:B:903:LEU:HD13	1.91	0.70
1:A:795:VAL:O	1:A:799:LYS:HG3	1.92	0.70
1:A:876:TYR:O	1:A:880:VAL:HG23	1.91	0.70
1:B:957:ILE:HD12	1:B:957:ILE:N	2.07	0.70
1:A:696:SER:HA	1:A:701:THR:HA	1.73	0.70
1:A:722:GLU:O	1:A:722:GLU:HG2	1.92	0.70
1:A:787:SER:HA	1:A:955:LEU:HD12	1.74	0.70
2:D:339:PRO:HB3	2:D:341:TYR:CE1	2.20	0.69
1:A:916:THR:HG23	1:A:954:TYR:O	1.92	0.69
1:A:689:LYS:O	1:A:705:GLY:HA3	1.92	0.69
1:A:789:TYR:HA	1:A:792:ASN:HD22	1.58	0.69
1:B:741:VAL:HG11	1:B:809:LEU:HD21	1.74	0.69
1:B:771:PHE:HE2	1:B:823:THR:HA	1.56	0.69
1:A:775:LEU:CG	1:A:779:ARG:HE	2.06	0.68
1:A:721:LYS:O	1:A:763:GLN:HA	1.93	0.68
1:B:874:TRP:CE3	1:B:927:TRP:HA	2.29	0.68
1:A:789:TYR:O	1:A:792:ASN:HB2	1.94	0.68
1:B:869:HIS:O	1:B:872:ASP:HB2	1.93	0.68
1:B:909:LEU:H	1:B:909:LEU:HD12	1.59	0.68
1:B:814:LEU:HD23	1:B:876:TYR:HA	1.74	0.68
1:B:855:LYS:HE2	1:B:891:TYR:HB2	1.75	0.68
1:B:917:ILE:O	1:B:921:MET:HG2	1.93	0.68
1:A:785:ILE:HD13	1:A:793:TRP:HH2	1.59	0.67
1:A:809:LEU:CD1	1:A:810:VAL:H	2.08	0.67
1:A:729:PRO:O	1:A:731:ALA:N	2.28	0.67
1:A:770:PRO:HG2	1:A:771:PHE:H	1.60	0.67
1:B:684:LYS:C	1:B:686:THR:H	1.98	0.67
1:A:775:LEU:HG	1:A:779:ARG:NE	2.08	0.66
1:A:790:LEU:HD23	1:A:793:TRP:CZ3	2.29	0.66
1:B:809:LEU:HD22	1:B:837:LEU:HD13	1.77	0.66
1:B:710:GLU:HG2	1:B:710:GLU:O	1.95	0.66
1:B:762:VAL:HG22	1:B:763:GLN:N	2.11	0.66
1:A:687:GLU:O	1:A:707:TRP:HA	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:GLU:HA	1:A:763:GLN:HG2	1.78	0.66
1:A:753:LEU:HD21	1:A:764:LEU:CD2	2.27	0.65
1:A:791:LEU:O	1:A:794:CYS:HB2	1.96	0.65
1:A:912:PRO:HB2	1:A:915:CYS:SG	2.37	0.65
1:B:911:GLN:HA	1:B:920:TYR:CE1	2.32	0.65
1:A:687:GLU:O	1:A:707:TRP:CD1	2.49	0.65
1:A:791:LEU:HD21	1:A:955:LEU:HD21	1.79	0.65
1:A:788:GLN:CD	1:A:792:ASN:HD21	2.00	0.65
1:A:792:ASN:O	1:A:793:TRP:C	2.34	0.65
1:A:881:TRP:N	1:A:923:MET:HE1	2.11	0.65
1:B:745:VAL:HA	1:B:803:TYR:OH	1.97	0.65
1:A:880:VAL:HB	1:A:923:MET:HE3	1.79	0.64
1:A:709:PRO:HB2	1:A:712:GLU:HB2	1.78	0.64
1:A:815:ALA:O	1:A:819:VAL:HG23	1.96	0.64
2:D:341:TYR:HD2	2:D:345:VAL:O	1.80	0.63
1:A:908:ARG:HB3	1:A:927:TRP:CE3	2.34	0.63
1:B:864:HIS:O	1:B:866:ILE:HG13	1.98	0.63
1:B:873:VAL:O	1:B:876:TYR:HB3	1.97	0.63
1:B:910:PRO:HG3	2:D:347:PRO:O	1.98	0.63
1:A:909:LEU:HD12	1:A:909:LEU:H	1.61	0.63
1:B:859:LEU:HG	1:B:863:LEU:HG	1.79	0.63
1:B:901:SER:HA	1:B:904:GLU:OE1	1.99	0.63
1:A:917:ILE:HG12	2:C:337:SER:HB2	1.79	0.63
1:B:930:ASP:HB3	1:B:933:SER:CB	2.28	0.63
1:A:788:GLN:HE21	1:A:788:GLN:HA	1.62	0.62
1:A:785:ILE:HD13	1:A:793:TRP:CH2	2.34	0.62
1:A:792:ASN:O	1:A:795:VAL:N	2.31	0.62
1:A:812:ARG:HG3	1:A:867:TYR:CE2	2.35	0.62
1:A:917:ILE:HG12	2:C:337:SER:CB	2.30	0.62
1:B:917:ILE:HG22	2:D:337:SER:HB2	1.81	0.62
1:A:712:GLU:O	1:A:714:VAL:N	2.33	0.62
1:A:881:TRP:HZ2	2:C:346:MET:HE3	1.63	0.62
1:B:788:GLN:HE21	1:B:792:ASN:HD21	1.48	0.61
1:B:876:TYR:CE2	1:B:940:LEU:HD13	2.35	0.61
1:A:734:GLU:O	1:A:735:ILE:C	2.37	0.61
1:A:799:LYS:O	1:A:802:ASN:HB3	2.00	0.61
1:A:732:ASN:HA	1:A:735:ILE:HG12	1.82	0.61
1:B:930:ASP:HB3	1:B:933:SER:HB2	1.83	0.61
1:A:854:ILE:HA	1:A:857:MET:SD	2.41	0.60
1:A:747:ASN:OD1	1:A:749:HIS:N	2.34	0.60
1:A:919:VAL:HG22	1:A:954:TYR:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:907:GLU:O	1:B:908:ARG:NH1	2.34	0.60
1:B:909:LEU:HD12	1:B:909:LEU:N	2.16	0.60
2:D:344:GLY:O	2:D:345:VAL:C	2.39	0.60
1:B:721:LYS:O	1:B:763:GLN:HA	2.01	0.60
1:B:925:LYS:O	1:B:928:MET:HG3	2.02	0.60
1:B:881:TRP:CA	1:B:923:MET:HE3	2.32	0.60
2:C:345:VAL:HG23	2:C:345:VAL:O	2.02	0.60
1:B:852:VAL:N	1:B:853:PRO:HD3	2.16	0.59
1:B:947:MET:HA	1:B:954:TYR:HE1	1.65	0.59
1:B:702:VAL:HG13	1:B:703:TYR:N	2.16	0.59
1:A:911:GLN:CD	2:C:339:PRO:HG3	2.22	0.59
1:B:796:GLN:O	1:B:799:LYS:HB2	2.03	0.59
1:A:805:GLU:HG3	1:A:869:HIS:ND1	2.18	0.59
1:B:758:LEU:CD2	1:B:762:VAL:HG23	2.30	0.59
1:B:909:LEU:HD13	1:B:927:TRP:CH2	2.37	0.59
1:A:770:PRO:HG2	1:A:771:PHE:CD1	2.38	0.59
2:C:355:ASP:OD1	2:C:357:LYS:N	2.29	0.59
1:A:753:LEU:HD21	1:A:764:LEU:HD22	1.83	0.59
1:A:937:PHE:O	1:A:938:ARG:C	2.40	0.59
1:B:870:GLN:HG3	1:B:931:ALA:O	2.02	0.59
1:B:917:ILE:CG2	2:D:337:SER:HB2	2.33	0.59
1:A:729:PRO:C	1:A:731:ALA:N	2.54	0.58
1:A:943:GLU:O	1:A:947:MET:HG3	2.02	0.58
1:A:730:LYS:C	1:A:732:ASN:H	2.04	0.58
1:A:876:TYR:HE2	1:A:940:LEU:HD22	1.68	0.58
1:B:912:PRO:HD2	1:B:915:CYS:HB2	1.85	0.58
1:B:745:VAL:CG2	1:B:752:ARG:HA	2.34	0.58
1:B:811:HIS:O	1:B:812:ARG:HB2	2.02	0.58
1:A:910:PRO:HB3	2:C:347:PRO:O	2.02	0.58
1:B:898:GLU:O	1:B:901:SER:N	2.37	0.58
1:B:917:ILE:O	1:B:917:ILE:HG13	2.04	0.58
1:A:881:TRP:CD2	1:A:909:LEU:HD23	2.39	0.58
1:B:805:GLU:HG3	1:B:869:HIS:ND1	2.19	0.58
1:B:837:LEU:HD12	1:B:838:LEU:H	1.69	0.58
1:B:700:GLY:O	1:B:701:THR:HG23	2.04	0.58
1:B:741:VAL:HG11	1:B:809:LEU:CD2	2.32	0.58
1:B:769:MET:HG3	1:B:820:LEU:CD1	2.33	0.58
1:B:946:LYS:O	1:B:949:ARG:N	2.36	0.58
1:A:723:LEU:HD23	1:A:723:LEU:H	1.69	0.57
1:B:937:PHE:O	1:B:941:ILE:HG13	2.04	0.57
1:B:764:LEU:O	1:B:765:ILE:HD13	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:LEU:H	1:A:909:LEU:CD1	2.17	0.57
1:A:809:LEU:HD13	1:A:810:VAL:H	1.70	0.57
1:B:766:THR:O	1:B:768:LEU:N	2.37	0.57
1:B:861:SER:HA	1:B:866:ILE:O	2.04	0.57
1:B:912:PRO:HB2	1:B:915:CYS:SG	2.45	0.57
1:B:707:TRP:O	1:B:709:PRO:HD3	2.05	0.57
1:A:921:MET:O	1:A:925:LYS:HB2	2.04	0.57
1:B:919:VAL:HG22	1:B:947:MET:SD	2.45	0.56
1:B:731:ALA:C	1:B:733:LYS:H	2.07	0.56
1:B:881:TRP:HB2	1:B:923:MET:CE	2.36	0.56
1:B:759:THR:OG1	1:B:760:SER:N	2.38	0.56
1:B:731:ALA:O	1:B:733:LYS:N	2.35	0.56
1:A:739:ALA:HB1	1:A:753:LEU:HD23	1.87	0.55
1:B:900:SER:O	1:B:904:GLU:HG3	2.06	0.55
1:A:845:TYR:HE2	1:A:847:ALA:HB2	1.72	0.55
1:A:712:GLU:C	1:A:714:VAL:H	2.08	0.55
1:B:855:LYS:HZ3	1:B:889:LYS:HE2	1.70	0.55
1:B:870:GLN:HA	1:B:873:VAL:HG23	1.89	0.55
1:A:700:GLY:HA3	1:A:723:LEU:HA	1.88	0.55
1:B:722:GLU:O	1:B:722:GLU:HG2	2.06	0.55
1:A:911:GLN:HA	1:A:920:TYR:CE1	2.42	0.54
1:A:874:TRP:HZ2	1:A:903:LEU:HD11	1.73	0.54
1:A:756:ILE:HD12	1:A:764:LEU:HD21	1.88	0.54
1:B:957:ILE:HG22	1:B:958:GLN:H	1.72	0.54
1:B:805:GLU:HG3	1:B:869:HIS:CE1	2.43	0.54
1:A:783:ASP:O	1:A:784:ASN:ND2	2.41	0.54
1:B:873:VAL:O	1:B:876:TYR:N	2.39	0.54
1:A:691:ILE:HG22	1:A:692:LYS:N	2.22	0.54
1:A:788:GLN:HA	1:A:788:GLN:NE2	2.23	0.54
1:B:799:LYS:HA	1:B:941:ILE:HD13	1.90	0.53
1:A:732:ASN:HA	1:A:735:ILE:CG1	2.39	0.53
1:A:914:ILE:O	1:A:955:LEU:HA	2.09	0.53
1:B:684:LYS:C	1:B:686:THR:N	2.62	0.53
1:A:750:VAL:O	1:A:752:ARG:N	2.41	0.53
1:A:898:GLU:O	1:A:902:ILE:HG12	2.08	0.53
1:A:788:GLN:HG3	1:A:789:TYR:N	2.23	0.53
1:A:858:ALA:HA	1:A:874:TRP:CD2	2.43	0.53
1:B:808:ARG:O	1:B:837:LEU:HD12	2.08	0.53
1:B:687:GLU:O	1:B:688:PHE:HB3	2.08	0.53
1:B:807:ARG:O	1:B:809:LEU:HD23	2.09	0.53
1:B:767:GLN:O	1:B:768:LEU:C	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:814:LEU:O	1:B:815:ALA:HB2	2.09	0.52
1:A:864:HIS:O	1:A:865:ARG:C	2.48	0.52
1:B:790:LEU:HA	1:B:793:TRP:CE3	2.44	0.52
1:B:937:PHE:CD2	1:B:940:LEU:HD12	2.43	0.52
1:A:777:TYR:OH	1:A:824:PRO:HG3	2.09	0.52
1:A:789:TYR:CA	1:A:792:ASN:HD22	2.21	0.52
1:A:908:ARG:HB3	1:A:927:TRP:HE3	1.74	0.52
1:B:732:ASN:O	1:B:736:LEU:HG	2.09	0.52
1:B:890:PRO:HB2	1:B:891:TYR:HD1	1.74	0.52
1:B:733:LYS:HA	1:B:736:LEU:HD12	1.91	0.52
1:B:790:LEU:HD23	1:B:793:TRP:CZ3	2.45	0.52
1:A:688:PHE:HD2	1:A:720:ILE:HD11	1.74	0.52
1:B:947:MET:HA	1:B:954:TYR:CD1	2.45	0.52
1:A:704:LYS:HA	1:A:719:ALA:HA	1.92	0.52
1:A:709:PRO:HD2	1:A:714:VAL:O	2.09	0.52
1:A:911:GLN:NE2	2:C:339:PRO:CG	2.73	0.52
1:B:794:CYS:HA	1:B:797:ILE:CD1	2.35	0.52
1:B:823:THR:OG1	1:B:824:PRO:HD2	2.09	0.52
1:B:748:PRO:O	1:B:828:LYS:HE2	2.09	0.51
1:A:941:ILE:O	1:A:945:SER:N	2.31	0.51
1:A:946:LYS:O	1:A:949:ARG:N	2.43	0.51
1:B:881:TRP:CE2	1:B:885:THR:HG21	2.45	0.51
1:B:898:GLU:O	1:B:899:ILE:C	2.49	0.51
1:B:891:TYR:O	1:B:894:ILE:HB	2.10	0.51
1:B:902:ILE:HB	1:B:907:GLU:CG	2.35	0.51
1:A:734:GLU:O	1:A:737:ASP:N	2.44	0.51
1:B:858:ALA:HA	1:B:874:TRP:CE2	2.45	0.51
1:A:909:LEU:HB2	1:A:927:TRP:HH2	1.75	0.51
1:B:702:VAL:HG22	1:B:721:LYS:HG2	1.91	0.51
1:B:938:ARG:O	1:B:942:ILE:HG13	2.11	0.51
1:B:947:MET:HG2	1:B:954:TYR:CE1	2.46	0.51
1:A:741:VAL:C	1:A:743:ALA:H	2.14	0.51
1:A:809:LEU:HD12	1:A:810:VAL:H	1.75	0.51
1:A:909:LEU:N	1:A:909:LEU:CD1	2.71	0.51
1:A:790:LEU:HA	1:A:793:TRP:CE3	2.46	0.51
1:A:947:MET:HA	1:A:954:TYR:HE1	1.72	0.51
2:C:342:LEU:O	2:C:343:ASN:CB	2.58	0.51
1:A:912:PRO:O	1:A:915:CYS:HB2	2.10	0.51
1:A:916:THR:C	1:A:918:ASP:H	2.14	0.51
1:A:823:THR:HG23	1:A:826:HIS:N	2.26	0.51
1:A:890:PRO:O	1:A:891:TYR:HD1	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:834:LEU:O	1:B:836:LYS:HE3	2.11	0.51
1:A:730:LYS:C	1:A:732:ASN:N	2.62	0.50
1:B:815:ALA:HA	1:B:879:THR:HG23	1.93	0.50
1:A:768:LEU:HD12	1:A:769:MET:H	1.77	0.50
1:A:790:LEU:HD23	1:A:793:TRP:HZ3	1.73	0.50
1:A:938:ARG:O	1:A:941:ILE:HG13	2.11	0.50
1:B:795:VAL:O	1:B:799:LYS:HG3	2.11	0.50
1:A:709:PRO:O	1:A:710:GLU:C	2.49	0.50
1:A:739:ALA:HA	1:A:742:MET:CB	2.33	0.50
1:B:798:ALA:O	1:B:802:ASN:N	2.43	0.50
1:A:790:LEU:CD2	1:A:793:TRP:HZ3	2.25	0.50
1:B:793:TRP:CD1	1:B:827:VAL:HG21	2.46	0.50
1:A:917:ILE:HG12	2:C:337:SER:OG	2.11	0.50
1:B:890:PRO:HB2	1:B:891:TYR:CD1	2.46	0.50
1:A:711:GLY:O	1:A:712:GLU:C	2.49	0.50
1:B:812:ARG:HH21	1:B:836:LYS:HE3	1.77	0.50
1:B:719:ALA:O	1:B:765:ILE:HA	2.12	0.50
1:B:912:PRO:HG2	1:B:915:CYS:SG	2.52	0.50
1:B:921:MET:O	1:B:925:LYS:HE3	2.12	0.50
1:B:858:ALA:HA	1:B:874:TRP:CD2	2.47	0.50
1:B:876:TYR:HA	1:B:879:THR:OG1	2.12	0.50
1:B:894:ILE:HD11	2:D:348:PRO:HB3	1.94	0.50
1:A:880:VAL:CB	1:A:923:MET:HE1	2.42	0.49
1:B:858:ALA:HB1	1:B:860:GLU:OE1	2.12	0.49
1:A:775:LEU:HD21	1:A:779:ARG:HH21	1.76	0.49
1:B:820:LEU:O	1:B:827:VAL:HG12	2.12	0.49
1:B:912:PRO:HD2	1:B:915:CYS:CB	2.41	0.49
1:B:917:ILE:HG22	2:D:337:SER:CB	2.42	0.49
1:A:753:LEU:HA	1:A:766:THR:CG2	2.43	0.49
1:A:753:LEU:HA	1:A:766:THR:HG22	1.93	0.49
1:A:787:SER:OG	1:A:951:PRO:HB2	2.13	0.49
1:A:934:ARG:HB3	1:A:935:PRO:CD	2.43	0.49
1:B:735:ILE:HD12	1:B:833:GLY:CA	2.42	0.49
1:B:793:TRP:HD1	1:B:827:VAL:CG2	2.25	0.49
1:A:845:TYR:HB3	1:A:867:TYR:HB2	1.95	0.49
1:A:879:THR:O	1:A:883:LEU:HG	2.12	0.49
1:B:793:TRP:O	1:B:796:GLN:HB2	2.12	0.49
1:B:958:GLN:O	1:B:959:GLY:O	2.30	0.49
1:A:781:HIS:HB3	1:A:784:ASN:HB2	1.95	0.49
1:B:902:ILE:O	1:B:907:GLU:HB2	2.13	0.49
1:B:821:VAL:HA	1:B:827:VAL:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:885:THR:CB	1:B:888:SER:HB2	2.43	0.49
1:A:909:LEU:HB2	1:A:927:TRP:CH2	2.48	0.49
1:B:677:GLN:O	1:B:678:ALA:HB2	2.13	0.49
1:B:919:VAL:HG21	1:B:955:LEU:CD2	2.40	0.49
1:A:683:LEU:HD11	1:A:765:ILE:HG13	1.95	0.48
1:B:814:LEU:HD23	1:B:876:TYR:CA	2.43	0.48
1:A:741:VAL:O	1:A:744:SER:N	2.45	0.48
1:A:890:PRO:C	1:A:891:TYR:CD1	2.87	0.48
1:B:748:PRO:HB2	1:B:826:HIS:NE2	2.29	0.48
1:B:846:HIS:HA	1:B:865:ARG:O	2.13	0.48
1:A:874:TRP:CZ2	1:A:903:LEU:HD21	2.48	0.48
1:B:835:ALA:O	1:B:836:LYS:HD3	2.13	0.48
1:A:790:LEU:HD23	1:A:793:TRP:CE3	2.49	0.48
1:A:830:THR:CG2	1:A:831:ASP:H	2.18	0.48
1:A:854:ILE:O	1:A:857:MET:HG3	2.13	0.48
1:A:775:LEU:CD2	1:A:779:ARG:HE	2.26	0.48
1:B:794:CYS:SG	1:B:880:VAL:HG13	2.53	0.48
1:B:939:GLU:O	1:B:942:ILE:N	2.47	0.48
1:A:762:VAL:C	1:A:763:GLN:HG3	2.34	0.48
1:B:691:ILE:HG13	1:B:705:GLY:HA2	1.96	0.48
1:B:762:VAL:HG22	1:B:763:GLN:H	1.75	0.48
1:B:868:THR:H	1:B:871:SER:CB	2.26	0.48
1:B:685:GLU:HA	1:B:688:PHE:CZ	2.48	0.48
1:A:792:ASN:O	1:A:794:CYS:N	2.47	0.48
1:A:874:TRP:C	1:A:874:TRP:CD1	2.87	0.48
1:B:930:ASP:CB	1:B:933:SER:HB2	2.44	0.48
1:A:912:PRO:HD3	1:A:920:TYR:CD1	2.49	0.48
1:B:741:VAL:CG1	1:B:809:LEU:HD21	2.43	0.47
1:B:775:LEU:CD1	1:B:779:ARG:HE	2.23	0.47
1:A:751:CYS:O	1:A:752:ARG:C	2.53	0.47
1:A:898:GLU:HA	1:A:901:SER:OG	2.14	0.47
1:B:695:GLY:O	1:B:702:VAL:N	2.47	0.47
1:B:868:THR:H	1:B:871:SER:HB3	1.79	0.47
1:A:688:PHE:HD2	1:A:720:ILE:CD1	2.27	0.47
1:A:795:VAL:HG12	1:A:799:LYS:HE3	1.96	0.47
1:A:823:THR:CG2	1:A:826:HIS:HB2	2.45	0.47
1:B:813:ASP:CG	1:B:813:ASP:O	2.51	0.47
2:D:341:TYR:N	2:D:341:TYR:CD1	2.82	0.47
1:A:810:VAL:O	1:A:835:ALA:HA	2.14	0.47
1:A:753:LEU:HD21	1:A:764:LEU:HD21	1.97	0.47
1:B:879:THR:O	1:B:883:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:909:LEU:HD13	1:B:927:TRP:CZ3	2.50	0.47
1:A:752:ARG:O	1:A:766:THR:HG22	2.14	0.47
1:B:735:ILE:HD12	1:B:833:GLY:HA2	1.95	0.47
1:B:762:VAL:CG2	1:B:763:GLN:N	2.77	0.47
1:B:947:MET:HG2	1:B:954:TYR:CD1	2.49	0.47
1:B:870:GLN:HA	1:B:873:VAL:CG2	2.45	0.47
1:A:708:ILE:O	1:A:710:GLU:N	2.48	0.46
2:D:341:TYR:CD2	2:D:347:PRO:CD	2.97	0.46
1:A:776:ASP:O	1:A:779:ARG:HB2	2.15	0.46
1:B:799:LYS:HA	1:B:941:ILE:CD1	2.45	0.46
1:B:814:LEU:HD23	1:B:876:TYR:HB2	1.96	0.46
1:B:957:ILE:N	1:B:957:ILE:CD1	2.76	0.46
1:B:745:VAL:O	1:B:745:VAL:HG23	2.16	0.46
1:A:811:HIS:O	1:A:812:ARG:HB3	2.15	0.46
1:A:718:VAL:HG21	1:A:765:ILE:HG23	1.98	0.46
1:A:707:TRP:CE3	1:A:716:ILE:HD12	2.51	0.46
1:A:721:LYS:NZ	1:A:830:THR:CG2	2.75	0.46
1:B:823:THR:HG22	1:B:826:HIS:HB3	1.96	0.46
1:B:742:MET:HA	1:B:745:VAL:HG13	1.97	0.46
1:B:891:TYR:OH	1:B:909:LEU:HD11	2.16	0.46
1:A:811:HIS:CE1	1:A:813:ASP:O	2.69	0.46
1:B:864:HIS:HB2	1:B:866:ILE:CD1	2.46	0.46
1:A:809:LEU:CD1	1:A:835:ALA:HB1	2.46	0.46
1:B:796:GLN:O	1:B:799:LYS:N	2.48	0.45
1:B:864:HIS:HB2	1:B:866:ILE:HD12	1.96	0.45
1:B:794:CYS:O	1:B:795:VAL:C	2.53	0.45
1:B:889:LYS:HG2	1:B:890:PRO:N	2.31	0.45
1:B:764:LEU:HD23	1:B:764:LEU:HA	1.74	0.45
1:B:793:TRP:HD1	1:B:827:VAL:HG21	1.81	0.45
1:A:734:GLU:O	1:A:738:GLU:N	2.35	0.45
1:A:778:VAL:HG12	1:A:785:ILE:CD1	2.45	0.45
1:A:907:GLU:C	1:A:908:ARG:HD3	2.33	0.45
1:B:745:VAL:HG21	1:B:752:ARG:HA	1.97	0.45
1:B:749:HIS:HA	1:B:828:LYS:HG2	1.97	0.45
1:B:803:TYR:O	1:B:806:ASP:HB2	2.16	0.45
1:B:830:THR:HG22	1:B:831:ASP:O	2.16	0.45
1:B:854:ILE:C	1:B:856:TRP:H	2.20	0.45
1:B:925:LYS:HE3	1:B:925:LYS:HB2	1.61	0.45
1:B:930:ASP:CG	1:B:933:SER:HB2	2.37	0.45
1:A:712:GLU:C	1:A:714:VAL:N	2.69	0.45
1:A:831:ASP:CG	1:A:833:GLY:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:803:TYR:HA	1:B:806:ASP:HB2	1.98	0.45
1:A:874:TRP:CD1	1:A:874:TRP:O	2.70	0.45
1:A:814:LEU:HD12	1:A:815:ALA:N	2.32	0.45
1:A:823:THR:C	1:A:825:GLN:N	2.68	0.45
1:B:687:GLU:O	1:B:688:PHE:CB	2.64	0.45
1:A:768:LEU:HD12	1:A:769:MET:N	2.32	0.45
1:A:911:GLN:HE21	2:C:339:PRO:HD3	1.82	0.45
1:A:917:ILE:CG1	2:C:337:SER:HB2	2.47	0.45
1:B:719:ALA:O	1:B:765:ILE:HD13	2.17	0.45
1:A:708:ILE:O	1:A:708:ILE:HG23	2.17	0.44
1:A:940:LEU:O	1:A:944:PHE:HD2	2.00	0.44
1:A:787:SER:N	1:A:957:ILE:CD1	2.81	0.44
1:B:884:MET:HE1	1:B:919:VAL:HG11	1.99	0.44
1:A:743:ALA:C	1:A:745:VAL:H	2.21	0.44
1:A:830:THR:CG2	1:A:831:ASP:N	2.75	0.44
1:A:876:TYR:CE2	1:A:940:LEU:HD13	2.52	0.44
1:A:924:VAL:O	2:C:358:TYR:HE2	1.99	0.44
1:B:939:GLU:O	1:B:940:LEU:C	2.55	0.44
1:B:690:LYS:O	1:B:690:LYS:HE3	2.18	0.44
1:B:798:ALA:HA	1:B:801:MET:HB2	1.98	0.44
1:B:891:TYR:O	1:B:892:ASP:C	2.56	0.44
1:A:774:LEU:HD12	1:A:774:LEU:O	2.18	0.44
1:B:748:PRO:HB2	1:B:826:HIS:CE1	2.53	0.44
2:D:341:TYR:CD2	2:D:347:PRO:HD3	2.52	0.44
1:A:696:SER:CB	1:A:701:THR:HG23	2.43	0.44
1:A:946:LYS:O	1:A:947:MET:C	2.54	0.44
1:B:880:VAL:HA	1:B:883:LEU:CD1	2.48	0.44
1:B:913:PRO:HD3	2:D:346:MET:SD	2.57	0.44
1:A:684:LYS:O	1:A:686:THR:N	2.42	0.44
1:A:741:VAL:C	1:A:743:ALA:N	2.70	0.44
1:B:700:GLY:O	1:B:701:THR:CG2	2.66	0.44
1:B:821:VAL:HG13	1:B:827:VAL:HG13	2.00	0.44
1:B:891:TYR:O	1:B:892:ASP:O	2.36	0.44
1:A:753:LEU:CD1	1:A:764:LEU:HD22	2.43	0.44
1:A:891:TYR:O	1:A:892:ASP:C	2.56	0.44
1:B:881:TRP:CZ2	1:B:885:THR:HG21	2.53	0.44
1:B:891:TYR:CZ	1:B:909:LEU:HG	2.53	0.44
1:B:770:PRO:HG2	1:B:771:PHE:H	1.82	0.43
1:B:873:VAL:O	1:B:874:TRP:C	2.55	0.43
1:A:741:VAL:O	1:A:743:ALA:N	2.51	0.43
1:A:855:LYS:HG2	1:A:899:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:874:TRP:CZ3	1:B:927:TRP:HA	2.53	0.43
1:A:787:SER:O	1:A:788:GLN:C	2.56	0.43
1:A:852:VAL:O	1:A:853:PRO:C	2.57	0.43
1:A:756:ILE:HG13	1:A:763:GLN:O	2.19	0.43
1:A:775:LEU:O	1:A:779:ARG:HD2	2.17	0.43
1:B:796:GLN:OE1	1:B:827:VAL:HG23	2.18	0.43
1:B:872:ASP:O	1:B:873:VAL:C	2.57	0.43
1:A:685:GLU:O	1:A:686:THR:HG23	2.18	0.43
1:A:711:GLY:O	1:A:713:LYS:N	2.51	0.43
1:A:811:HIS:O	1:A:812:ARG:CB	2.66	0.43
1:A:880:VAL:O	1:A:881:TRP:C	2.56	0.43
1:B:912:PRO:HA	1:B:913:PRO:HD3	1.90	0.43
1:A:707:TRP:O	1:A:709:PRO:HD3	2.19	0.43
1:A:716:ILE:HA	1:A:717:PRO:HD3	1.66	0.43
1:B:935:PRO:HA	1:B:939:GLU:OE1	2.19	0.43
1:A:707:TRP:N	1:A:716:ILE:O	2.49	0.43
1:B:959:GLY:C	1:B:961:GLU:H	2.21	0.43
1:A:773:CYS:HA	1:A:819:VAL:O	2.19	0.43
1:A:788:GLN:NE2	1:A:788:GLN:CA	2.80	0.43
1:B:854:ILE:C	1:B:856:TRP:N	2.72	0.43
1:B:924:VAL:O	1:B:927:TRP:N	2.40	0.43
1:A:940:LEU:O	1:A:944:PHE:HB2	2.18	0.42
1:B:810:VAL:HG12	1:B:810:VAL:O	2.18	0.42
1:B:903:LEU:HG	1:B:908:ARG:HH12	1.85	0.42
1:A:748:PRO:HB2	1:A:826:HIS:NE2	2.34	0.42
1:A:759:THR:C	1:A:761:THR:H	2.23	0.42
1:A:787:SER:CB	1:A:951:PRO:HB2	2.49	0.42
1:A:944:PHE:C	1:A:946:LYS:H	2.22	0.42
1:B:691:ILE:HG22	1:B:692:LYS:N	2.34	0.42
1:B:911:GLN:HA	1:B:920:TYR:CD1	2.54	0.42
1:B:951:PRO:HG2	1:B:952:GLN:H	1.84	0.42
2:D:339:PRO:HB2	2:D:341:TYR:CD1	2.51	0.42
1:A:777:TYR:CE1	1:A:781:HIS:CD2	3.08	0.42
1:A:791:LEU:O	1:A:795:VAL:HG23	2.19	0.42
1:A:906:GLY:HA2	1:A:908:ARG:NH1	2.34	0.42
1:A:722:GLU:CA	1:A:763:GLN:HG2	2.47	0.42
1:A:813:ASP:HB2	1:A:852:VAL:HG22	2.02	0.42
1:A:876:TYR:CD2	1:A:940:LEU:HD13	2.54	0.42
1:A:953:ARG:O	1:A:953:ARG:HG2	2.19	0.42
1:A:764:LEU:HD23	1:A:764:LEU:HA	1.88	0.42
1:B:702:VAL:CG1	1:B:703:TYR:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:881:TRP:CZ3	1:B:888:SER:O	2.73	0.42
2:C:354:PRO:HB2	2:D:339:PRO:HA	2.02	0.42
1:A:777:TYR:CD1	1:A:781:HIS:CD2	3.07	0.42
1:A:788:GLN:O	1:A:792:ASN:ND2	2.52	0.42
1:A:890:PRO:O	1:A:891:TYR:CD1	2.71	0.42
1:B:770:PRO:HG2	1:B:771:PHE:N	2.34	0.42
1:B:788:GLN:HE21	1:B:792:ASN:ND2	2.14	0.42
1:A:819:VAL:CG1	1:A:828:LYS:O	2.68	0.41
1:A:823:THR:C	1:A:825:GLN:H	2.22	0.41
1:A:874:TRP:O	1:A:874:TRP:HD1	2.03	0.41
1:B:916:THR:HG23	1:B:954:TYR:O	2.19	0.41
2:D:354:PRO:O	2:D:355:ASP:C	2.56	0.41
1:A:819:VAL:HG12	1:A:828:LYS:O	2.19	0.41
1:B:731:ALA:C	1:B:733:LYS:N	2.73	0.41
1:B:870:GLN:O	1:B:873:VAL:HB	2.20	0.41
1:B:880:VAL:HG12	1:B:884:MET:CE	2.50	0.41
1:A:785:ILE:HG21	1:A:790:LEU:HG	2.03	0.41
1:B:914:ILE:O	1:B:914:ILE:HG13	2.20	0.41
1:B:912:PRO:CG	1:B:915:CYS:SG	3.09	0.41
1:A:859:LEU:HD12	1:A:859:LEU:HA	1.71	0.41
1:A:876:TYR:CE1	1:A:880:VAL:CG2	3.04	0.41
1:A:878:VAL:O	1:A:881:TRP:HB3	2.19	0.41
1:A:920:TYR:CE2	1:A:924:VAL:HG21	2.56	0.41
1:B:690:LYS:O	1:B:690:LYS:HD2	2.21	0.41
1:B:748:PRO:O	1:B:828:LYS:HG2	2.21	0.41
1:A:877:GLY:O	1:A:923:MET:CE	2.69	0.41
1:A:885:THR:HB	1:A:888:SER:OG	2.21	0.41
1:B:815:ALA:CA	1:B:879:THR:HG23	2.50	0.41
1:A:770:PRO:CG	1:A:771:PHE:H	2.31	0.41
1:A:904:GLU:C	1:A:906:GLY:H	2.25	0.41
1:A:957:ILE:H	1:A:957:ILE:HG13	1.77	0.41
2:D:341:TYR:CE2	2:D:347:PRO:HD3	2.52	0.41
2:D:341:TYR:CD2	2:D:345:VAL:O	2.68	0.41
2:D:346:MET:HA	2:D:347:PRO:HD2	1.81	0.41
1:A:788:GLN:CG	1:A:789:TYR:N	2.83	0.41
1:A:917:ILE:HG23	2:C:337:SER:O	2.21	0.41
1:B:784:ASN:HD22	1:B:784:ASN:HA	1.55	0.41
1:B:909:LEU:H	1:B:909:LEU:CD1	2.32	0.41
1:A:796:GLN:HA	1:A:799:LYS:HD2	2.04	0.40
1:A:916:THR:HA	2:C:337:SER:O	2.21	0.40
1:B:756:ILE:O	1:B:756:ILE:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:341:TYR:N	2:D:341:TYR:HD1	2.18	0.40
1:A:890:PRO:O	1:A:891:TYR:HB2	2.22	0.40
1:B:742:MET:HA	1:B:745:VAL:CG1	2.51	0.40
1:B:771:PHE:HD2	1:B:821:VAL:O	2.04	0.40
1:B:774:LEU:O	1:B:777:TYR:HB3	2.21	0.40
1:B:790:LEU:HD23	1:B:793:TRP:HZ3	1.86	0.40
1:A:850:GLY:O	1:A:851:LYS:HB3	2.22	0.40
1:B:793:TRP:CD1	1:B:827:VAL:CG2	3.02	0.40
1:B:855:LYS:NZ	1:B:889:LYS:HE2	2.35	0.40
2:C:346:MET:HA	2:C:347:PRO:HD2	1.96	0.40
1:A:762:VAL:HG22	1:A:763:GLN:N	2.37	0.40
1:A:777:TYR:C	1:A:779:ARG:H	2.24	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	274/330 (83%)	188 (69%)	57 (21%)	29 (11%)	0 7
1	B	259/330 (78%)	183 (71%)	54 (21%)	22 (8%)	1 9
2	C	25/65 (38%)	21 (84%)	3 (12%)	1 (4%)	3 24
2	D	24/65 (37%)	15 (62%)	8 (33%)	1 (4%)	3 23
All	All	582/790 (74%)	407 (70%)	122 (21%)	53 (9%)	1 8

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	713	LYS
1	A	730	LYS
1	A	751	CYS

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Mol	Chain	Res	Type
1	A	788	GLN
1	A	835	ALA
1	A	840	ALA
1	A	851	LYS
1	B	678	ALA
1	B	679	LEU
1	B	767	GLN
1	B	892	ASP
1	B	959	GLY
2	C	343	ASN
2	D	345	VAL
1	A	685	GLU
1	A	712	GLU
1	A	767	GLN
1	A	770	PRO
1	A	836	LYS
1	A	895	PRO
1	B	691	ILE
1	B	732	ASN
1	B	873	VAL
1	A	710	GLU
1	A	735	ILE
1	A	792	ASN
1	A	808	ARG
1	A	852	VAL
1	A	858	ALA
1	A	892	ASP
1	B	688	PHE
1	B	768	LEU
1	B	815	ALA
1	B	855	LYS
1	A	679	LEU
1	A	742	MET
1	A	744	SER
1	A	793	TRP
1	B	687	GLU
1	B	770	PRO
1	A	676	ASN
1	A	709	PRO
1	A	855	LYS
1	B	680	LEU
1	B	685	GLU

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Mol	Chain	Res	Type
1	B	885	THR
1	B	951	PRO
1	B	960	ASP
1	B	717	PRO
1	B	797	ILE
1	B	913	PRO
1	A	917	ILE
1	A	691	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	203/288 (70%)	188 (93%)	15 (7%)	13	44
1	B	200/288 (69%)	184 (92%)	16 (8%)	12	41
2	C	18/58 (31%)	18 (100%)	0	100	100
2	D	16/58 (28%)	14 (88%)	2 (12%)	4	23
All	All	437/692 (63%)	404 (92%)	33 (8%)	13	43

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	745	VAL
1	A	761	THR
1	A	766	THR
1	A	809	LEU
1	A	814	LEU
1	A	823	THR
1	A	827	VAL
1	A	834	LEU
1	A	857	MET
1	A	865	ARG
1	A	895	PRO
1	A	901	SER
1	A	913	PRO

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Mol	Chain	Res	Type
1	A	918	ASP
1	A	957	ILE
1	B	690	LYS
1	B	702	VAL
1	B	707	TRP
1	B	723	LEU
1	B	734	GLU
1	B	741	VAL
1	B	751	CYS
1	B	784	ASN
1	B	827	VAL
1	B	862	ILE
1	B	875	SER
1	B	879	THR
1	B	909	LEU
1	B	914	ILE
1	B	932	ASP
1	B	957	ILE
2	D	341	TYR
2	D	346	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	788	GLN
1	A	792	ASN
1	A	911	GLN
1	B	749	HIS
1	B	781	HIS
1	B	784	ASN
1	B	788	GLN
1	B	802	ASN
1	B	811	HIS
1	B	911	GLN

5.3.3 RNA (i)

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	280/330 (84%)	-0.38	1 (0%)	92	90	24, 62, 106, 126	0
1	B	269/330 (81%)	-0.28	2 (0%)	87	83	41, 71, 102, 111	0
2	C	27/65 (41%)	0.00	0	100	100	71, 84, 98, 100	0
2	D	26/65 (40%)	-0.37	0	100	100	68, 83, 92, 102	0
All	All	602/790 (76%)	-0.32	3 (0%)	91	88	24, 70, 102, 126	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	953	ARG	2.2
1	B	952	GLN	2.2
1	A	676	ASN	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.