Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:44 PM GMT

PDB ID	:	3UR1
Title	:	The structure of a ternary complex between CheA domains P4 and P5 with CheW and with a truncated fragment of TM14, a chemoreceptor analog from Thermotoga maritima.
Authors	:	Li, X.; Crane, B.R.; Bilwes, A.M.
Deposited on	:	2011-11-21
Resolution	:	4.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

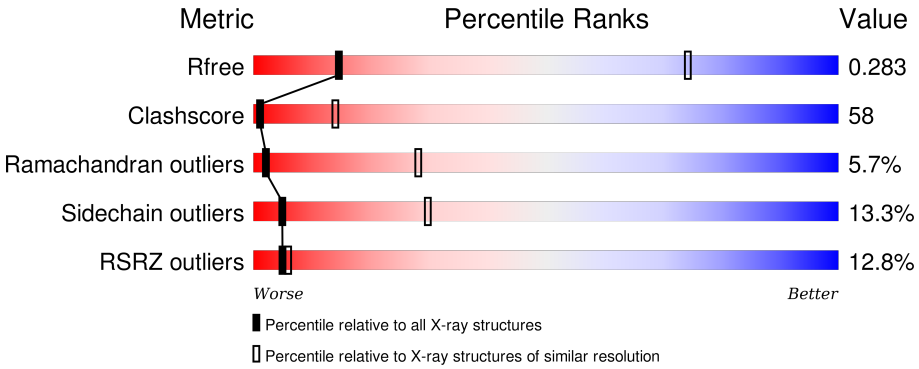
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 4.50 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}	91344	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

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	320	22% 23% 50% 9% 18%
2	B	139	39% 48% 13%
3	C	85	29% 59% 12%
3	D	85	4% 13% 76% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4488 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 Chemotaxis protein CheA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2063	1312	354	392	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	352	GLY	-	EXPRESSION TAG	UNP Q56310
A	353	SER	-	EXPRESSION TAG	UNP Q56310
A	354	HIS	-	EXPRESSION TAG	UNP Q56310

- Molecule 2 is a protein called Chemotaxis protein CheW.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total	C	N	O	S	0	0	0
			1105	710	183	210	2			

- Molecule 3 is a protein called Methyl-accepting chemotaxis protein.

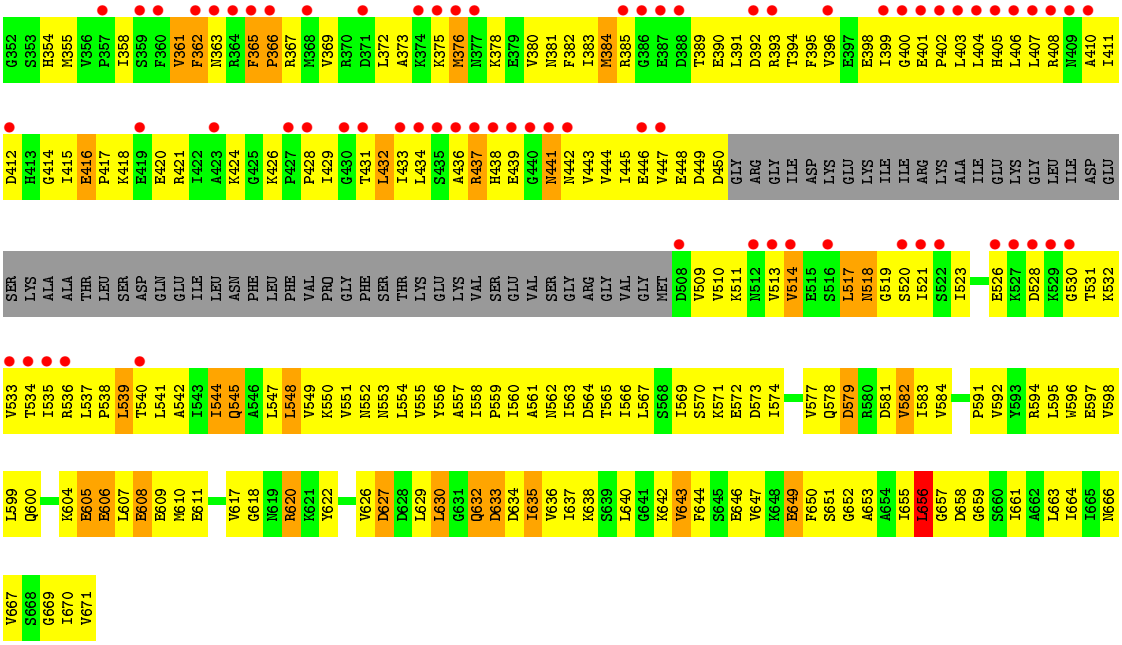
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	85	Total	C	N	O	S	0	0	0
			660	402	120	136	2			
3	D	85	Total	C	N	O	S	0	0	0
			660	402	120	136	2			

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.

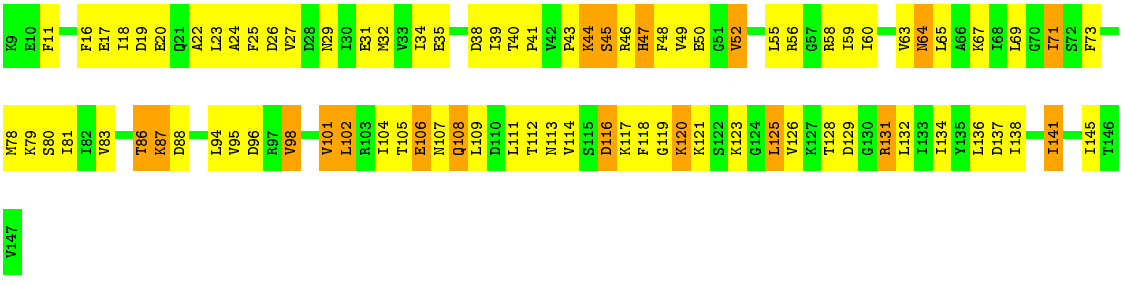
- Molecule 1: Chemotaxis protein CheA

Chain A:



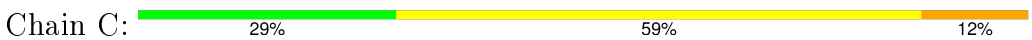
- Molecule 2: Chemotaxis protein CheW

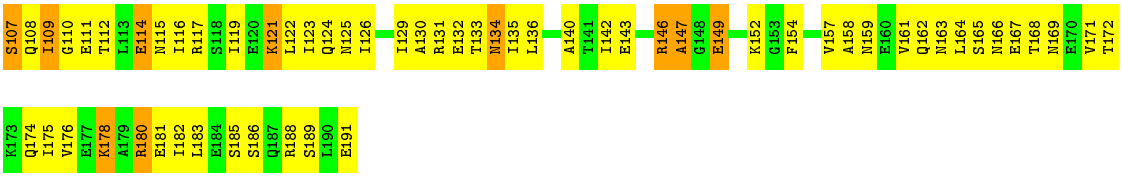
Chain B:



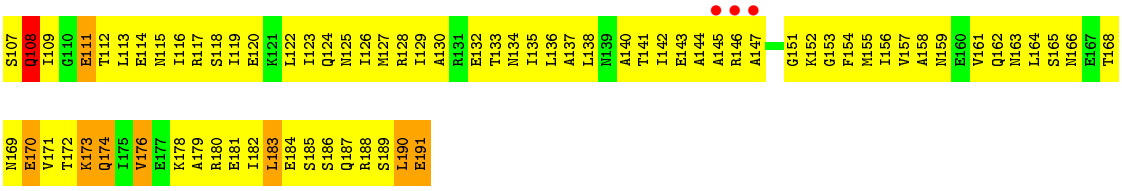
- Molecule 3: Methyl-accepting chemotaxis protein

Chain C:





- Molecule 3: Methyl-accepting chemotaxis protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	213.99Å 213.99Å 208.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.75 – 4.50 49.90 – 4.49	Depositor EDS
% Data completeness (in resolution range)	86.0 (29.75-4.50) 86.0 (49.90-4.49)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.00 (at 4.45Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.266 , 0.291 0.240 , 0.283	Depositor DCC
R_{free} test set	983 reflections (10.34%)	DCC
Wilson B-factor (Å^2)	177.6	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 220.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 10933 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4488	wwPDB-VP
Average B, all atoms (Å^2)	245.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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	0.42	0/2087	0.63	1/2818 (0.0%)
2	B	0.44	0/1116	0.59	0/1501
3	C	0.55	0/660	0.66	0/884
3	D	0.51	0/660	0.61	0/884
All	All	0.46	0/4523	0.62	1/6087 (0.0%)

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	542	ALA	N-CA-C	10.20	138.54	111.00

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	2063	0	2147	272	0
2	B	1105	0	1166	91	0
3	C	660	0	678	105	0
3	D	660	0	678	122	1
All	All	4488	0	4669	534	1

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 58.

All (534) 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:402:PRO:HB3	1:A:514:VAL:HG22	1.43	1.00
1:A:443:VAL:CG2	1:A:539:LEU:HB3	1.92	0.99
3:C:115:ASN:HD21	3:D:178:LYS:HD2	1.25	0.97
1:A:653:ALA:HB2	1:A:663:LEU:HD23	1.46	0.96
1:A:365:PHE:H	1:A:366:PRO:HD2	1.34	0.93
1:A:539:LEU:HD22	1:A:539:LEU:O	1.69	0.92
2:B:86:THR:HG22	2:B:87:LYS:HD3	1.51	0.92
1:A:604:LYS:HG3	1:A:605:GLU:H	1.37	0.90
2:B:123:LYS:HG3	2:B:137:ASP:HB2	1.53	0.89
1:A:443:VAL:HG23	1:A:539:LEU:HB3	1.55	0.89
1:A:402:PRO:HG3	1:A:513:VAL:HG12	1.55	0.88
3:C:182:ILE:HG21	3:D:182:ILE:HD13	1.55	0.88
1:A:441:ASN:C	1:A:441:ASN:HD22	1.77	0.88
3:D:123:ILE:HD13	3:D:176:VAL:HG22	1.56	0.88
3:C:117:ARG:HH22	3:C:183:LEU:HD13	1.39	0.87
1:A:514:VAL:HG11	1:A:535:ILE:HD13	1.57	0.87
1:A:380:VAL:HG21	1:A:411:ILE:HA	1.57	0.86
3:D:108:GLN:N	3:D:111:GLU:HB2	1.93	0.84
1:A:545:GLN:HB3	1:A:560:ILE:HD12	1.61	0.83
1:A:381:ASN:HB3	1:A:431:THR:HA	1.61	0.82
1:A:398:GLU:HG3	1:A:517:LEU:HD12	1.62	0.81
1:A:521:ILE:HG22	1:A:535:ILE:HG12	1.63	0.81
1:A:391:LEU:HB2	1:A:443:VAL:HG21	1.63	0.81
3:C:174:GLN:HB3	3:D:122:LEU:HD13	1.63	0.81
3:C:174:GLN:NE2	3:D:122:LEU:HD22	1.96	0.81
1:A:358:ILE:HG13	1:A:391:LEU:HD22	1.64	0.80
1:A:640:LEU:HD22	1:A:652:GLY:HA2	1.62	0.80
1:A:436:ALA:HA	1:A:445:ILE:HA	1.63	0.79
1:A:373:ALA:HA	1:A:411:ILE:HG21	1.65	0.79
3:D:141:THR:HG23	3:D:155:MET:HB3	1.66	0.79
3:D:144:ALA:HB3	3:D:155:MET:HG2	1.64	0.78
1:A:372:LEU:HD13	1:A:408:ARG:HG2	1.67	0.77
1:A:358:ILE:HD12	1:A:389:THR:HB	1.66	0.77
3:C:123:ILE:HD13	3:D:171:VAL:HB	1.65	0.76
1:A:523:ILE:HG23	1:A:531:THR:HG21	1.68	0.76
1:A:604:LYS:HG3	1:A:605:GLU:N	2.00	0.75
2:B:27:VAL:HG21	3:C:146:ARG:HD3	1.67	0.75
1:A:620:ARG:NH1	1:A:622:TYR:HB3	2.02	0.74
1:A:635:ILE:HD13	1:A:635:ILE:H	1.53	0.74
1:A:598:VAL:HG21	1:A:670:ILE:HG23	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:LEU:HD13	1:A:445:ILE:HD11	1.68	0.74
1:A:653:ALA:HA	1:A:663:LEU:HA	1.70	0.73
1:A:441:ASN:ND2	1:A:441:ASN:C	2.39	0.73
3:D:140:ALA:O	3:D:144:ALA:HB2	1.88	0.73
3:D:183:LEU:HD12	3:D:183:LEU:H	1.52	0.73
1:A:443:VAL:HG22	1:A:539:LEU:HB3	1.70	0.73
1:A:406:LEU:HD22	1:A:533:VAL:HG11	1.71	0.73
1:A:548:LEU:HD11	1:A:656:LEU:HD11	1.70	0.73
2:B:101:VAL:HG22	3:C:142:ILE:HG23	1.71	0.72
1:A:415:ILE:HG23	1:A:421:ARG:NH1	2.04	0.72
2:B:56:ARG:HH21	3:D:152:LYS:HE3	1.54	0.72
1:A:391:LEU:HD11	1:A:399:ILE:HG21	1.71	0.72
1:A:550:LYS:HE3	1:A:553:ASN:HA	1.72	0.71
1:A:550:LYS:HB2	1:A:630:LEU:HD13	1.71	0.71
1:A:511:LYS:O	1:A:511:LYS:HD3	1.91	0.71
3:D:112:THR:HB	3:D:183:LEU:HG	1.73	0.71
1:A:640:LEU:H	1:A:640:LEU:HD23	1.56	0.70
1:A:355:MET:CE	1:A:541:LEU:HD22	2.21	0.70
1:A:437:ARG:HE	1:A:439:GLU:HB2	1.56	0.70
1:A:436:ALA:HB2	1:A:445:ILE:HG23	1.72	0.70
2:B:56:ARG:HH22	3:D:156:ILE:HD12	1.55	0.70
1:A:399:ILE:HD13	1:A:537:LEU:HD13	1.73	0.70
1:A:549:VAL:HG22	1:A:629:LEU:HD23	1.74	0.70
3:C:115:ASN:ND2	3:D:178:LYS:HD2	2.04	0.69
3:C:164:LEU:O	3:C:167:GLU:HB3	1.92	0.69
1:A:438:HIS:CD2	1:A:539:LEU:HG	2.26	0.69
1:A:551:VAL:HA	1:A:627:ASP:HB2	1.73	0.69
1:A:559:PRO:HB2	1:A:562:ASN:HD22	1.58	0.69
1:A:547:LEU:HD11	1:A:566:ILE:HD11	1.73	0.69
1:A:355:MET:HE2	1:A:541:LEU:HD13	1.73	0.69
3:C:182:ILE:HD13	3:D:182:ILE:CD1	2.23	0.69
3:C:119:ILE:O	3:C:123:ILE:HG22	1.93	0.69
2:B:87:LYS:HD3	2:B:87:LYS:H	1.57	0.69
1:A:380:VAL:HB	1:A:411:ILE:HG13	1.75	0.69
1:A:545:GLN:CB	1:A:560:ILE:HD12	2.23	0.69
1:A:544:ILE:HD13	1:A:637:ILE:HD13	1.75	0.69
1:A:551:VAL:HG21	1:A:595:LEU:HD23	1.75	0.68
3:D:152:LYS:NZ	3:D:156:ILE:HD11	2.09	0.68
3:C:166:ASN:HA	3:C:169:ASN:HD22	1.59	0.68
1:A:355:MET:HE3	1:A:541:LEU:HD22	1.76	0.68
1:A:560:ILE:HA	1:A:563:ILE:HD12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:SER:OG	2:B:49:VAL:HG21	1.95	0.67
2:B:46:ARG:O	2:B:49:VAL:HG22	1.93	0.67
1:A:606:GLU:HG3	1:A:610:MET:SD	2.35	0.67
3:C:168:THR:HG22	3:C:172:THR:OG1	1.96	0.66
2:B:87:LYS:HB2	2:B:87:LYS:NZ	2.11	0.66
3:D:107:SER:HA	3:D:111:GLU:CD	2.16	0.66
2:B:11:PHE:HB2	2:B:104:ILE:HB	1.76	0.66
3:D:123:ILE:HD12	3:D:176:VAL:HG13	1.78	0.65
1:A:442:ASN:HA	1:A:538:PRO:HA	1.78	0.65
3:C:123:ILE:O	3:C:126:ILE:HD13	1.96	0.65
1:A:450:ASP:HA	1:A:530:GLY:HA3	1.79	0.64
1:A:560:ILE:HD11	1:A:632:GLN:HG3	1.79	0.64
3:C:154:PHE:CE2	3:D:151:GLY:HA2	2.33	0.64
1:A:544:ILE:HD11	1:A:637:ILE:HG12	1.78	0.64
2:B:22:ALA:HB3	2:B:132:LEU:O	1.97	0.64
1:A:406:LEU:HB3	1:A:533:VAL:HG11	1.80	0.64
2:B:52:VAL:HB	2:B:59:ILE:HG23	1.80	0.64
1:A:399:ILE:HG12	1:A:445:ILE:HD12	1.80	0.64
1:A:549:VAL:HG11	1:A:626:VAL:HG11	1.81	0.63
1:A:380:VAL:HG22	1:A:415:ILE:HD12	1.81	0.63
1:A:407:LEU:HD11	1:A:434:LEU:HD22	1.79	0.63
1:A:438:HIS:CE1	1:A:539:LEU:HG	2.33	0.63
1:A:432:LEU:HB2	1:A:449:ASP:HA	1.81	0.63
3:C:108:GLN:HA	3:C:111:GLU:HB2	1.80	0.63
3:C:132:GLU:O	3:C:135:ILE:HG12	1.99	0.63
1:A:441:ASN:ND2	1:A:441:ASN:O	2.31	0.62
1:A:651:SER:HB3	1:A:666:ASN:HB2	1.81	0.62
3:C:175:ILE:HD11	3:D:126:ILE:HG13	1.80	0.62
1:A:446:GLU:HG2	1:A:534:THR:HG23	1.80	0.62
3:C:168:THR:HG22	3:C:172:THR:HG1	1.65	0.62
3:D:107:SER:C	3:D:111:GLU:HB2	2.20	0.62
3:C:188:ARG:O	3:C:191:GLU:HB2	1.99	0.62
3:C:108:GLN:O	3:C:111:GLU:HB2	2.00	0.62
2:B:34:ILE:HG13	2:B:81:ILE:HB	1.81	0.61
1:A:443:VAL:HG12	1:A:445:ILE:HG13	1.82	0.61
1:A:395:PHE:HD1	1:A:517:LEU:HD13	1.65	0.61
1:A:401:GLU:HB3	1:A:402:PRO:HD3	1.82	0.61
1:A:547:LEU:HD12	1:A:563:ILE:HD13	1.82	0.61
3:C:186:SER:HA	3:C:189:SER:HB3	1.82	0.61
1:A:545:GLN:HB3	1:A:560:ILE:CD1	2.29	0.61
3:C:131:ARG:HD3	3:C:134:ASN:ND2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:108:GLN:O	3:D:112:THR:HG23	2.01	0.60
2:B:132:LEU:H	2:B:132:LEU:HD23	1.67	0.60
3:D:181:GLU:HA	3:D:184:GLU:HB3	1.83	0.60
3:D:118:SER:O	3:D:122:LEU:HG	2.01	0.60
1:A:380:VAL:HG13	1:A:415:ILE:HD12	1.84	0.60
1:A:438:HIS:NE2	1:A:539:LEU:HG	2.16	0.60
1:A:405:HIS:CD2	1:A:510:VAL:HG21	2.36	0.59
2:B:56:ARG:HE	3:D:152:LYS:HG3	1.67	0.59
3:C:178:LYS:HG2	3:D:118:SER:O	2.02	0.59
1:A:391:LEU:CB	1:A:443:VAL:HG21	2.32	0.59
1:A:571:LYS:CE	1:A:608:GLU:HA	2.33	0.59
3:D:116:ILE:O	3:D:119:ILE:HG22	2.02	0.59
3:D:144:ALA:HB3	3:D:155:MET:CG	2.32	0.59
1:A:594:ARG:HB2	1:A:597:GLU:HG3	1.85	0.59
3:C:178:LYS:NZ	3:D:122:LEU:HD11	2.18	0.59
1:A:358:ILE:HB	1:A:389:THR:O	2.02	0.59
3:C:140:ALA:HA	3:C:143:GLU:OE1	2.03	0.59
1:A:582:VAL:HG12	1:A:591:PRO:HA	1.85	0.59
3:C:166:ASN:HA	3:C:169:ASN:ND2	2.18	0.58
1:A:399:ILE:HB	1:A:537:LEU:HD22	1.85	0.58
3:C:171:VAL:HG12	3:D:126:ILE:HG12	1.85	0.58
1:A:635:ILE:CD1	1:A:635:ILE:H	2.17	0.58
1:A:514:VAL:HG11	1:A:535:ILE:HG21	1.84	0.58
1:A:385:ARG:CZ	1:A:433:ILE:HD13	2.33	0.58
1:A:650:PHE:HE2	2:B:43:PRO:HD2	1.69	0.58
2:B:56:ARG:NH2	3:D:156:ILE:HD12	2.19	0.58
3:C:121:LYS:HA	3:C:124:GLN:HB2	1.86	0.58
1:A:395:PHE:HE1	1:A:517:LEU:HD22	1.69	0.58
2:B:55:LEU:HD23	2:B:56:ARG:CG	2.34	0.58
1:A:638:LYS:HD2	2:B:59:ILE:HD13	1.85	0.58
1:A:547:LEU:HD11	1:A:566:ILE:CD1	2.34	0.57
1:A:358:ILE:HD11	1:A:445:ILE:HD13	1.87	0.57
3:D:132:GLU:HG3	3:D:133:THR:N	2.20	0.57
1:A:557:ALA:HB3	1:A:664:ILE:HG13	1.85	0.57
1:A:571:LYS:HE2	1:A:608:GLU:OE1	2.05	0.57
3:D:116:ILE:HG23	3:D:117:ARG:N	2.18	0.57
1:A:545:GLN:O	1:A:560:ILE:HB	2.04	0.57
3:C:123:ILE:CD1	3:D:171:VAL:HB	2.34	0.57
3:C:111:GLU:O	3:C:115:ASN:HB2	2.04	0.57
3:C:107:SER:O	3:C:111:GLU:N	2.39	0.56
3:D:109:ILE:N	3:D:109:ILE:HD12	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ARG:HH22	1:A:426:LYS:NZ	2.02	0.56
3:C:171:VAL:CG1	3:D:126:ILE:HG12	2.34	0.56
2:B:22:ALA:C	2:B:23:LEU:HD12	2.25	0.56
2:B:32:MET:H	2:B:83:VAL:HG23	1.70	0.56
3:D:116:ILE:HB	3:D:183:LEU:HD21	1.87	0.56
1:A:582:VAL:HA	1:A:592:VAL:HG22	1.87	0.56
1:A:395:PHE:O	1:A:399:ILE:HG22	2.06	0.56
1:A:381:ASN:ND2	1:A:382:PHE:H	2.03	0.56
1:A:646:GLU:HG2	1:A:647:VAL:N	2.21	0.56
1:A:406:LEU:HD21	1:A:521:ILE:HG21	1.86	0.56
3:D:124:GLN:HG2	3:D:127:MET:HE1	1.88	0.56
1:A:447:VAL:HB	1:A:533:VAL:HB	1.88	0.56
1:A:569:ILE:HD13	1:A:583:ILE:HD13	1.87	0.55
1:A:437:ARG:NE	1:A:439:GLU:HB2	2.20	0.55
2:B:48:PHE:CZ	2:B:145:ILE:HG23	2.42	0.55
1:A:399:ILE:HB	1:A:537:LEU:CD2	2.37	0.55
1:A:523:ILE:HG23	1:A:531:THR:CG2	2.35	0.55
1:A:404:LEU:O	1:A:408:ARG:HG3	2.06	0.55
1:A:541:LEU:HD23	1:A:541:LEU:H	1.71	0.55
2:B:109:LEU:HD12	2:B:109:LEU:O	2.07	0.55
3:C:111:GLU:O	3:C:115:ASN:CB	2.55	0.55
2:B:123:LYS:HE2	2:B:137:ASP:OD1	2.07	0.55
1:A:544:ILE:CD1	1:A:637:ILE:HG12	2.37	0.55
2:B:119:GLY:O	2:B:121:LYS:N	2.39	0.55
1:A:514:VAL:CG1	1:A:535:ILE:HG21	2.37	0.55
3:C:178:LYS:HZ2	3:D:122:LEU:HD11	1.72	0.55
1:A:549:VAL:HG22	1:A:629:LEU:CD2	2.37	0.55
1:A:640:LEU:H	1:A:640:LEU:CD2	2.20	0.54
3:C:146:ARG:HD2	3:C:147:ALA:N	2.22	0.54
1:A:376:MET:SD	1:A:412:ASP:HB2	2.46	0.54
1:A:567:LEU:O	1:A:567:LEU:HD12	2.07	0.54
1:A:365:PHE:H	1:A:366:PRO:CD	2.15	0.54
1:A:421:ARG:HH12	1:A:426:LYS:NZ	2.05	0.54
3:D:116:ILE:CG2	3:D:117:ARG:N	2.70	0.54
1:A:554:LEU:HD11	2:B:41:PRO:HG2	1.90	0.54
3:C:165:SER:C	3:C:167:GLU:H	2.10	0.54
3:D:125:ASN:O	3:D:128:ARG:HB3	2.08	0.54
1:A:436:ALA:HB1	1:A:445:ILE:HG12	1.89	0.54
1:A:632:GLN:HG2	1:A:633:ASP:N	2.22	0.54
3:D:138:LEU:O	3:D:142:ILE:HG12	2.08	0.54
3:D:141:THR:HG23	3:D:155:MET:CB	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:109:ILE:HG21	3:D:190:LEU:HD12	1.89	0.53
3:C:185:SER:OG	3:D:111:GLU:HB3	2.08	0.53
2:B:55:LEU:HD23	2:B:56:ARG:HG3	1.90	0.53
3:D:183:LEU:O	3:D:187:GLN:N	2.42	0.53
3:C:131:ARG:HH21	3:C:131:ARG:HG2	1.73	0.53
2:B:105:THR:HG23	2:B:107:ASN:H	1.73	0.53
1:A:570:SER:C	1:A:572:GLU:H	2.10	0.53
2:B:118:PHE:HD1	2:B:121:LYS:HB2	1.72	0.53
2:B:125:LEU:HD22	2:B:126:VAL:N	2.23	0.53
3:C:135:ILE:HG13	3:C:136:LEU:N	2.23	0.53
3:D:151:GLY:O	3:D:155:MET:HG3	2.08	0.53
1:A:548:LEU:CD1	1:A:656:LEU:HD11	2.37	0.53
1:A:562:ASN:CB	1:A:667:VAL:HG21	2.38	0.53
1:A:355:MET:CE	1:A:541:LEU:HD13	2.39	0.53
3:D:116:ILE:O	3:D:120:GLU:HG3	2.09	0.53
3:C:116:ILE:HD13	3:C:182:ILE:HD12	1.92	0.52
2:B:106:GLU:HA	2:B:109:LEU:CD2	2.39	0.52
2:B:138:ILE:O	2:B:141:ILE:HG22	2.09	0.52
2:B:18:ILE:HG21	2:B:71:ILE:HD11	1.90	0.52
3:D:116:ILE:HB	3:D:183:LEU:HD11	1.91	0.52
1:A:372:LEU:CD1	1:A:408:ARG:HG2	2.37	0.52
3:C:172:THR:O	3:C:176:VAL:HG23	2.10	0.52
1:A:574:ILE:HG21	1:A:581:ASP:OD2	2.09	0.52
2:B:56:ARG:NH2	3:D:152:LYS:HE3	2.21	0.52
3:C:134:ASN:CG	3:C:135:ILE:N	2.63	0.52
3:C:165:SER:C	3:C:167:GLU:N	2.63	0.52
2:B:31:GLU:HB2	2:B:83:VAL:HG23	1.90	0.52
3:C:176:VAL:O	3:C:180:ARG:HB3	2.10	0.52
1:A:393:ARG:O	1:A:396:VAL:HG13	2.10	0.52
1:A:642:LYS:C	1:A:644:PHE:H	2.12	0.52
1:A:547:LEU:CD1	1:A:566:ILE:HD11	2.40	0.52
3:C:126:ILE:HG23	3:C:130:ALA:HB3	1.92	0.52
2:B:101:VAL:HG22	3:C:142:ILE:CG2	2.39	0.52
3:C:126:ILE:HG23	3:C:130:ALA:CB	2.40	0.51
2:B:17:GLU:O	2:B:96:ASP:HB2	2.10	0.51
1:A:380:VAL:HG11	1:A:410:ALA:O	2.11	0.51
3:D:182:ILE:O	3:D:186:SER:HB2	2.10	0.51
1:A:405:HIS:CB	1:A:510:VAL:HG11	2.41	0.51
3:C:131:ARG:HD3	3:C:134:ASN:HD22	1.74	0.51
1:A:635:ILE:HD13	1:A:635:ILE:N	2.22	0.51
1:A:418:LYS:HE3	1:A:428:PRO:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:HIS:HB3	1:A:510:VAL:HG11	1.92	0.51
1:A:549:VAL:HG12	1:A:550:LYS:N	2.26	0.51
3:D:161:VAL:O	3:D:165:SER:HB2	2.11	0.51
3:D:107:SER:C	3:D:111:GLU:H	2.14	0.51
3:C:146:ARG:HD2	3:C:146:ARG:C	2.31	0.51
3:C:166:ASN:CA	3:C:169:ASN:HD22	2.23	0.51
1:A:375:LYS:HB3	1:A:376:MET:HE3	1.91	0.51
1:A:410:ALA:HB1	1:A:432:LEU:HD22	1.93	0.51
3:C:182:ILE:CG2	3:D:182:ILE:HD13	2.35	0.51
2:B:87:LYS:HB2	2:B:87:LYS:HZ2	1.74	0.51
3:C:154:PHE:HE2	3:D:151:GLY:HA2	1.76	0.50
1:A:358:ILE:HD11	1:A:445:ILE:CD1	2.42	0.50
1:A:514:VAL:HG21	1:A:521:ILE:HG23	1.93	0.50
1:A:410:ALA:HB1	1:A:449:ASP:HB3	1.93	0.50
1:A:369:VAL:HG21	1:A:407:LEU:HD13	1.94	0.50
1:A:563:ILE:HG22	1:A:564:ASP:N	2.27	0.50
3:D:145:ALA:HB2	3:D:155:MET:CE	2.41	0.50
1:A:544:ILE:CD1	1:A:637:ILE:HD13	2.41	0.50
1:A:517:LEU:O	1:A:518:ASN:HB2	2.11	0.50
3:D:113:LEU:C	3:D:115:ASN:H	2.14	0.50
1:A:383:ILE:HD12	1:A:385:ARG:HH21	1.77	0.50
3:D:168:THR:HG22	3:D:172:THR:OG1	2.12	0.50
1:A:650:PHE:CE2	2:B:43:PRO:HD2	2.47	0.49
1:A:380:VAL:HG12	1:A:432:LEU:HD23	1.93	0.49
3:D:113:LEU:C	3:D:115:ASN:N	2.65	0.49
3:C:157:VAL:HG21	3:D:140:ALA:HB1	1.94	0.49
3:D:124:GLN:O	3:D:127:MET:HB3	2.12	0.49
1:A:365:PHE:N	1:A:366:PRO:HD2	2.15	0.49
3:C:111:GLU:O	3:C:115:ASN:N	2.34	0.49
1:A:523:ILE:HD13	1:A:533:VAL:HG22	1.95	0.49
3:D:112:THR:O	3:D:115:ASN:HB2	2.12	0.49
3:C:131:ARG:O	3:C:134:ASN:ND2	2.45	0.49
3:C:129:ILE:O	3:C:132:GLU:HB3	2.13	0.49
1:A:510:VAL:HA	1:A:513:VAL:HG23	1.95	0.49
1:A:535:ILE:HG22	1:A:536:ARG:H	1.77	0.49
3:D:141:THR:C	3:D:143:GLU:H	2.16	0.49
1:A:637:ILE:HG13	1:A:637:ILE:O	2.12	0.49
1:A:647:VAL:CG2	2:B:45:SER:HA	2.42	0.49
2:B:32:MET:HG2	2:B:83:VAL:HG21	1.94	0.49
2:B:105:THR:HG23	2:B:107:ASN:HB2	1.94	0.49
3:D:113:LEU:HA	3:D:116:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:VAL:HG21	2:B:45:SER:HA	1.94	0.49
2:B:11:PHE:CB	2:B:104:ILE:HB	2.42	0.49
1:A:581:ASP:O	1:A:582:VAL:HG13	2.13	0.49
3:C:154:PHE:O	3:C:158:ALA:HB2	2.13	0.49
1:A:415:ILE:HG23	1:A:421:ARG:CZ	2.43	0.49
3:D:123:ILE:HG21	3:D:176:VAL:CG2	2.43	0.49
1:A:617:VAL:HG23	1:A:620:ARG:HG3	1.95	0.49
3:C:123:ILE:C	3:C:125:ASN:N	2.65	0.48
2:B:31:GLU:HB2	2:B:83:VAL:CG2	2.43	0.48
1:A:380:VAL:CB	1:A:411:ILE:HG13	2.43	0.48
3:C:129:ILE:HG23	3:D:164:LEU:HD23	1.96	0.48
3:D:132:GLU:O	3:D:136:LEU:HB2	2.12	0.48
1:A:391:LEU:CD1	1:A:399:ILE:HG21	2.42	0.48
3:C:180:ARG:O	3:C:180:ARG:HD2	2.13	0.48
3:D:162:GLN:O	3:D:165:SER:HB3	2.14	0.48
2:B:16:PHE:HE2	2:B:95:VAL:HG11	1.77	0.48
1:A:432:LEU:HD13	1:A:448:GLU:O	2.13	0.48
3:D:109:ILE:H	3:D:109:ILE:CD1	2.25	0.48
3:C:114:GLU:O	3:C:117:ARG:N	2.46	0.48
2:B:63:VAL:HG12	2:B:64:ASN:N	2.28	0.48
1:A:406:LEU:HB2	1:A:447:VAL:HG21	1.95	0.48
1:A:442:ASN:OD1	1:A:538:PRO:HG3	2.12	0.48
2:B:47:HIS:C	2:B:67:LYS:HZ1	2.17	0.48
2:B:47:HIS:HB3	2:B:67:LYS:HZ1	1.79	0.48
1:A:640:LEU:CD2	1:A:652:GLY:HA2	2.41	0.48
1:A:438:HIS:CG	1:A:539:LEU:HG	2.48	0.48
3:C:182:ILE:HD13	3:D:182:ILE:HD13	1.95	0.48
3:D:152:LYS:HA	3:D:155:MET:HE3	1.95	0.48
2:B:48:PHE:HE2	2:B:145:ILE:HG12	1.79	0.48
1:A:395:PHE:CD1	1:A:517:LEU:HD13	2.47	0.47
2:B:125:LEU:HD13	2:B:125:LEU:O	2.14	0.47
1:A:424:LYS:HE2	1:A:528:ASP:OD2	2.14	0.47
1:A:584:VAL:HG13	1:A:584:VAL:O	2.13	0.47
1:A:363:ASN:O	1:A:366:PRO:HD2	2.14	0.47
1:A:361:VAL:HG13	1:A:361:VAL:O	2.13	0.47
1:A:555:VAL:HG12	1:A:630:LEU:HD22	1.97	0.47
2:B:101:VAL:H	3:C:142:ILE:HG21	1.79	0.47
1:A:415:ILE:HD11	1:A:450:ASP:OD1	2.14	0.47
1:A:604:LYS:HE2	1:A:607:LEU:HD21	1.96	0.47
3:D:108:GLN:HE21	3:D:109:ILE:HD13	1.80	0.47
2:B:128:THR:OG1	2:B:131:ARG:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:109:ILE:HD12	3:D:109:ILE:H	1.77	0.47
3:C:174:GLN:HE22	3:D:122:LEU:HD22	1.76	0.47
3:C:123:ILE:HB	3:D:171:VAL:CG1	2.45	0.47
3:D:153:GLY:O	3:D:157:VAL:HG23	2.14	0.47
1:A:606:GLU:HG3	1:A:610:MET:CE	2.45	0.47
1:A:373:ALA:CA	1:A:411:ILE:HG21	2.40	0.47
1:A:438:HIS:CE1	1:A:539:LEU:CD2	2.98	0.47
1:A:361:VAL:O	1:A:361:VAL:HG22	2.15	0.47
1:A:358:ILE:HG13	1:A:391:LEU:CD2	2.38	0.47
1:A:434:LEU:CD1	1:A:447:VAL:HG22	2.45	0.47
2:B:27:VAL:HG21	3:C:146:ARG:CD	2.42	0.47
1:A:571:LYS:HE2	1:A:608:GLU:HA	1.96	0.47
3:D:146:ARG:HG2	3:D:146:ARG:HH11	1.78	0.47
1:A:509:VAL:O	1:A:513:VAL:HG23	2.15	0.47
1:A:594:ARG:HB3	1:A:596:TRP:CZ2	2.50	0.47
3:D:183:LEU:C	3:D:185:SER:N	2.68	0.47
3:D:109:ILE:HG21	3:D:190:LEU:CD1	2.45	0.47
2:B:35:GLU:HG3	2:B:79:LYS:O	2.15	0.47
1:A:411:ILE:N	1:A:411:ILE:HD12	2.30	0.46
1:A:437:ARG:HH21	1:A:444:VAL:HG21	1.81	0.46
2:B:56:ARG:HH21	3:D:152:LYS:HG3	1.80	0.46
1:A:420:GLU:HG2	1:A:420:GLU:O	2.15	0.46
1:A:402:PRO:HB3	1:A:514:VAL:CG2	2.31	0.46
1:A:406:LEU:HD13	1:A:533:VAL:CG1	2.46	0.46
3:D:130:ALA:O	3:D:134:ASN:HB2	2.15	0.46
1:A:539:LEU:O	1:A:539:LEU:CD2	2.53	0.46
1:A:578:GLN:O	1:A:579:ASP:HB2	2.14	0.46
1:A:448:GLU:HG3	1:A:532:LYS:HA	1.96	0.46
3:D:127:MET:HA	3:D:169:ASN:HD21	1.80	0.46
1:A:649:GLU:HA	1:A:669:GLY:O	2.16	0.46
1:A:521:ILE:O	1:A:521:ILE:HG13	2.15	0.46
3:D:108:GLN:HB2	3:D:109:ILE:H	1.46	0.46
1:A:378:LYS:NZ	1:A:417:PRO:HD3	2.31	0.46
1:A:358:ILE:HG12	1:A:362:PHE:HB2	1.97	0.46
1:A:398:GLU:O	1:A:402:PRO:HG2	2.15	0.46
1:A:410:ALA:C	1:A:411:ILE:HD12	2.36	0.46
3:C:159:ASN:O	3:C:162:GLN:HB2	2.16	0.46
2:B:16:PHE:HB3	2:B:98:VAL:HG12	1.98	0.46
1:A:550:LYS:CE	1:A:553:ASN:HA	2.45	0.46
1:A:544:ILE:CD1	1:A:637:ILE:CD1	2.94	0.46
3:C:186:SER:HA	3:C:189:SER:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ILE:HG23	1:A:400:GLY:N	2.31	0.46
3:C:114:GLU:HA	3:C:117:ARG:HB2	1.98	0.46
1:A:551:VAL:HG13	1:A:627:ASP:OD2	2.16	0.46
1:A:562:ASN:HB3	1:A:667:VAL:HG21	1.98	0.45
3:D:129:ILE:HA	3:D:132:GLU:HG2	1.98	0.45
3:C:126:ILE:O	3:C:130:ALA:HB3	2.16	0.45
1:A:551:VAL:O	1:A:554:LEU:HB2	2.17	0.45
3:D:179:ALA:HA	3:D:182:ILE:CD1	2.46	0.45
1:A:547:LEU:HB3	1:A:558:ILE:HB	1.98	0.45
1:A:643:VAL:HG12	2:B:145:ILE:HG22	1.97	0.45
2:B:78:MET:HB3	2:B:94:LEU:HG	1.98	0.45
1:A:611:GLU:OE2	1:A:629:LEU:HD12	2.16	0.45
3:D:183:LEU:O	3:D:184:GLU:C	2.55	0.45
3:C:114:GLU:HA	3:C:117:ARG:CB	2.47	0.45
1:A:655:ILE:O	1:A:655:ILE:HD12	2.17	0.45
3:C:149:GLU:O	3:C:152:LYS:HB2	2.17	0.45
1:A:406:LEU:HD13	1:A:533:VAL:HG12	1.99	0.45
2:B:58:ARG:HE	2:B:60:ILE:HD11	1.82	0.45
1:A:402:PRO:HG3	1:A:513:VAL:CG1	2.38	0.45
3:C:121:LYS:HD2	3:C:121:LYS:O	2.17	0.45
3:D:135:ILE:HG13	3:D:136:LEU:N	2.31	0.45
1:A:403:LEU:HD23	1:A:406:LEU:HD12	1.99	0.45
3:D:123:ILE:CD1	3:D:176:VAL:HG13	2.45	0.45
1:A:560:ILE:HG22	1:A:561:ALA:N	2.31	0.45
3:C:181:GLU:O	3:C:182:ILE:C	2.54	0.44
3:D:183:LEU:O	3:D:185:SER:N	2.50	0.44
3:C:122:LEU:HD12	3:D:171:VAL:CG1	2.48	0.44
3:D:173:LYS:O	3:D:176:VAL:HG23	2.18	0.44
1:A:650:PHE:CZ	1:A:663:LEU:HD13	2.52	0.44
1:A:547:LEU:HB2	1:A:563:ILE:HD11	2.00	0.44
3:C:125:ASN:HD21	3:C:129:ILE:HD12	1.83	0.44
3:C:161:VAL:HA	3:C:164:LEU:HB2	1.99	0.44
1:A:444:VAL:HG12	1:A:446:GLU:CG	2.48	0.44
3:C:126:ILE:HG12	3:D:168:THR:HG23	1.99	0.44
1:A:548:LEU:HD22	1:A:630:LEU:HD22	2.00	0.44
3:D:132:GLU:CG	3:D:133:THR:N	2.81	0.44
1:A:608:GLU:HG3	1:A:609:GLU:N	2.32	0.44
1:A:405:HIS:CG	1:A:510:VAL:HG11	2.53	0.44
1:A:549:VAL:HG11	1:A:626:VAL:CG1	2.47	0.44
2:B:111:LEU:H	2:B:111:LEU:HD12	1.83	0.44
1:A:394:THR:O	1:A:394:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:116:ILE:HD11	3:D:180:ARG:HG3	1.98	0.44
3:D:156:ILE:O	3:D:159:ASN:HB3	2.18	0.44
1:A:421:ARG:HG3	1:A:421:ARG:HH11	1.83	0.44
3:D:119:ILE:HG23	3:D:123:ILE:HD12	2.00	0.44
3:C:161:VAL:HG22	3:D:161:VAL:HG11	1.98	0.44
2:B:125:LEU:C	2:B:125:LEU:HD13	2.38	0.44
2:B:18:ILE:O	2:B:19:ASP:HB2	2.18	0.44
1:A:552:ASN:O	1:A:553:ASN:HB2	2.18	0.43
1:A:519:GLY:HA2	1:A:536:ARG:HG3	2.00	0.43
3:C:123:ILE:HB	3:D:171:VAL:HG12	1.99	0.43
1:A:375:LYS:HB3	1:A:376:MET:CE	2.48	0.43
3:C:178:LYS:O	3:C:180:ARG:N	2.51	0.43
3:D:187:GLN:O	3:D:190:LEU:HB2	2.18	0.43
2:B:112:THR:O	2:B:112:THR:HG22	2.18	0.43
3:C:182:ILE:N	3:D:115:ASN:ND2	2.67	0.43
1:A:655:ILE:HG23	2:B:59:ILE:HD11	1.99	0.43
2:B:118:PHE:HB2	2:B:121:LYS:HG3	2.00	0.43
3:C:185:SER:HB2	3:D:111:GLU:HG2	2.00	0.43
1:A:550:LYS:HE3	1:A:553:ASN:CA	2.47	0.43
1:A:365:PHE:HB3	1:A:382:PHE:CZ	2.54	0.43
1:A:640:LEU:HG	1:A:640:LEU:O	2.18	0.43
1:A:553:ASN:O	1:A:554:LEU:HD22	2.19	0.43
2:B:105:THR:HG22	2:B:108:GLN:CD	2.38	0.43
2:B:64:ASN:CG	2:B:73:PHE:HZ	2.22	0.43
1:A:416:GLU:O	1:A:421:ARG:HB2	2.19	0.43
3:D:115:ASN:O	3:D:118:SER:N	2.51	0.43
2:B:101:VAL:H	3:C:142:ILE:CG2	2.32	0.43
1:A:421:ARG:HG3	1:A:421:ARG:NH1	2.34	0.43
1:A:402:PRO:CB	1:A:514:VAL:HG13	2.49	0.43
3:D:158:ALA:O	3:D:161:VAL:HB	2.18	0.43
1:A:608:GLU:HG3	1:A:609:GLU:HG3	2.01	0.43
2:B:65:LEU:O	2:B:65:LEU:HD12	2.19	0.43
1:A:661:ILE:HD12	2:B:40:THR:CG2	2.49	0.43
1:A:438:HIS:CE1	1:A:539:LEU:CG	3.02	0.42
1:A:432:LEU:CB	1:A:449:ASP:HA	2.47	0.42
3:D:109:ILE:N	3:D:109:ILE:CD1	2.81	0.42
3:D:123:ILE:HG21	3:D:176:VAL:HG22	2.01	0.42
1:A:550:LYS:O	1:A:627:ASP:HB2	2.19	0.42
1:A:369:VAL:HG21	1:A:382:PHE:CE2	2.54	0.42
1:A:437:ARG:NH2	1:A:444:VAL:HG21	2.34	0.42
3:C:178:LYS:HG3	3:D:118:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:LEU:HD22	1:A:657:GLY:H	1.84	0.42
3:D:169:ASN:O	3:D:170:GLU:C	2.57	0.42
1:A:376:MET:HG2	1:A:412:ASP:OD1	2.19	0.42
1:A:367:ARG:O	1:A:367:ARG:HD2	2.19	0.42
1:A:354:HIS:HB3	1:A:541:LEU:HD13	2.01	0.42
2:B:32:MET:H	2:B:83:VAL:CG2	2.32	0.42
1:A:421:ARG:NH2	1:A:426:LYS:NZ	2.67	0.42
1:A:382:PHE:CD2	1:A:432:LEU:HD11	2.55	0.42
3:D:107:SER:O	3:D:108:GLN:C	2.57	0.42
1:A:384:MET:H	1:A:384:MET:CE	2.33	0.42
3:C:143:GLU:HA	3:C:146:ARG:HG3	2.02	0.42
2:B:65:LEU:HD23	2:B:95:VAL:HG11	2.00	0.42
1:A:661:ILE:HB	2:B:40:THR:HG21	2.02	0.42
3:C:165:SER:O	3:C:169:ASN:ND2	2.52	0.42
2:B:69:LEU:HD13	2:B:118:PHE:CE1	2.54	0.42
2:B:105:THR:HG22	2:B:108:GLN:CG	2.50	0.42
2:B:112:THR:C	2:B:114:VAL:H	2.23	0.42
1:A:391:LEU:HD13	1:A:445:ILE:CD1	2.44	0.42
1:A:395:PHE:CE1	1:A:517:LEU:HD22	2.52	0.42
1:A:544:ILE:HD11	1:A:637:ILE:CG1	2.48	0.42
1:A:583:ILE:HG13	1:A:583:ILE:O	2.20	0.42
3:C:109:ILE:HG22	3:C:110:GLY:N	2.34	0.42
1:A:369:VAL:CG2	1:A:407:LEU:HD13	2.50	0.42
3:C:134:ASN:ND2	3:C:135:ILE:HG23	2.35	0.42
3:C:140:ALA:HA	3:C:143:GLU:CG	2.50	0.42
1:A:559:PRO:HB2	1:A:562:ASN:ND2	2.30	0.42
1:A:540:THR:CG2	1:A:540:THR:O	2.68	0.42
1:A:389:THR:HG21	1:A:443:VAL:HG13	2.02	0.41
1:A:437:ARG:HD2	1:A:438:HIS:N	2.35	0.41
1:A:560:ILE:HA	1:A:563:ILE:CD1	2.49	0.41
1:A:549:VAL:CG1	1:A:550:LYS:N	2.83	0.41
1:A:544:ILE:CD1	1:A:637:ILE:CG1	2.98	0.41
1:A:383:ILE:HG13	1:A:433:ILE:HG12	2.02	0.41
1:A:380:VAL:HG22	1:A:415:ILE:HB	2.02	0.41
3:C:131:ARG:O	3:C:134:ASN:HB3	2.20	0.41
1:A:636:VAL:O	1:A:636:VAL:HG23	2.20	0.41
1:A:402:PRO:HB2	1:A:514:VAL:HG13	2.01	0.41
2:B:86:THR:CG2	2:B:87:LYS:HD3	2.37	0.41
3:C:122:LEU:HD12	3:D:171:VAL:HG13	2.02	0.41
2:B:59:ILE:N	2:B:59:ILE:HD12	2.35	0.41
2:B:32:MET:O	2:B:83:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:124:GLN:HG2	3:D:127:MET:CE	2.49	0.41
2:B:64:ASN:O	2:B:67:LYS:N	2.46	0.41
3:D:189:SER:C	3:D:191:GLU:N	2.68	0.41
1:A:369:VAL:HG21	1:A:382:PHE:CZ	2.55	0.41
3:C:174:GLN:CB	3:D:122:LEU:HD13	2.42	0.41
2:B:116:ASP:OD1	2:B:117:LYS:N	2.54	0.41
3:D:183:LEU:O	3:D:187:GLN:HB2	2.21	0.41
3:D:144:ALA:HB1	3:D:154:PHE:HD2	1.85	0.41
3:C:143:GLU:HA	3:C:146:ARG:NE	2.35	0.41
2:B:23:LEU:O	2:B:24:ALA:HB2	2.20	0.41
2:B:119:GLY:O	2:B:120:LYS:C	2.59	0.41
1:A:652:GLY:O	1:A:664:ILE:HD13	2.21	0.41
1:A:636:VAL:O	1:A:638:LYS:HG2	2.20	0.41
3:D:135:ILE:C	3:D:137:ALA:H	2.24	0.41
1:A:406:LEU:HD21	1:A:521:ILE:CG2	2.50	0.41
3:C:178:LYS:C	3:C:180:ARG:N	2.73	0.41
3:C:157:VAL:C	3:C:159:ASN:N	2.74	0.41
1:A:670:ILE:O	1:A:671:VAL:C	2.59	0.41
2:B:105:THR:HG22	2:B:108:GLN:HG2	2.02	0.41
2:B:125:LEU:HD23	2:B:134:ILE:HA	2.03	0.41
3:D:188:ARG:O	3:D:188:ARG:HD2	2.21	0.41
1:A:432:LEU:HB2	1:A:448:GLU:O	2.20	0.41
3:C:119:ILE:HD13	3:D:174:GLN:O	2.21	0.41
3:D:157:VAL:O	3:D:161:VAL:HG23	2.21	0.41
3:D:125:ASN:O	3:D:129:ILE:HG12	2.21	0.41
2:B:39:ILE:HG21	2:B:50:GLU:HG3	2.03	0.41
3:C:112:THR:C	3:C:114:GLU:H	2.24	0.40
1:A:514:VAL:HG21	1:A:521:ILE:CG2	2.51	0.40
1:A:556:TYR:CE1	1:A:599:LEU:HD13	2.56	0.40
1:A:381:ASN:OD1	1:A:431:THR:HG23	2.21	0.40
1:A:395:PHE:CD1	1:A:537:LEU:HD23	2.56	0.40
3:C:108:GLN:HA	3:C:111:GLU:HG3	2.03	0.40
2:B:43:PRO:O	2:B:44:LYS:C	2.60	0.40
3:C:112:THR:C	3:C:114:GLU:N	2.74	0.40
3:C:114:GLU:O	3:C:117:ARG:HB3	2.21	0.40
3:C:133:THR:HG21	3:D:161:VAL:HA	2.03	0.40
3:D:142:ILE:O	3:D:142:ILE:HG22	2.22	0.40
2:B:55:LEU:O	2:B:58:ARG:HG2	2.21	0.40
1:A:598:VAL:O	1:A:598:VAL:HG22	2.21	0.40
1:A:657:GLY:O	1:A:659:GLY:N	2.54	0.40
1:A:544:ILE:HD12	1:A:637:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:PHE:CE2	2:B:145:ILE:HG12	2.57	0.40
3:C:123:ILE:O	3:C:125:ASN:N	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:188:ARG:NH1	3:D:188:ARG:NH1[12_555]	2.14	0.06

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	259/320 (81%)	177 (68%)	65 (25%)	17 (7%)	1 25
2	B	137/139 (99%)	93 (68%)	33 (24%)	11 (8%)	1 19
3	C	83/85 (98%)	63 (76%)	18 (22%)	2 (2%)	7 49
3	D	83/85 (98%)	57 (69%)	24 (29%)	2 (2%)	7 49
All	All	562/629 (89%)	390 (69%)	140 (25%)	32 (6%)	2 28

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	VAL
1	A	579	ASP
1	A	605	GLU
1	A	608	GLU
3	C	147	ALA
1	A	365	PHE
1	A	606	GLU
1	A	618	GLY

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Mol	Chain	Res	Type
1	A	630	LEU
1	A	656	LEU
2	B	44	LYS
2	B	45	SER
2	B	47	HIS
2	B	88	ASP
2	B	120	LYS
1	A	390	GLU
1	A	518	ASN
2	B	38	ASP
3	D	108	GLN
1	A	362	PHE
1	A	414	GLY
1	A	520	SER
2	B	113	ASN
3	D	147	ALA
2	B	102	LEU
2	B	116	ASP
1	A	577	VAL
2	B	101	VAL
3	C	149	GLU
1	A	643	VAL
2	B	71	ILE
1	A	366	PRO

5.3.2 Protein sidechains

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	233/280 (83%)	205 (88%)	28 (12%)	6 33
2	B	127/127 (100%)	109 (86%)	18 (14%)	4 28
3	C	72/72 (100%)	63 (88%)	9 (12%)	6 31
3	D	72/72 (100%)	60 (83%)	12 (17%)	3 20
All	All	504/551 (92%)	437 (87%)	67 (13%)	5 30

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	376	MET
1	A	384	MET
1	A	392	ASP
1	A	416	GLU
1	A	429	ILE
1	A	432	LEU
1	A	437	ARG
1	A	441	ASN
1	A	514	VAL
1	A	517	LEU
1	A	526	GLU
1	A	539	LEU
1	A	544	ILE
1	A	545	GLN
1	A	548	LEU
1	A	565	THR
1	A	573	ASP
1	A	582	VAL
1	A	600	GLN
1	A	620	ARG
1	A	627	ASP
1	A	632	GLN
1	A	633	ASP
1	A	634	ASP
1	A	635	ILE
1	A	649	GLU
1	A	656	LEU
1	A	658	ASP
2	B	20	GLU
2	B	25	PHE
2	B	26	ASP
2	B	29	ASN
2	B	52	VAL
2	B	64	ASN
2	B	80	SER
2	B	86	THR
2	B	87	LYS
2	B	98	VAL
2	B	102	LEU
2	B	106	GLU
2	B	108	GLN
2	B	125	LEU

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Mol	Chain	Res	Type
2	B	129	ASP
2	B	131	ARG
2	B	136	LEU
2	B	141	ILE
3	C	107	SER
3	C	109	ILE
3	C	114	GLU
3	C	121	LYS
3	C	134	ASN
3	C	146	ARG
3	C	163	ASN
3	C	178	LYS
3	C	180	ARG
3	D	108	GLN
3	D	111	GLU
3	D	114	GLU
3	D	163	ASN
3	D	166	ASN
3	D	170	GLU
3	D	173	LYS
3	D	174	GLN
3	D	176	VAL
3	D	183	LEU
3	D	190	LEU
3	D	191	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	HIS
1	A	381	ASN
1	A	409	ASN
1	A	438	HIS
1	A	441	ASN
1	A	442	ASN
1	A	512	ASN
1	A	545	GLN
1	A	552	ASN
1	A	562	ASN
1	A	578	GLN
1	A	600	GLN
1	A	603	HIS

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Mol	Chain	Res	Type
1	A	632	GLN
2	B	64	ASN
2	B	107	ASN
3	C	115	ASN
3	C	134	ASN
3	C	159	ASN
3	C	162	GLN
3	C	166	ASN
3	C	169	ASN
3	C	174	GLN
3	D	108	GLN
3	D	115	ASN
3	D	163	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	263/320 (82%)	1.15	70 (26%) 1 2	125, 296, 446, 623	0
2	B	139/139 (100%)	-0.03	0 100 100	137, 195, 260, 313	0
3	C	85/85 (100%)	-0.06	0 100 100	93, 202, 269, 332	0
3	D	85/85 (100%)	0.07	3 (3%) 48 38	152, 215, 295, 365	0
All	All	572/629 (90%)	0.52	73 (12%) 5 6	93, 212, 418, 623	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	435	SER	6.7
3	D	146	ARG	5.8
1	A	385	ARG	5.3
1	A	375	LYS	5.3
1	A	409	ASN	5.1
1	A	439	GLU	5.1
1	A	386	GLY	4.9
1	A	405	HIS	4.8
1	A	534	THR	4.8
1	A	527	LYS	4.5
1	A	363	ASN	4.2
1	A	436	ALA	4.2
1	A	406	LEU	4.2
1	A	438	HIS	4.1
1	A	437	ARG	4.0
1	A	401	GLU	4.0
1	A	376	MET	4.0
1	A	366	PRO	4.0
1	A	446	GLU	4.0
1	A	528	ASP	3.9
1	A	371	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
3	D	147	ALA	3.8
1	A	431	THR	3.7
1	A	520	SER	3.4
1	A	433	ILE	3.4
1	A	359	SER	3.3
1	A	407	LEU	3.3
1	A	364	ARG	3.2
1	A	419	GLU	3.2
1	A	377	ASN	3.2
1	A	362	PHE	3.1
1	A	400	GLY	3.1
1	A	521	ILE	3.1
1	A	516	SER	3.1
1	A	412	ASP	3.0
1	A	393	ARG	3.0
1	A	529	LYS	3.0
1	A	530	GLY	3.0
1	A	514	VAL	3.0
1	A	404	LEU	3.0
1	A	540	THR	2.9
1	A	374	LYS	2.9
1	A	408	ARG	2.8
1	A	526	GLU	2.8
1	A	396	VAL	2.8
1	A	440	GLY	2.8
1	A	365	PHE	2.8
1	A	402	PRO	2.7
1	A	441	ASN	2.6
1	A	442	ASN	2.6
3	D	145	ALA	2.5
1	A	522	SER	2.5
1	A	403	LEU	2.5
1	A	533	VAL	2.5
1	A	360	PHE	2.4
1	A	427	PRO	2.4
1	A	434	LEU	2.4
1	A	447	VAL	2.4
1	A	512	ASN	2.4
1	A	368	MET	2.3
1	A	388	ASP	2.3
1	A	399	ILE	2.3
1	A	428	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	392	ASP	2.3
1	A	513	VAL	2.3
1	A	423	ALA	2.3
1	A	535	ILE	2.2
1	A	410	ALA	2.2
1	A	430	GLY	2.2
1	A	357	PRO	2.2
1	A	536	ARG	2.1
1	A	387	GLU	2.1
1	A	508	ASP	2.1

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.