Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 11:42 AM EST

PDB ID	:	4K0E
Title	:	X-ray crystal structure of a heavy metal efflux pump, crystal form II
Authors	:	Pak, J.E.; Ngonlong Ekende, E.; Vandenbussche, G.; Stroud, R.M.; Center for Structures of Membrane Proteins (CSMP)
Deposited on	:	2013-04-03
Resolution	:	3.71 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

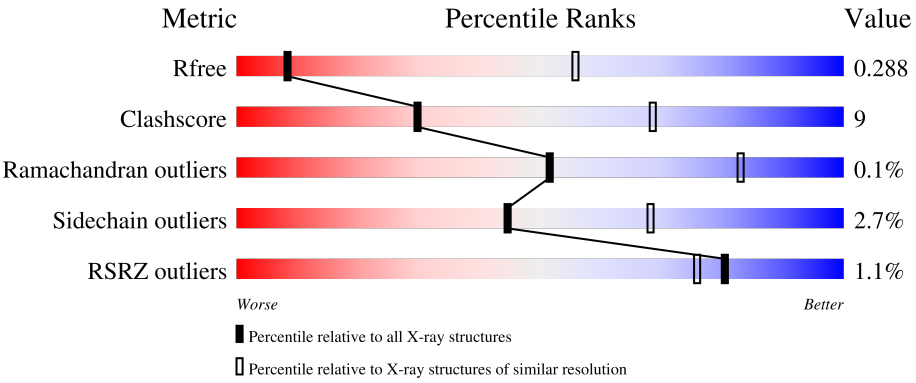
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1089 (3.90-3.54)
Clashscore	141614	1012 (3.88-3.56)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1045	70% 23% 7%
1	B	1045	69% 21% 8%
1	C	1045	68% 21% 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 22061 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 Heavy metal cation tricomponent efflux pump ZneA(CzcA-like).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	977	Total	C	N	O	S	0	0	0
			7489	4809	1303	1345	32			
1	B	957	Total	C	N	O	S	0	0	0
			7329	4710	1271	1317	31			
1	C	942	Total	C	N	O	S	0	0	0
			7239	4644	1261	1302	32			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1040	HIS	-	expression tag	UNP Q1LCD8
A	1041	HIS	-	expression tag	UNP Q1LCD8
A	1042	HIS	-	expression tag	UNP Q1LCD8
A	1043	HIS	-	expression tag	UNP Q1LCD8
A	1044	HIS	-	expression tag	UNP Q1LCD8
A	1045	HIS	-	expression tag	UNP Q1LCD8
B	1040	HIS	-	expression tag	UNP Q1LCD8
B	1041	HIS	-	expression tag	UNP Q1LCD8
B	1042	HIS	-	expression tag	UNP Q1LCD8
B	1043	HIS	-	expression tag	UNP Q1LCD8
B	1044	HIS	-	expression tag	UNP Q1LCD8
B	1045	HIS	-	expression tag	UNP Q1LCD8
C	1040	HIS	-	expression tag	UNP Q1LCD8
C	1041	HIS	-	expression tag	UNP Q1LCD8
C	1042	HIS	-	expression tag	UNP Q1LCD8
C	1043	HIS	-	expression tag	UNP Q1LCD8
C	1044	HIS	-	expression tag	UNP Q1LCD8
C	1045	HIS	-	expression tag	UNP Q1LCD8

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

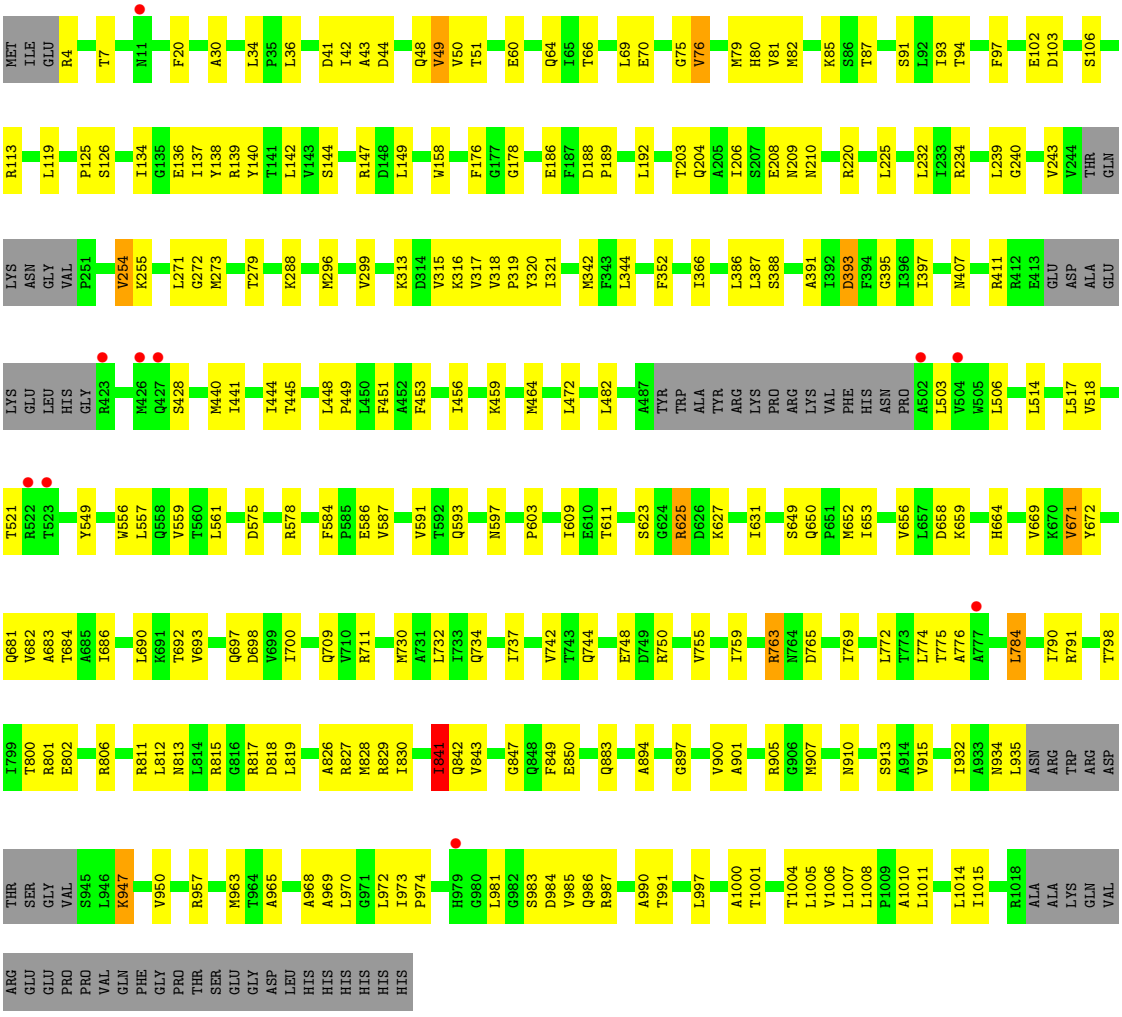
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

3 Residue-property plots (i)

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

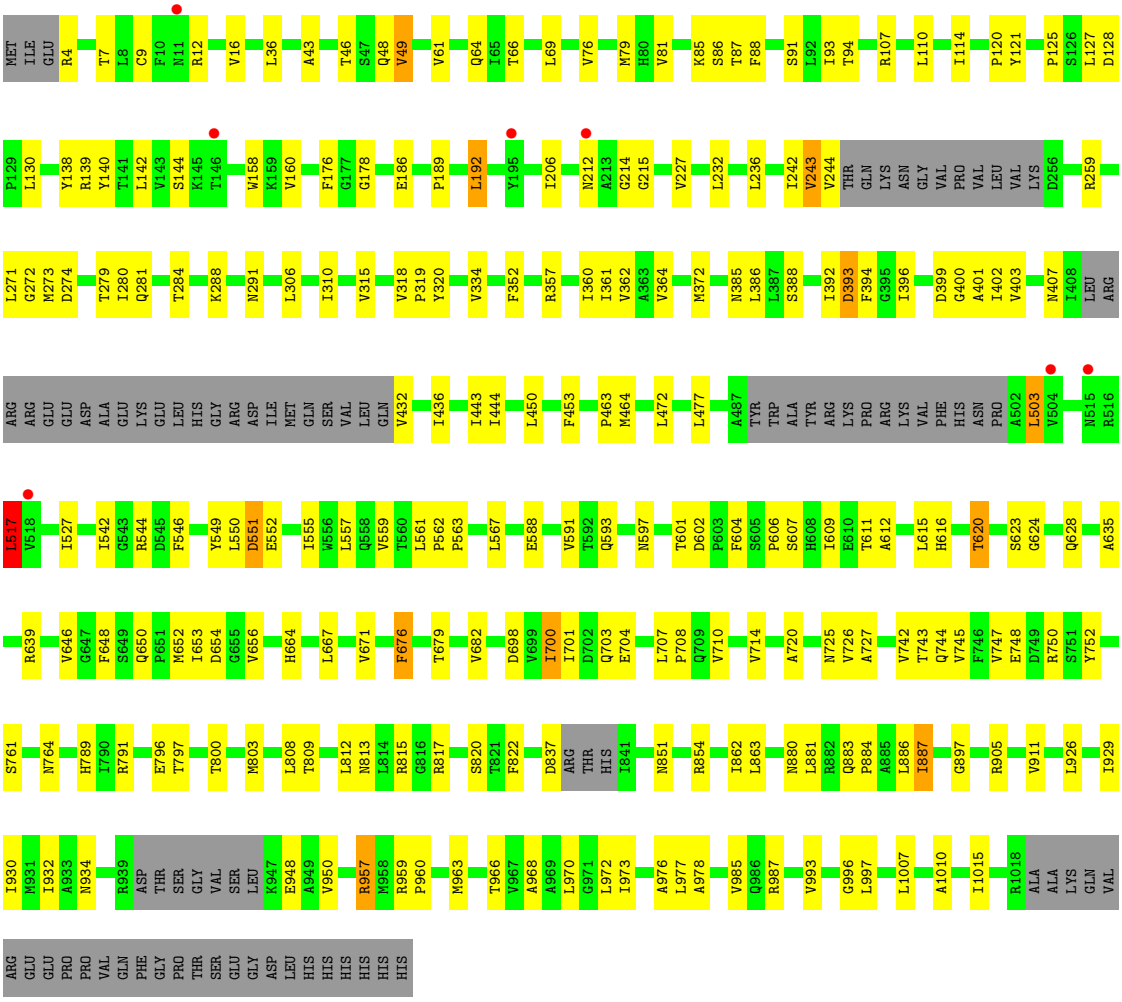
• Molecule 1: Heavy metal cation tricomponent efflux pump ZneA(CzcA-like)

Chain A:



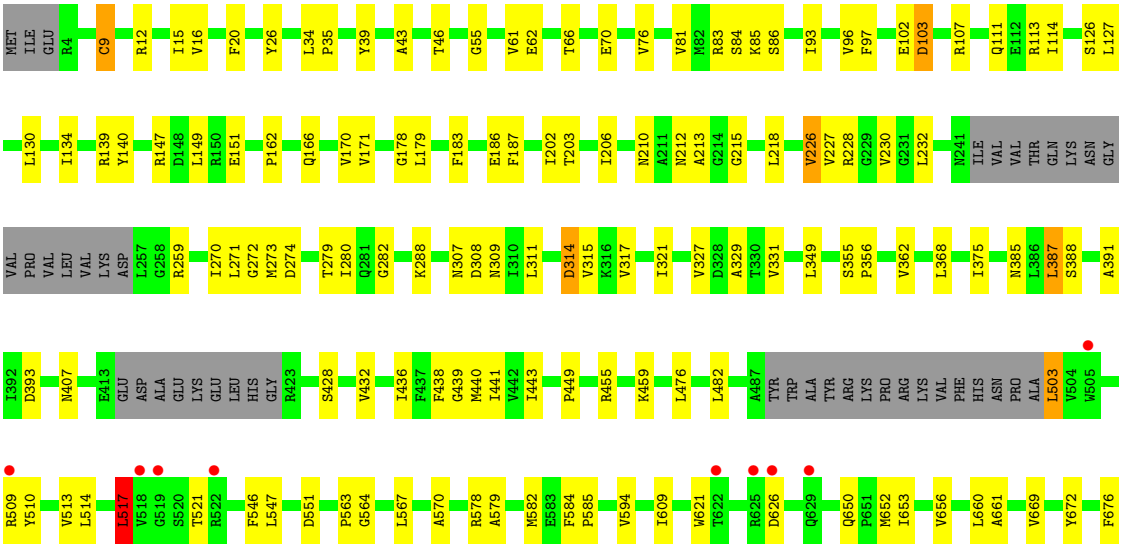
• Molecule 1: Heavy metal cation tricomponent efflux pump ZneA(CzcA-like)

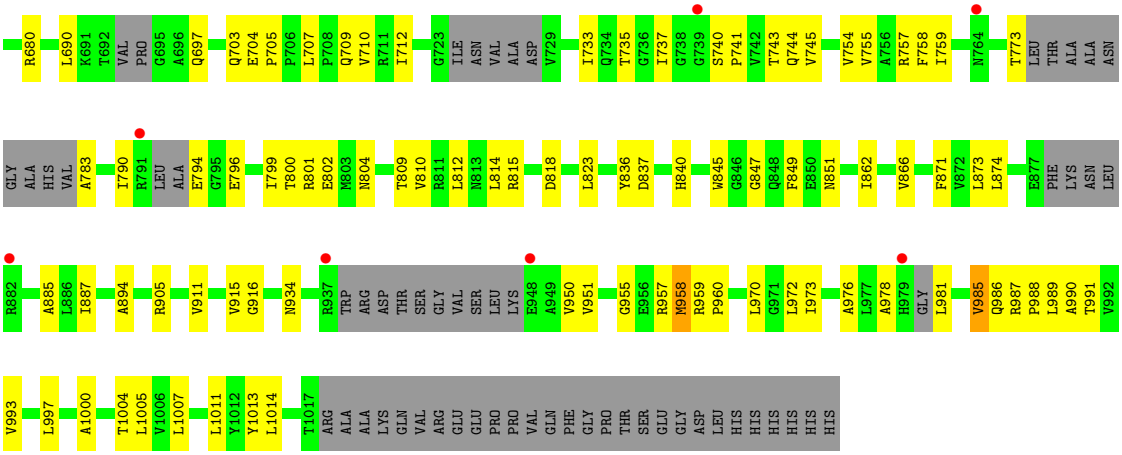
Chain B:



• Molecule 1: Heavy metal cation tricomponent efflux pump ZneA(CzcA-like)

Chain C:




R680 L690 K691 T692 VAL PRO G695 A696 Q697 Q703 E704 P705 P706 L707 P708 Q709 V710 R711 I712 G723 ILE ASN VAL ALA ASP V729 I733 Q734 T735 G736 I737 G738 G739 S740 P741 V742 T743 Q744 V745 V754 V755 A756 R757 F758 I759 N764 T773 LEU THR ALA ALA ASN
GLY ALA HIS VAL A783 I790 R791 LEU ALA E794 G795 E796 I799 T800 R801 E802 M803 N804 T809 V810 H811 L812 N813 L814 R815 D818 L823 Y836 D837 H840 W845 G846 G847 Q848 F849 E850 N851 I862 V866 F871 V872 L873 L874 E877 PHE LYS ASN LEU
R882 A885 L886 I887 A894 R905 V911 V915 G916 N934 R937 TRP ARG ASP THR SER GLY VAL SER LEU LYS E948 A949 V950 V951 G955 E956 R957 M958 R959 P960 L970 G971 L972 I973 A976 L977 A978 H979 GLY L981 V985 Q986 R987 P988 L989 A990 T991 V992
V993 L997 A1000 T1004 L1005 V1006 L1007 L1011 Y1012 Y1013 L1014 T1017 ARG ALA ALA LYS GLN VAL ARG GLU GLU PRO PRO VAL GLN PHE GLY PRO THR SER GLU GLY ASP LEU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	215.34Å 127.07Å 163.33Å 90.00° 93.12° 90.00°	Depositor
Resolution (Å)	19.94 – 3.71 20.02 – 3.71	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.94-3.71) 85.5 (20.02-3.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 3.71Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.229 , 0.283 0.238 , 0.288	Depositor DCC
R_{free} test set	2162 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	94.6	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.014 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.018 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	22061	wwPDB-VP
Average B, all atoms (Å^2)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.24	0/7618	0.45	0/10362
1	B	0.23	0/7457	0.44	1/10146 (0.0%)
1	C	0.22	0/7358	0.43	1/9996 (0.0%)
All	All	0.23	0/22433	0.44	2/30504 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	517	LEU	CA-CB-CG	5.41	127.74	115.30
1	B	517	LEU	CA-CB-CG	5.34	127.59	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7489	0	7783	153	0
1	B	7329	0	7597	146	0
1	C	7239	0	7499	137	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	22061	0	22879	423	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 9.

All (423) 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:70:GLU:HA	1:A:82:MET:HE1	1.62	0.81
1:A:984:ASP:HB3	1:A:987:ARG:HE	1.51	0.75
1:B:623:SER:OG	1:B:624:GLY:N	2.15	0.75
1:C:735:THR:HA	1:C:740:SER:HB3	1.71	0.73
1:B:978:ALA:HA	1:B:987:ARG:HE	1.55	0.71
1:A:559:VAL:HB	1:A:609:ILE:HB	1.72	0.71
1:B:206:ILE:HB	1:B:742:VAL:HG11	1.73	0.71
1:A:49:VAL:HG13	1:A:93:ILE:HB	1.72	0.71
1:B:930:ILE:O	1:B:934:ASN:ND2	2.25	0.70
1:B:557:LEU:HB2	1:B:611:THR:HB	1.74	0.69
1:B:271:LEU:HD23	1:B:279:THR:HG23	1.74	0.68
1:A:209:ASN:HB2	1:B:726:VAL:HB	1.76	0.68
1:B:551:ASP:HB2	1:B:650:GLN:HE22	1.58	0.67
1:C:130:LEU:HG	1:C:288:LYS:HB2	1.77	0.67
1:B:602:ASP:HB3	1:B:604:PHE:HD1	1.59	0.67
1:B:957:ARG:HD2	1:B:960:PRO:HG2	1.75	0.67
1:A:557:LEU:HB2	1:A:611:THR:HB	1.77	0.66
1:C:563:PRO:HG3	1:C:705:PRO:HG2	1.78	0.66
1:C:147:ARG:HD3	1:C:151:GLU:HG2	1.77	0.66
1:C:773:THR:HG1	1:C:783:ALA:N	1.94	0.66
1:A:549:TYR:OH	1:A:627:LYS:NZ	2.29	0.65
1:B:396:ILE:HG12	1:B:443:ILE:HG12	1.79	0.65
1:C:349:LEU:HD13	1:C:362:VAL:HG13	1.79	0.64
1:C:905:ARG:NH2	1:C:991:THR:OG1	2.29	0.64
1:C:514:LEU:HD13	1:C:951:VAL:HA	1.80	0.64
1:C:271:LEU:HD23	1:C:279:THR:HG23	1.79	0.64
1:C:690:LEU:HD13	1:C:812:LEU:HD13	1.79	0.64
1:A:85:LYS:HG2	1:A:800:THR:HG22	1.80	0.63
1:B:550:LEU:HD21	1:B:985:VAL:HG23	1.79	0.63
1:B:817:ARG:HD3	1:B:822:PHE:HB2	1.80	0.63
1:C:139:ARG:HB2	1:C:321:ILE:HB	1.79	0.63
1:C:12:ARG:HB3	1:C:16:VAL:HG23	1.80	0.63
1:C:186:GLU:HB2	1:C:259:ARG:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:733:ILE:HG13	1:C:737:ILE:HD12	1.81	0.63
1:A:934:ASN:HB2	1:A:957:ARG:HE	1.63	0.62
1:C:407:ASN:ND2	1:C:428:SER:O	2.33	0.62
1:B:884:PRO:HA	1:B:887:ILE:HG22	1.82	0.62
1:B:49:VAL:HG13	1:B:93:ILE:HB	1.81	0.62
1:C:111:GLN:HG2	1:C:127:LEU:HD22	1.82	0.62
1:B:698:ASP:OD2	1:B:815:ARG:NH2	2.32	0.62
1:C:510:TYR:HE2	1:C:955:GLY:HA2	1.66	0.61
1:A:897:GLY:HA2	1:A:900:VAL:HG22	1.82	0.60
1:A:36:LEU:HD12	1:A:386:LEU:HD11	1.81	0.60
1:C:441:ILE:HG23	1:C:873:LEU:HD13	1.84	0.60
1:C:672:TYR:OH	1:C:802:GLU:OE1	2.14	0.60
1:B:385:ASN:HB2	1:B:463:PRO:HG2	1.83	0.60
1:A:732:LEU:HD22	1:A:774:LEU:HD23	1.85	0.59
1:A:271:LEU:HD23	1:A:279:THR:HG23	1.83	0.59
1:C:972:LEU:HD13	1:C:990:ALA:HA	1.85	0.59
1:A:186:GLU:HB3	1:A:759:ILE:HD13	1.85	0.59
1:B:64:GLN:HB3	1:B:120:PRO:HG2	1.84	0.59
1:A:210:ASN:ND2	1:A:744:GLN:O	2.36	0.59
1:C:680:ARG:NH2	1:C:796:GLU:OE1	2.35	0.59
1:C:521:THR:HB	1:C:1014:LEU:HD22	1.84	0.59
1:A:139:ARG:HB2	1:A:321:ILE:HB	1.84	0.58
1:C:385:ASN:HB2	1:C:388:SER:HB3	1.85	0.58
1:C:823:LEU:HD13	1:C:849:PHE:HD1	1.69	0.58
1:B:48:GLN:HB3	1:B:94:THR:HA	1.86	0.58
1:B:851:ASN:HD22	1:B:854:ARG:HH12	1.50	0.58
1:C:76:VAL:HG23	1:C:113:ARG:HD2	1.85	0.57
1:C:206:ILE:O	1:C:210:ASN:ND2	2.37	0.57
1:A:734:GLN:HB2	1:C:213:ALA:HB1	1.86	0.57
1:C:455:ARG:NH1	1:C:851:ASN:OD1	2.38	0.57
1:B:76:VAL:HG13	1:B:79:MET:HB2	1.86	0.57
1:A:575:ASP:OD1	1:A:578:ARG:NH2	2.32	0.57
1:B:61:VAL:HG12	1:B:86:SER:HB3	1.87	0.56
1:B:648:PHE:HB2	1:B:815:ARG:NH2	2.20	0.56
1:B:107:ARG:NH1	1:B:128:ASP:O	2.32	0.56
1:B:700:ILE:HG22	1:B:701:ILE:H	1.70	0.56
1:C:308:ASP:OD2	1:C:309:ASN:ND2	2.38	0.56
1:A:243:VAL:HG22	1:B:720:ALA:HA	1.87	0.56
1:A:448:LEU:HA	1:A:451:PHE:HD2	1.70	0.56
1:B:897:GLY:HA3	1:B:996:GLY:HA2	1.88	0.56
1:A:972:LEU:HD13	1:A:990:ALA:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:880:ASN:ND2	1:B:883:GLN:OE1	2.38	0.56
1:B:107:ARG:HD2	1:B:130:LEU:HD13	1.88	0.56
1:C:85:LYS:HG2	1:C:800:THR:HG22	1.88	0.56
1:B:396:ILE:HG21	1:B:443:ILE:HG21	1.88	0.55
1:A:209:ASN:ND2	1:B:725:ASN:OD1	2.39	0.55
1:A:232:LEU:HD23	1:A:234:ARG:HH12	1.72	0.55
1:B:559:VAL:HG22	1:B:646:VAL:HG22	1.87	0.55
1:C:183:PHE:HB2	1:C:754:VAL:HG22	1.89	0.55
1:A:395:GLY:HA3	1:A:968:ALA:HA	1.88	0.55
1:B:212:ASN:HD21	1:B:232:LEU:HB2	1.71	0.54
1:B:399:ASP:HA	1:B:402:ILE:HG12	1.87	0.54
1:B:555:ILE:HG13	1:B:615:LEU:HD21	1.90	0.54
1:B:64:GLN:NE2	1:B:121:TYR:OH	2.38	0.54
1:C:551:ASP:HA	1:C:650:GLN:HE22	1.73	0.54
1:A:225:LEU:HD23	1:B:708:PRO:HB2	1.90	0.54
1:B:559:VAL:HB	1:B:609:ILE:HB	1.89	0.54
1:C:712:ILE:HG12	1:C:790:ILE:HG13	1.89	0.54
1:A:817:ARG:HG2	1:A:818:ASP:H	1.73	0.54
1:C:391:ALA:HB2	1:C:986:GLN:HG3	1.90	0.54
1:A:1005:LEU:HD12	1:A:1006:VAL:HG23	1.89	0.53
1:A:119:LEU:HD22	1:A:125:PRO:HD3	1.90	0.53
1:A:698:ASP:O	1:A:812:LEU:HA	2.07	0.53
1:C:986:GLN:HB2	1:C:989:LEU:HD22	1.90	0.53
1:B:393:ASP:OD1	1:B:968:ALA:HA	2.09	0.53
1:C:438:PHE:HA	1:C:441:ILE:HG22	1.90	0.53
1:A:709:GLN:HG2	1:C:226:VAL:HG13	1.91	0.53
1:B:396:ILE:HB	1:B:472:LEU:HD11	1.90	0.53
1:B:407:ASN:HD22	1:B:432:VAL:HG22	1.73	0.53
1:B:588:GLU:HB3	1:B:616:HIS:CE1	2.44	0.53
1:B:789:HIS:HE1	1:B:791:ARG:HD3	1.72	0.53
1:A:140:TYR:HA	1:A:319:PRO:HA	1.91	0.53
1:B:178:GLY:HA3	1:B:280:ILE:HD13	1.91	0.53
1:C:510:TYR:HE1	1:C:1005:LEU:HB3	1.73	0.53
1:A:134:ILE:HB	1:A:652:MET:HE3	1.91	0.53
1:A:910:ASN:H	1:A:913:SER:HB2	1.74	0.53
1:C:9:CYS:HA	1:C:12:ARG:HB2	1.91	0.53
1:C:874:LEU:HD22	1:C:887:ILE:HD12	1.91	0.53
1:A:60:GLU:OE2	1:C:228:ARG:NE	2.41	0.52
1:A:445:THR:HA	1:A:448:LEU:HD13	1.90	0.52
1:B:212:ASN:ND2	1:B:232:LEU:HB2	2.25	0.52
1:B:527:ILE:HG22	1:B:1007:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ILE:HG22	1:B:394:PHE:H	1.75	0.52
1:A:671:VAL:HG21	1:A:683:ALA:HB2	1.91	0.52
1:A:969:ALA:HB2	1:A:997:LEU:HD22	1.92	0.52
1:B:12:ARG:HB3	1:B:16:VAL:HG23	1.90	0.52
1:A:48:GLN:HG2	1:A:94:THR:HA	1.90	0.51
1:A:240:GLY:HA2	1:A:254:VAL:HG12	1.92	0.51
1:A:698:ASP:HB2	1:A:813:ASN:HD22	1.74	0.51
1:A:737:ILE:HG23	1:A:763:ARG:HH21	1.75	0.51
1:A:521:THR:HG21	1:A:1014:LEU:HD13	1.93	0.51
1:A:784:LEU:HD11	1:A:790:ILE:HD11	1.91	0.51
1:A:983:SER:O	1:A:986:GLN:NE2	2.34	0.51
1:C:871:PHE:HE2	1:C:885:ALA:HB2	1.75	0.51
1:A:142:LEU:HD23	1:A:142:LEU:H	1.74	0.51
1:A:76:VAL:HG12	1:A:79:MET:HB2	1.91	0.51
1:B:36:LEU:O	1:B:291:ASN:ND2	2.42	0.51
1:A:189:PRO:O	1:A:192:LEU:HG	2.11	0.51
1:A:204:GLN:O	1:A:208:GLU:HB2	2.11	0.51
1:A:503:LEU:HD23	1:A:506:LEU:HD12	1.93	0.51
1:A:693:VAL:HG11	1:A:826:ALA:HB2	1.92	0.51
1:C:84:SER:HB3	1:C:93:ILE:HG23	1.92	0.51
1:B:271:LEU:HD22	1:B:281:GLN:HB3	1.94	0.50
1:B:279:THR:OG1	1:B:280:ILE:N	2.44	0.50
1:B:667:LEU:HB2	1:B:812:LEU:HG	1.93	0.50
1:B:959:ARG:HB2	1:B:960:PRO:HD3	1.93	0.50
1:C:449:PRO:HG2	1:C:866:VAL:HG22	1.92	0.50
1:A:627:LYS:O	1:A:631:ILE:HG12	2.11	0.50
1:A:209:ASN:HB3	1:B:727:ALA:H	1.76	0.50
1:A:518:VAL:HG22	1:A:947:LYS:HD3	1.93	0.50
1:B:9:CYS:HA	1:B:12:ARG:HB2	1.92	0.50
1:C:626:ASP:OD2	1:C:626:ASP:N	2.43	0.50
1:A:827:ARG:H	1:A:830:ILE:HD13	1.76	0.50
1:B:66:THR:OG1	1:B:91:SER:HB2	2.11	0.50
1:A:901:ALA:HB1	1:A:991:THR:HG22	1.94	0.50
1:B:393:ASP:HB2	1:B:972:LEU:HG	1.93	0.50
1:B:714:VAL:HG11	1:B:726:VAL:HG22	1.93	0.50
1:A:206:ILE:HD11	1:A:239:LEU:HD11	1.94	0.50
1:A:296:MET:HA	1:A:299:VAL:HG12	1.94	0.50
1:C:34:LEU:HD12	1:C:35:PRO:HD2	1.94	0.50
1:C:503:LEU:HD13	1:C:959:ARG:HH22	1.77	0.50
1:A:352:PHE:HD2	1:A:963:MET:HG3	1.77	0.50
1:B:352:PHE:CZ	1:B:963:MET:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:743:THR:OG1	1:C:744:GLN:N	2.45	0.50
1:C:212:ASN:HD21	1:C:232:LEU:HB2	1.76	0.49
1:C:563:PRO:HB3	1:C:704:GLU:HB2	1.92	0.49
1:A:391:ALA:HB2	1:A:986:GLN:HB2	1.94	0.49
1:A:671:VAL:HG12	1:A:843:VAL:HG12	1.94	0.49
1:C:970:LEU:HD22	1:C:973:ILE:HD11	1.94	0.49
1:B:698:ASP:HB2	1:B:813:ASN:HB2	1.94	0.49
1:C:178:GLY:HA3	1:C:280:ILE:HD12	1.93	0.49
1:C:594:VAL:HG23	1:C:609:ILE:HG12	1.94	0.49
1:C:837:ASP:OD2	1:C:840:HIS:ND1	2.31	0.49
1:C:985:VAL:HG13	1:C:986:GLN:H	1.77	0.49
1:A:682:VAL:HG21	1:A:841:ILE:HD12	1.94	0.49
1:B:227:VAL:HG22	1:C:710:VAL:HG13	1.94	0.49
1:A:44:ASP:OD2	1:A:44:ASP:N	2.46	0.49
1:A:970:LEU:HD12	1:A:973:ILE:HD12	1.95	0.49
1:B:87:THR:OG1	1:B:88:PHE:N	2.46	0.49
1:C:894:ALA:HA	1:C:1000:ALA:HB2	1.95	0.49
1:C:510:TYR:HA	1:C:513:VAL:HG22	1.94	0.49
1:B:388:SER:HB3	1:B:464:MET:HB2	1.95	0.48
1:B:400:GLY:HA2	1:B:436:ILE:HD12	1.96	0.48
1:B:176:PHE:CZ	1:B:593:GLN:HB3	2.49	0.48
1:A:748:GLU:OE1	1:A:750:ARG:NH1	2.46	0.48
1:B:650:GLN:HB2	1:B:653:ILE:HG22	1.94	0.48
1:C:950:VAL:HG21	1:C:1013:TYR:HB2	1.96	0.48
1:A:139:ARG:NH1	1:A:320:TYR:OH	2.41	0.48
1:B:242:ILE:HG22	1:B:243:VAL:HG12	1.95	0.48
1:B:517:LEU:HD23	1:B:1010:ALA:HA	1.95	0.48
1:C:279:THR:OG1	1:C:280:ILE:N	2.46	0.48
1:A:97:PHE:CZ	1:A:106:SER:HB2	2.48	0.48
1:A:711:ARG:NH1	1:A:791:ARG:HH21	2.12	0.48
1:B:620:THR:O	1:B:620:THR:OG1	2.32	0.48
1:A:41:ASP:HB3	1:A:459:LYS:HE3	1.95	0.48
1:A:775:THR:OG1	1:A:776:ALA:N	2.46	0.48
1:A:826:ALA:C	1:A:828:MET:H	2.17	0.48
1:B:306:LEU:HD23	1:B:310:ILE:HD12	1.96	0.48
1:B:654:ASP:OD2	1:B:664:HIS:HB3	2.14	0.47
1:C:187:PHE:CZ	1:C:202:ILE:HG21	2.48	0.47
1:A:158:TRP:CD1	1:A:750:ARG:HD2	2.49	0.47
1:A:763:ARG:O	1:A:763:ARG:NE	2.47	0.47
1:B:747:VAL:HG12	1:B:748:GLU:HG2	1.95	0.47
1:B:789:HIS:CE1	1:B:791:ARG:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:GLY:HA3	1:C:227:VAL:HB	1.97	0.47
1:C:916:GLY:HA2	1:C:989:LEU:HG	1.95	0.47
1:A:586:GLU:OE2	1:A:623:SER:OG	2.23	0.47
1:A:672:TYR:OH	1:A:802:GLU:OE1	2.32	0.47
1:B:761:SER:O	1:B:764:ASN:ND2	2.47	0.47
1:B:597:ASN:HD21	1:B:601:THR:HG22	1.80	0.47
1:C:43:ALA:HB2	1:C:656:VAL:HG12	1.95	0.47
1:A:650:GLN:HB2	1:A:653:ILE:HG22	1.96	0.47
1:B:372:MET:HE1	1:B:477:LEU:HD23	1.96	0.47
1:C:387:LEU:HB2	1:C:985:VAL:HG11	1.97	0.47
1:C:440:MET:HG3	1:C:476:LEU:HD13	1.96	0.47
1:B:676:PHE:CD2	1:B:796:GLU:HG3	2.50	0.47
1:C:570:ALA:HB1	1:C:594:VAL:HG21	1.97	0.47
1:B:138:TYR:OH	1:B:319:PRO:HG3	2.15	0.47
1:B:214:GLY:HA3	1:C:55:GLY:O	2.14	0.47
1:A:387:LEU:HD22	1:A:985:VAL:HG21	1.97	0.46
1:C:455:ARG:HH22	1:C:851:ASN:HA	1.78	0.46
1:B:236:LEU:HD12	1:B:236:LEU:H	1.80	0.46
1:B:567:LEU:HD13	1:B:606:PRO:HB3	1.98	0.46
1:B:142:LEU:HD11	1:B:160:VAL:HG21	1.97	0.46
1:B:243:VAL:HG22	1:B:244:VAL:H	1.79	0.46
1:A:144:SER:HB2	1:A:315:VAL:HG22	1.97	0.46
1:C:972:LEU:HB3	1:C:990:ALA:HB1	1.97	0.46
1:A:669:VAL:HG11	1:A:686:ILE:HG21	1.96	0.46
1:C:203:THR:HG21	1:C:735:THR:HG21	1.97	0.46
1:C:934:ASN:CB	1:C:957:ARG:HG3	2.46	0.46
1:A:313:LYS:O	1:A:316:LYS:NZ	2.49	0.46
1:B:635:ALA:O	1:B:639:ARG:HG2	2.16	0.46
1:B:957:ARG:HA	1:B:960:PRO:HD2	1.98	0.46
1:C:61:VAL:HG13	1:C:86:SER:HB3	1.98	0.46
1:A:905:ARG:HB3	1:A:907:MET:HG3	1.98	0.46
1:A:137:ILE:HG13	1:A:138:TYR:H	1.82	0.46
1:B:905:ARG:NH1	1:B:976:ALA:O	2.44	0.46
1:C:546:PHE:HD1	1:C:547:LEU:HG	1.81	0.46
1:A:894:ALA:HA	1:A:1000:ALA:HB2	1.98	0.45
1:A:984:ASP:HA	1:A:987:ARG:HG3	1.97	0.45
1:C:650:GLN:HB2	1:C:653:ILE:HG22	1.98	0.45
1:A:43:ALA:HB2	1:A:656:VAL:HG12	1.98	0.45
1:B:970:LEU:HG	1:B:973:ILE:HD12	1.97	0.45
1:C:270:ILE:HD11	1:C:567:LEU:HB3	1.98	0.45
1:B:43:ALA:HB2	1:B:656:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:948:GLU:HB2	1:B:950:VAL:HG22	1.99	0.45
1:B:676:PHE:CE2	1:B:796:GLU:HG3	2.52	0.45
1:B:745:VAL:HG13	1:B:752:TYR:HB2	1.98	0.45
1:C:669:VAL:HB	1:C:810:VAL:HB	1.98	0.45
1:C:905:ARG:NH1	1:C:976:ALA:O	2.38	0.45
1:B:450:LEU:HD13	1:B:453:PHE:HZ	1.81	0.45
1:C:314:ASP:OD1	1:C:315:VAL:HG23	2.17	0.45
1:A:288:LYS:HD2	1:A:288:LYS:HA	1.53	0.45
1:A:763:ARG:HG2	1:C:218:LEU:HD12	1.98	0.45
1:A:763:ARG:HB2	1:A:769:ILE:HG12	1.99	0.45
1:A:149:LEU:HD11	1:A:178:GLY:HA2	1.99	0.45
1:B:36:LEU:HD11	1:B:386:LEU:HD21	1.98	0.45
1:B:138:TYR:HB3	1:B:284:THR:HB	1.99	0.45
1:C:162:PRO:O	1:C:166:GLN:HG3	2.17	0.45
1:B:4:ARG:O	1:B:7:THR:OG1	2.31	0.45
1:B:562:PRO:HA	1:B:563:PRO:HD3	1.79	0.45
1:C:579:ALA:HA	1:C:582:MET:HE2	1.99	0.45
1:A:69:LEU:HD13	1:A:119:LEU:HD11	1.99	0.44
1:A:393:ASP:HB3	1:A:972:LEU:HG	1.99	0.44
1:B:158:TRP:CD1	1:B:750:ARG:HD3	2.52	0.44
1:C:987:ARG:HB3	1:C:988:PRO:HD3	1.99	0.44
1:B:557:LEU:HD23	1:B:646:VAL:HG11	1.98	0.44
1:C:76:VAL:HG11	1:C:97:PHE:HE2	1.82	0.44
1:C:697:GLN:HG2	1:C:815:ARG:NH1	2.32	0.44
1:B:648:PHE:HB2	1:B:815:ARG:HH22	1.82	0.44
1:C:149:LEU:HD23	1:C:179:LEU:HD23	1.99	0.44
1:B:743:THR:OG1	1:B:744:GLN:N	2.50	0.44
1:B:926:LEU:O	1:B:929:ILE:HG22	2.18	0.44
1:C:959:ARG:HB3	1:C:960:PRO:HD3	2.00	0.44
1:B:679:THR:HB	1:B:808:LEU:HB2	1.98	0.44
1:C:703:GLN:HE22	1:C:809:THR:H	1.63	0.44
1:C:709:GLN:HB2	1:C:794:GLU:N	2.33	0.44
1:C:796:GLU:HB3	1:C:799:ILE:HG12	2.00	0.44
1:A:407:ASN:O	1:A:411:ARG:HB2	2.18	0.44
1:A:1011:LEU:O	1:A:1015:ILE:HG22	2.17	0.44
1:B:69:LEU:HD12	1:B:69:LEU:HA	1.80	0.44
1:C:455:ARG:O	1:C:459:LYS:HG2	2.16	0.44
1:A:441:ILE:HA	1:A:444:ILE:HG22	2.00	0.44
1:C:70:GLU:OE2	1:C:84:SER:OG	2.23	0.44
1:C:978:ALA:HA	1:C:987:ARG:HH11	1.82	0.44
1:A:102:GLU:OE1	1:A:103:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:TRP:HB3	1:A:649:SER:HB2	2.00	0.44
1:B:886:LEU:HD22	1:B:1015:ILE:HG13	2.00	0.44
1:C:564:GLY:HA2	1:C:707:LEU:HD22	2.00	0.44
1:C:690:LEU:HD21	1:C:845:TRP:HH2	1.81	0.44
1:A:769:ILE:HA	1:A:772:LEU:HG	1.98	0.43
1:C:801:ARG:NH2	1:C:804:ASN:O	2.51	0.43
1:A:586:GLU:OE2	1:A:625:ARG:NH1	2.51	0.43
1:A:847:GLY:O	1:A:850:GLU:HG2	2.18	0.43
1:A:932:ILE:HD11	1:A:1008:LEU:HG	2.00	0.43
1:A:514:LEU:HA	1:A:517:LEU:HD12	1.99	0.43
1:A:344:LEU:HD12	1:A:974:PRO:HD3	2.01	0.43
1:A:1001:THR:HA	1:A:1004:THR:HG22	2.00	0.43
1:B:85:LYS:HG2	1:B:800:THR:HG22	2.00	0.43
1:B:714:VAL:HG21	1:B:726:VAL:HG13	1.99	0.43
1:A:4:ARG:O	1:A:7:THR:OG1	2.32	0.43
1:A:51:THR:HB	1:A:91:SER:HB3	2.00	0.43
1:A:87:THR:HB	1:A:798:THR:HG22	2.00	0.43
1:A:517:LEU:HD22	1:A:1010:ALA:HB2	2.01	0.43
1:A:883:GLN:HG3	1:A:932:ILE:HG21	2.01	0.43
1:C:329:ALA:HB1	1:C:981:LEU:HB2	2.00	0.43
1:C:1000:ALA:O	1:C:1004:THR:OG1	2.25	0.43
1:B:139:ARG:HB3	1:B:320:TYR:CZ	2.54	0.43
1:C:407:ASN:HD22	1:C:432:VAL:HB	1.84	0.43
1:C:757:ARG:HG2	1:C:758:PHE:H	1.84	0.43
1:C:874:LEU:HD13	1:C:887:ILE:HB	2.01	0.43
1:B:881:LEU:HA	1:B:881:LEU:HD23	1.87	0.43
1:C:741:PRO:HB3	1:C:755:VAL:HG22	2.00	0.43
1:A:819:LEU:HD21	1:A:849:PHE:HA	2.01	0.43
1:B:561:LEU:HB2	1:B:607:SER:O	2.19	0.43
1:B:48:GLN:NE2	1:B:94:THR:OG1	2.51	0.43
1:B:703:GLN:HE22	1:B:809:THR:H	1.67	0.43
1:A:203:THR:HA	1:A:206:ILE:HG22	2.01	0.43
1:A:690:LEU:HD13	1:A:812:LEU:HD13	2.00	0.43
1:A:972:LEU:HD23	1:A:972:LEU:HA	1.89	0.43
1:B:215:GLY:HA3	1:B:227:VAL:HB	2.00	0.43
1:C:551:ASP:OD1	1:C:551:ASP:N	2.52	0.43
1:A:66:THR:O	1:A:70:GLU:HG3	2.19	0.42
1:B:138:TYR:CE1	1:B:140:TYR:HB3	2.54	0.42
1:C:836:TYR:HA	1:C:837:ASP:HA	1.60	0.42
1:C:911:VAL:O	1:C:915:VAL:HG23	2.19	0.42
1:A:681:GLN:O	1:A:684:THR:OG1	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:ILE:HG23	1:A:763:ARG:HD2	1.99	0.42
1:B:186:GLU:HB2	1:B:259:ARG:HB2	2.00	0.42
1:A:147:ARG:HD2	1:A:315:VAL:HG23	2.01	0.42
1:A:448:LEU:N	1:A:449:PRO:HD2	2.34	0.42
1:C:126:SER:OG	1:C:127:LEU:N	2.52	0.42
1:A:801:ARG:HG2	1:A:806:ARG:HG2	2.00	0.42
1:B:114:ILE:HD12	1:B:125:PRO:HB2	2.00	0.42
1:C:12:ARG:HG2	1:C:15:ILE:HD12	2.00	0.42
1:A:30:ALA:O	1:A:34:LEU:HB2	2.20	0.42
1:A:697:GLN:HG2	1:A:815:ARG:CZ	2.50	0.42
1:C:20:PHE:HD2	1:C:482:LEU:HD13	1.84	0.42
1:C:273:MET:O	1:C:578:ARG:HD3	2.20	0.42
1:B:271:LEU:HG	1:B:272:GLY:N	2.34	0.42
1:B:993:VAL:O	1:B:997:LEU:HB2	2.20	0.42
1:C:26:TYR:HE2	1:C:375:ILE:HG23	1.85	0.42
1:C:134:ILE:HB	1:C:652:MET:HE3	2.01	0.42
1:C:355:SER:HA	1:C:356:PRO:HD3	1.89	0.42
1:B:140:TYR:O	1:B:281:GLN:HB2	2.19	0.42
1:B:966:THR:HG23	1:B:970:LEU:HD13	2.01	0.42
1:C:271:LEU:HG	1:C:272:GLY:N	2.34	0.42
1:C:584:PHE:HA	1:C:585:PRO:HD3	1.83	0.42
1:C:140:TYR:CZ	1:C:282:GLY:HA3	2.54	0.42
1:C:958:MET:HG3	1:C:959:ARG:N	2.35	0.42
1:A:730:MET:SD	1:C:212:ASN:HA	2.59	0.42
1:B:318:VAL:HA	1:B:319:PRO:HD3	1.90	0.42
1:B:334:VAL:HG21	1:B:386:LEU:HB3	2.02	0.42
1:B:544:ARG:HB2	1:B:820:SER:HB2	2.01	0.42
1:B:862:ILE:H	1:B:862:ILE:HG13	1.69	0.42
1:A:79:MET:SD	1:A:82:MET:HB2	2.60	0.42
1:B:362:VAL:HG12	1:B:401:ALA:HB1	2.02	0.42
1:C:514:LEU:HA	1:C:517:LEU:HB3	2.01	0.42
1:A:342:MET:HG2	1:A:366:ILE:HG21	2.01	0.41
1:A:464:MET:HE1	1:A:915:VAL:HG11	2.02	0.41
1:A:692:THR:HG21	1:A:829:ARG:HH22	1.85	0.41
1:A:734:GLN:HB2	1:C:213:ALA:CB	2.49	0.41
1:A:765:ASP:OD1	1:A:765:ASP:N	2.53	0.41
1:A:965:ALA:HB1	1:A:997:LEU:HD21	2.02	0.41
1:B:81:VAL:HA	1:B:803:MET:HE1	2.02	0.41
1:C:111:GLN:HA	1:C:114:ILE:HG12	2.02	0.41
1:A:41:ASP:HA	1:A:134:ILE:HD13	2.02	0.41
1:C:187:PHE:O	1:C:759:ILE:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:PHE:CZ	1:A:593:GLN:HB3	2.56	0.41
1:A:968:ALA:HB3	1:A:997:LEU:HD11	2.02	0.41
1:C:449:PRO:HB2	1:C:862:ILE:HG23	2.02	0.41
1:C:1007:LEU:O	1:C:1011:LEU:HG	2.20	0.41
1:A:176:PHE:HD1	1:A:597:ASN:HB3	1.86	0.41
1:A:387:LEU:HD12	1:A:388:SER:N	2.35	0.41
1:B:357:ARG:O	1:B:361:ILE:HG13	2.19	0.41
1:B:403:VAL:HB	1:B:436:ILE:HD11	2.02	0.41
1:B:957:ARG:HH11	1:B:960:PRO:HG2	1.84	0.41
1:A:20:PHE:CE2	1:A:482:LEU:HB2	2.55	0.41
1:A:42:ILE:HG23	1:A:456:ILE:HG23	2.03	0.41
1:A:50:VAL:N	1:A:126:SER:O	2.41	0.41
1:A:75:GLY:O	1:A:113:ARG:NH2	2.51	0.41
1:A:440:MET:HG2	1:A:472:LEU:HD12	2.02	0.41
1:A:981:LEU:HD23	1:A:981:LEU:HA	1.92	0.41
1:B:144:SER:HB2	1:B:315:VAL:HA	2.02	0.41
1:B:602:ASP:HB3	1:B:604:PHE:CD1	2.45	0.41
1:B:887:ILE:HB	1:B:932:ILE:HD13	2.02	0.41
1:A:220:ARG:HB3	1:A:225:LEU:HD11	2.02	0.41
1:A:658:ASP:HB2	1:A:664:HIS:CD2	2.55	0.41
1:B:360:ILE:O	1:B:364:VAL:HG13	2.19	0.41
1:B:503:LEU:H	1:B:503:LEU:HD23	1.85	0.41
1:C:103:ASP:OD1	1:C:103:ASP:N	2.53	0.41
1:A:271:LEU:HG	1:A:272:GLY:N	2.36	0.41
1:A:669:VAL:HG21	1:A:690:LEU:HD11	2.03	0.41
1:B:552:GLU:OE1	1:B:652:MET:HB2	2.21	0.41
1:B:704:GLU:CD	1:B:704:GLU:H	2.20	0.41
1:C:741:PRO:HA	1:C:755:VAL:HA	2.03	0.41
1:B:130:LEU:HG	1:B:288:LYS:HB2	2.02	0.41
1:B:546:PHE:O	1:B:911:VAL:HG22	2.21	0.41
1:B:863:LEU:HD12	1:B:863:LEU:HA	1.91	0.41
1:C:993:VAL:O	1:C:997:LEU:HB2	2.21	0.41
1:A:273:MET:HG3	1:A:591:VAL:HG22	2.02	0.41
1:A:407:ASN:OD1	1:A:428:SER:OG	2.39	0.41
1:A:659:LYS:HD3	1:A:659:LYS:HA	1.88	0.41
1:B:444:ILE:HD13	1:B:444:ILE:HA	1.96	0.41
1:B:671:VAL:HG11	1:B:682:VAL:HB	2.03	0.41
1:C:46:THR:HB	1:C:96:VAL:HG23	2.02	0.41
1:C:62:GLU:HA	1:C:66:THR:HB	2.03	0.41
1:C:436:ILE:O	1:C:440:MET:HG2	2.21	0.41
1:C:704:GLU:CD	1:C:704:GLU:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LEU:HB3	1:A:317:VAL:HG22	2.03	0.41
1:A:397:ILE:H	1:A:397:ILE:HG13	1.63	0.41
1:A:700:ILE:HD13	1:A:811:ARG:NH2	2.36	0.41
1:A:935:LEU:HD11	1:A:950:VAL:HA	2.02	0.41
1:C:107:ARG:NE	1:C:127:LEU:HD23	2.36	0.41
1:A:80:HIS:CD2	1:A:81:VAL:HG23	2.56	0.40
1:A:85:LYS:HD3	1:A:603:PRO:HG3	2.04	0.40
1:B:189:PRO:HA	1:B:192:LEU:HD23	2.03	0.40
1:B:591:VAL:HB	1:B:612:ALA:HB3	2.03	0.40
1:B:704:GLU:HG2	1:B:797:THR:OG1	2.22	0.40
1:C:307:ASN:HA	1:C:311:LEU:HB2	2.03	0.40
1:B:243:VAL:HG13	1:B:244:VAL:N	2.36	0.40
1:B:883:GLN:HE21	1:B:932:ILE:HB	1.86	0.40
1:C:83:ARG:NH2	1:C:660:LEU:O	2.55	0.40
1:C:327:VAL:O	1:C:331:VAL:HG13	2.21	0.40
1:C:407:ASN:ND2	1:C:432:VAL:HB	2.36	0.40
1:C:661:ALA:HB2	1:C:847:GLY:HA2	2.04	0.40
1:A:255:LYS:HA	1:A:255:LYS:HD2	1.88	0.40
1:A:584:PHE:O	1:A:587:VAL:HG22	2.22	0.40
1:B:110:LEU:HB3	1:B:127:LEU:HD21	2.02	0.40
1:C:439:GLY:O	1:C:443:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	967/1045 (92%)	909 (94%)	57 (6%)	1 (0%)	51	83
1	B	945/1045 (90%)	882 (93%)	61 (6%)	2 (0%)	47	78
1	C	920/1045 (88%)	855 (93%)	64 (7%)	1 (0%)	51	83
All	All	2832/3135 (90%)	2646 (93%)	182 (6%)	4 (0%)	51	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	243	VAL
1	B	542	ILE
1	A	841	ILE
1	C	171	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	805/864 (93%)	785 (98%)	20 (2%)	47	70
1	B	785/864 (91%)	765 (98%)	20 (2%)	47	70
1	C	778/864 (90%)	754 (97%)	24 (3%)	40	65
All	All	2368/2592 (91%)	2304 (97%)	64 (3%)	44	68

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	VAL
1	A	64	GLN
1	A	76	VAL
1	A	136	GLU
1	A	188	ASP
1	A	254	VAL
1	A	318	VAL
1	A	393	ASP
1	A	453	PHE
1	A	561	LEU
1	A	625	ARG
1	A	671	VAL
1	A	742	VAL
1	A	755	VAL
1	A	763	ARG
1	A	784	LEU
1	A	841	ILE

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Mol	Chain	Res	Type
1	A	842	GLN
1	A	947	LYS
1	A	1007	LEU
1	B	46	THR
1	B	49	VAL
1	B	192	LEU
1	B	273	MET
1	B	274	ASP
1	B	393	ASP
1	B	503	LEU
1	B	517	LEU
1	B	549	TYR
1	B	551	ASP
1	B	620	THR
1	B	628	GLN
1	B	676	PHE
1	B	700	ILE
1	B	707	LEU
1	B	710	VAL
1	B	837	ASP
1	B	887	ILE
1	B	957	ARG
1	B	977	LEU
1	C	9	CYS
1	C	39	TYR
1	C	81	VAL
1	C	102	GLU
1	C	103	ASP
1	C	170	VAL
1	C	226	VAL
1	C	230	VAL
1	C	274	ASP
1	C	314	ASP
1	C	317	VAL
1	C	368	LEU
1	C	387	LEU
1	C	393	ASP
1	C	503	LEU
1	C	509	ARG
1	C	517	LEU
1	C	621	TRP
1	C	676	PHE

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Mol	Chain	Res	Type
1	C	745	VAL
1	C	814	LEU
1	C	818	ASP
1	C	958	MET
1	C	985	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	63	GLN
1	A	64	GLN
1	A	124	GLN
1	A	182	GLN
1	A	196	ASN
1	A	209	ASN
1	A	281	GLN
1	A	597	ASN
1	A	650	GLN
1	A	753	ASN
1	A	789	HIS
1	A	813	ASN
1	A	842	GLN
1	A	848	GLN
1	B	48	GLN
1	B	52	GLN
1	B	63	GLN
1	B	64	GLN
1	B	166	GLN
1	B	223	GLN
1	B	558	GLN
1	B	597	ASN
1	B	616	HIS
1	B	674	ASN
1	B	703	GLN
1	B	764	ASN
1	B	786	GLN
1	B	789	HIS
1	B	842	GLN
1	B	848	GLN
1	B	851	ASN
1	B	852	GLN

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Mol	Chain	Res	Type
1	B	903	HIS
1	B	986	GLN
1	C	48	GLN
1	C	54	ASN
1	C	108	GLN
1	C	182	GLN
1	C	223	GLN
1	C	268	HIS
1	C	309	ASN
1	C	407	ASN
1	C	650	GLN
1	C	753	ASN
1	C	842	GLN
1	C	848	GLN
1	C	852	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	977/1045 (93%)	-0.55	10 (1%)	82	78	59, 104, 178, 228	0
1	B	957/1045 (91%)	-0.51	7 (0%)	87	85	61, 109, 168, 213	0
1	C	942/1045 (90%)	-0.31	16 (1%)	70	64	78, 140, 198, 251	0
All	All	2876/3135 (91%)	-0.46	33 (1%)	80	76	59, 118, 187, 251	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	ASN	4.5
1	A	427	GLN	3.9
1	A	502	ALA	3.6
1	C	764	ASN	3.5
1	C	509	ARG	3.4
1	C	739	GLY	3.3
1	C	882	ARG	3.2
1	C	522	ARG	3.0
1	A	423	ARG	3.0
1	B	518	VAL	2.9
1	A	979	HIS	2.9
1	C	518	VAL	2.9
1	C	622	THR	2.8
1	A	504	VAL	2.7
1	C	505	TRP	2.7
1	C	948	GLU	2.7
1	C	791	ARG	2.5
1	A	522	ARG	2.3
1	C	629	GLN	2.3
1	A	523	THR	2.2
1	C	626	ASP	2.2
1	B	515	ASN	2.2
1	C	625	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	777	ALA	2.2
1	C	979	HIS	2.2
1	C	519	GLY	2.2
1	B	146	THR	2.1
1	B	195	TYR	2.1
1	B	212	ASN	2.1
1	B	504	VAL	2.1
1	B	11	ASN	2.0
1	A	426	MET	2.0
1	C	937	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	C	1101	1/1	0.82	0.17	151,151,151,151	0
2	ZN	A	1102	1/1	0.90	0.07	138,138,138,138	0
2	ZN	B	1101	1/1	0.97	0.09	99,99,99,99	0
2	ZN	A	1101	1/1	0.97	0.20	107,107,107,107	0

6.5 Other polymers (i)

There are no such residues in this entry.