Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:37 AM GMT

PDB ID	:	2RFE
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	:	2.90 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:

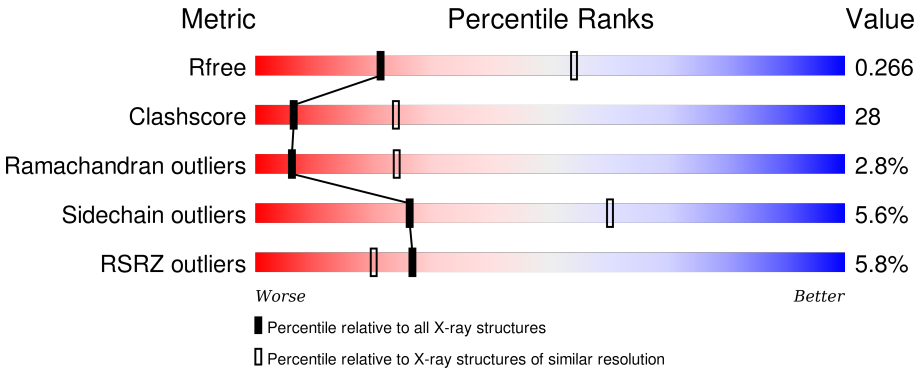
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 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.



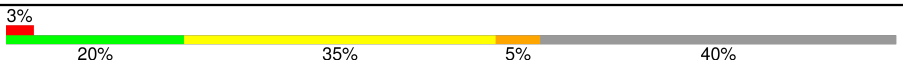
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	324	2% 45% 40% 12%
1	B	324	3% 45% 35% 16%
1	C	324	8% 43% 35% 19%
1	D	324	7% 49% 35% 14%
2	E	40	5% 38% 23% 5% 35%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	40	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8889 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	286	Total	C	N	O	S	0	0	0
			2210	1426	371	398	15			
1	B	273	Total	C	N	O	S	0	0	0
			2116	1367	358	376	15			
1	C	262	Total	C	N	O	S	0	0	0
			2028	1309	344	360	15			
1	D	278	Total	C	N	O	S	0	0	0
			2130	1376	358	381	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	675	GLY	-	EXPRESSION TAG	UNP P00533
A	676	ALA	-	EXPRESSION TAG	UNP P00533
A	677	MET	-	EXPRESSION TAG	UNP P00533
A	799	GLU	LYS	ENGINEERED	UNP P00533
B	675	GLY	-	EXPRESSION TAG	UNP P00533
B	676	ALA	-	EXPRESSION TAG	UNP P00533
B	677	MET	-	EXPRESSION TAG	UNP P00533
B	799	GLU	LYS	ENGINEERED	UNP P00533
C	675	GLY	-	EXPRESSION TAG	UNP P00533
C	676	ALA	-	EXPRESSION TAG	UNP P00533
C	677	MET	-	EXPRESSION TAG	UNP P00533
C	799	GLU	LYS	ENGINEERED	UNP P00533
D	675	GLY	-	EXPRESSION TAG	UNP P00533
D	676	ALA	-	EXPRESSION TAG	UNP P00533
D	677	MET	-	EXPRESSION TAG	UNP P00533
D	799	GLU	LYS	ENGINEERED	UNP P00533

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	26	Total	C	N	O	S	0	0	0
			190	122	29	38	1			
2	F	24	Total	C	N	O	S	0	0	0
			179	116	27	35	1			

- Molecule 3 is water.

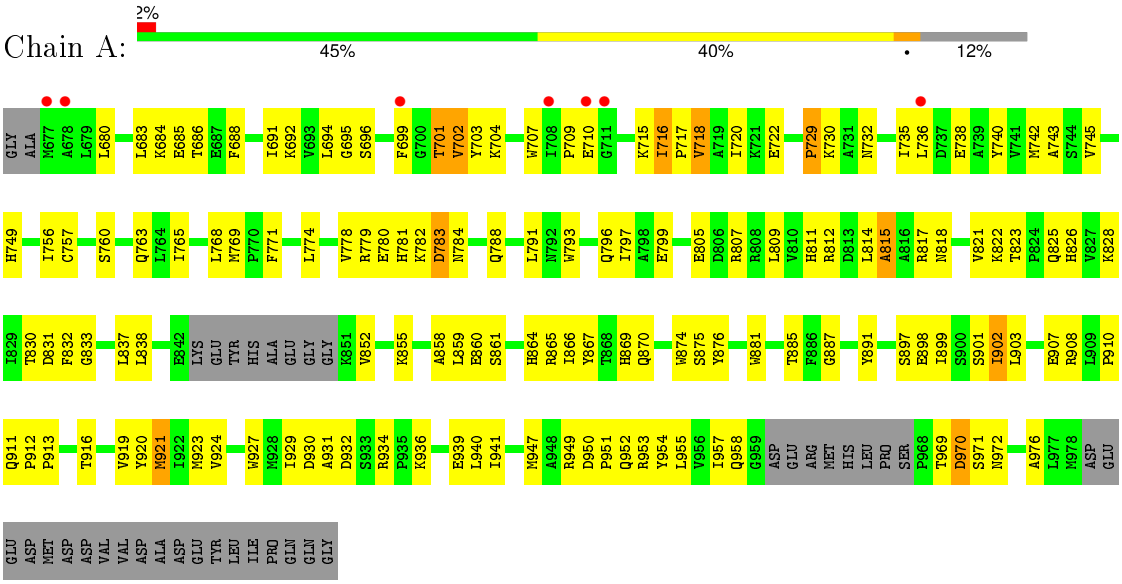
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		
3	B	7	Total	O	0	0
			7	7		
3	C	9	Total	O	0	0
			9	9		
3	D	7	Total	O	0	0
			7	7		
3	E	1	Total	O	0	0
			1	1		

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.

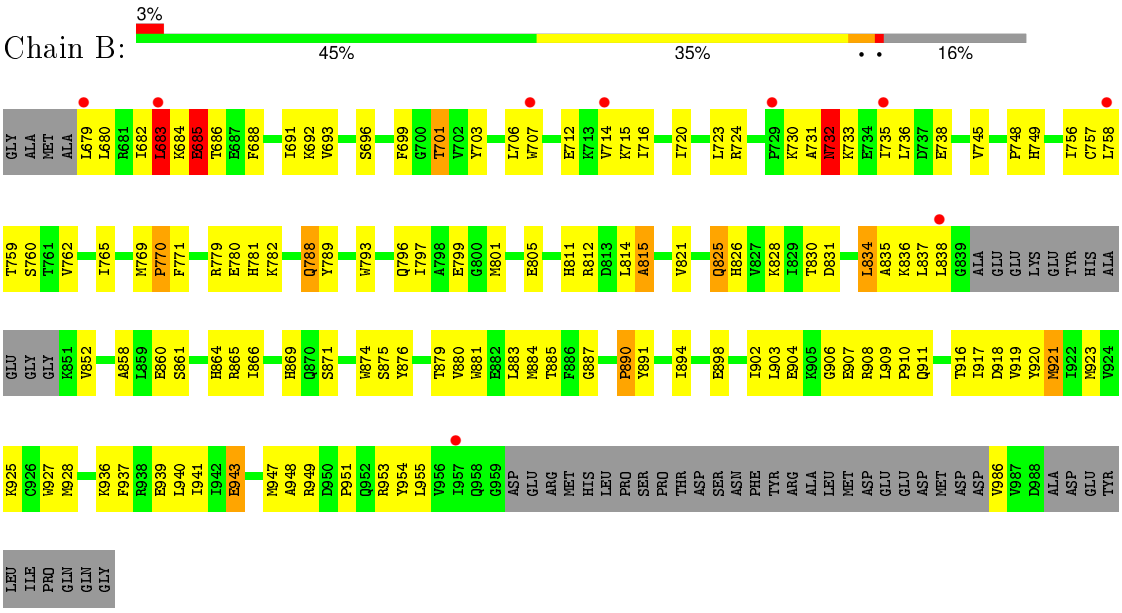
- Molecule 1: Epidermal growth factor receptor

Chain A:



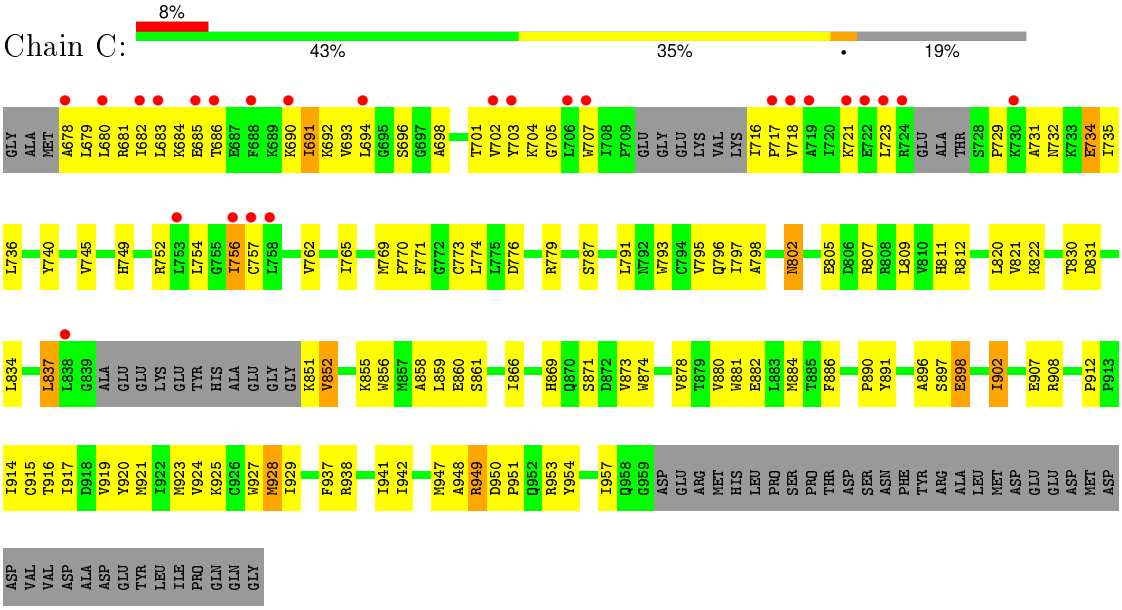
- Molecule 1: Epidermal growth factor receptor

Chain B:



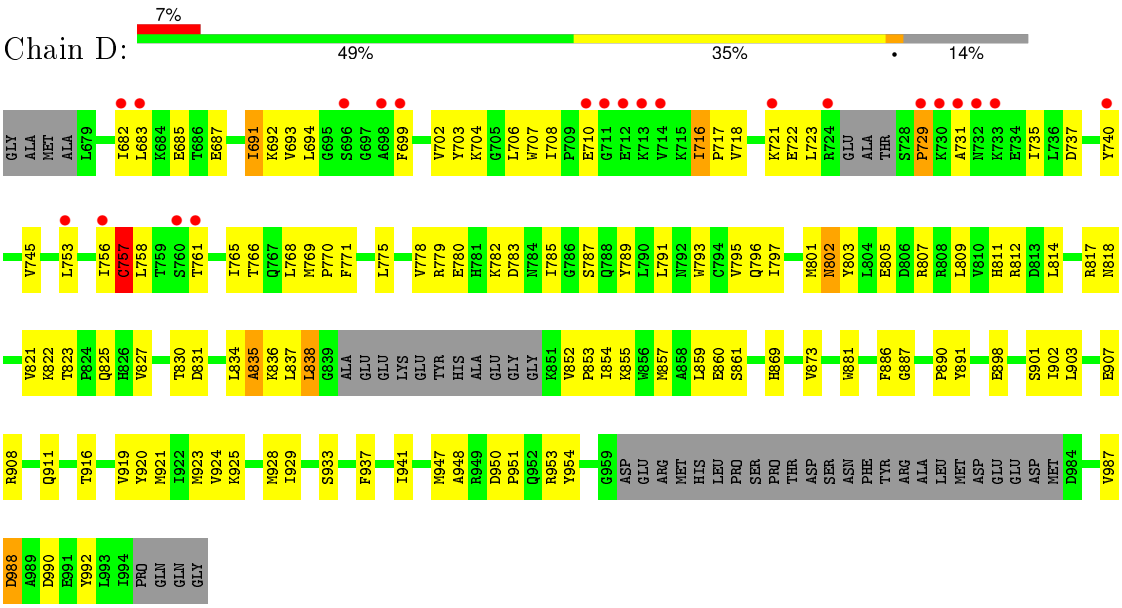
• Molecule 1: Epidermal growth factor receptor

Chain C:



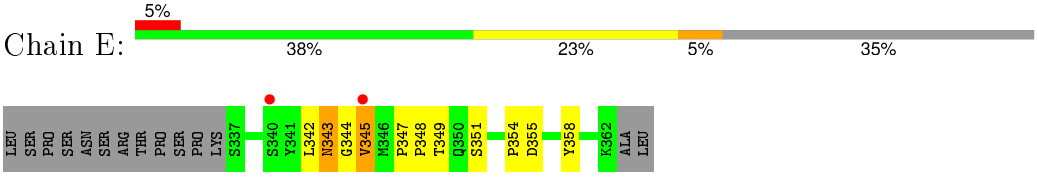
• Molecule 1: Epidermal growth factor receptor

Chain D:



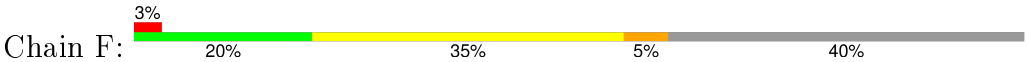
• Molecule 2: ERBB receptor feedback inhibitor 1

Chain E:



• Molecule 2: ERBB receptor feedback inhibitor 1

Chain F:




LEU
SER
PRO
SER
ASN
SER
ARG
THR
PRO
SER
PRO
LYS
S337
L338
P339
S340
Y341
L342
N343
G344
V345
M346
P347
P348
T349
Q350
A353
P354
K357
Y358
V359
S360
SER
LYS
ALA
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.51Å 98.42Å 101.50Å 90.00° 112.59° 90.00°	Depositor
Resolution (Å)	49.85 – 2.90 49.84 – 2.91	Depositor EDS
% Data completeness (in resolution range)	82.6 (49.85-2.90) 83.4 (49.84-2.91)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.271 0.227 , 0.266	Depositor DCC
R_{free} test set	1514 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	46.2	Xtriage
Anisotropy	0.864	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 58.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 32539 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8889	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% 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	0.45	0/2258	0.67	1/3069 (0.0%)
1	B	0.43	0/2161	0.68	0/2935
1	C	0.45	0/2071	0.68	1/2812 (0.0%)
1	D	0.41	0/2175	0.64	1/2959 (0.0%)
2	E	0.53	0/197	0.82	0/271
2	F	0.49	0/186	0.67	0/256
All	All	0.44	0/9048	0.67	3/12302 (0.0%)

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	C	729	PRO	N-CA-CB	5.83	110.30	103.30
1	A	729	PRO	N-CA-CB	5.71	110.15	103.30
1	D	729	PRO	N-CA-CB	5.57	109.98	103.30

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	2210	0	2171	117	0
1	B	2116	0	2108	131	0
1	C	2028	0	2000	119	0
1	D	2130	0	2078	111	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	190	0	174	9	0
2	F	179	0	167	19	0
3	A	12	0	0	0	0
3	B	7	0	0	0	0
3	C	9	0	0	0	0
3	D	7	0	0	0	0
3	E	1	0	0	0	0
All	All	8889	0	8698	483	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 28.

All (483) 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:949:ARG:HG2	1:B:826:HIS:HB2	1.41	1.03
1:D:769:MET:HE1	1:D:822:LYS:HB2	1.45	0.98
1:A:716:ILE:H	1:A:716:ILE:HD13	1.31	0.94
1:D:716:ILE:HG22	1:D:987:VAL:O	1.69	0.93
1:D:707:TRP:HB3	1:D:716:ILE:HG13	1.54	0.89
1:C:949:ARG:HG2	1:C:949:ARG:HH11	1.34	0.89
1:C:690:LYS:HD2	1:C:703:TYR:CD1	2.08	0.88
1:C:769:MET:HE3	1:C:822:LYS:HA	1.54	0.88
1:B:683:LEU:H	1:B:683:LEU:HD23	1.36	0.88
1:B:691:ILE:HD11	1:B:706:LEU:HG	1.56	0.87
1:C:683:LEU:HD12	1:C:765:ILE:HG13	1.59	0.84
1:C:680:LEU:HD11	1:C:756:ILE:HG22	1.58	0.83
1:B:696:SER:HB2	1:B:701:THR:HG23	1.59	0.83
1:D:771:PHE:HB2	1:D:821:VAL:HB	1.59	0.83
1:C:680:LEU:HD12	1:C:681:ARG:H	1.44	0.82
1:D:699:PHE:CD1	1:D:721:LYS:HE3	2.15	0.82
1:A:699:PHE:HD2	1:A:838:LEU:HD12	1.44	0.82
1:A:837:LEU:O	1:A:837:LEU:HD23	1.79	0.81
1:C:716:ILE:CB	1:C:717:PRO:HD2	2.09	0.80
1:C:802:ASN:HB2	1:C:941:ILE:HD11	1.65	0.78
1:D:723:LEU:O	1:D:761:THR:HG23	1.84	0.77
1:B:679:LEU:HG	1:B:680:LEU:N	1.98	0.77
1:B:906:GLY:HA2	2:F:358:TYR:O	1.85	0.77
1:A:699:PHE:CD2	1:A:838:LEU:HD12	2.19	0.77
1:A:921:MET:CE	1:A:921:MET:HA	2.15	0.75
1:D:722:GLU:HG2	1:D:761:THR:HG21	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:953:ARG:HG2	1:B:953:ARG:O	1.88	0.74
1:B:861:SER:O	1:B:865:ARG:HD3	1.88	0.73
1:A:903:LEU:HD12	1:A:908:ARG:NH1	2.04	0.73
1:B:780:GLU:HG2	1:B:780:GLU:O	1.88	0.72
1:B:683:LEU:HD11	1:B:765:ILE:HD12	1.71	0.72
1:C:690:LYS:HD2	1:C:703:TYR:CE1	2.25	0.71
1:C:723:LEU:HD12	1:C:762:VAL:HG11	1.72	0.71
1:A:780:GLU:OE2	1:A:971:SER:HA	1.90	0.71
1:D:802:ASN:HB2	1:D:941:ILE:HD11	1.72	0.71
1:A:881:TRP:HA	1:A:923:MET:HE1	1.72	0.71
1:B:916:THR:HG23	1:B:954:TYR:O	1.91	0.71
1:A:793:TRP:O	1:A:797:ILE:HG13	1.91	0.71
1:B:928:MET:HG2	2:F:358:TYR:CE2	2.26	0.70
1:A:716:ILE:N	1:A:716:ILE:HD13	2.04	0.70
1:C:756:ILE:HG12	1:C:757:CYS:N	2.06	0.70
1:D:683:LEU:HD21	1:D:707:TRP:HZ2	1.54	0.70
1:A:805:GLU:HG3	1:A:869:HIS:CG	2.26	0.70
1:D:898:GLU:O	1:D:902:ILE:HG23	1.92	0.70
1:D:855:LYS:HD3	1:D:891:TYR:HB2	1.73	0.70
1:C:690:LYS:HD2	1:C:703:TYR:HD1	1.57	0.69
1:C:731:ALA:HB3	1:C:734:GLU:CD	2.11	0.69
1:C:680:LEU:HD21	1:C:756:ILE:CG2	2.22	0.69
1:A:771:PHE:HB2	1:A:821:VAL:HB	1.75	0.69
1:A:953:ARG:HG2	1:A:953:ARG:O	1.91	0.69
1:D:817:ARG:C	1:D:818:ASN:HD22	1.96	0.69
1:C:771:PHE:HB2	1:C:821:VAL:HB	1.74	0.69
1:C:917:ILE:O	1:C:921:MET:HG3	1.93	0.69
1:C:701:THR:HG22	1:C:703:TYR:CE2	2.28	0.69
1:C:680:LEU:HD21	1:C:756:ILE:HG21	1.74	0.68
1:A:695:GLY:O	1:A:702:VAL:HG23	1.93	0.68
1:D:756:ILE:HG12	1:D:757:CYS:H	1.59	0.68
2:E:342:LEU:O	2:E:343:ASN:HB2	1.94	0.67
1:D:683:LEU:HD12	1:D:765:ILE:HG13	1.77	0.67
1:C:937:PHE:O	1:C:941:ILE:HG13	1.95	0.67
1:D:691:ILE:HG22	1:D:692:LYS:N	2.07	0.67
1:A:826:HIS:HB2	1:B:949:ARG:HG2	1.77	0.67
1:A:718:VAL:O	1:A:768:LEU:HB2	1.94	0.67
1:B:907:GLU:O	1:B:908:ARG:HD3	1.94	0.66
1:C:834:LEU:O	1:C:837:LEU:HB3	1.96	0.66
1:A:769:MET:HE1	1:A:822:LYS:HB2	1.77	0.66
1:C:769:MET:HE3	1:C:822:LYS:CA	2.23	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:837:LEU:O	1:B:837:LEU:HD23	1.96	0.66
1:B:793:TRP:O	1:B:797:ILE:HG13	1.95	0.66
1:A:720:ILE:HG12	1:A:765:ILE:HD12	1.78	0.65
1:C:701:THR:HG22	1:C:703:TYR:HE2	1.61	0.65
1:C:696:SER:HB3	1:C:701:THR:HG23	1.78	0.65
1:A:903:LEU:HD12	1:A:908:ARG:HH11	1.59	0.65
1:D:902:ILE:O	1:D:907:GLU:HB2	1.97	0.65
1:C:869:HIS:O	1:C:873:VAL:HG23	1.95	0.65
1:D:769:MET:HE1	1:D:822:LYS:CB	2.24	0.64
1:A:722:GLU:HG3	1:A:763:GLN:HG2	1.79	0.64
1:D:805:GLU:HG3	1:D:869:HIS:CG	2.33	0.64
1:D:937:PHE:O	1:D:941:ILE:HG13	1.98	0.64
1:A:730:LYS:HB2	1:A:735:ILE:HD11	1.81	0.63
1:C:683:LEU:HD22	1:C:707:TRP:HE1	1.63	0.63
1:A:811:HIS:O	1:A:812:ARG:HB2	1.97	0.63
1:A:707:TRP:HB3	1:A:716:ILE:HG12	1.81	0.62
1:A:969:THR:O	1:A:970:ASP:HB2	1.99	0.62
1:D:793:TRP:O	1:D:797:ILE:HG13	1.99	0.62
1:C:948:ALA:O	1:C:951:PRO:HD3	1.99	0.62
1:C:949:ARG:NH1	1:C:949:ARG:HG2	2.09	0.62
1:A:919:VAL:HG22	1:A:947:MET:HE2	1.82	0.62
1:B:723:LEU:N	1:B:723:LEU:HD12	2.15	0.62
1:C:805:GLU:HG3	1:C:869:HIS:CG	2.35	0.61
1:D:925:LYS:O	1:D:928:MET:HG3	1.99	0.61
1:D:791:LEU:O	1:D:795:VAL:HG23	1.99	0.61
1:B:801:MET:HB3	1:B:937:PHE:CE1	2.36	0.61
1:C:731:ALA:O	1:C:735:ILE:HG12	1.99	0.61
1:D:869:HIS:O	1:D:873:VAL:HG23	2.00	0.61
1:D:731:ALA:O	1:D:735:ILE:HG12	2.00	0.61
1:A:805:GLU:HG3	1:A:869:HIS:CD2	2.36	0.61
1:A:910:PRO:HG3	2:E:347:PRO:O	2.01	0.61
1:C:795:VAL:O	1:C:798:ALA:HB3	2.01	0.60
1:B:699:PHE:CD2	1:B:838:LEU:HD12	2.37	0.60
1:C:686:THR:HG22	1:C:686:THR:O	2.00	0.60
1:A:916:THR:HG23	1:A:954:TYR:O	2.01	0.60
1:A:949:ARG:HG2	1:B:826:HIS:CB	2.24	0.60
1:A:885:THR:HG22	1:A:912:PRO:HB3	1.82	0.60
1:B:682:ILE:O	1:B:682:ILE:HG22	2.01	0.60
1:A:874:TRP:CE3	1:A:927:TRP:HA	2.37	0.60
1:D:692:LYS:O	1:D:703:TYR:HB3	2.01	0.60
1:B:693:VAL:HG12	1:B:703:TYR:CE2	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:920:TYR:O	1:C:924:VAL:HG23	2.02	0.60
1:B:881:TRP:HA	1:B:923:MET:HE1	1.83	0.59
1:A:861:SER:O	1:A:865:ARG:HD3	2.02	0.59
1:A:696:SER:HA	1:A:701:THR:HA	1.84	0.59
1:C:856:TRP:HZ2	1:C:882:GLU:OE1	1.85	0.59
1:C:683:LEU:HD21	1:C:707:TRP:HZ2	1.68	0.59
1:A:858:ALA:HA	1:A:874:TRP:CE2	2.38	0.59
2:F:342:LEU:O	2:F:343:ASN:HB2	2.03	0.59
1:B:738:GLU:OE1	1:B:837:LEU:HA	2.03	0.59
1:B:715:LYS:O	1:B:986:VAL:HA	2.02	0.59
1:B:916:THR:HA	2:F:338:LEU:HD23	1.84	0.59
1:A:809:LEU:HD22	1:A:832:PHE:HZ	1.68	0.59
1:B:723:LEU:HD23	1:B:838:LEU:HD21	1.84	0.58
1:D:707:TRP:O	1:D:716:ILE:HG12	2.03	0.58
1:D:837:LEU:HD22	1:D:838:LEU:HD23	1.85	0.58
1:B:771:PHE:HB2	1:B:821:VAL:HB	1.86	0.58
1:A:837:LEU:O	1:A:838:LEU:HD23	2.04	0.58
1:D:779:ARG:HG2	1:D:887:GLY:HA3	1.85	0.58
1:B:779:ARG:HG2	1:B:887:GLY:HA3	1.86	0.58
1:D:756:ILE:HG12	1:D:757:CYS:N	2.20	0.57
1:B:910:PRO:HG3	2:F:347:PRO:O	2.04	0.57
1:D:881:TRP:HA	1:D:923:MET:HE1	1.85	0.57
1:A:855:LYS:HD3	1:A:891:TYR:HB2	1.84	0.57
1:D:920:TYR:O	1:D:924:VAL:HG23	2.04	0.57
1:C:691:ILE:HG22	1:C:692:LYS:N	2.20	0.57
1:C:682:ILE:HA	1:C:756:ILE:O	2.05	0.57
1:B:814:LEU:HD12	1:B:815:ALA:H	1.70	0.57
1:B:911:GLN:NE2	2:F:339:PRO:HG3	2.20	0.57
1:C:683:LEU:HD21	1:C:707:TRP:CZ2	2.39	0.57
1:B:723:LEU:CD1	1:B:723:LEU:N	2.67	0.57
1:B:858:ALA:HA	1:B:874:TRP:CD2	2.39	0.57
1:B:902:ILE:O	1:B:907:GLU:HB2	2.05	0.56
1:C:793:TRP:O	1:C:797:ILE:HG13	2.05	0.56
1:B:707:TRP:HB3	1:B:716:ILE:HB	1.87	0.56
1:B:811:HIS:O	1:B:812:ARG:HB2	2.05	0.56
1:C:902:ILE:O	1:C:907:GLU:HB2	2.06	0.56
1:D:780:GLU:HG2	1:D:780:GLU:O	2.05	0.56
1:D:902:ILE:HB	1:D:907:GLU:HG3	1.87	0.56
1:C:749:HIS:CE1	1:C:796:GLN:HG2	2.40	0.56
1:A:730:LYS:HB2	1:A:735:ILE:CD1	2.35	0.56
1:D:707:TRP:CE3	1:D:716:ILE:CD1	2.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:707:TRP:CE3	1:D:716:ILE:HD11	2.40	0.56
1:D:722:GLU:HG2	1:D:761:THR:CG2	2.35	0.56
1:B:837:LEU:O	1:B:838:LEU:HD23	2.05	0.56
1:C:762:VAL:HG13	1:C:762:VAL:O	2.06	0.55
1:B:688:PHE:HD2	1:B:720:ILE:HD13	1.71	0.55
1:A:907:GLU:OE1	2:E:351:SER:HB2	2.07	0.55
1:B:911:GLN:CD	2:F:339:PRO:HG3	2.27	0.55
1:A:817:ARG:HG3	1:A:818:ASN:OD1	2.07	0.55
1:C:716:ILE:CB	1:C:717:PRO:CD	2.83	0.55
1:B:738:GLU:OE2	1:B:836:LYS:HG2	2.07	0.55
1:B:864:HIS:CD2	1:D:693:VAL:HG11	2.42	0.55
1:D:916:THR:HG23	1:D:954:TYR:O	2.07	0.55
1:D:803:TYR:CE2	1:D:807:ARG:HD3	2.42	0.55
1:D:745:VAL:O	1:D:745:VAL:HG23	2.07	0.55
1:D:805:GLU:HG3	1:D:869:HIS:ND1	2.22	0.55
1:B:693:VAL:HG12	1:B:703:TYR:CD2	2.42	0.55
1:A:749:HIS:CE1	1:A:796:GLN:HG2	2.42	0.54
1:C:693:VAL:HG23	1:C:693:VAL:O	2.07	0.54
1:B:858:ALA:HA	1:B:874:TRP:CE2	2.43	0.54
1:A:814:LEU:HD12	1:A:815:ALA:H	1.73	0.54
1:B:928:MET:CE	2:F:357:LYS:HB3	2.38	0.54
1:B:928:MET:HE2	2:F:357:LYS:HB3	1.89	0.54
1:A:899:ILE:O	1:A:903:LEU:HB2	2.07	0.54
1:A:898:GLU:O	1:A:902:ILE:HG23	2.07	0.54
2:F:349:THR:OG1	2:F:350:GLN:N	2.40	0.54
1:C:881:TRP:HA	1:C:923:MET:HE1	1.89	0.54
1:C:736:LEU:HG	1:C:740:TYR:OH	2.08	0.54
1:D:707:TRP:HB3	1:D:716:ILE:CG1	2.32	0.54
1:C:683:LEU:CD1	1:C:765:ILE:HG13	2.34	0.54
1:D:753:LEU:HA	1:D:766:THR:HG22	1.90	0.54
1:C:694:LEU:HD11	1:C:704:LYS:HB2	1.89	0.53
1:B:948:ALA:O	1:B:951:PRO:HD3	2.08	0.53
1:C:754:LEU:HB2	1:C:765:ILE:O	2.08	0.53
1:A:720:ILE:HG12	1:A:765:ILE:CD1	2.38	0.53
1:A:860:GLU:HG2	1:A:861:SER:N	2.22	0.53
1:B:759:THR:HG22	1:B:760:SER:H	1.73	0.53
1:A:688:PHE:HD2	1:A:720:ILE:HD13	1.72	0.53
1:B:730:LYS:HD3	1:B:735:ILE:HD13	1.90	0.53
1:B:911:GLN:HA	1:B:920:TYR:CD1	2.44	0.53
1:B:758:LEU:CD2	1:B:762:VAL:HG22	2.38	0.53
1:A:814:LEU:O	1:A:815:ALA:HB2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:SER:O	1:A:876:TYR:C	2.46	0.53
1:B:921:MET:CE	1:B:921:MET:HA	2.39	0.53
1:D:950:ASP:N	1:D:951:PRO:CD	2.72	0.53
1:B:799:GLU:HA	1:B:941:ILE:HD11	1.91	0.53
1:A:799:GLU:HA	1:A:941:ILE:HD11	1.91	0.53
1:B:866:ILE:HD11	1:D:693:VAL:HB	1.90	0.53
1:B:714:VAL:O	1:B:716:ILE:HG13	2.08	0.52
1:C:769:MET:HE1	1:C:822:LYS:HB2	1.92	0.52
1:A:969:THR:HG22	1:A:969:THR:O	2.10	0.52
1:D:683:LEU:HD21	1:D:707:TRP:CZ2	2.41	0.52
1:C:902:ILE:HG13	1:C:907:GLU:HB2	1.92	0.52
1:A:774:LEU:O	1:A:778:VAL:HG13	2.10	0.52
1:A:781:HIS:O	1:A:783:ASP:N	2.43	0.52
1:C:880:VAL:O	1:C:884:MET:HG2	2.10	0.52
2:E:343:ASN:C	2:E:345:VAL:H	2.13	0.52
1:D:837:LEU:CD2	1:D:838:LEU:HD23	2.40	0.52
1:A:921:MET:HE3	1:A:924:VAL:HG21	1.91	0.52
1:D:687:GLU:HB3	1:D:708:ILE:O	2.10	0.52
1:B:815:ALA:HA	1:B:879:THR:OG1	2.10	0.51
1:B:770:PRO:HG2	1:B:771:PHE:HD2	1.75	0.51
1:B:881:TRP:CZ3	1:B:890:PRO:HA	2.45	0.51
1:C:684:LYS:C	1:C:686:THR:H	2.14	0.51
1:D:948:ALA:O	1:D:951:PRO:HD3	2.10	0.51
1:A:911:GLN:HA	1:A:920:TYR:CD1	2.46	0.51
1:C:680:LEU:CD1	1:C:756:ILE:HG22	2.37	0.51
1:D:704:LYS:HG3	1:D:768:LEU:HD22	1.91	0.51
1:A:691:ILE:HB	1:A:704:LYS:O	2.10	0.51
1:C:682:ILE:HD13	1:C:682:ILE:N	2.25	0.51
1:A:902:ILE:HG13	1:A:907:GLU:HB2	1.92	0.51
1:D:707:TRP:N	1:D:716:ILE:O	2.38	0.51
1:C:860:GLU:HG2	1:C:861:SER:N	2.26	0.51
2:F:341:TYR:CE1	2:F:347:PRO:HD2	2.46	0.51
1:C:723:LEU:HD12	1:C:762:VAL:CG1	2.37	0.51
1:C:680:LEU:CD1	1:C:681:ARG:H	2.20	0.50
1:C:949:ARG:CG	1:C:949:ARG:HH11	2.13	0.50
1:B:756:ILE:HG12	1:B:757:CYS:N	2.25	0.50
2:F:353:ALA:HA	2:F:359:VAL:HG21	1.93	0.50
1:C:679:LEU:HG	1:C:680:LEU:N	2.26	0.50
1:C:683:LEU:HD12	1:C:765:ILE:CG1	2.37	0.50
1:C:757:CYS:O	1:C:757:CYS:SG	2.69	0.50
1:D:911:GLN:HA	1:D:920:TYR:CD1	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:947:MET:HE2	1:D:954:TYR:CD2	2.45	0.50
1:C:745:VAL:HG23	1:C:745:VAL:O	2.10	0.50
1:D:835:ALA:O	1:D:836:LYS:C	2.50	0.50
1:B:871:SER:O	1:B:874:TRP:HB3	2.12	0.50
1:C:774:LEU:HD11	1:C:793:TRP:CE3	2.47	0.50
1:D:947:MET:HG2	1:D:954:TYR:CD2	2.47	0.50
1:D:822:LYS:O	1:D:823:THR:HG22	2.11	0.50
1:D:775:LEU:O	1:D:778:VAL:HG22	2.12	0.50
1:C:871:SER:O	1:C:874:TRP:HB3	2.12	0.50
1:C:680:LEU:HD12	1:C:681:ARG:N	2.19	0.50
1:A:951:PRO:CD	1:B:825:GLN:HG3	2.42	0.50
1:A:833:GLY:O	1:A:837:LEU:HB2	2.12	0.49
1:D:911:GLN:HG3	1:D:920:TYR:HB2	1.94	0.49
1:C:874:TRP:CE3	1:C:927:TRP:HA	2.47	0.49
1:A:692:LYS:NZ	1:A:976:ALA:O	2.45	0.49
1:D:859:LEU:CD2	1:D:929:ILE:HD12	2.42	0.49
1:C:717:PRO:O	1:C:718:VAL:HG13	2.12	0.49
1:B:779:ARG:HD3	1:B:887:GLY:O	2.11	0.49
1:D:822:LYS:HG2	1:D:823:THR:HG23	1.95	0.49
1:D:782:LYS:HG2	1:D:886:PHE:HB3	1.94	0.49
1:B:830:THR:OG1	1:B:831:ASP:N	2.44	0.49
1:B:831:ASP:OD1	1:B:834:LEU:HD12	2.11	0.49
1:A:680:LEU:HD13	1:A:743:ALA:HB2	1.94	0.49
1:D:928:MET:SD	1:D:933:SER:HB3	2.52	0.49
1:C:811:HIS:O	1:C:812:ARG:HB2	2.13	0.49
1:A:742:MET:O	1:A:745:VAL:HG22	2.12	0.49
1:C:770:PRO:HG2	1:C:771:PHE:HD2	1.78	0.49
1:A:921:MET:HA	1:A:921:MET:HE3	1.91	0.49
1:B:730:LYS:HB3	1:B:735:ILE:HD11	1.95	0.49
1:C:680:LEU:HD23	1:C:740:TYR:CE2	2.48	0.49
1:C:680:LEU:HD23	1:C:740:TYR:HE2	1.77	0.49
1:B:679:LEU:CG	1:B:680:LEU:N	2.73	0.49
1:A:953:ARG:CG	1:A:953:ARG:O	2.59	0.49
1:B:748:PRO:O	1:B:828:LYS:HE2	2.12	0.49
1:B:911:GLN:HA	1:B:920:TYR:CE1	2.47	0.49
1:C:898:GLU:O	1:C:902:ILE:HG23	2.12	0.49
1:B:860:GLU:HG2	1:B:861:SER:N	2.28	0.49
1:D:802:ASN:CB	1:D:941:ILE:HD11	2.43	0.49
1:D:811:HIS:O	1:D:812:ARG:HB2	2.13	0.49
1:C:925:LYS:O	1:C:928:MET:HG3	2.12	0.49
1:C:683:LEU:HD13	1:C:707:TRP:NE1	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:817:ARG:HG3	1:D:818:ASN:ND2	2.29	0.48
1:D:789:TYR:HE2	1:D:825:GLN:HE21	1.59	0.48
1:A:902:ILE:HB	1:A:907:GLU:HG3	1.94	0.48
2:E:343:ASN:O	2:E:345:VAL:N	2.46	0.48
1:B:881:TRP:CA	1:B:923:MET:HE1	2.43	0.48
1:A:812:ARG:HD3	1:A:867:TYR:CG	2.48	0.48
1:D:683:LEU:HB2	1:D:757:CYS:HB2	1.95	0.48
1:D:718:VAL:C	1:D:768:LEU:HB2	2.34	0.48
1:D:723:LEU:O	1:D:761:THR:CG2	2.60	0.48
1:B:904:GLU:HB3	2:F:360:SER:HB3	1.96	0.48
1:B:928:MET:HG2	2:F:358:TYR:HE2	1.76	0.48
1:B:954:TYR:O	1:B:955:LEU:HD23	2.14	0.48
1:C:694:LEU:HD21	1:C:704:LYS:HB2	1.95	0.48
1:C:858:ALA:HA	1:C:874:TRP:CE2	2.49	0.48
1:A:683:LEU:HD21	1:A:707:TRP:CZ2	2.49	0.48
1:D:911:GLN:HG3	1:D:920:TYR:CG	2.48	0.48
1:A:924:VAL:HA	1:A:927:TRP:CE3	2.49	0.48
1:A:899:ILE:HG22	1:A:903:LEU:HD22	1.96	0.48
1:B:911:GLN:CG	2:F:339:PRO:HG3	2.44	0.48
1:A:684:LYS:O	1:A:686:THR:N	2.42	0.48
1:D:859:LEU:HD23	1:D:929:ILE:HG23	1.96	0.47
1:A:780:GLU:HG2	1:A:780:GLU:O	2.14	0.47
1:C:684:LYS:O	1:C:686:THR:N	2.48	0.47
1:D:947:MET:CE	1:D:954:TYR:CD2	2.97	0.47
1:B:756:ILE:HG12	1:B:757:CYS:H	1.79	0.47
1:B:732:ASN:O	1:B:736:LEU:HB2	2.15	0.47
1:D:881:TRP:CA	1:D:923:MET:HE1	2.44	0.47
1:C:949:ARG:NH1	1:C:949:ARG:CG	2.74	0.47
1:B:801:MET:SD	1:B:814:LEU:HD22	2.55	0.47
1:B:879:THR:O	1:B:883:LEU:HG	2.15	0.47
1:D:807:ARG:O	1:D:809:LEU:HG	2.15	0.47
1:B:936:LYS:O	1:B:939:GLU:HB2	2.15	0.47
1:D:693:VAL:O	1:D:693:VAL:HG13	2.15	0.47
1:B:805:GLU:HG3	1:B:869:HIS:CG	2.49	0.47
1:D:830:THR:O	1:D:831:ASP:HB2	2.15	0.47
1:C:683:LEU:O	1:C:757:CYS:HB2	2.15	0.47
1:B:917:ILE:HG23	1:B:918:ASP:N	2.29	0.47
1:A:683:LEU:HD22	1:A:707:TRP:HE1	1.80	0.46
1:B:925:LYS:O	1:B:928:MET:HG3	2.15	0.46
1:A:951:PRO:HD2	1:B:825:GLN:HG3	1.96	0.46
1:C:902:ILE:HB	1:C:907:GLU:HG3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:GLN:HA	1:A:958:GLN:OE1	2.14	0.46
2:E:354:PRO:O	2:E:355:ASP:C	2.52	0.46
1:A:858:ALA:HA	1:A:874:TRP:CD2	2.50	0.46
1:A:709:PRO:O	1:A:710:GLU:C	2.54	0.46
1:D:834:LEU:O	1:D:835:ALA:C	2.53	0.46
1:A:769:MET:CE	1:A:822:LYS:HB2	2.45	0.46
1:C:861:SER:HA	1:C:866:ILE:H	1.80	0.46
1:C:736:LEU:HG	1:C:740:TYR:CZ	2.51	0.46
1:B:730:LYS:O	1:B:731:ALA:C	2.54	0.46
1:A:694:LEU:HD11	1:A:704:LYS:HB2	1.97	0.46
1:C:798:ALA:HB1	1:C:941:ILE:HG12	1.98	0.46
1:A:876:TYR:CD2	1:A:940:LEU:HD13	2.50	0.46
1:A:684:LYS:C	1:A:686:THR:H	2.17	0.46
1:D:682:ILE:HG23	1:D:682:ILE:O	2.16	0.46
1:D:683:LEU:HD13	1:D:707:TRP:HE1	1.82	0.45
1:C:802:ASN:CB	1:C:941:ILE:HD11	2.39	0.45
2:F:341:TYR:HE1	2:F:346:MET:HG3	1.80	0.45
1:D:853:PRO:O	1:D:857:MET:HG3	2.16	0.45
1:B:876:TYR:O	1:B:880:VAL:HG23	2.16	0.45
1:B:723:LEU:CD1	1:B:723:LEU:H	2.28	0.45
1:B:801:MET:HB3	1:B:937:PHE:CZ	2.51	0.45
1:C:881:TRP:CZ3	1:C:890:PRO:HA	2.52	0.45
1:A:859:LEU:HD23	1:A:929:ILE:HD12	1.98	0.45
1:A:954:TYR:O	1:A:955:LEU:HD23	2.17	0.45
1:D:775:LEU:O	1:D:779:ARG:HG3	2.16	0.45
1:C:691:ILE:HB	1:C:705:GLY:HA2	1.99	0.45
1:D:722:GLU:CG	1:D:761:THR:CG2	2.94	0.45
1:B:679:LEU:HG	1:B:680:LEU:H	1.76	0.45
1:D:837:LEU:HD23	1:D:837:LEU:C	2.37	0.45
1:D:903:LEU:HD12	1:D:908:ARG:HH11	1.82	0.45
1:D:694:LEU:HB2	1:D:702:VAL:HG12	1.99	0.45
1:D:903:LEU:HD12	1:D:903:LEU:HA	1.77	0.45
1:D:796:GLN:OE1	1:D:827:VAL:HG22	2.17	0.45
1:D:801:MET:SD	1:D:814:LEU:HD22	2.57	0.45
1:C:769:MET:HA	1:C:770:PRO:HD2	1.77	0.44
1:A:736:LEU:O	1:A:740:TYR:HD1	2.00	0.44
1:B:749:HIS:CE1	1:B:796:GLN:HG2	2.52	0.44
1:A:870:GLN:HA	1:A:870:GLN:OE1	2.16	0.44
1:A:811:HIS:O	1:A:812:ARG:CB	2.65	0.44
1:C:907:GLU:C	1:C:908:ARG:HG2	2.37	0.44
1:D:771:PHE:CD2	1:D:771:PHE:N	2.84	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:925:LYS:HE3	1:D:925:LYS:HB2	1.76	0.44
2:E:355:ASP:C	2:E:355:ASP:OD1	2.56	0.44
1:D:769:MET:HA	1:D:770:PRO:HD2	1.77	0.44
1:D:854:ILE:HD13	1:D:857:MET:SD	2.58	0.44
1:C:953:ARG:HD3	1:C:954:TYR:CE1	2.53	0.44
1:C:702:VAL:O	1:C:703:TYR:HD2	2.01	0.44
1:C:771:PHE:CD2	1:C:771:PHE:N	2.86	0.44
1:B:953:ARG:CG	1:B:953:ARG:O	2.63	0.44
1:D:737:ASP:O	1:D:740:TYR:HB2	2.18	0.44
1:B:683:LEU:H	1:B:683:LEU:CD2	2.15	0.44
1:B:874:TRP:CE3	1:B:927:TRP:HA	2.53	0.44
1:B:758:LEU:HD22	1:B:762:VAL:HG22	2.00	0.44
1:A:907:GLU:O	1:A:908:ARG:HD3	2.17	0.44
1:B:936:LYS:HG2	1:B:939:GLU:OE2	2.18	0.44
1:A:732:ASN:O	1:A:736:LEU:HB2	2.18	0.43
1:B:903:LEU:HD12	1:B:903:LEU:HA	1.89	0.43
1:C:773:CYS:HA	1:C:820:LEU:HD23	2.00	0.43
1:C:769:MET:CE	1:C:822:LYS:CA	2.94	0.43
1:A:864:HIS:HB2	1:A:866:ILE:HG13	1.99	0.43
1:C:938:ARG:O	1:C:942:ILE:HG13	2.18	0.43
1:B:723:LEU:CD2	1:B:837:LEU:HD22	2.48	0.43
1:B:881:TRP:HB2	1:B:923:MET:CE	2.48	0.43
1:C:774:LEU:HD11	1:C:793:TRP:CZ3	2.54	0.43
1:C:947:MET:CE	1:C:954:TYR:CD2	3.01	0.43
1:D:860:GLU:HG2	1:D:861:SER:N	2.34	0.43
1:C:851:LYS:HG2	1:C:852:VAL:N	2.33	0.43
1:C:950:ASP:N	1:C:951:PRO:CD	2.81	0.43
1:A:861:SER:HA	1:A:866:ILE:H	1.83	0.43
1:B:826:HIS:NE2	1:B:828:LYS:HE3	2.34	0.43
1:A:912:PRO:HA	1:A:913:PRO:HD3	1.91	0.43
1:D:778:VAL:HA	1:D:785:ILE:CD1	2.48	0.43
1:A:707:TRP:O	1:A:709:PRO:HD3	2.19	0.43
1:C:769:MET:CE	1:C:822:LYS:HB2	2.49	0.43
1:B:947:MET:HE2	1:B:954:TYR:HD2	1.83	0.43
1:A:969:THR:O	1:A:970:ASP:CB	2.65	0.43
1:A:738:GLU:O	1:A:742:MET:HG3	2.19	0.43
1:A:936:LYS:O	1:A:939:GLU:HB2	2.19	0.43
1:B:891:TYR:HB3	1:B:894:ILE:HD12	2.00	0.43
1:C:834:LEU:HD23	1:C:834:LEU:HA	1.86	0.43
2:F:341:TYR:O	2:F:343:ASN:N	2.52	0.43
1:B:880:VAL:O	1:B:884:MET:HG2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:891:TYR:CZ	1:B:909:LEU:HG	2.53	0.43
1:B:684:LYS:O	1:B:686:THR:N	2.52	0.43
1:B:811:HIS:O	1:B:812:ARG:CB	2.67	0.43
1:D:919:VAL:HG22	1:D:947:MET:CE	2.48	0.43
1:A:950:ASP:N	1:A:951:PRO:CD	2.82	0.43
1:B:788:GLN:NE2	1:B:789:TYR:HD2	2.16	0.43
1:A:902:ILE:O	1:A:907:GLU:HB2	2.19	0.42
1:C:830:THR:OG1	1:C:831:ASP:N	2.51	0.42
1:A:716:ILE:HA	1:A:717:PRO:HD3	1.75	0.42
1:A:860:GLU:OE2	1:A:934:ARG:NH1	2.48	0.42
1:C:896:ALA:O	1:C:898:GLU:N	2.52	0.42
1:D:787:SER:OG	1:D:951:PRO:HB2	2.19	0.42
1:C:855:LYS:HD3	1:C:891:TYR:HB2	2.00	0.42
1:B:685:GLU:HG2	1:B:685:GLU:H	1.60	0.42
1:A:828:LYS:HB3	1:A:828:LYS:HE2	1.86	0.42
1:A:874:TRP:CZ3	1:A:927:TRP:HA	2.53	0.42
1:B:861:SER:O	1:B:865:ARG:HA	2.19	0.42
1:B:875:SER:O	1:B:876:TYR:C	2.54	0.42
1:C:953:ARG:O	1:C:953:ARG:HG2	2.19	0.42
1:D:699:PHE:HD1	1:D:721:LYS:HE3	1.76	0.42
1:B:919:VAL:HG22	1:B:947:MET:HE2	2.01	0.42
1:C:807:ARG:O	1:C:809:LEU:HG	2.19	0.42
1:C:878:VAL:O	1:C:881:TRP:HB3	2.20	0.42
1:C:773:CYS:SG	1:C:776:ASP:OD2	2.76	0.42
1:A:807:ARG:O	1:A:809:LEU:HG	2.19	0.42
1:D:992:TYR:CD1	1:D:992:TYR:O	2.73	0.42
1:A:716:ILE:N	1:A:716:ILE:CD1	2.74	0.42
1:D:881:TRP:CZ3	1:D:890:PRO:HA	2.54	0.42
1:C:859:LEU:HD23	1:C:929:ILE:HD12	2.01	0.42
1:C:701:THR:CG2	1:C:703:TYR:HE2	2.30	0.42
1:B:731:ALA:C	1:B:733:LYS:H	2.22	0.42
1:B:799:GLU:HA	1:B:941:ILE:CD1	2.50	0.42
1:B:745:VAL:O	1:B:745:VAL:HG23	2.20	0.42
2:F:342:LEU:O	2:F:343:ASN:CB	2.67	0.41
1:A:947:MET:C	1:A:949:ARG:N	2.74	0.41
1:A:707:TRP:O	1:A:715:LYS:HA	2.20	0.41
1:A:907:GLU:O	1:A:908:ARG:NH1	2.52	0.41
1:D:837:LEU:HD22	1:D:838:LEU:CD2	2.49	0.41
1:D:947:MET:HE2	1:D:954:TYR:HD2	1.86	0.41
1:C:912:PRO:HB2	1:C:915:CYS:SG	2.60	0.41
1:B:814:LEU:HD12	1:B:815:ALA:N	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:911:GLN:HA	1:D:920:TYR:CE1	2.56	0.41
1:B:876:TYR:CD2	1:B:940:LEU:HD13	2.56	0.41
1:A:930:ASP:O	1:A:931:ALA:C	2.57	0.41
1:B:814:LEU:O	1:B:815:ALA:HB2	2.19	0.41
1:C:721:LYS:HE3	1:C:721:LYS:HB2	1.93	0.41
1:B:781:HIS:O	1:B:782:LYS:C	2.58	0.41
1:C:787:SER:OG	1:C:951:PRO:HB2	2.19	0.41
1:D:779:ARG:NH1	1:D:887:GLY:O	2.53	0.41
1:A:830:THR:O	1:A:831:ASP:HB2	2.20	0.41
1:A:703:TYR:CD1	1:A:703:TYR:N	2.88	0.41
1:C:678:ALA:HB1	1:C:752:ARG:CZ	2.50	0.41
1:B:771:PHE:CD2	1:B:771:PHE:N	2.88	0.41
1:B:866:ILE:CD1	1:D:693:VAL:HB	2.51	0.41
1:B:731:ALA:C	1:B:733:LYS:N	2.74	0.41
1:D:694:LEU:HD11	1:D:704:LYS:HB2	2.03	0.41
1:A:957:ILE:HG22	1:A:958:GLN:N	2.35	0.41
1:C:914:ILE:HG21	1:C:957:ILE:HG12	2.01	0.41
1:B:830:THR:O	1:B:831:ASP:HB2	2.20	0.41
1:B:788:GLN:HE21	1:B:788:GLN:HB3	1.60	0.41
1:C:692:LYS:O	1:C:703:TYR:HB3	2.21	0.41
1:B:943:GLU:O	1:B:947:MET:HG3	2.21	0.41
1:B:881:TRP:O	1:B:885:THR:HG23	2.21	0.41
1:D:903:LEU:HD12	1:D:908:ARG:NH1	2.35	0.41
1:C:916:THR:HG23	1:C:954:TYR:O	2.21	0.41
1:D:706:LEU:HD23	1:D:717:PRO:HA	2.01	0.41
1:C:791:LEU:HD23	1:C:791:LEU:HA	1.92	0.41
1:B:947:MET:HE2	1:B:954:TYR:CD2	2.56	0.41
1:B:731:ALA:O	1:B:733:LYS:N	2.54	0.41
1:B:769:MET:HA	1:B:770:PRO:HD2	1.78	0.40
1:D:881:TRP:CB	1:D:923:MET:HE1	2.51	0.40
1:C:858:ALA:HA	1:C:874:TRP:CD2	2.56	0.40
1:A:791:LEU:HD12	1:A:951:PRO:HB3	2.01	0.40
1:B:683:LEU:CD1	1:B:765:ILE:HD12	2.45	0.40
2:E:347:PRO:HA	2:E:348:PRO:HD3	1.95	0.40
1:A:809:LEU:HD22	1:A:832:PHE:CZ	2.54	0.40
1:A:876:TYR:CE2	1:A:940:LEU:HD13	2.56	0.40
1:B:904:GLU:HA	2:F:360:SER:HB2	2.03	0.40
1:A:823:THR:O	1:A:825:GLN:N	2.54	0.40
1:A:756:ILE:HG12	1:A:757:CYS:N	2.36	0.40
1:A:779:ARG:HG2	1:A:887:GLY:HA3	2.02	0.40
1:D:987:VAL:HG12	1:D:988:ASP:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:924:VAL:HG12	2:E:358:TYR:CE2	2.56	0.40
1:B:788:GLN:NE2	1:B:789:TYR:CD2	2.90	0.40
1:B:699:PHE:N	1:B:699:PHE:CD1	2.88	0.40
1:C:919:VAL:HG22	1:C:947:MET:CE	2.51	0.40
1:B:684:LYS:O	1:B:685:GLU:C	2.60	0.40
1:D:953:ARG:O	1:D:953:ARG:HG2	2.21	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	280/324 (86%)	229 (82%)	45 (16%)	6 (2%)	9 32
1	B	267/324 (82%)	224 (84%)	36 (14%)	7 (3%)	7 26
1	C	254/324 (78%)	222 (87%)	27 (11%)	5 (2%)	9 33
1	D	270/324 (83%)	231 (86%)	31 (12%)	8 (3%)	5 22
2	E	24/40 (60%)	17 (71%)	4 (17%)	3 (12%)	0 1
2	F	22/40 (55%)	17 (77%)	3 (14%)	2 (9%)	1 2
All	All	1117/1376 (81%)	940 (84%)	146 (13%)	31 (3%)	6 24

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	729	PRO
1	B	685	GLU
1	B	890	PRO
1	C	685	GLU
1	C	698	ALA
1	D	691	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	729	PRO
2	F	342	LEU
1	A	685	GLU
1	A	782	LYS
1	C	691	ILE
1	C	886	PHE
1	D	835	ALA
2	E	344	GLY
1	C	897	SER
1	D	990	ASP
2	E	343	ASN
1	A	815	ALA
1	A	952	GLN
1	B	683	LEU
1	D	685	GLU
1	D	757	CYS
1	B	732	ASN
1	B	835	ALA
1	D	710	GLU
1	D	838	LEU
1	B	815	ALA
2	F	345	VAL
1	B	770	PRO
2	E	345	VAL
1	A	718	VAL

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	230/284 (81%)	215 (94%)	15 (6%)	21	52
1	B	223/284 (78%)	209 (94%)	14 (6%)	22	54
1	C	211/284 (74%)	200 (95%)	11 (5%)	29	64
1	D	220/284 (78%)	211 (96%)	9 (4%)	37	73
2	E	22/37 (60%)	21 (96%)	1 (4%)	34	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	21/37 (57%)	19 (90%)	2 (10%)	11 31
All	All	927/1210 (77%)	875 (94%)	52 (6%)	26 60

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	701	THR
1	A	702	VAL
1	A	716	ILE
1	A	760	SER
1	A	783	ASP
1	A	784	ASN
1	A	788	GLN
1	A	852	VAL
1	A	897	SER
1	A	901	SER
1	A	902	ILE
1	A	921	MET
1	A	932	ASP
1	A	970	ASP
1	A	972	ASN
1	B	683	LEU
1	B	685	GLU
1	B	692	LYS
1	B	701	THR
1	B	712	GLU
1	B	724	ARG
1	B	732	ASN
1	B	788	GLN
1	B	825	GLN
1	B	834	LEU
1	B	852	VAL
1	B	898	GLU
1	B	921	MET
1	B	943	GLU
1	C	732	ASN
1	C	734	GLU
1	C	756	ILE
1	C	779	ARG
1	C	802	ASN
1	C	837	LEU
1	C	852	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	898	GLU
1	C	902	ILE
1	C	928	MET
1	C	949	ARG
1	D	716	ILE
1	D	757	CYS
1	D	758	LEU
1	D	783	ASP
1	D	802	ASN
1	D	852	VAL
1	D	901	SER
1	D	921	MET
1	D	988	ASP
2	E	349	THR
2	F	349	THR
2	F	354	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	784	ASN
1	A	802	ASN
1	A	869	HIS
1	A	952	GLN
1	A	972	ASN
1	B	781	HIS
1	B	784	ASN
1	B	788	GLN
1	B	792	ASN
1	B	864	HIS
1	B	869	HIS
1	B	952	GLN
1	C	781	HIS
1	C	952	GLN
1	D	781	HIS
1	D	788	GLN
1	D	792	ASN
1	D	818	ASN
1	D	952	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	286/324 (88%)	0.23	7 (2%) 62 57	28, 50, 96, 104	0
1	B	273/324 (84%)	0.27	9 (3%) 50 42	30, 55, 93, 107	0
1	C	262/324 (80%)	0.47	26 (9%) 9 5	22, 56, 115, 125	0
1	D	278/324 (85%)	0.48	22 (7%) 15 10	29, 66, 103, 118	0
2	E	26/40 (65%)	0.47	2 (7%) 16 11	48, 61, 87, 90	0
2	F	24/40 (60%)	0.56	1 (4%) 40 33	66, 71, 88, 90	0
All	All	1149/1376 (83%)	0.37	67 (5%) 26 20	22, 57, 104, 125	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	723	LEU	4.7
1	B	714	VAL	4.7
1	D	699	PHE	4.3
1	C	683	LEU	4.1
1	D	683	LEU	4.1
1	D	760	SER	4.0
1	C	758	LEU	4.0
1	C	724	ARG	3.8
1	C	688	PHE	3.7
1	C	753	LEU	3.4
1	B	735	ILE	3.4
1	C	707	TRP	3.3
1	C	718	VAL	3.2
1	A	678	ALA	3.2
2	F	337	SER	3.1
1	C	838	LEU	2.9
1	C	682	ILE	2.9
1	D	756	ILE	2.9
1	C	719	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	733	LYS	2.8
1	A	677	MET	2.8
1	D	711	GLY	2.7
1	C	685	GLU	2.7
1	D	730	LYS	2.6
1	B	683	LEU	2.6
1	C	686	THR	2.6
1	C	680	LEU	2.6
1	C	690	LYS	2.6
1	D	721	LYS	2.5
1	C	730	LYS	2.5
1	C	706	LEU	2.5
1	B	957	ILE	2.5
1	A	710	GLU	2.5
1	D	698	ALA	2.5
1	D	714	VAL	2.4
1	C	721	LYS	2.4
1	C	757	CYS	2.4
1	D	710	GLU	2.4
1	D	732	ASN	2.4
1	B	679	LEU	2.4
1	B	707	TRP	2.3
1	D	712	GLU	2.3
1	A	711	GLY	2.3
1	D	729	PRO	2.3
1	C	756	ILE	2.3
1	D	713	LYS	2.3
1	D	753	LEU	2.3
1	A	736	LEU	2.3
1	C	694	LEU	2.3
1	D	682	ILE	2.3
1	B	758	LEU	2.3
1	C	702	VAL	2.2
1	D	761	THR	2.2
1	C	678	ALA	2.2
1	C	717	PRO	2.2
1	D	731	ALA	2.2
1	B	729	PRO	2.2
1	C	722	GLU	2.2
2	E	345	VAL	2.1
1	A	708	ILE	2.1
1	D	696	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	838	LEU	2.1
2	E	340	SER	2.0
1	D	724	ARG	2.0
1	C	703	TYR	2.0
1	D	740	TYR	2.0
1	A	699	PHE	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 carbohydrates 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.