Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:51 PM GMT

PDB ID	:	4DOP
Title	:	Crystal structure of the CusBA heavy-metal efflux complex from Escherichia coli, R mutant
Authors	:	Su, C.-C.; Long, F.; Yu, E.
Deposited on	:	2012-02-10
Resolution	:	4.20 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 ⓘ symbol.

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

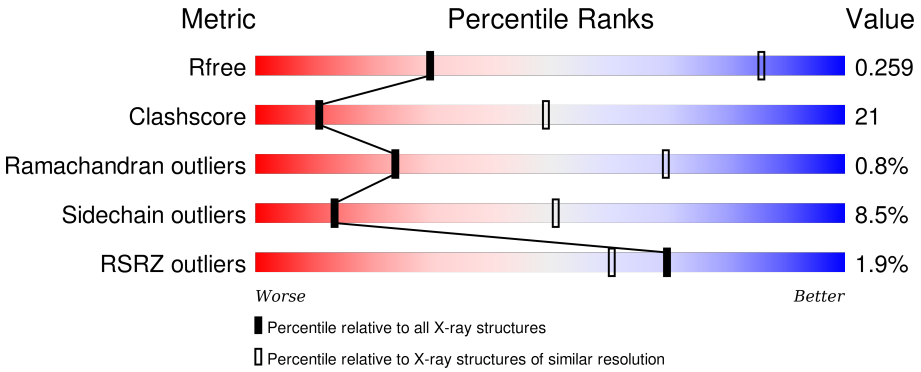
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 4.20 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	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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	B	413	52% 22% • 22%
1	C	413	52% 24% • 22%
2	A	1054	3% 51% 42% 5% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12891 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 Cation efflux system protein CusB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	322	Total	C	N	O	S	0	0	0
			2458	1555	428	469	6			
1	C	324	Total	C	N	O	S	0	0	0
			2473	1563	430	474	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	408	HIS	-	EXPRESSION TAG	UNP P77239
B	409	HIS	-	EXPRESSION TAG	UNP P77239
B	410	HIS	-	EXPRESSION TAG	UNP P77239
B	411	HIS	-	EXPRESSION TAG	UNP P77239
B	412	HIS	-	EXPRESSION TAG	UNP P77239
B	413	HIS	-	EXPRESSION TAG	UNP P77239
C	408	HIS	-	EXPRESSION TAG	UNP P77239
C	409	HIS	-	EXPRESSION TAG	UNP P77239
C	410	HIS	-	EXPRESSION TAG	UNP P77239
C	411	HIS	-	EXPRESSION TAG	UNP P77239
C	412	HIS	-	EXPRESSION TAG	UNP P77239
C	413	HIS	-	EXPRESSION TAG	UNP P77239

- Molecule 2 is a protein called Cation efflux system protein CusA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1031	Total	C	N	O	S	0	0	0
			7942	5137	1330	1438	37			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	EXPRESSION TAG	UNP P38054
A	-5	HIS	-	EXPRESSION TAG	UNP P38054

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	EXPRESSION TAG	UNP P38054
A	-3	HIS	-	EXPRESSION TAG	UNP P38054
A	-2	HIS	-	EXPRESSION TAG	UNP P38054
A	-1	HIS	-	EXPRESSION TAG	UNP P38054
A	0	HIS	-	EXPRESSION TAG	UNP P38054
A	669	ALA	ARG	ENGINEERED MUTATION	UNP P38054

- Molecule 3 is water.

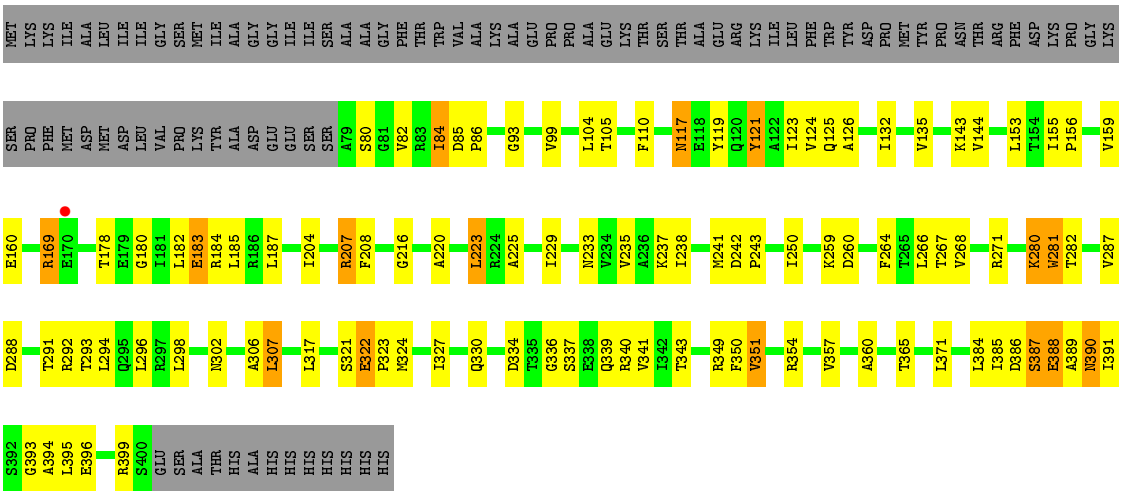
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	4	Total O 4 4	0	0
3	C	11	Total O 11 11	0	0
3	A	3	Total O 3 3	0	0

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.

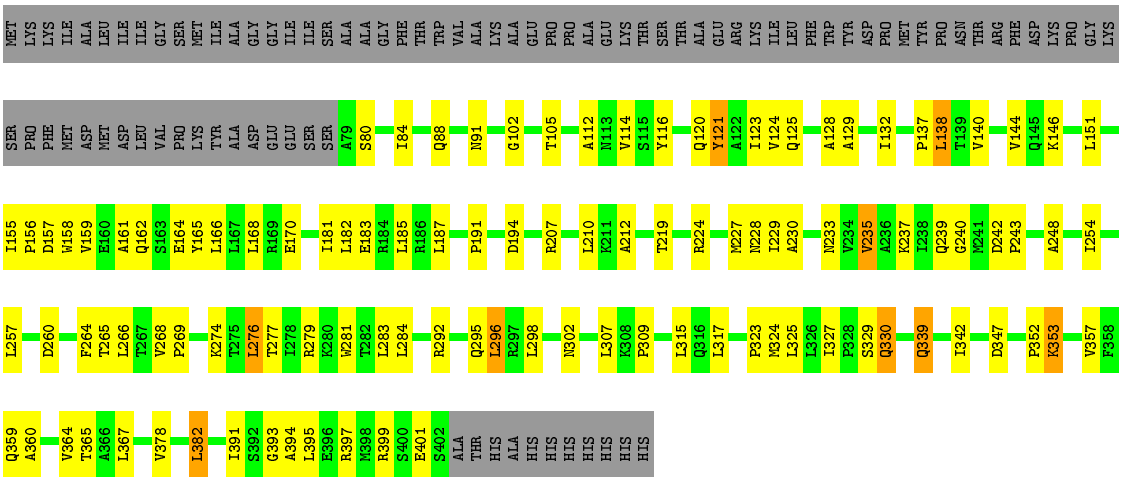
- Molecule 1: Cation efflux system protein CusB

Chain B:



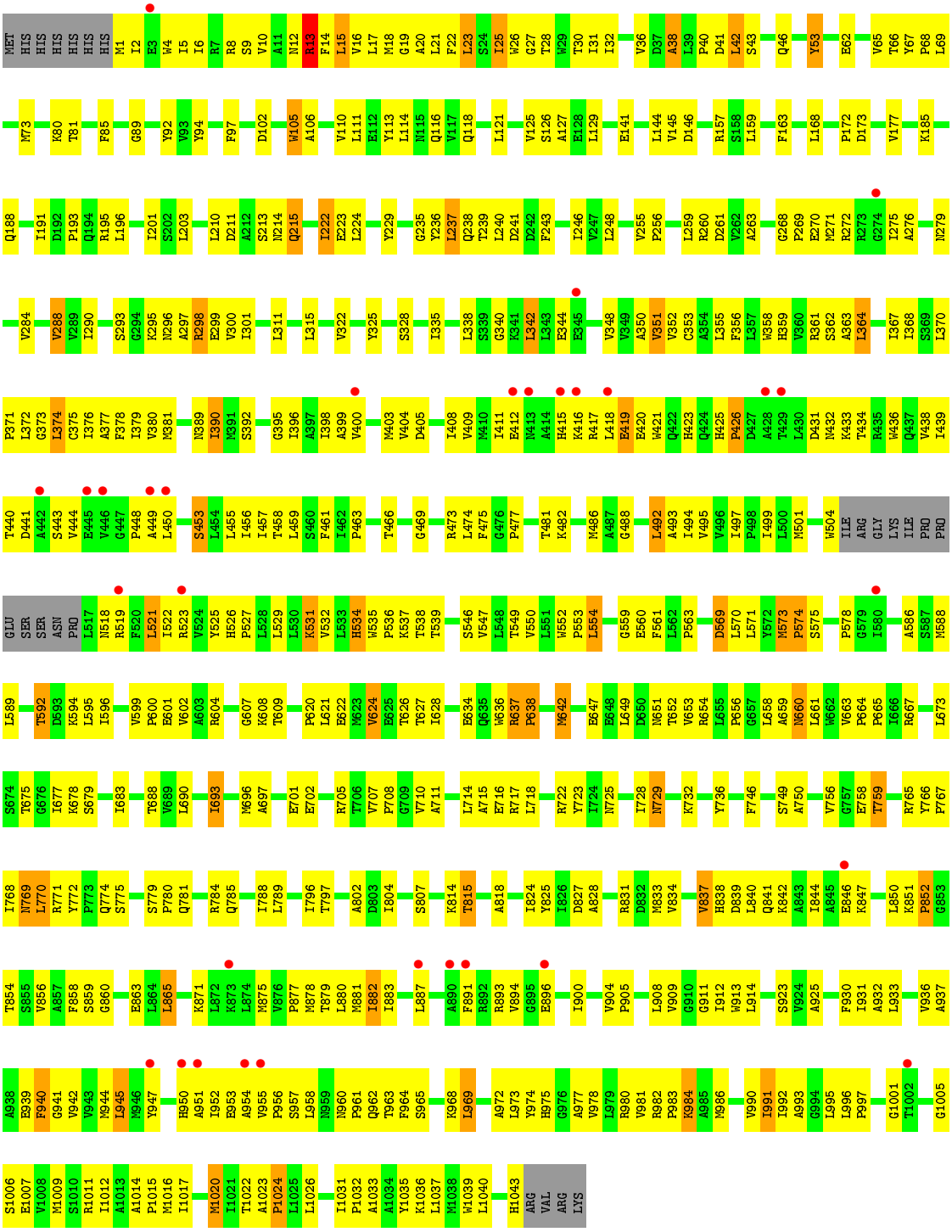
- Molecule 1: Cation efflux system protein CusB

Chain C:



- Molecule 2: Cation efflux system protein CusA

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	160.52Å 160.52Å 681.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.31 – 4.20 136.21 – 4.20	Depositor EDS
% Data completeness (in resolution range)	92.2 (97.31-4.20) 99.9 (136.21-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.33	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 4.15Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.222 , 0.268 0.202 , 0.259	Depositor DCC
R_{free} test set	1281 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	86.2	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 128.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 25302 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	12891	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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	B	0.22	0/2498	0.43	0/3401
1	C	0.22	0/2513	0.42	0/3421
2	A	0.22	0/8108	0.41	0/11041
All	All	0.22	0/13119	0.41	0/17863

There are no bond length outliers.

There are no bond angle outliers.

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	B	2458	0	2522	92	0
1	C	2473	0	2533	80	0
2	A	7942	0	8187	399	0
3	A	3	0	0	0	0
3	B	4	0	0	0	0
3	C	11	0	0	0	0
All	All	12891	0	13242	550	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 21.

All (550) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:573:MET:HG2	2:A:678:LYS:NZ	1.80	0.96
1:C:242:ASP:HB3	1:C:243:PRO:HD3	1.49	0.94
2:A:696:MET:HG3	2:A:854:THR:HG21	1.50	0.93
2:A:573:MET:SD	2:A:678:LYS:HD2	2.11	0.90
2:A:574:PRO:HB2	2:A:658:LEU:HD11	1.52	0.89
2:A:574:PRO:HG2	2:A:624:VAL:HG13	1.55	0.89
2:A:459:LEU:HB3	2:A:882:ILE:HD11	1.58	0.84
1:B:117:ASN:HD22	1:B:119:TYR:H	1.23	0.83
2:A:573:MET:HG2	2:A:678:LYS:HZ2	1.37	0.83
1:B:242:ASP:HB3	1:B:243:PRO:HD3	1.61	0.82
1:B:82:VAL:HG11	2:A:652:THR:HG23	1.62	0.80
2:A:851:LYS:HB3	2:A:852:PRO:HD2	1.63	0.80
2:A:43:SER:HB2	2:A:673:LEU:HD23	1.63	0.79
2:A:950:HIS:HA	2:A:953:GLU:HB2	1.63	0.79
2:A:550:VAL:HB	2:A:909:VAL:HG13	1.65	0.79
2:A:191:ILE:HD13	2:A:263:ALA:HB2	1.65	0.77
2:A:550:VAL:HG11	2:A:909:VAL:HG22	1.65	0.77
1:C:339:GLN:HG3	1:C:357:VAL:HG23	1.67	0.76
1:C:80:SER:HA	1:C:397:ARG:HD2	1.67	0.76
2:A:518:ASN:HA	2:A:521:LEU:HD21	1.69	0.75
1:B:117:ASN:ND2	1:B:119:TYR:H	1.85	0.74
2:A:118:GLN:HE22	2:A:127:ALA:H	1.35	0.74
2:A:6:ILE:HD13	2:A:443:SER:HB3	1.70	0.74
1:B:159:VAL:HG23	1:B:204:ILE:HG21	1.70	0.74
1:C:283:LEU:HD23	1:C:296:LEU:HD12	1.69	0.74
1:B:125:GLN:NE2	1:C:228:ASN:H	1.88	0.72
1:B:125:GLN:HE21	1:C:228:ASN:H	1.38	0.71
2:A:20:ALA:HA	2:A:23:LEU:HD23	1.71	0.71
2:A:275:ILE:HD13	2:A:586:ALA:HB2	1.71	0.71
2:A:529:LEU:O	2:A:532:VAL:HG12	1.92	0.70
2:A:27:GLY:HA3	2:A:375:CYS:HB3	1.72	0.70
2:A:409:VAL:HB	2:A:450:LEU:HD11	1.73	0.70
2:A:784:ARG:HG3	2:A:804:ILE:HD11	1.73	0.70
2:A:425:HIS:HB3	2:A:426:PRO:HD2	1.71	0.70
2:A:377:ALA:O	2:A:381:MET:HG3	1.93	0.69
2:A:466:THR:O	2:A:871:LYS:HE2	1.92	0.69
2:A:609:THR:HG22	2:A:624:VAL:HB	1.75	0.69
2:A:493:ALA:HA	2:A:497:ILE:HB	1.74	0.69
2:A:42:LEU:HA	2:A:473:ARG:HD2	1.75	0.68
2:A:80:LYS:HG2	2:A:81:THR:HG23	1.74	0.68
2:A:991:ILE:O	2:A:995:LEU:HB2	1.93	0.68
2:A:573:MET:CG	2:A:678:LYS:HD2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:TYR:HB2	1:C:181:ILE:HG21	1.76	0.68
2:A:279:ASN:HD21	2:A:604:ARG:HA	1.57	0.68
1:B:360:ALA:HA	1:B:365:THR:HA	1.74	0.67
2:A:980:ARG:O	2:A:984:LYS:HB2	1.94	0.67
2:A:547:VAL:O	2:A:550:VAL:HG12	1.95	0.66
2:A:964:PHE:CZ	2:A:1043:HIS:HB3	2.30	0.66
2:A:690:LEU:HD22	2:A:718:LEU:HD23	1.76	0.66
2:A:552:TRP:HB3	2:A:553:PRO:HD3	1.76	0.66
2:A:977:ALA:HA	2:A:980:ARG:NE	2.10	0.66
2:A:65:VAL:O	2:A:69:LEU:HB2	1.96	0.66
2:A:940:PHE:CE1	2:A:1024:PRO:HA	2.32	0.65
2:A:986:MET:O	2:A:990:VAL:HG22	1.97	0.65
1:C:254:ILE:HG22	1:C:257:LEU:HB2	1.77	0.65
1:C:219:THR:OG1	1:C:237:LYS:HD2	1.95	0.65
2:A:707:VAL:HG21	2:A:840:LEU:HD23	1.77	0.65
2:A:573:MET:HG2	2:A:678:LYS:HD2	1.78	0.65
2:A:364:LEU:O	2:A:368:ILE:HG12	1.96	0.65
2:A:482:LYS:O	2:A:486:MET:HG2	1.96	0.64
1:C:302:ASN:HD21	1:C:307:LEU:H	1.45	0.64
2:A:573:MET:HG2	2:A:678:LYS:CE	2.28	0.64
1:B:280:LYS:HA	1:B:280:LYS:HE3	1.80	0.63
2:A:601:GLU:OE2	2:A:637:ARG:HD3	1.99	0.63
2:A:982:ARG:HB3	2:A:983:PRO:HD3	1.79	0.63
2:A:532:VAL:HG23	2:A:539:THR:HG21	1.81	0.63
2:A:370:LEU:HB2	2:A:371:PRO:HD3	1.81	0.63
2:A:569:ASP:HB3	2:A:628:ILE:O	1.98	0.63
2:A:224:LEU:HB2	2:A:229:TYR:CE1	2.34	0.63
2:A:361:ARG:HB3	2:A:504:TRP:HB3	1.79	0.63
1:B:341:VAL:HG21	1:B:371:LEU:HD11	1.79	0.63
2:A:398:ILE:HD11	2:A:482:LYS:HG3	1.82	0.62
2:A:955:VAL:HG12	2:A:956:PRO:HD3	1.81	0.62
2:A:960:ASN:HB2	2:A:961:PRO:HD3	1.81	0.62
2:A:550:VAL:HG21	2:A:909:VAL:HA	1.80	0.62
1:B:385:ILE:HG22	1:B:389:ALA:HB2	1.82	0.62
2:A:834:VAL:HG22	2:A:838:HIS:CD2	2.34	0.62
1:B:84:ILE:HD11	2:A:594:LYS:HD2	1.80	0.62
1:B:360:ALA:HB2	1:B:365:THR:HG22	1.82	0.62
2:A:891:PHE:HE2	2:A:942:VAL:HG13	1.64	0.62
2:A:1023:ALA:HB3	2:A:1024:PRO:HD3	1.81	0.61
2:A:1001:GLY:HA2	2:A:1006:SER:HB2	1.82	0.61
2:A:660:ASN:HD22	2:A:660:ASN:N	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:940:PHE:CD2	2:A:940:PHE:C	2.73	0.61
2:A:877:PRO:O	2:A:881:MET:HG2	2.00	0.61
2:A:570:LEU:HA	2:A:665:PRO:HD3	1.83	0.60
2:A:707:VAL:HG13	2:A:708:PRO:HD2	1.83	0.60
2:A:696:MET:CE	2:A:851:LYS:HG3	2.31	0.60
2:A:519:ARG:O	2:A:523:ARG:HG3	2.01	0.60
2:A:418:LEU:HD21	2:A:438:VAL:HG11	1.83	0.60
2:A:370:LEU:O	2:A:374:LEU:HB2	2.01	0.60
1:C:327:ILE:HG12	1:C:367:LEU:HD21	1.83	0.59
2:A:338:LEU:HD21	2:A:390:ILE:HG13	1.85	0.59
1:C:279:ARG:NH1	1:C:279:ARG:HB2	2.16	0.59
2:A:2:ILE:HD12	2:A:2:ILE:H	1.68	0.59
2:A:573:MET:HG2	2:A:678:LYS:CD	2.32	0.59
2:A:416:LYS:HD2	2:A:419:GLU:HB3	1.84	0.59
2:A:969:LEU:O	2:A:973:LEU:HD13	2.02	0.59
2:A:563:PRO:HG3	2:A:1011:ARG:HG2	1.85	0.58
2:A:599:VAL:HG21	2:A:649:LEU:HD12	1.84	0.58
2:A:904:VAL:HG12	2:A:937:ALA:HB3	1.84	0.58
2:A:340:GLY:O	2:A:344:GLU:HG3	2.03	0.58
2:A:995:LEU:O	2:A:1017:ILE:HD11	2.04	0.58
2:A:188:GLN:HA	2:A:769:ASN:ND2	2.18	0.58
2:A:276:ALA:HB3	2:A:284:VAL:O	2.03	0.58
1:B:287:VAL:HG12	1:B:294:LEU:HD23	1.84	0.58
1:C:342:ILE:HB	1:C:378:VAL:CG1	2.34	0.58
2:A:588:MET:HE1	2:A:658:LEU:HD13	1.86	0.58
2:A:38:ALA:O	2:A:390:ILE:HG22	2.03	0.58
2:A:729:ASN:HD22	2:A:729:ASN:C	2.07	0.58
1:B:110:PHE:CG	1:B:250:ILE:HG12	2.38	0.58
2:A:168:LEU:HB3	2:A:177:VAL:HG21	1.86	0.57
2:A:804:ILE:HG13	2:A:804:ILE:O	2.04	0.57
2:A:2:ILE:HD13	2:A:448:PRO:HB3	1.86	0.57
2:A:535:TRP:O	2:A:538:THR:HG22	2.05	0.57
2:A:746:PHE:CZ	2:A:788:ILE:HG23	2.40	0.57
2:A:912:ILE:HD12	2:A:930:PHE:CZ	2.40	0.57
2:A:188:GLN:HA	2:A:769:ASN:HD21	1.70	0.57
1:C:342:ILE:HB	1:C:378:VAL:HG12	1.86	0.57
2:A:756:VAL:HG21	2:A:770:LEU:HD22	1.87	0.57
2:A:222:ILE:HG12	2:A:223:GLU:N	2.20	0.56
2:A:28:THR:O	2:A:32:ILE:HG13	2.05	0.56
2:A:534:HIS:C	2:A:534:HIS:CD2	2.78	0.56
2:A:141:GLU:HB3	2:A:325:TYR:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:893:ARG:HB3	2:A:896:GLU:HB3	1.87	0.56
1:B:390:ASN:HD22	1:B:393:GLY:H	1.53	0.56
2:A:4:TRP:O	2:A:8:ARG:HG2	2.06	0.56
2:A:900:ILE:HG23	2:A:941:GLY:HA3	1.88	0.56
1:C:116:TYR:CE2	1:C:309:PRO:HG2	2.40	0.56
2:A:390:ILE:HD12	2:A:1005:GLY:HA3	1.88	0.56
2:A:933:LEU:HB2	2:A:1016:MET:HG2	1.87	0.55
1:B:330:GLN:HA	1:B:330:GLN:HE21	1.71	0.55
2:A:607:GLY:HA2	2:A:626:THR:HG22	1.88	0.55
2:A:488:GLY:O	2:A:492:LEU:HB2	2.07	0.55
2:A:351:VAL:O	2:A:355:LEU:HG	2.06	0.55
2:A:449:ALA:O	2:A:453:SER:HB2	2.05	0.55
1:B:220:ALA:HB3	1:B:237:LYS:HB2	1.88	0.55
2:A:696:MET:HE2	2:A:851:LYS:HG3	1.88	0.55
1:B:123:ILE:CD1	1:B:237:LYS:HG3	2.37	0.55
1:C:359:GLN:HG3	1:C:360:ALA:N	2.22	0.55
2:A:954:ALA:HB3	2:A:956:PRO:HD2	1.87	0.55
1:B:322:GLU:HG3	1:B:323:PRO:HD2	1.89	0.55
1:C:123:ILE:HG12	1:C:237:LYS:HG3	1.87	0.55
1:B:144:VAL:HG21	1:B:238:ILE:HD13	1.88	0.55
2:A:1031:ILE:HB	2:A:1032:PRO:HD3	1.88	0.54
2:A:536:PRO:HB3	2:A:1033:ALA:HB1	1.89	0.54
2:A:40:PRO:O	2:A:42:LEU:HG	2.06	0.54
1:B:268:VAL:HG23	1:B:271:ARG:H	1.72	0.54
2:A:573:MET:CG	2:A:678:LYS:HZ2	2.17	0.54
2:A:1007:GLU:O	2:A:1011:ARG:HD3	2.08	0.54
1:B:387:SER:HA	2:A:771:ARG:HH12	1.72	0.54
1:C:242:ASP:HB3	1:C:243:PRO:CD	2.30	0.54
2:A:363:ALA:O	2:A:367:ILE:HG13	2.08	0.54
2:A:53:TYR:O	2:A:89:GLY:HA2	2.08	0.54
2:A:955:VAL:HA	2:A:958:LEU:HD13	1.90	0.54
2:A:972:ALA:HA	2:A:975:HIS:HD2	1.73	0.54
2:A:880:LEU:HA	2:A:883:ILE:HG22	1.89	0.54
1:B:242:ASP:CB	1:B:243:PRO:HD3	2.37	0.54
1:B:123:ILE:HD12	1:B:237:LYS:HG3	1.89	0.54
2:A:522:ILE:HG12	2:A:981:VAL:HG11	1.90	0.53
1:B:135:VAL:HG12	1:B:225:ALA:HB2	1.89	0.53
1:B:123:ILE:HB	1:C:227:MET:CG	2.38	0.53
2:A:842:LYS:O	2:A:846:GLU:HG2	2.08	0.53
1:C:164:GLU:O	1:C:168:LEU:HD13	2.09	0.53
1:B:155:ILE:HB	1:B:208:PHE:HE1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:441:ASP:HA	2:A:444:VAL:HG23	1.89	0.53
2:A:940:PHE:HD2	2:A:940:PHE:C	2.09	0.53
2:A:620:PRO:HG2	2:A:622:GLU:HG2	1.91	0.53
1:B:126:ALA:HB2	1:B:229:ILE:HD13	1.91	0.53
2:A:459:LEU:HB3	2:A:882:ILE:CD1	2.34	0.53
2:A:421:TRP:O	2:A:421:TRP:HD1	1.92	0.53
2:A:9:SER:HA	2:A:12:ASN:ND2	2.24	0.53
1:C:317:LEU:HD12	1:C:317:LEU:C	2.30	0.53
1:C:102:GLY:O	1:C:323:PRO:HA	2.09	0.53
2:A:43:SER:HB2	2:A:673:LEU:CD2	2.35	0.52
2:A:248:LEU:HD11	2:A:259:LEU:HA	1.91	0.52
2:A:301:ILE:HD12	2:A:328:SER:HB3	1.91	0.52
2:A:239:THR:HG22	2:A:241:ASP:H	1.72	0.52
1:B:180:GLY:O	1:B:184:ARG:HG3	2.09	0.52
1:B:156:PRO:O	1:B:159:VAL:HG12	2.09	0.52
2:A:955:VAL:N	2:A:956:PRO:CD	2.72	0.52
1:C:325:LEU:H	1:C:325:LEU:HD12	1.73	0.52
2:A:474:LEU:HD23	2:A:475:PHE:CE1	2.45	0.52
2:A:338:LEU:HG	2:A:390:ILE:HA	1.91	0.52
1:B:266:LEU:HD13	1:B:267:THR:N	2.25	0.52
1:B:223:LEU:HD11	1:B:235:VAL:HA	1.90	0.52
2:A:977:ALA:O	2:A:981:VAL:HG23	2.10	0.52
2:A:759:THR:HG22	2:A:768:ILE:HD11	1.91	0.52
2:A:904:VAL:N	2:A:905:PRO:CD	2.73	0.52
2:A:710:VAL:HA	2:A:828:ALA:HB2	1.92	0.51
2:A:546:SER:O	2:A:549:THR:HG22	2.10	0.51
1:B:143:LYS:HD2	1:B:216:GLY:O	2.10	0.51
2:A:975:HIS:C	2:A:977:ALA:H	2.13	0.51
2:A:891:PHE:CE2	2:A:942:VAL:HG13	2.44	0.51
2:A:1022:THR:O	2:A:1026:LEU:HB2	2.09	0.51
2:A:214:ASN:OD1	2:A:237:LEU:HB2	2.09	0.51
2:A:964:PHE:CE2	2:A:1043:HIS:HB3	2.46	0.51
1:B:259:LYS:HG3	1:B:260:ASP:N	2.25	0.51
2:A:361:ARG:HA	2:A:364:LEU:HB2	1.92	0.51
1:B:124:VAL:HB	1:B:235:VAL:HG22	1.92	0.51
2:A:844:ILE:HD12	2:A:858:PHE:HZ	1.76	0.51
2:A:214:ASN:H	2:A:215:GLN:NE2	2.09	0.51
1:B:340:ARG:HB3	1:B:354:ARG:HA	1.92	0.51
2:A:914:LEU:HD23	2:A:1014:ALA:O	2.10	0.51
2:A:342:LEU:HD21	2:A:396:ILE:HG22	1.93	0.51
2:A:102:ASP:HB3	2:A:105:TRP:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ASP:HB3	1:B:243:PRO:CD	2.37	0.51
2:A:522:ILE:HG23	2:A:526:HIS:HE2	1.75	0.51
1:C:156:PRO:O	1:C:159:VAL:HG22	2.11	0.51
1:C:254:ILE:HD11	2:A:797:THR:HG21	1.93	0.50
2:A:850:LEU:HD21	2:A:856:VAL:HG23	1.94	0.50
2:A:746:PHE:O	2:A:750:ALA:HB3	2.11	0.50
1:C:128:ALA:HB3	1:C:155:ILE:HG21	1.93	0.50
2:A:97:PHE:CE1	2:A:106:ALA:HB1	2.46	0.50
1:C:80:SER:HB3	1:C:401:GLU:OE2	2.11	0.50
1:B:384:LEU:N	1:B:384:LEU:HD12	2.26	0.50
2:A:16:VAL:HG11	2:A:495:VAL:HG12	1.93	0.50
1:B:385:ILE:HG13	2:A:272:ARG:H	1.77	0.50
2:A:725:ASN:O	2:A:804:ILE:HA	2.12	0.50
2:A:359:HIS:HB3	2:A:362:SER:OG	2.12	0.50
2:A:392:SER:O	2:A:481:THR:HG21	2.11	0.50
1:B:117:ASN:HD21	1:B:119:TYR:HB2	1.77	0.50
2:A:1:MET:O	2:A:5:ILE:HG13	2.12	0.50
1:C:138:LEU:HD21	1:C:144:VAL:HG11	1.94	0.50
2:A:19:GLY:O	2:A:23:LEU:HB3	2.12	0.50
2:A:26:TRP:O	2:A:30:THR:HG23	2.12	0.50
1:B:336:GLY:HA3	2:A:775:SER:HB2	1.94	0.50
2:A:121:LEU:HB3	2:A:125:VAL:CG2	2.42	0.50
2:A:878:MET:O	2:A:882:ILE:HG22	2.11	0.49
2:A:932:ALA:O	2:A:936:VAL:HG23	2.12	0.49
2:A:964:PHE:HZ	2:A:1043:HIS:HB3	1.73	0.49
2:A:111:LEU:HD13	2:A:129:LEU:HD22	1.94	0.49
2:A:21:LEU:O	2:A:25:ILE:HG22	2.12	0.49
1:B:169:ARG:HA	1:B:169:ARG:HE	1.77	0.49
2:A:405:ASP:OD2	2:A:991:ILE:HG12	2.12	0.49
2:A:596:ILE:HG12	2:A:653:VAL:HG21	1.93	0.49
1:B:391:ILE:HG12	2:A:774:GLN:OE1	2.12	0.49
2:A:697:ALA:HA	2:A:824:ILE:HD11	1.93	0.49
2:A:458:THR:HA	2:A:482:LYS:NZ	2.27	0.49
1:B:389:ALA:O	1:B:390:ASN:C	2.50	0.49
2:A:390:ILE:HD12	2:A:1005:GLY:CA	2.43	0.49
2:A:5:ILE:HA	2:A:8:ARG:HG3	1.94	0.49
2:A:42:LEU:H	2:A:42:LEU:HD12	1.77	0.49
2:A:23:LEU:HD12	2:A:23:LEU:O	2.13	0.49
1:C:166:LEU:O	1:C:170:GLU:HG2	2.12	0.49
1:B:153:LEU:H	1:B:153:LEU:HD23	1.76	0.49
2:A:113:TYR:HA	2:A:116:GLN:HE21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:14:PHE:O	2:A:17:LEU:HB3	2.12	0.49
1:C:242:ASP:CB	1:C:243:PRO:HD3	2.33	0.49
2:A:526:HIS:HA	2:A:529:LEU:HB3	1.94	0.49
2:A:421:TRP:CD1	2:A:421:TRP:O	2.66	0.49
2:A:592:THR:O	2:A:596:ILE:HG13	2.13	0.49
2:A:596:ILE:HD13	2:A:628:ILE:HD11	1.94	0.49
2:A:550:VAL:HG23	2:A:913:TRP:CD1	2.48	0.49
2:A:947:TYR:O	2:A:951:ALA:HB2	2.12	0.49
2:A:399:ALA:O	2:A:403:MET:HG3	2.12	0.48
2:A:458:THR:HA	2:A:482:LYS:HZ3	1.79	0.48
1:C:302:ASN:ND2	1:C:307:LEU:H	2.11	0.48
2:A:338:LEU:O	2:A:342:LEU:HB2	2.12	0.48
1:B:121:TYR:CG	1:C:224:ARG:HD3	2.48	0.48
2:A:779:SER:HB2	2:A:780:PRO:HD2	1.95	0.48
1:B:220:ALA:HB3	1:B:237:LYS:CB	2.43	0.48
2:A:526:HIS:N	2:A:527:PRO:CD	2.77	0.48
2:A:356:PHE:HD2	2:A:986:MET:CB	2.27	0.48
2:A:683:ILE:HB	2:A:824:ILE:HB	1.95	0.48
2:A:945:LEU:O	2:A:945:LEU:HD13	2.14	0.48
2:A:270:GLU:HG2	2:A:271:MET:H	1.79	0.48
2:A:173:ASP:HB2	2:A:300:VAL:CG2	2.44	0.48
2:A:900:ILE:HD12	2:A:941:GLY:O	2.14	0.48
2:A:925:ALA:O	2:A:1012:ILE:HG13	2.14	0.48
2:A:436:TRP:C	2:A:436:TRP:CD1	2.87	0.48
2:A:882:ILE:HD13	2:A:882:ILE:C	2.35	0.48
2:A:522:ILE:HG23	2:A:526:HIS:NE2	2.29	0.48
2:A:784:ARG:HG3	2:A:804:ILE:CD1	2.44	0.48
1:B:84:ILE:HG22	1:C:91:ASN:OD1	2.14	0.48
2:A:270:GLU:HG2	2:A:271:MET:N	2.28	0.48
1:C:158:TRP:O	1:C:162:GLN:HG3	2.13	0.48
1:B:390:ASN:ND2	1:B:393:GLY:H	2.12	0.48
1:C:360:ALA:HB2	1:C:365:THR:HG22	1.96	0.48
2:A:85:PHE:HB2	2:A:92:TYR:HB2	1.96	0.48
2:A:550:VAL:O	2:A:553:PRO:HD2	2.14	0.47
2:A:2:ILE:N	2:A:2:ILE:HD12	2.28	0.47
2:A:736:TYR:CE1	2:A:796:ILE:HG21	2.49	0.47
2:A:661:LEU:HD21	2:A:663:VAL:HG13	1.96	0.47
2:A:6:ILE:HG12	2:A:494:ILE:HG13	1.96	0.47
2:A:27:GLY:O	2:A:31:ILE:HG22	2.14	0.47
2:A:368:ILE:O	2:A:372:LEU:HD13	2.14	0.47
1:B:124:VAL:O	1:B:235:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:SER:HB3	1:B:82:VAL:HG12	1.96	0.47
1:C:394:ALA:HA	1:C:397:ARG:NH1	2.30	0.47
2:A:421:TRP:CE3	2:A:438:VAL:HB	2.49	0.47
1:B:178:THR:O	1:B:182:LEU:HB2	2.15	0.47
2:A:574:PRO:HD2	2:A:624:VAL:HG22	1.95	0.47
2:A:911:GLY:HA3	2:A:930:PHE:HE2	1.80	0.47
2:A:408:ILE:HG13	2:A:409:VAL:N	2.29	0.47
1:C:279:ARG:HH11	1:C:279:ARG:HB2	1.79	0.47
2:A:6:ILE:HG21	2:A:443:SER:HB3	1.97	0.47
1:C:114:VAL:O	1:C:309:PRO:HA	2.14	0.47
2:A:715:ALA:HB2	2:A:824:ILE:HG12	1.97	0.47
2:A:833:MET:O	2:A:837:VAL:HG12	2.15	0.47
1:C:264:PHE:HB3	1:C:315:LEU:HD11	1.97	0.47
1:B:85:ASP:HA	1:B:86:PRO:HD3	1.78	0.47
1:B:99:VAL:HG22	1:B:327:ILE:HG22	1.95	0.47
2:A:951:ALA:HB1	2:A:972:ALA:O	2.14	0.47
2:A:213:SER:O	2:A:237:LEU:HD13	2.14	0.47
2:A:574:PRO:HA	2:A:659:ALA:O	2.15	0.47
2:A:461:PHE:CE2	2:A:932:ALA:HB2	2.49	0.47
2:A:571:LEU:CD1	2:A:665:PRO:HA	2.45	0.47
2:A:846:GLU:HG3	2:A:847:LYS:HG3	1.97	0.47
2:A:589:LEU:HD13	2:A:609:THR:HG23	1.95	0.47
2:A:837:VAL:O	2:A:841:GLN:HG3	2.14	0.47
1:B:343:THR:OG1	1:B:351:VAL:HG23	2.15	0.47
2:A:463:PRO:CB	2:A:875:MET:HG3	2.45	0.47
1:B:93:GLY:HA3	2:A:146:ASP:O	2.15	0.47
1:B:339:GLN:N	1:B:339:GLN:OE1	2.47	0.46
1:C:284:LEU:HB2	1:C:295:GLN:HB2	1.97	0.46
2:A:419:GLU:O	2:A:423:HIS:HD2	1.97	0.46
2:A:859:SER:HA	2:A:863:GLU:HB2	1.97	0.46
1:B:386:ASP:HB2	2:A:269:PRO:O	2.16	0.46
2:A:702:GLU:HA	2:A:705:ARG:HH21	1.80	0.46
2:A:1036:LYS:HG2	2:A:1036:LYS:O	2.15	0.46
1:B:264:PHE:CE2	1:B:317:LEU:HD22	2.50	0.46
2:A:433:LYS:HA	2:A:436:TRP:HB3	1.96	0.46
2:A:1014:ALA:HB3	2:A:1015:PRO:HD3	1.98	0.46
1:C:121:TYR:HE1	1:C:237:LYS:HD3	1.81	0.46
1:B:121:TYR:HE1	1:B:123:ILE:HD11	1.81	0.46
1:B:259:LYS:HE3	1:B:259:LYS:HB2	1.81	0.46
1:C:125:GLN:HG2	1:C:233:ASN:O	2.14	0.46
2:A:678:LYS:HE2	2:A:825:TYR:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:378:PHE:HA	2:A:381:MET:HE2	1.96	0.46
1:C:352:PRO:O	1:C:353:LYS:HG3	2.16	0.46
1:B:121:TYR:CE1	1:B:123:ILE:HD11	2.50	0.46
1:B:384:LEU:HD23	1:B:394:ALA:HB3	1.97	0.46
2:A:647:GLU:O	2:A:651:ASN:HB2	2.16	0.46
2:A:550:VAL:CB	2:A:909:VAL:HG13	2.41	0.46
2:A:693:ILE:HD11	2:A:718:LEU:HD22	1.98	0.46
2:A:785:GLN:HA	2:A:797:THR:HB	1.98	0.46
2:A:537:LYS:HD3	2:A:1037:LEU:HD11	1.98	0.46
1:C:281:TRP:HB2	1:C:298:LEU:HD23	1.97	0.46
2:A:728:ILE:HA	2:A:802:ALA:HB2	1.97	0.46
2:A:759:THR:HG23	2:A:766:TYR:HB2	1.98	0.46
2:A:758:GLU:HA	2:A:766:TYR:O	2.16	0.46
2:A:952:ILE:HG22	2:A:952:ILE:O	2.16	0.46
1:C:165:TYR:HB2	1:C:181:ILE:CG2	2.44	0.45
2:A:769:ASN:N	2:A:769:ASN:HD22	2.15	0.45
2:A:534:HIS:O	2:A:535:TRP:C	2.55	0.45
2:A:395:GLY:O	2:A:398:ILE:HG12	2.16	0.45
2:A:13:ARG:HA	2:A:499:ILE:HD13	1.98	0.45
2:A:930:PHE:CE1	2:A:1015:PRO:HB3	2.51	0.45
2:A:525:TYR:OH	2:A:980:ARG:NH2	2.49	0.45
2:A:887:LEU:HD13	2:A:900:ILE:HB	1.98	0.45
1:C:391:ILE:C	1:C:393:GLY:H	2.19	0.45
2:A:418:LEU:HD12	2:A:439:ILE:HD11	1.98	0.45
2:A:844:ILE:HD12	2:A:858:PHE:CZ	2.51	0.45
1:B:183:GLU:O	1:B:187:LEU:HG	2.16	0.45
1:B:207:ARG:HG3	1:B:207:ARG:O	2.13	0.45
2:A:348:VAL:HG12	2:A:993:ALA:HB1	1.98	0.45
2:A:42:LEU:HD21	2:A:474:LEU:HD13	1.98	0.45
2:A:474:LEU:O	2:A:477:PRO:HD2	2.16	0.45
2:A:637:ARG:HB3	2:A:638:PRO:HD2	1.99	0.45
2:A:453:SER:OG	2:A:939:GLU:HA	2.15	0.45
2:A:675:THR:HG21	2:A:860:GLY:O	2.16	0.45
2:A:421:TRP:HE1	2:A:425:HIS:CD2	2.34	0.45
1:C:266:LEU:HB3	1:C:276:LEU:HD12	1.97	0.45
2:A:2:ILE:O	2:A:6:ILE:HG13	2.15	0.45
2:A:18:MET:HA	2:A:21:LEU:HB3	1.99	0.45
2:A:411:ILE:HA	2:A:501:MET:CE	2.47	0.45
1:C:395:LEU:HB3	1:C:399:ARG:HH12	1.82	0.45
1:C:329:SER:HA	1:C:365:THR:HG23	1.99	0.45
2:A:297:ALA:O	2:A:301:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:463:PRO:HB2	2:A:875:MET:HG3	1.99	0.45
2:A:875:MET:CE	2:A:931:ILE:HG21	2.47	0.45
1:C:230:ALA:H	1:C:233:ASN:ND2	2.15	0.45
2:A:195:ARG:HD3	2:A:261:ASP:O	2.17	0.45
2:A:38:ALA:O	2:A:389:ASN:HB2	2.16	0.45
1:B:387:SER:HB2	2:A:271:MET:HG3	1.98	0.45
2:A:298:ARG:NE	2:A:328:SER:HB2	2.32	0.45
2:A:701:GLU:HG2	2:A:705:ARG:HH22	1.80	0.45
1:C:323:PRO:O	1:C:324:MET:HE3	2.17	0.44
2:A:952:ILE:C	2:A:957:SER:HB3	2.37	0.44
1:C:397:ARG:O	1:C:401:GLU:HG3	2.17	0.44
2:A:554:LEU:CD2	2:A:912:ILE:HG12	2.48	0.44
2:A:118:GLN:HE22	2:A:127:ALA:N	2.11	0.44
2:A:301:ILE:CD1	2:A:328:SER:HB3	2.46	0.44
2:A:350:ALA:HA	2:A:353:CYS:SG	2.58	0.44
2:A:716:GLU:OE1	2:A:814:LYS:HE3	2.17	0.44
2:A:482:LYS:C	2:A:482:LYS:HD3	2.38	0.44
2:A:559:GLY:H	2:A:834:VAL:HG12	1.81	0.44
1:B:121:TYR:CD1	1:C:224:ARG:HD3	2.52	0.44
2:A:6:ILE:O	2:A:10:VAL:HG23	2.17	0.44
1:C:281:TRP:CB	1:C:298:LEU:HD23	2.47	0.44
2:A:561:PHE:HA	2:A:865:LEU:HG	1.99	0.44
1:C:151:LEU:HD11	1:C:210:LEU:HD12	2.00	0.44
2:A:116:GLN:H	2:A:116:GLN:HG2	1.65	0.44
2:A:1009:MET:O	2:A:1012:ILE:HG22	2.17	0.44
1:C:298:LEU:HD11	1:C:315:LEU:HD22	1.99	0.44
1:B:288:ASP:O	1:B:292:ARG:N	2.50	0.44
1:C:330:GLN:O	1:C:382:LEU:HD12	2.18	0.44
2:A:420:GLU:HG3	2:A:421:TRP:N	2.33	0.44
2:A:723:TYR:HB2	2:A:807:SER:OG	2.18	0.44
2:A:711:ALA:HB3	2:A:827:ASP:O	2.18	0.44
2:A:118:GLN:NE2	2:A:126:SER:HA	2.33	0.44
2:A:969:LEU:HD12	2:A:969:LEU:O	2.18	0.44
2:A:288:VAL:HG22	2:A:290:ILE:HD12	2.00	0.44
2:A:73:MET:HE3	2:A:110:VAL:HG13	2.00	0.44
2:A:574:PRO:HG2	2:A:624:VAL:CG1	2.37	0.43
1:C:183:GLU:O	1:C:187:LEU:HG	2.18	0.43
1:B:117:ASN:HD22	1:B:117:ASN:C	2.21	0.43
2:A:196:LEU:HD22	2:A:201:ILE:O	2.17	0.43
1:C:146:LYS:HA	1:C:212:ALA:O	2.18	0.43
2:A:431:ASP:CG	2:A:432:ASN:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:GLN:NE2	1:C:243:PRO:HD2	2.32	0.43
2:A:940:PHE:CE1	2:A:984:LYS:HE3	2.54	0.43
2:A:571:LEU:HD11	2:A:665:PRO:HA	2.00	0.43
2:A:492:LEU:HA	2:A:492:LEU:HD22	1.81	0.43
1:C:88:GLN:HE21	2:A:654:ARG:HG3	1.82	0.43
2:A:595:LEU:HD23	2:A:595:LEU:HA	1.86	0.43
2:A:661:LEU:CD2	2:A:663:VAL:HG13	2.48	0.43
1:C:191:PRO:HG2	1:C:194:ASP:OD2	2.19	0.43
2:A:40:PRO:O	2:A:41:ASP:C	2.56	0.43
1:B:396:GLU:HG2	1:B:399:ARG:HH21	1.83	0.43
2:A:550:VAL:CG1	2:A:909:VAL:HG22	2.43	0.43
1:B:287:VAL:CG1	1:B:294:LEU:HD23	2.47	0.43
2:A:965:SER:OG	2:A:968:LYS:HB3	2.19	0.43
2:A:526:HIS:HB3	2:A:974:TYR:OH	2.18	0.43
2:A:834:VAL:HG22	2:A:838:HIS:NE2	2.33	0.43
2:A:996:LEU:N	2:A:997:PRO:CD	2.82	0.43
1:C:132:ILE:CD1	1:C:229:ILE:HB	2.48	0.43
1:B:104:LEU:HB2	1:B:321:SER:OG	2.19	0.43
2:A:461:PHE:CD1	2:A:482:LYS:HD2	2.53	0.43
2:A:42:LEU:HD12	2:A:42:LEU:N	2.33	0.43
2:A:1036:LYS:O	2:A:1040:LEU:HG	2.19	0.43
2:A:677:ILE:HG22	2:A:679:SER:H	1.82	0.43
2:A:642:MET:HA	2:A:642:MET:HE3	2.00	0.43
1:C:84:ILE:HG21	2:A:656:PRO:HG3	2.01	0.43
1:C:181:ILE:O	1:C:185:LEU:HD13	2.18	0.43
2:A:891:PHE:CE1	2:A:945:LEU:HD12	2.54	0.43
1:B:334:ASP:OD2	1:B:339:GLN:HB3	2.19	0.43
2:A:636:TRP:CD1	2:A:636:TRP:N	2.87	0.43
2:A:526:HIS:HB3	2:A:974:TYR:CZ	2.54	0.43
1:C:254:ILE:HD11	2:A:797:THR:CG2	2.49	0.43
1:C:121:TYR:CE1	1:C:237:LYS:HD3	2.54	0.43
1:B:340:ARG:HD2	1:B:395:LEU:HD13	1.99	0.43
2:A:940:PHE:CE2	2:A:944:MET:HG3	2.54	0.42
1:B:385:ILE:HG23	1:B:385:ILE:O	2.19	0.42
2:A:522:ILE:CG1	2:A:981:VAL:HG11	2.48	0.42
2:A:425:HIS:HB3	2:A:426:PRO:CD	2.46	0.42
2:A:325:TYR:HB2	2:A:627:THR:HG21	2.00	0.42
2:A:348:VAL:O	2:A:352:VAL:HG23	2.19	0.42
2:A:575:SER:O	2:A:714:LEU:HD22	2.19	0.42
1:C:268:VAL:HA	1:C:269:PRO:HD3	1.85	0.42
2:A:240:LEU:HA	2:A:240:LEU:HD23	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:LEU:HD23	1:B:298:LEU:N	2.34	0.42
2:A:469:GLY:O	2:A:473:ARG:HG3	2.18	0.42
1:B:390:ASN:HA	2:A:774:GLN:HE22	1.85	0.42
2:A:904:VAL:O	2:A:908:LEU:HG	2.19	0.42
2:A:185:LYS:O	2:A:767:PRO:HD2	2.19	0.42
2:A:534:HIS:CD2	2:A:534:HIS:O	2.72	0.42
2:A:715:ALA:CB	2:A:824:ILE:HG12	2.49	0.42
2:A:110:VAL:O	2:A:114:LEU:HB2	2.19	0.42
2:A:376:ILE:O	2:A:380:VAL:HG23	2.19	0.42
2:A:718:LEU:HD12	2:A:718:LEU:HA	1.84	0.42
2:A:222:ILE:CD1	2:A:224:LEU:HG	2.49	0.42
1:B:322:GLU:O	1:B:324:MET:HG3	2.20	0.42
2:A:311:LEU:O	2:A:315:LEU:HG	2.19	0.42
1:C:367:LEU:N	1:C:367:LEU:HD22	2.35	0.42
2:A:531:LYS:O	2:A:534:HIS:HB3	2.19	0.42
1:B:291:THR:O	1:B:293:THR:HG23	2.19	0.42
2:A:295:LYS:HD3	2:A:295:LYS:HA	1.88	0.42
1:B:125:GLN:HG2	1:B:233:ASN:O	2.19	0.42
2:A:421:TRP:HE3	2:A:438:VAL:HB	1.84	0.42
1:C:161:ALA:HB3	1:C:185:LEU:HD11	2.01	0.42
2:A:933:LEU:HD23	2:A:1016:MET:HA	2.02	0.42
2:A:62:GLU:HA	2:A:66:THR:HB	2.00	0.42
2:A:67:TYR:N	2:A:68:PRO:HD2	2.34	0.42
2:A:399:ALA:HA	2:A:486:MET:HE1	2.00	0.42
2:A:534:HIS:HD2	2:A:534:HIS:O	2.02	0.42
2:A:770:LEU:O	2:A:771:ARG:HB2	2.18	0.42
2:A:550:VAL:C	2:A:553:PRO:HD2	2.40	0.42
2:A:97:PHE:CZ	2:A:106:ALA:HB1	2.55	0.42
2:A:172:PRO:O	2:A:173:ASP:HB2	2.20	0.42
2:A:729:ASN:HB3	2:A:732:LYS:HB2	2.01	0.42
1:B:132:ILE:HD11	1:B:229:ILE:HB	2.01	0.42
1:B:389:ALA:O	1:B:391:ILE:N	2.53	0.41
1:B:121:TYR:OH	1:B:237:LYS:HE2	2.20	0.41
2:A:114:LEU:HA	2:A:114:LEU:HD12	1.95	0.41
2:A:275:ILE:O	2:A:608:LYS:HA	2.20	0.41
2:A:375:CYS:O	2:A:379:ILE:HG13	2.20	0.41
1:B:280:LYS:HE3	1:B:281:TRP:H	1.84	0.41
2:A:1016:MET:O	2:A:1020:MET:HB2	2.20	0.41
2:A:992:ILE:O	2:A:996:LEU:HB2	2.20	0.41
1:C:274:LYS:HB3	1:C:274:LYS:HE2	1.72	0.41
1:B:302:ASN:HD21	1:B:306:ALA:N	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:972:ALA:HA	2:A:975:HIS:CD2	2.55	0.41
2:A:404:VAL:O	2:A:408:ILE:HG12	2.19	0.41
2:A:599:VAL:HG12	2:A:601:GLU:H	1.86	0.41
1:B:391:ILE:HG12	2:A:774:GLN:CD	2.40	0.41
2:A:992:ILE:HD11	2:A:1020:MET:O	2.20	0.41
2:A:15:LEU:HA	2:A:15:LEU:HD22	1.92	0.41
1:B:159:VAL:HG13	1:B:160:GLU:N	2.36	0.41
2:A:904:VAL:HG22	2:A:905:PRO:HD3	2.03	0.41
2:A:188:GLN:NE2	2:A:268:GLY:HA3	2.35	0.41
2:A:578:PRO:HG2	2:A:717:ARG:HB2	2.02	0.41
2:A:193:PRO:HG3	2:A:772:TYR:CD2	2.54	0.41
1:B:110:PHE:CD1	1:B:250:ILE:HG12	2.56	0.41
2:A:535:TRP:NE1	2:A:537:LYS:HB3	2.35	0.41
2:A:214:ASN:HB2	2:A:237:LEU:HD22	2.03	0.41
1:C:129:ALA:O	1:C:155:ILE:HG23	2.20	0.41
2:A:1020:MET:HA	2:A:1020:MET:CE	2.51	0.41
1:C:395:LEU:O	1:C:399:ARG:HG3	2.20	0.41
2:A:574:PRO:CD	2:A:624:VAL:HG22	2.51	0.41
2:A:418:LEU:CD2	2:A:438:VAL:HG11	2.51	0.41
2:A:456:ILE:HG23	2:A:883:ILE:HD13	2.02	0.41
1:C:112:ALA:HB2	1:C:248:ALA:HB2	2.02	0.41
2:A:962:GLN:HG3	2:A:963:THR:N	2.34	0.41
2:A:911:GLY:HA3	2:A:930:PHE:CE2	2.56	0.41
2:A:494:ILE:HG12	2:A:494:ILE:O	2.21	0.41
2:A:22:PHE:O	2:A:25:ILE:HG23	2.21	0.41
1:B:296:LEU:HD23	1:B:296:LEU:C	2.41	0.41
2:A:159:LEU:O	2:A:163:PHE:HB3	2.20	0.41
1:C:120:GLN:OE1	1:C:240:GLY:HA3	2.21	0.41
2:A:574:PRO:HD2	2:A:624:VAL:O	2.21	0.41
2:A:459:LEU:C	2:A:461:PHE:H	2.24	0.41
2:A:595:LEU:CB	2:A:653:VAL:HG22	2.50	0.41
1:B:350:PHE:O	1:B:351:VAL:HG13	2.20	0.41
1:C:266:LEU:HD23	1:C:266:LEU:HA	1.93	0.41
2:A:373:GLY:HA2	2:A:376:ILE:HG22	2.02	0.41
2:A:560:GLU:HG3	2:A:923:SER:HB3	2.02	0.41
2:A:243:PHE:O	2:A:246:ILE:HG13	2.21	0.41
1:C:124:VAL:O	1:C:235:VAL:HG13	2.21	0.41
2:A:440:THR:O	2:A:440:THR:HG22	2.21	0.41
2:A:945:LEU:HD22	2:A:945:LEU:HA	1.96	0.40
2:A:769:ASN:H	2:A:769:ASN:HD22	1.69	0.40
2:A:535:TRP:O	2:A:537:LYS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:815:THR:HG22	2:A:818:ALA:HA	2.03	0.40
2:A:296:ASN:HB3	2:A:299:GLU:CB	2.51	0.40
2:A:36:VAL:HG21	2:A:335:ILE:HG12	2.02	0.40
2:A:664:PRO:HA	2:A:665:PRO:HD3	1.99	0.40
2:A:553:PRO:HB2	2:A:912:ILE:HG22	2.02	0.40
1:C:161:ALA:CB	1:C:185:LEU:HD11	2.51	0.40
2:A:1031:ILE:N	2:A:1032:PRO:CD	2.85	0.40
1:C:156:PRO:O	1:C:157:ASP:C	2.60	0.40
1:B:307:LEU:H	1:B:307:LEU:HD22	1.85	0.40
2:A:46:GLN:OE1	2:A:94:TYR:HD2	2.04	0.40
2:A:522:ILE:HD13	2:A:978:VAL:HG23	2.04	0.40
2:A:599:VAL:HA	2:A:600:PRO:HD3	1.85	0.40
2:A:390:ILE:O	2:A:390:ILE:HG12	2.16	0.40
1:C:360:ALA:CB	1:C:365:THR:HG22	2.52	0.40
2:A:831:ARG:HH22	2:A:839:ASP:CG	2.24	0.40
2:A:255:VAL:HA	2:A:256:PRO:HD3	1.87	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	B	320/413 (78%)	281 (88%)	36 (11%)	3 (1%)	21	67
1	C	322/413 (78%)	300 (93%)	21 (6%)	1 (0%)	46	83
2	A	1027/1054 (97%)	922 (90%)	95 (9%)	10 (1%)	19	65
All	All	1669/1880 (89%)	1503 (90%)	152 (9%)	14 (1%)	24	69

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	388	GLU

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Mol	Chain	Res	Type
2	A	638	PRO
1	B	337	SER
1	B	390	ASN
2	A	894	VAL
2	A	574	PRO
2	A	13	ARG
2	A	238	GLN
1	C	137	PRO
2	A	38	ALA
2	A	235	GLY
2	A	852	PRO
2	A	1024	PRO
2	A	426	PRO

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	B	263/338 (78%)	243 (92%)	20 (8%)	16	56
1	C	265/338 (78%)	245 (92%)	20 (8%)	17	56
2	A	849/871 (98%)	772 (91%)	77 (9%)	12	47
All	All	1377/1547 (89%)	1260 (92%)	117 (8%)	13	51

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	84	ILE
1	B	105	THR
1	B	117	ASN
1	B	121	TYR
1	B	169	ARG
1	B	183	GLU
1	B	185	LEU
1	B	207	ARG
1	B	223	LEU

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Mol	Chain	Res	Type
1	B	241	MET
1	B	280	LYS
1	B	281	TRP
1	B	282	THR
1	B	307	LEU
1	B	322	GLU
1	B	349	ARG
1	B	351	VAL
1	B	357	VAL
1	B	387	SER
1	B	388	GLU
1	C	105	THR
1	C	121	TYR
1	C	138	LEU
1	C	140	VAL
1	C	182	LEU
1	C	207	ARG
1	C	235	VAL
1	C	239	GLN
1	C	260	ASP
1	C	265	THR
1	C	276	LEU
1	C	277	THR
1	C	292	ARG
1	C	296	LEU
1	C	330	GLN
1	C	339	GLN
1	C	347	ASP
1	C	353	LYS
1	C	364	VAL
1	C	382	LEU
2	A	13	ARG
2	A	15	LEU
2	A	23	LEU
2	A	25	ILE
2	A	42	LEU
2	A	53	TYR
2	A	105	TRP
2	A	144	LEU
2	A	145	VAL
2	A	157	ARG
2	A	203	LEU

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Mol	Chain	Res	Type
2	A	210	LEU
2	A	211	ASP
2	A	215	GLN
2	A	222	ILE
2	A	236	TYR
2	A	237	LEU
2	A	260	ARG
2	A	288	VAL
2	A	293	SER
2	A	298	ARG
2	A	322	VAL
2	A	342	LEU
2	A	351	VAL
2	A	358	TRP
2	A	364	LEU
2	A	374	LEU
2	A	390	ILE
2	A	400	VAL
2	A	412	GLU
2	A	415	HIS
2	A	417	ARG
2	A	419	GLU
2	A	434	THR
2	A	453	SER
2	A	455	LEU
2	A	457	ILE
2	A	492	LEU
2	A	521	LEU
2	A	531	LYS
2	A	534	HIS
2	A	554	LEU
2	A	569	ASP
2	A	573	MET
2	A	592	THR
2	A	602	VAL
2	A	621	LEU
2	A	624	VAL
2	A	634	GLU
2	A	637	ARG
2	A	642	MET
2	A	660	ASN
2	A	667	ARG

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Mol	Chain	Res	Type
2	A	688	THR
2	A	693	ILE
2	A	722	ARG
2	A	729	ASN
2	A	749	SER
2	A	759	THR
2	A	765	ARG
2	A	769	ASN
2	A	770	LEU
2	A	781	GLN
2	A	789	LEU
2	A	815	THR
2	A	837	VAL
2	A	865	LEU
2	A	879	THR
2	A	882	ILE
2	A	940	PHE
2	A	945	LEU
2	A	969	LEU
2	A	984	LYS
2	A	991	ILE
2	A	1020	MET
2	A	1035	TYR
2	A	1039	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	113	ASN
1	B	117	ASN
1	B	125	GLN
1	B	177	GLN
1	B	302	ASN
1	B	330	GLN
1	B	359	GLN
1	B	390	ASN
1	C	88	GLN
1	C	177	GLN
1	C	233	ASN
1	C	263	GLN
1	C	302	ASN
2	A	116	GLN

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Mol	Chain	Res	Type
2	A	118	GLN
2	A	151	HIS
2	A	215	GLN
2	A	238	GLN
2	A	279	ASN
2	A	329	GLN
2	A	359	HIS
2	A	423	HIS
2	A	470	GLN
2	A	534	HIS
2	A	629	GLN
2	A	633	GLN
2	A	635	GLN
2	A	651	ASN
2	A	660	ASN
2	A	729	ASN
2	A	744	GLN
2	A	769	ASN
2	A	795	GLN
2	A	838	HIS

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	B	322/413 (77%)	0.08	1 (0%) 94 92	36, 86, 147, 228	0
1	C	324/413 (78%)	0.16	0 100 100	35, 88, 138, 217	0
2	A	1031/1054 (97%)	0.33	31 (3%) 54 42	30, 110, 226, 401	0
All	All	1677/1880 (89%)	0.25	32 (1%) 70 60	30, 99, 210, 401	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	446	VAL	7.2
2	A	445	GLU	5.3
2	A	954	ALA	4.9
2	A	429	THR	4.2
2	A	890	ALA	3.9
2	A	450	LEU	3.9
2	A	3	GLU	2.9
2	A	449	ALA	2.9
2	A	428	ALA	2.7
2	A	416	LYS	2.7
2	A	413	ASN	2.5
2	A	523	ARG	2.5
2	A	400	VAL	2.4
2	A	896	GLU	2.4
2	A	345	GLU	2.3
2	A	412	GLU	2.3
2	A	873	LYS	2.3
2	A	1002	THR	2.2
2	A	442	ALA	2.2
2	A	955	VAL	2.1
2	A	947	TYR	2.1
2	A	950	HIS	2.1
2	A	887	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	A	846	GLU	2.1
2	A	891	PHE	2.1
1	B	170	GLU	2.1
2	A	274	GLY	2.1
2	A	519	ARG	2.1
2	A	418	LEU	2.0
2	A	415	HIS	2.0
2	A	951	ALA	2.0
2	A	580	ILE	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.