Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:21 PM GMT

PDB ID	:	1JX7
Title	:	Crystal structure of ychN protein from E.coli
Authors	:	Shin, D.H.; Yokota, H.; Kim, R.; Kim, S.-H.; Berkeley Structural Genomics Center (BSGC)
Deposited on	:	2001-09-05
Resolution	:	2.80 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:

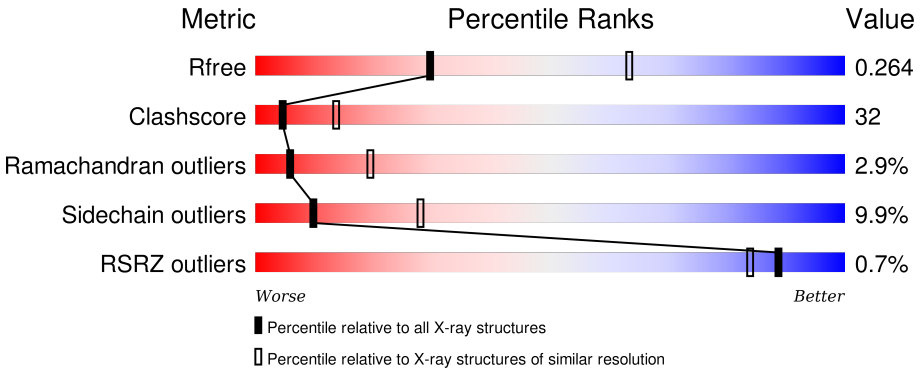
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	117	44% 43% 14%
1	B	117	3% 47% 46% 7%
1	C	117	49% 44% 8%
1	D	117	% 52% 42% 5%
1	E	117	50% 42% 9%

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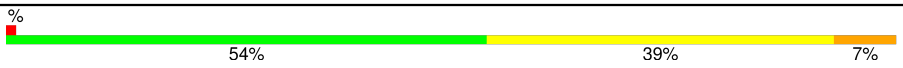
Mol	Chain	Length	Quality of chain
1	F	117	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5420 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 HYPOTHETICAL PROTEIN YCHN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	S	Se	0	0	0
			889	563	150	171	2	3			
1	B	117	Total	C	N	O	S	Se	0	0	0
			889	563	150	171	2	3			
1	C	117	Total	C	N	O	S	Se	0	0	0
			889	563	150	171	2	3			
1	D	117	Total	C	N	O	S	Se	0	0	0
			889	563	150	171	2	3			
1	E	117	Total	C	N	O	S	Se	0	0	0
			889	563	150	171	2	3			
1	F	117	Total	C	N	O	S	Se	0	0	0
			889	563	150	171	2	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	CLONING ARTIFACT	UNP P0AB52
A	42	MSE	MET	CLONING ARTIFACT	UNP P0AB52
A	64	MSE	MET	CLONING ARTIFACT	UNP P0AB52
B	201	MSE	MET	CLONING ARTIFACT	UNP P0AB52
B	242	MSE	MET	CLONING ARTIFACT	UNP P0AB52
B	264	MSE	MET	CLONING ARTIFACT	UNP P0AB52
C	401	MSE	MET	CLONING ARTIFACT	UNP P0AB52
C	442	MSE	MET	CLONING ARTIFACT	UNP P0AB52
C	464	MSE	MET	CLONING ARTIFACT	UNP P0AB52
D	601	MSE	MET	CLONING ARTIFACT	UNP P0AB52
D	642	MSE	MET	CLONING ARTIFACT	UNP P0AB52
D	664	MSE	MET	CLONING ARTIFACT	UNP P0AB52
E	801	MSE	MET	CLONING ARTIFACT	UNP P0AB52
E	842	MSE	MET	CLONING ARTIFACT	UNP P0AB52
E	864	MSE	MET	CLONING ARTIFACT	UNP P0AB52
F	1001	MSE	MET	CLONING ARTIFACT	UNP P0AB52
F	1042	MSE	MET	CLONING ARTIFACT	UNP P0AB52

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1064	MSE	MET	CLONING ARTIFACT	UNP P0AB52

- Molecule 2 is water.

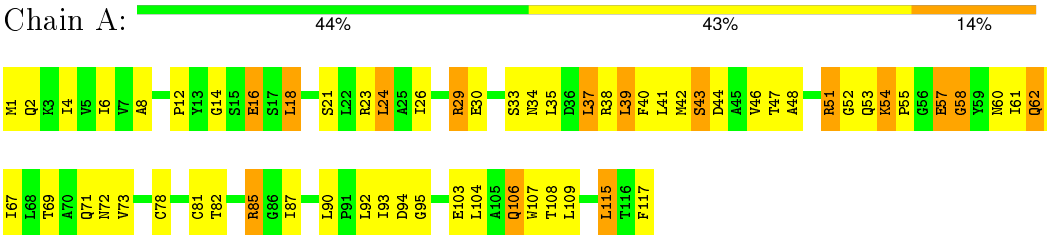
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	16	Total O 16 16	0	0
2	B	14	Total O 14 14	0	0
2	C	10	Total O 10 10	0	0
2	D	13	Total O 13 13	0	0
2	E	21	Total O 21 21	0	0
2	F	12	Total O 12 12	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

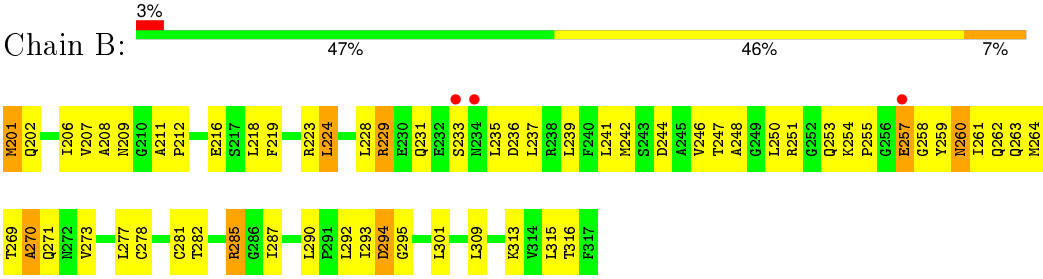
- Molecule 1: HYPOTHETICAL PROTEIN YCHN

Chain A:



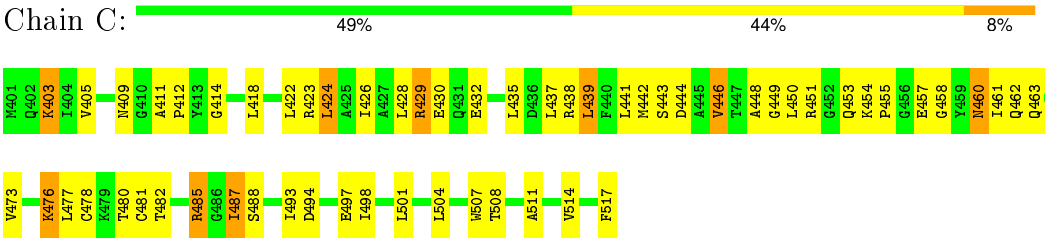
- Molecule 1: HYPOTHETICAL PROTEIN YCHN

Chain B:



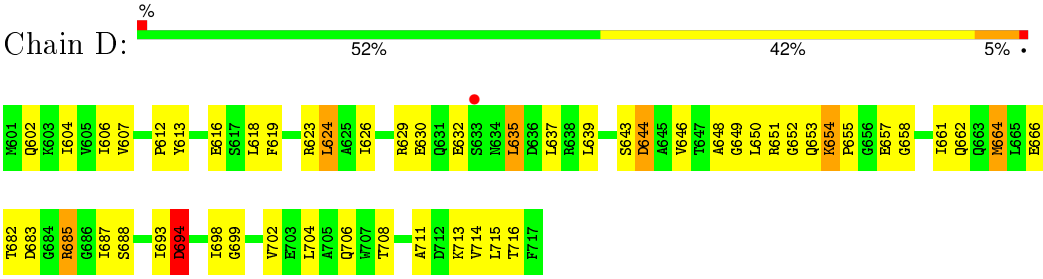
- Molecule 1: HYPOTHETICAL PROTEIN YCHN

Chain C:



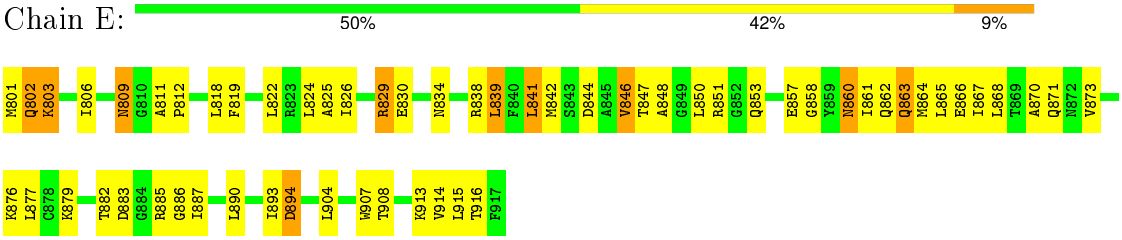
- Molecule 1: HYPOTHETICAL PROTEIN YCHN

Chain D:



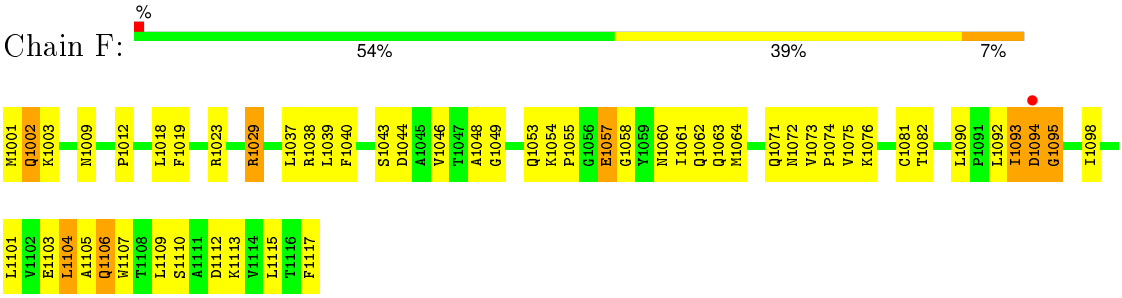
• Molecule 1: HYPOTHETICAL PROTEIN YCHN

Chain E:



• Molecule 1: HYPOTHETICAL PROTEIN YCHN

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.21Å 80.46Å 140.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.80 69.78 – 2.69	Depositor EDS
% Data completeness (in resolution range)	95.4 (19.98-2.80) 94.8 (69.78-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.68 (at 2.69Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.229 , 0.265 0.229 , 0.264	Depositor DCC
R_{free} test set	1806 reflections (9.95%)	DCC
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 36.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 20429 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5420	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.31% 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	0.53	1/897 (0.1%)	0.70	0/1210
1	B	0.52	1/897 (0.1%)	0.66	0/1210
1	C	0.49	0/897	0.63	0/1210
1	D	0.52	1/897 (0.1%)	0.65	0/1210
1	E	0.50	0/897	0.71	0/1210
1	F	0.49	0/897	0.74	1/1210 (0.1%)
All	All	0.51	3/5382 (0.1%)	0.68	1/7260 (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	F	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	664	MSE	SE-CE	-5.32	1.64	1.95
1	B	201	MSE	CG-SE	-5.21	1.77	1.95
1	A	64	MSE	SE-CE	-5.09	1.65	1.95

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	1095	GLY	N-CA-C	-9.34	89.74	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	1095	GLY	Peptide

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	889	0	924	77	0
1	B	889	0	921	70	0
1	C	889	0	921	63	0
1	D	889	0	921	58	0
1	E	889	0	921	59	0
1	F	889	0	921	60	0
2	A	16	0	0	1	0
2	B	14	0	0	1	0
2	C	10	0	0	1	0
2	D	13	0	0	3	0
2	E	21	0	0	2	0
2	F	12	0	0	2	0
All	All	5420	0	5529	349	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 32.

All (349) 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:F:1117:PHE:OXT	2:F:2068:HOH:O	1.68	1.12
1:F:1060:ASN:ND2	1:F:1063:GLN:H	1.50	1.07
1:B:246:VAL:HG11	1:B:282:THR:HG22	1.37	1.05
1:B:294:ASP:O	2:B:2067:HOH:O	1.77	1.01
1:B:246:VAL:CG1	1:B:282:THR:HG22	1.99	0.92
1:D:685:ARG:HB2	1:D:687:ILE:HD13	1.53	0.89
1:A:12:PRO:HG3	1:A:48:ALA:HB2	1.54	0.88
1:B:207:VAL:HG22	1:B:316:THR:HG22	1.58	0.86
1:A:1:MSE:HG2	1:A:2:GLN:H	1.39	0.83
1:D:612:PRO:HG3	1:D:648:ALA:HB2	1.61	0.83
1:F:1060:ASN:HD21	1:F:1063:GLN:H	1.24	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:LEU:HD21	1:B:287:ILE:HG23	1.62	0.80
1:A:60:ASN:HD22	1:A:63:GLN:H	1.30	0.79
1:A:108:THR:O	1:B:313:LYS:HE3	1.84	0.78
1:A:29:ARG:HH12	1:A:71:GLN:HB3	1.49	0.78
1:F:1019:PHE:HD1	1:F:1064:MSE:HE1	1.50	0.77
1:B:262:GLN:O	1:B:266:GLU:HG3	1.83	0.77
1:C:462:GLN:O	1:C:466:GLU:HG3	1.84	0.76
1:D:651:ARG:HG2	1:D:652:GLY:H	1.50	0.76
1:B:211:ALA:HB2	1:B:244:ASP:HB3	1.67	0.76
1:A:51:ARG:HH11	1:A:51:ARG:HB2	1.49	0.76
1:F:1009:ASN:ND2	2:F:2040:HOH:O	2.18	0.76
1:D:606:ILE:HB	1:D:639:LEU:HD12	1.68	0.76
1:B:290:LEU:HD13	1:E:890:LEU:HD23	1.66	0.76
1:A:46:VAL:CG1	1:A:82:THR:HG22	2.17	0.75
1:B:257:GLU:HG2	1:F:1058:GLY:HA2	1.69	0.75
1:C:418:LEU:HD12	1:C:461:ILE:HD13	1.70	0.74
1:B:260:ASN:HD21	1:B:262:GLN:HB3	1.52	0.74
1:B:257:GLU:CD	1:B:258:GLY:H	1.91	0.74
1:C:412:PRO:HG3	1:C:448:ALA:HB2	1.69	0.74
1:D:651:ARG:HG2	1:D:652:GLY:N	2.03	0.74
1:B:218:LEU:HD12	1:B:261:ILE:HD13	1.70	0.73
1:D:711:ALA:O	1:E:913:LYS:HE2	1.89	0.73
1:D:661:ILE:HA	1:D:664:MSE:HE3	1.71	0.72
1:A:61:ILE:HA	1:A:64:MSE:HE3	1.70	0.72
1:A:109:LEU:HD23	1:B:202:GLN:NE2	2.05	0.71
1:B:278:CYS:O	1:B:282:THR:HG23	1.90	0.71
1:A:53:GLN:H	1:A:62:GLN:HE21	1.36	0.71
1:A:35:LEU:CD1	1:A:37:LEU:HB2	2.21	0.71
1:F:1060:ASN:HD22	1:F:1063:GLN:H	1.37	0.71
1:E:860:ASN:HD22	1:E:860:ASN:C	1.93	0.71
1:F:1093:ILE:O	1:F:1094:ASP:OD2	2.09	0.70
1:C:458:GLY:HA3	1:E:857:GLU:HG2	1.73	0.70
1:A:16:GLU:HG2	1:C:443:SER:OG	1.91	0.70
1:B:260:ASN:ND2	1:B:263:GLN:H	1.88	0.70
1:D:624:LEU:O	1:D:624:LEU:HD22	1.91	0.70
1:D:618:LEU:HD12	1:D:661:ILE:HD13	1.73	0.70
1:B:212:PRO:HG3	1:B:248:ALA:HB2	1.74	0.70
1:A:29:ARG:HH11	1:A:71:GLN:NE2	1.88	0.70
1:A:23:ARG:HG2	1:C:501:LEU:CD2	2.23	0.69
1:C:411:ALA:HB2	1:C:444:ASP:HB3	1.73	0.69
1:D:623:ARG:HG2	1:F:1101:LEU:CD2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HD13	1:F:1090:LEU:HD13	1.72	0.69
1:E:853:GLN:HB2	1:E:862:GLN:HE21	1.56	0.69
1:A:6:ILE:HB	1:A:39:LEU:HD22	1.75	0.69
1:D:646:VAL:HG13	1:D:682:THR:HG22	1.74	0.69
1:F:1105:ALA:O	1:F:1106:GLN:HB2	1.91	0.68
1:D:702:VAL:O	1:D:706:GLN:HG3	1.93	0.68
1:A:35:LEU:HD13	1:A:37:LEU:HB2	1.76	0.68
1:B:218:LEU:HD12	1:B:261:ILE:CD1	2.24	0.67
1:F:1012:PRO:HG3	1:F:1048:ALA:HB2	1.77	0.67
1:B:206:ILE:HB	1:B:239:LEU:CD2	2.25	0.67
1:D:679:LYS:HE2	1:D:683:ASP:OD2	1.95	0.67
1:C:446:VAL:HG13	1:C:482:THR:HG22	1.77	0.67
1:B:207:VAL:CG2	1:B:316:THR:HG22	2.25	0.67
1:F:1093:ILE:O	1:F:1094:ASP:CG	2.33	0.67
1:D:688:SER:HA	1:D:698:ILE:HD11	1.75	0.67
1:D:623:ARG:HG2	1:F:1101:LEU:HD21	1.77	0.66
1:B:301:LEU:HD22	1:C:423:ARG:HG2	1.78	0.66
1:C:460:ASN:C	1:C:460:ASN:HD22	1.98	0.66
1:A:47:THR:HG22	1:A:87:ILE:CD1	2.26	0.65
1:C:482:THR:HB	1:C:487:ILE:HG22	1.78	0.65
1:E:861:ILE:HD13	1:E:864:MSE:HE3	1.78	0.65
1:B:301:LEU:CD2	1:C:423:ARG:HG2	2.26	0.65
1:F:1019:PHE:CD1	1:F:1064:MSE:HE1	2.31	0.65
1:E:862:GLN:HG3	1:E:893:ILE:CD1	2.27	0.64
1:A:29:ARG:NH1	1:A:71:GLN:HB3	2.13	0.64
1:A:51:ARG:CB	1:A:51:ARG:HH11	2.09	0.64
1:E:862:GLN:O	1:E:866:GLU:HG3	1.98	0.64
1:D:646:VAL:CG1	1:D:682:THR:HG22	2.28	0.64
1:A:47:THR:HG22	1:A:87:ILE:HD11	1.80	0.63
1:A:46:VAL:HG13	1:A:82:THR:HG22	1.81	0.63
1:B:269:THR:HB	1:B:295:GLY:HA3	1.81	0.63
1:A:46:VAL:HG11	1:A:82:THR:HG22	1.81	0.63
1:C:450:LEU:HD11	1:C:487:ILE:HD11	1.79	0.63
1:C:460:ASN:HD21	1:C:462:GLN:HB3	1.64	0.63
1:F:1057:GLU:HG2	1:F:1058:GLY:N	2.13	0.63
1:D:653:GLN:H	1:D:662:GLN:NE2	1.95	0.63
1:A:61:ILE:HA	1:A:64:MSE:CE	2.28	0.62
1:C:457:GLU:HG2	1:E:858:GLY:HA3	1.79	0.62
1:A:37:LEU:HD23	1:A:38:ARG:N	2.14	0.62
1:E:826:ILE:O	1:E:830:GLU:HG3	2.00	0.62
1:A:65:LEU:O	1:A:69:THR:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:508:THR:HG23	1:C:514:VAL:HG21	1.80	0.61
1:D:607:VAL:HB	1:D:716:THR:HG22	1.82	0.61
1:C:409:ASN:OD1	1:C:442:MSE:HB2	2.01	0.61
1:C:424:LEU:O	1:C:428:LEU:HG	2.00	0.61
1:A:1:MSE:HG2	1:A:2:GLN:N	2.15	0.61
1:F:1060:ASN:ND2	1:F:1063:GLN:N	2.35	0.60
1:B:253:GLN:H	1:B:262:GLN:NE2	1.98	0.60
1:D:632:GLU:HG2	1:F:1109:LEU:HD13	1.84	0.60
1:A:62:GLN:HG2	1:A:93:ILE:CD1	2.31	0.60
1:A:109:LEU:HD23	1:B:202:GLN:HE22	1.65	0.59
1:E:812:PRO:HG3	1:E:848:ALA:HB2	1.83	0.59
1:A:62:GLN:HG2	1:A:93:ILE:HD13	1.84	0.59
1:D:616:GLU:O	1:D:619:PHE:HB3	2.03	0.59
1:E:838:ARG:HD3	1:E:907:TRP:CE2	2.38	0.59
1:D:604:ILE:HG12	1:D:713:LYS:CG	2.33	0.59
1:B:267:ILE:O	1:B:271:GLN:HG3	2.03	0.59
1:A:26:ILE:O	1:A:30:GLU:HG3	2.03	0.58
1:E:908:THR:O	1:F:1113:LYS:HE3	2.03	0.57
1:C:460:ASN:ND2	1:C:463:GLN:H	2.02	0.57
1:A:12:PRO:HB3	1:A:61:ILE:HD13	1.85	0.57
1:B:290:LEU:HD13	1:E:890:LEU:CD2	2.33	0.57
1:E:879:LYS:HE2	1:E:883:ASP:OD2	2.05	0.56
1:F:1046:VAL:CG1	1:F:1082:THR:HG22	2.35	0.56
1:F:1071:GLN:O	1:F:1072:ASN:HB2	2.05	0.56
1:E:819:PHE:HD1	1:E:864:MSE:HE1	1.70	0.56
1:A:54:LYS:O	1:A:54:LYS:HD3	2.05	0.56
1:B:259:TYR:HB2	1:B:264:MSE:CE	2.35	0.56
1:E:819:PHE:CD1	1:E:864:MSE:HE1	2.41	0.56
1:D:643:SER:O	1:D:646:VAL:HB	2.06	0.56
1:A:12:PRO:CG	1:A:48:ALA:HB2	2.33	0.56
1:E:801:MSE:O	1:E:802:GLN:HB2	2.05	0.55
1:E:860:ASN:HD21	1:E:862:GLN:HB3	1.71	0.55
1:F:1046:VAL:HG13	1:F:1082:THR:HG22	1.87	0.55
1:F:1019:PHE:CE2	1:F:1023:ARG:HD2	2.41	0.55
1:B:260:ASN:HD22	1:B:263:GLN:H	1.53	0.55
1:B:212:PRO:HB3	1:B:261:ILE:HD12	1.88	0.55
1:F:1093:ILE:O	1:F:1094:ASP:CB	2.55	0.55
1:A:60:ASN:ND2	1:A:63:GLN:H	1.99	0.55
1:A:14:GLY:HA3	1:F:1044:ASP:OD2	2.06	0.55
1:C:446:VAL:CG1	1:C:482:THR:HG22	2.35	0.55
1:B:259:TYR:HB2	1:B:264:MSE:HE1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1002:GLN:OE1	1:F:1113:LYS:HE2	2.07	0.54
1:D:644:ASP:N	1:D:644:ASP:OD1	2.39	0.54
1:A:62:GLN:O	1:A:66:GLU:HG3	2.06	0.54
1:D:604:ILE:HG12	1:D:713:LYS:HG3	1.88	0.54
1:B:247:THR:HG22	1:B:287:ILE:HD11	1.88	0.54
1:A:43:SER:HB2	1:B:216:GLU:OE1	2.08	0.54
1:E:838:ARG:HD3	1:E:907:TRP:CZ2	2.43	0.54
1:D:635:LEU:HD21	1:D:637:LEU:HB2	1.90	0.54
1:F:1072:ASN:O	1:F:1074:PRO:HD3	2.07	0.54
1:D:651:ARG:CB	1:D:651:ARG:HH11	2.21	0.54
1:D:693:ILE:CG2	1:D:694:ASP:N	2.70	0.54
1:E:811:ALA:HB2	1:E:844:ASP:HB3	1.89	0.53
1:A:57:GLU:HG2	1:A:58:GLY:H	1.74	0.53
1:A:57:GLU:HG2	1:A:58:GLY:N	2.23	0.53
1:B:260:ASN:C	1:B:260:ASN:HD22	2.12	0.53
1:D:651:ARG:HB3	1:D:651:ARG:HH11	1.73	0.53
1:D:708:THR:HG23	1:D:714:VAL:HG21	1.91	0.53
1:B:281:CYS:O	1:B:285:ARG:HG2	2.09	0.53
1:C:437:LEU:O	1:C:473:VAL:HG13	2.09	0.53
1:F:1055:PRO:HG2	1:F:1060:ASN:HA	1.90	0.52
1:E:809:ASN:OD1	1:E:842:MSE:HE3	2.09	0.52
1:E:851:ARG:O	1:E:862:GLN:NE2	2.42	0.52
1:F:1046:VAL:HG21	1:F:1081:CYS:HB2	1.91	0.52
1:D:714:VAL:HB	1:E:915:LEU:CD2	2.39	0.52
1:A:21:SER:OG	1:A:117:PHE:HB2	2.08	0.52
1:A:4:ILE:HD12	1:A:35:LEU:HD21	1.92	0.52
1:A:47:THR:HA	1:A:87:ILE:HD13	1.90	0.52
1:E:803:LYS:N	1:E:803:LYS:HD2	2.24	0.52
1:A:38:ARG:HD3	1:A:107:TRP:CD2	2.45	0.52
1:E:806:ILE:CD1	1:E:825:ALA:HB2	2.40	0.52
1:C:411:ALA:HB3	1:D:644:ASP:OD2	2.10	0.52
1:A:16:GLU:HG2	1:C:443:SER:HG	1.75	0.51
1:F:1003:LYS:HD3	1:F:1110:SER:O	2.09	0.51
1:E:838:ARG:HB3	1:E:907:TRP:CZ3	2.45	0.51
1:E:904:LEU:HD23	1:E:904:LEU:O	2.10	0.51
1:D:654:LYS:HD3	1:D:654:LYS:O	2.11	0.51
1:F:1076:LYS:HG3	1:F:1103:GLU:OE2	2.11	0.51
1:E:865:LEU:HD12	1:E:893:ILE:HD12	1.93	0.51
1:F:1093:ILE:O	1:F:1093:ILE:CG2	2.59	0.50
1:E:861:ILE:HD13	1:E:864:MSE:CE	2.40	0.50
1:C:403:LYS:HB3	1:C:511:ALA:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLN:NE2	2:A:2080:HOH:O	2.43	0.50
1:B:257:GLU:CD	1:B:258:GLY:N	2.61	0.50
1:C:418:LEU:HD12	1:C:461:ILE:CD1	2.39	0.50
1:F:1060:ASN:HD21	1:F:1063:GLN:N	2.01	0.50
1:A:63:GLN:O	1:A:67:ILE:HG13	2.11	0.50
1:A:52:GLY:H	1:A:62:GLN:NE2	2.09	0.50
1:A:51:ARG:NH1	1:A:51:ARG:HB2	2.24	0.49
1:B:257:GLU:CG	1:B:258:GLY:N	2.75	0.49
1:D:623:ARG:HG2	1:F:1101:LEU:HD22	1.93	0.49
1:A:23:ARG:HG2	1:C:501:LEU:HD22	1.95	0.49
1:C:480:THR:HG23	2:C:2015:HOH:O	2.11	0.49
1:C:424:LEU:HD12	1:C:517:PHE:HE2	1.78	0.49
1:C:451:ARG:HG2	1:C:451:ARG:HH11	1.77	0.49
1:D:680:THR:HG23	2:D:2022:HOH:O	2.13	0.49
1:D:685:ARG:NH1	2:D:2002:HOH:O	2.45	0.49
1:E:860:ASN:ND2	1:E:860:ASN:C	2.65	0.49
1:B:206:ILE:HB	1:B:239:LEU:HD23	1.93	0.49
1:C:426:ILE:O	1:C:430:GLU:HG3	2.12	0.49
1:A:85:ARG:NH1	1:F:1012:PRO:O	2.46	0.48
1:E:908:THR:HG21	1:F:1115:LEU:HD11	1.96	0.48
1:B:309:LEU:HD13	1:C:432:GLU:HG3	1.94	0.48
1:D:649:GLY:O	1:D:693:ILE:HG13	2.13	0.48
1:E:829:ARG:NH1	1:E:873:VAL:HG23	2.28	0.48
1:F:1012:PRO:CG	1:F:1048:ALA:HB2	2.42	0.48
1:D:693:ILE:HG22	1:D:694:ASP:N	2.28	0.48
1:D:651:ARG:CB	1:D:651:ARG:NH1	2.77	0.48
1:C:403:LYS:NZ	1:C:438:ARG:NH1	2.61	0.48
1:B:246:VAL:HG13	1:B:277:LEU:HB3	1.96	0.47
1:C:460:ASN:ND2	1:C:460:ASN:C	2.68	0.47
1:B:257:GLU:HG2	1:F:1058:GLY:CA	2.42	0.47
1:C:460:ASN:ND2	1:C:462:GLN:N	2.62	0.47
1:F:1060:ASN:ND2	1:F:1063:GLN:HB2	2.29	0.47
1:B:219:PHE:CZ	1:B:223:ARG:HD2	2.49	0.47
1:B:208:ALA:HB3	1:B:241:LEU:CD2	2.44	0.47
1:B:253:GLN:H	1:B:262:GLN:HE22	1.62	0.47
1:E:862:GLN:HG3	1:E:893:ILE:HD11	1.96	0.47
1:B:218:LEU:CD1	1:B:261:ILE:HD13	2.41	0.47
1:D:653:GLN:H	1:D:662:GLN:HE22	1.58	0.47
1:C:488:SER:HA	1:C:498:ILE:HD11	1.96	0.47
1:E:847:THR:HA	1:E:887:ILE:CD1	2.46	0.46
1:C:422:LEU:O	1:C:426:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ILE:HG22	1:B:287:ILE:O	2.14	0.46
1:A:53:GLN:HB2	1:A:62:GLN:HB2	1.98	0.46
1:B:281:CYS:O	1:B:285:ARG:CG	2.63	0.46
1:C:476:LYS:HG2	1:C:507:TRP:HH2	1.80	0.46
1:B:218:LEU:HD13	1:B:218:LEU:O	2.15	0.46
1:A:23:ARG:HG2	1:C:501:LEU:HD21	1.97	0.46
1:D:662:GLN:O	1:D:666:GLU:HG3	2.14	0.46
1:D:657:GLU:HG2	1:D:658:GLY:N	2.29	0.46
1:D:681:CYS:O	1:D:685:ARG:HG2	2.16	0.46
1:C:478:CYS:O	1:C:482:THR:HG23	2.16	0.46
1:A:24:LEU:HD23	1:A:24:LEU:O	2.16	0.46
1:A:57:GLU:CG	1:A:58:GLY:H	2.25	0.46
1:A:40:PHE:HE1	1:A:42:MSE:HG2	1.81	0.46
1:E:846:VAL:HG21	1:E:882:THR:HG23	1.97	0.46
1:C:460:ASN:ND2	1:C:462:GLN:H	2.13	0.46
1:C:444:ASP:OD1	1:C:485:ARG:NH1	2.48	0.46
1:B:229:ARG:O	1:B:233:SER:HA	2.16	0.46
1:A:29:ARG:HB3	1:A:71:GLN:HE22	1.81	0.46
1:B:262:GLN:HG3	1:B:293:ILE:CD1	2.46	0.46
1:E:860:ASN:ND2	1:E:862:GLN:H	2.14	0.46
1:E:846:VAL:CG2	1:E:877:LEU:HB3	2.45	0.46
1:E:876:LYS:NZ	2:E:2064:HOH:O	2.38	0.46
1:F:1019:PHE:CZ	1:F:1023:ARG:HD2	2.51	0.45
1:F:1071:GLN:O	1:F:1072:ASN:CB	2.63	0.45
1:C:466:GLU:HG2	1:C:493:ILE:CG2	2.45	0.45
1:C:454:LYS:HE2	1:D:683:ASP:HB3	1.98	0.45
1:B:260:ASN:ND2	1:B:262:GLN:H	2.14	0.45
1:F:1053:GLN:HB2	1:F:1062:GLN:HE21	1.81	0.45
1:B:260:ASN:ND2	1:B:262:GLN:N	2.64	0.45
1:B:241:LEU:HD12	1:B:277:LEU:CD2	2.47	0.45
1:E:861:ILE:HA	1:E:864:MSE:HE3	1.99	0.45
1:D:662:GLN:HG3	1:D:693:ILE:CD1	2.46	0.45
1:E:822:LEU:O	1:E:826:ILE:HG13	2.17	0.45
1:E:839:LEU:HD12	1:E:841:LEU:CD1	2.47	0.45
1:E:850:LEU:O	1:E:853:GLN:NE2	2.47	0.45
1:E:826:ILE:HG12	1:E:868:LEU:HD21	1.99	0.45
1:C:424:LEU:O	1:C:424:LEU:HD22	2.16	0.45
1:B:246:VAL:HG11	1:B:282:THR:CG2	2.28	0.45
1:F:1001:MSE:HB2	1:F:1002:GLN:H	1.61	0.45
1:F:1038:ARG:HB3	1:F:1107:TRP:CZ3	2.51	0.45
1:A:52:GLY:N	1:A:62:GLN:NE2	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:HA	1:B:315:LEU:O	2.17	0.44
1:C:446:VAL:HG22	1:C:477:LEU:HB3	2.00	0.44
1:D:616:GLU:OE1	1:F:1043:SER:HB2	2.17	0.44
1:F:1029:ARG:NH2	1:F:1071:GLN:O	2.50	0.44
1:A:103:GLU:O	1:A:106:GLN:HB3	2.17	0.44
1:D:715:LEU:N	1:D:715:LEU:HD12	2.32	0.44
1:F:1060:ASN:HD22	1:F:1063:GLN:CB	2.30	0.44
1:E:886:GLY:O	1:E:890:LEU:HD13	2.18	0.44
1:A:8:ALA:HB3	1:A:41:LEU:HD22	2.00	0.44
1:B:211:ALA:HB2	1:B:244:ASP:CB	2.44	0.44
1:E:867:ILE:O	1:E:871:GLN:HG3	2.18	0.44
1:C:439:LEU:HD12	1:C:441:LEU:CD1	2.47	0.44
1:F:1018:LEU:O	1:F:1018:LEU:HD23	2.18	0.44
1:D:651:ARG:NH1	1:D:651:ARG:HB2	2.33	0.44
1:C:457:GLU:CG	1:E:858:GLY:HA3	2.47	0.44
1:A:53:GLN:H	1:A:62:GLN:NE2	2.10	0.43
1:A:43:SER:N	1:A:81:CYS:SG	2.91	0.43
1:E:806:ILE:HB	1:E:839:LEU:HD22	1.99	0.43
1:C:412:PRO:O	1:C:414:GLY:N	2.51	0.43
1:C:476:LYS:HA	1:C:497:GLU:O	2.17	0.43
1:B:247:THR:HG22	1:B:287:ILE:CD1	2.48	0.43
1:B:266:GLU:O	1:B:270:ALA:HB2	2.18	0.43
1:F:1082:THR:HG21	1:F:1098:ILE:CD1	2.48	0.43
1:F:1073:VAL:O	1:F:1075:VAL:HG23	2.18	0.43
1:C:449:GLY:O	1:C:493:ILE:HG13	2.18	0.43
1:E:860:ASN:ND2	1:E:862:GLN:N	2.67	0.43
1:B:253:GLN:O	1:B:255:PRO:HD3	2.18	0.43
1:A:90:LEU:O	1:A:92:LEU:HD22	2.19	0.43
1:F:1029:ARG:HH21	1:F:1071:GLN:HB3	1.83	0.43
1:B:237:LEU:O	1:B:273:VAL:HG13	2.18	0.43
1:C:412:PRO:C	1:C:414:GLY:H	2.21	0.43
1:D:661:ILE:HA	1:D:664:MSE:CE	2.47	0.43
1:E:914:VAL:HB	1:F:1115:LEU:CD2	2.49	0.43
1:E:801:MSE:O	1:E:802:GLN:CB	2.67	0.43
1:B:224:LEU:HD22	1:B:228:LEU:HG	2.00	0.43
1:A:69:THR:HB	1:A:95:GLY:HA3	2.00	0.43
1:C:424:LEU:HD12	1:C:517:PHE:CE2	2.53	0.43
1:B:208:ALA:HB3	1:B:241:LEU:HD23	2.00	0.43
1:E:850:LEU:HA	1:E:850:LEU:HD23	1.92	0.43
1:D:653:GLN:O	1:D:655:PRO:HD3	2.19	0.42
1:E:826:ILE:CG1	1:E:868:LEU:HD21	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MSE:CG	1:A:2:GLN:N	2.79	0.42
1:C:463:GLN:O	1:C:467:ILE:HG13	2.19	0.42
1:A:78:CYS:O	1:A:82:THR:HG23	2.19	0.42
1:A:38:ARG:HB3	1:A:107:TRP:CZ3	2.54	0.42
1:F:1018:LEU:HD22	1:F:1061:ILE:CD1	2.50	0.42
1:C:460:ASN:HD22	1:C:462:GLN:N	2.17	0.42
1:C:446:VAL:HG21	1:C:481:CYS:HB2	2.00	0.42
1:D:626:ILE:O	1:D:630:GLU:HG3	2.18	0.42
1:A:37:LEU:O	1:A:73:VAL:HG13	2.19	0.42
1:C:409:ASN:OD1	1:C:442:MSE:HE3	2.18	0.42
1:B:212:PRO:CG	1:B:248:ALA:HB2	2.45	0.42
1:A:57:GLU:CG	1:A:58:GLY:N	2.83	0.42
1:C:429:ARG:HH11	1:C:429:ARG:HG2	1.84	0.42
1:E:860:ASN:ND2	1:E:863:GLN:H	2.18	0.42
1:C:438:ARG:HG3	1:C:438:ARG:HH11	1.84	0.42
1:E:890:LEU:HD12	1:E:890:LEU:N	2.35	0.41
1:B:219:PHE:CE1	1:B:264:MSE:HE1	2.55	0.41
1:A:14:GLY:HA3	1:F:1044:ASP:CG	2.40	0.41
1:C:405:VAL:HG21	1:C:507:TRP:HB3	2.01	0.41
1:C:476:LYS:HG2	1:C:507:TRP:CH2	2.55	0.41
1:D:662:GLN:HG3	1:D:693:ILE:HD13	2.02	0.41
1:E:824:LEU:HD23	1:E:824:LEU:O	2.20	0.41
1:B:263:GLN:O	1:B:267:ILE:HG13	2.20	0.41
1:E:860:ASN:HD22	1:E:862:GLN:N	2.18	0.41
1:D:679:LYS:N	1:D:699:GLY:O	2.52	0.41
1:A:18:LEU:HD23	1:A:18:LEU:O	2.21	0.41
1:B:201:MSE:HE3	1:B:236:ASP:HB2	2.03	0.41
1:A:55:PRO:HD2	1:A:60:ASN:OD1	2.21	0.41
1:A:29:ARG:HD3	1:A:29:ARG:HA	1.79	0.41
1:D:643:SER:HB3	1:D:644:ASP:H	1.39	0.41
1:D:632:GLU:HG3	1:F:1109:LEU:HD22	2.03	0.41
1:D:650:LEU:HD21	1:D:687:ILE:HG13	2.02	0.41
1:F:1049:GLY:O	1:F:1093:ILE:HG13	2.21	0.41
1:D:602:GLN:NE2	1:D:713:LYS:NZ	2.68	0.41
1:C:411:ALA:HB1	2:D:2002:HOH:O	2.21	0.41
1:F:1061:ILE:HA	1:F:1064:MSE:HE3	2.02	0.41
1:A:44:ASP:OD2	1:A:85:ARG:NH1	2.50	0.41
1:C:453:GLN:C	1:C:455:PRO:HD3	2.40	0.41
1:B:242:MSE:HE3	1:B:242:MSE:HB2	1.78	0.41
1:A:71:GLN:O	1:A:72:ASN:HB2	2.22	0.40
1:C:478:CYS:HB3	1:C:481:CYS:SG	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:714:VAL:HB	1:E:915:LEU:HD22	2.02	0.40
1:B:251:ARG:NH1	1:B:292:LEU:O	2.54	0.40
1:E:834:ASN:HB2	2:E:2065:HOH:O	2.21	0.40
1:B:260:ASN:HD22	1:B:262:GLN:N	2.20	0.40
1:A:115:LEU:N	1:A:115:LEU:HD13	2.37	0.40
1:B:257:GLU:CG	1:B:258:GLY:H	2.32	0.40
1:A:21:SER:OG	1:A:117:PHE:CB	2.69	0.40
1:D:616:GLU:OE1	1:F:1043:SER:CB	2.69	0.40
1:F:1003:LYS:N	1:F:1112:ASP:OD2	2.54	0.40
1:F:1040:PHE:CG	1:F:1104:LEU:HG	2.56	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	115/117 (98%)	105 (91%)	4 (4%)	6 (5%)	2 7
1	B	115/117 (98%)	106 (92%)	5 (4%)	4 (4%)	4 15
1	C	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	21 55
1	D	115/117 (98%)	109 (95%)	4 (4%)	2 (2%)	11 36
1	E	115/117 (98%)	101 (88%)	11 (10%)	3 (3%)	7 22
1	F	115/117 (98%)	105 (91%)	6 (5%)	4 (4%)	4 15
All	All	690/702 (98%)	632 (92%)	38 (6%)	20 (3%)	6 19

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ASP
1	B	257	GLU

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Mol	Chain	Res	Type
1	E	802	GLN
1	E	870	ALA
1	E	894	ASP
1	F	1094	ASP
1	F	1106	GLN
1	A	106	GLN
1	D	694	ASP
1	F	1002	GLN
1	B	270	ALA
1	B	294	ASP
1	C	494	ASP
1	D	613	TYR
1	A	33	SER
1	A	43	SER
1	A	57	GLU
1	B	231	GLN
1	A	58	GLY
1	F	1093	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	98/95 (103%)	85 (87%)	13 (13%)	5 14
1	B	98/95 (103%)	91 (93%)	7 (7%)	18 46
1	C	98/95 (103%)	87 (89%)	11 (11%)	7 22
1	D	98/95 (103%)	90 (92%)	8 (8%)	14 38
1	E	98/95 (103%)	86 (88%)	12 (12%)	6 18
1	F	98/95 (103%)	91 (93%)	7 (7%)	18 46
All	All	588/570 (103%)	530 (90%)	58 (10%)	10 28

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	18	LEU
1	A	24	LEU
1	A	29	ARG
1	A	34	ASN
1	A	37	LEU
1	A	39	LEU
1	A	51	ARG
1	A	54	LYS
1	A	62	GLN
1	A	85	ARG
1	A	104	LEU
1	A	115	LEU
1	B	209	ASN
1	B	224	LEU
1	B	229	ARG
1	B	235	LEU
1	B	254	LYS
1	B	260	ASN
1	B	285	ARG
1	C	403	LYS
1	C	424	LEU
1	C	429	ARG
1	C	435	LEU
1	C	439	LEU
1	C	446	VAL
1	C	460	ASN
1	C	476	LYS
1	C	485	ARG
1	C	487	ILE
1	C	504	LEU
1	D	624	LEU
1	D	629	ARG
1	D	635	LEU
1	D	644	ASP
1	D	654	LYS
1	D	685	ARG
1	D	694	ASP
1	D	704	LEU
1	E	803	LYS
1	E	809	ASN
1	E	818	LEU
1	E	829	ARG

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Mol	Chain	Res	Type
1	E	839	LEU
1	E	841	LEU
1	E	846	VAL
1	E	860	ASN
1	E	863	GLN
1	E	885	ARG
1	E	894	ASP
1	E	916	THR
1	F	1029	ARG
1	F	1037	LEU
1	F	1039	LEU
1	F	1054	LYS
1	F	1057	GLU
1	F	1092	LEU
1	F	1104	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	62	GLN
1	A	63	GLN
1	A	71	GLN
1	B	202	GLN
1	B	260	ASN
1	B	262	GLN
1	B	271	GLN
1	C	460	ASN
1	C	463	GLN
1	D	602	GLN
1	D	662	GLN
1	E	802	GLN
1	E	860	ASN
1	E	862	GLN
1	E	871	GLN
1	E	906	GLN
1	F	1020	ASN
1	F	1031	GLN
1	F	1060	ASN
1	F	1062	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	114/117 (97%)	-0.21	0 100 100	9, 24, 40, 64	0
1	B	114/117 (97%)	-0.00	3 (2%) 59 47	10, 25, 52, 86	0
1	C	114/117 (97%)	-0.32	0 100 100	12, 24, 55, 71	0
1	D	114/117 (97%)	-0.29	1 (0%) 85 79	9, 24, 48, 85	0
1	E	114/117 (97%)	-0.16	0 100 100	9, 24, 49, 58	0
1	F	114/117 (97%)	-0.01	1 (0%) 85 79	13, 25, 45, 68	0
All	All	684/702 (97%)	-0.17	5 (0%) 89 84	9, 24, 49, 86	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	633	SER	4.7
1	B	257	GLU	4.5
1	F	1094	ASP	3.2
1	B	234	ASN	2.1
1	B	233	SER	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 (i)

There are no such residues in this entry.