



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:19 PM UTC

PDB ID : 4K0E / pdb_00004k0e
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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

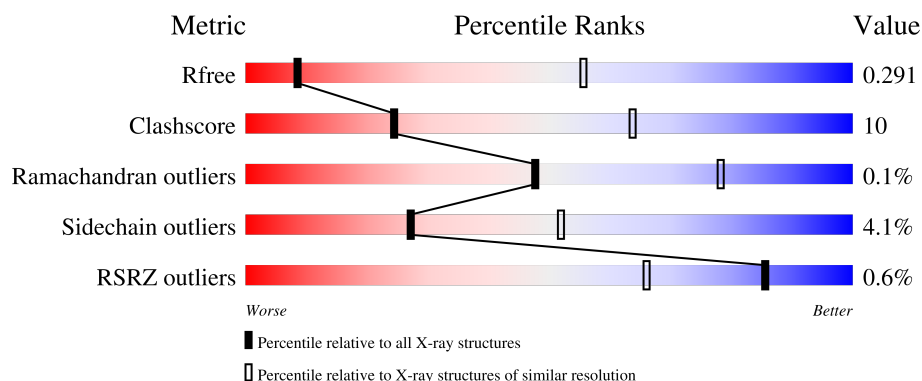
1 Overall quality at a glance

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}	180053	1182 (3.84-3.60)
Clashscore	190562	1222 (3.84-3.60)
Ramachandran outliers	187476	1178 (3.84-3.60)
Sidechain outliers	187428	1174 (3.84-3.60)
RSRZ outliers	180081	1181 (3.84-3.60)

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 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 $\leq 5\%$. 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	
1	B	1045	
1	C	1045	

2 Entry composition

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

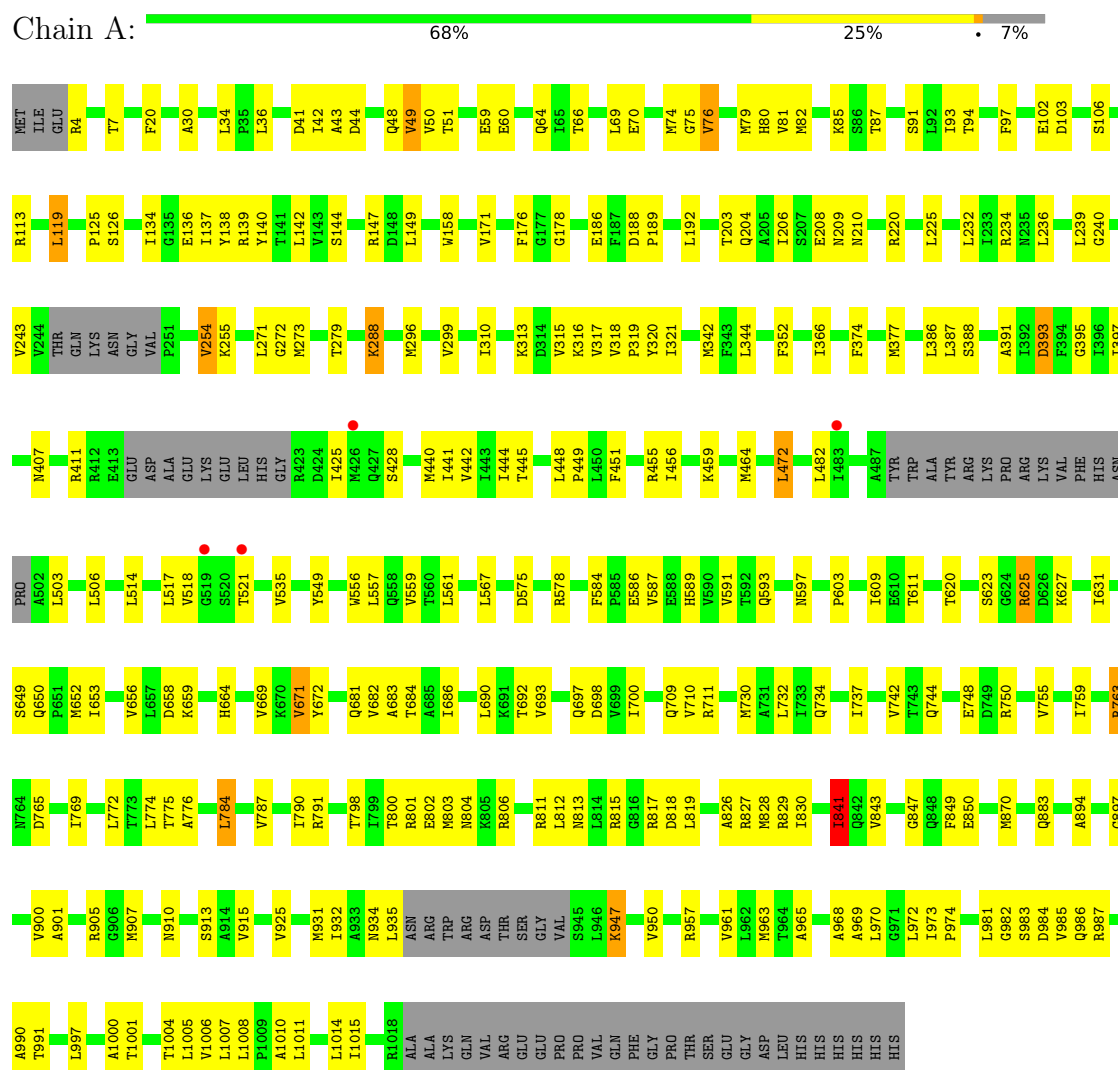
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

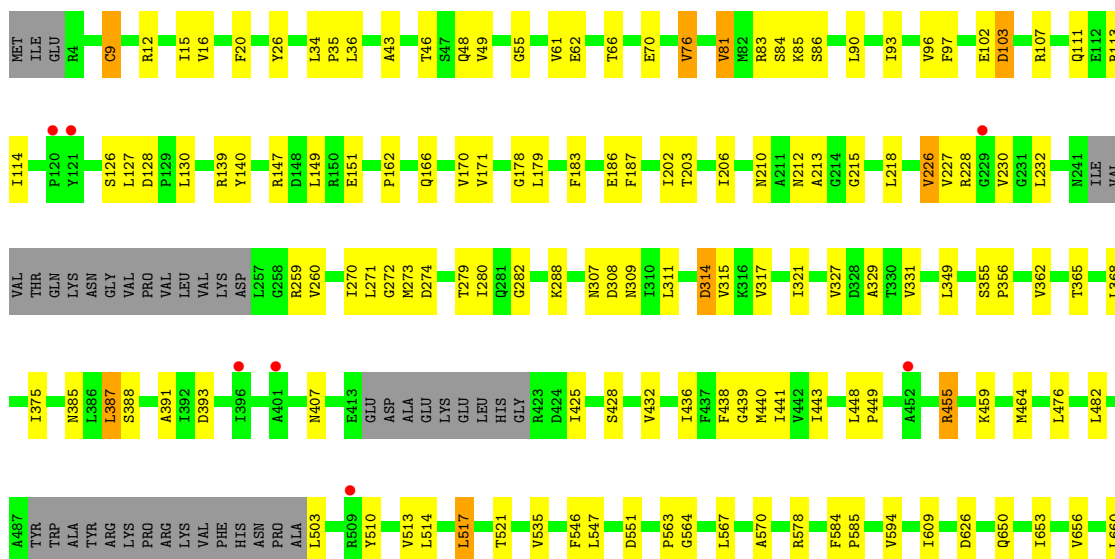
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0

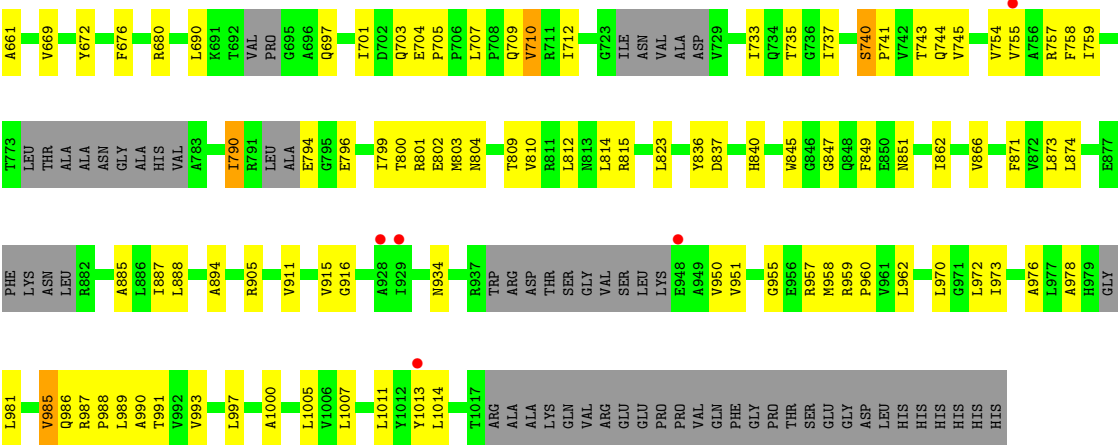
3 Residue-property plots

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)







4 Data and refinement statistics

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 19.94 – 3.71	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.94-3.71) 84.9 (19.94-3.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.71Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.229 , 0.283 0.240 , 0.291	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)	0.25 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.34	0/7618	0.80	5/10362 (0.0%)
1	B	0.33	0/7457	0.79	8/10146 (0.1%)
1	C	0.31	0/7358	0.78	5/9996 (0.1%)
All	All	0.33	0/22433	0.79	18/30504 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	448	LEU	CA-C-N	-7.16	114.42	121.65
1	C	448	LEU	C-N-CA	-7.16	114.42	121.65
1	A	119	LEU	CA-C-N	5.88	127.19	119.84
1	A	119	LEU	C-N-CA	5.88	127.19	119.84
1	B	90	LEU	N-CA-C	5.70	117.13	108.07
1	A	455	ARG	CB-CA-C	-5.68	110.04	116.63
1	C	740	SER	CA-C-N	5.52	125.79	119.83
1	C	740	SER	C-N-CA	5.52	125.79	119.83
1	A	982	GLY	N-CA-C	-5.32	107.90	115.30
1	B	455	ARG	CB-CA-C	-5.31	110.47	116.63
1	B	562	PRO	CA-C-N	5.28	125.53	119.83
1	B	562	PRO	C-N-CA	5.28	125.53	119.83
1	B	834	VAL	N-CA-C	5.22	113.04	107.76
1	B	74	MET	N-CA-C	5.20	117.35	111.11
1	C	90	LEU	N-CA-C	5.08	116.16	108.07
1	B	276	ASN	CA-C-N	5.06	124.67	119.05
1	B	276	ASN	C-N-CA	5.06	124.67	119.05
1	A	310	ILE	N-CA-C	5.03	115.26	110.53

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	167	0
1	B	7329	0	7597	155	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
All	All	22061	0	22879	446	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 10.

All (446) 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	1.63	0.80
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:81:VAL:HG23	1:C:803:MET:HE2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:586:GLU:OE2	1:A:623:SER:OG	2.23	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:A:931:MET:HE2	1:A:961:VAL:HG21	1.89	0.54
1:A:138:TYR:HD2	1:A:296:MET:HE1	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:442:VAL:HG13	1:A:870:MET:HE3	1.91	0.52
1:A:826:ALA:C	1:A:828:MET:H	2.17	0.52
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:704:GLU:CD	1:B:704:GLU:H	2.20	0.50
1:C:743:THR:OG1	1:C:744:GLN:N	2.45	0.50
1:A:440:MET:HE2	1:A:472:LEU:HB3	1.93	0.49
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:A:352:PHE:HB3	1:A:963:MET:HE2	1.93	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:A:134:ILE:HB	1:A:652:MET:HE3	1.95	0.48
1:A:870:MET:HE1	1:A:925:VAL:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:306:LEU:HD23	1:B:310:ILE:HD12	1.96	0.48
1:B:978:ALA:O	1:B:983:SER:OG	2.30	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:C:958:MET:HE3	1:C:962:LEU:HD12	1.95	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
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: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: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:C:391:ALA:HB3	1:C:464:MET:HE2	1.96	0.47
1:C:704:GLU:CD	1:C:704:GLU:H	2.23	0.47
1:A:81:VAL:HA	1:A:803:MET:HE2	1.98	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:372:MET:HE1	1:B:477:LEU:HD23	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:A:374:PHE:HD2	1:A:377:MET:HE2	1.80	0.46
1:A:464:MET:HE2	1:A:464:MET:HB3	1.82	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
1:A:82:MET:H	1:A:803:MET:HE2	1.81	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:464:MET:HE1	1:A:915:VAL:HG11	1.99	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:C:48:GLN:HG2	1:C:128:ASP:CG	2.43	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
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:B:878:PHE:C	1:B:880:ASN:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LEU:HD22	1:B:22:MET:HE2	2.01	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:A:34:LEU:HD11	1:A:377:MET:HE3	2.01	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:81:VAL:HA	1:B:803:MET:HE1	2.01	0.43
1:B:506:LEU:HB3	1:B:958:MET:HE1	2.01	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:76:VAL:HG12	1:A:79:MET:HE2	2.01	0.42
1:A:681:GLN:O	1:A:684:THR:OG1	2.27	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:905:ARG:HD3	1:B:907:MET:HE3	2.00	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: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:B:442:VAL:HB	1:B:870:MET:HE1	2.01	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:273:MET:HE2	1:A:589:HIS:CD2	2.56	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:405:MET:HE1	1:B:486:LEU:HD22	2.03	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: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:B:957:ARG:C	1:B:960:PRO:HD2	2.46	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: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:74:MET:HE3	1:A:804:ASN:HB2	2.03	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:82:MET:HE3	1:B:82:MET:HB2	1.99	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%)	48	78
1	B	945/1045 (90%)	882 (93%)	61 (6%)	2 (0%)	43	71
1	C	920/1045 (88%)	855 (93%)	64 (7%)	1 (0%)	48	78
All	All	2832/3135 (90%)	2646 (93%)	182 (6%)	4 (0%)	48	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	243	VAL
1	B	542	ILE

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Mol	Chain	Res	Type
1	A	841	ILE
1	C	171	VAL

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	805/864 (93%)	776 (96%)	29 (4%)	31	54
1	B	785/864 (91%)	748 (95%)	37 (5%)	23	48
1	C	778/864 (90%)	748 (96%)	30 (4%)	28	52
All	All	2368/2592 (91%)	2272 (96%)	96 (4%)	27	52

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	VAL
1	A	59	GLU
1	A	64	GLN
1	A	76	VAL
1	A	136	GLU
1	A	171	VAL
1	A	188	ASP
1	A	236	LEU
1	A	254	VAL
1	A	288	LYS
1	A	318	VAL
1	A	393	ASP
1	A	425	ILE
1	A	472	LEU
1	A	535	VAL
1	A	561	LEU
1	A	567	LEU
1	A	620	THR
1	A	625	ARG
1	A	671	VAL

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Mol	Chain	Res	Type
1	A	710	VAL
1	A	742	VAL
1	A	755	VAL
1	A	763	ARG
1	A	784	LEU
1	A	787	VAL
1	A	841	ILE
1	A	947	LYS
1	A	1007	LEU
1	B	46	THR
1	B	49	VAL
1	B	53	VAL
1	B	110	LEU
1	B	134	ILE
1	B	170	VAL
1	B	192	LEU
1	B	260	VAL
1	B	273	MET
1	B	274	ASP
1	B	393	ASP
1	B	456	ILE
1	B	472	LEU
1	B	503	LEU
1	B	517	LEU
1	B	535	VAL
1	B	549	TYR
1	B	551	ASP
1	B	620	THR
1	B	627	LYS
1	B	628	GLN
1	B	676	PHE
1	B	700	ILE
1	B	701	ILE
1	B	704	GLU
1	B	710	VAL
1	B	724	ILE
1	B	745	VAL
1	B	784	LEU
1	B	790	ILE
1	B	808	LEU
1	B	837	ASP
1	B	887	ILE

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Mol	Chain	Res	Type
1	B	918	ILE
1	B	952	ARG
1	B	957	ARG
1	B	977	LEU
1	C	9	CYS
1	C	36	LEU
1	C	49	VAL
1	C	76	VAL
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	260	VAL
1	C	274	ASP
1	C	314	ASP
1	C	317	VAL
1	C	365	THR
1	C	368	LEU
1	C	387	LEU
1	C	393	ASP
1	C	425	ILE
1	C	455	ARG
1	C	517	LEU
1	C	535	VAL
1	C	676	PHE
1	C	701	ILE
1	C	710	VAL
1	C	745	VAL
1	C	790	ILE
1	C	814	LEU
1	C	888	LEU
1	C	985	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	64	GLN
1	A	80	HIS
1	A	111	GLN

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Mol	Chain	Res	Type
1	A	124	GLN
1	A	182	GLN
1	A	209	ASN
1	A	276	ASN
1	A	291	ASN
1	A	378	HIS
1	A	650	GLN
1	A	753	ASN
1	A	789	HIS
1	A	804	ASN
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	80	HIS
1	B	124	GLN
1	B	166	GLN
1	B	223	GLN
1	B	325	ASN
1	B	378	HIS
1	B	558	GLN
1	B	597	ASN
1	B	616	HIS
1	B	674	ASN
1	B	703	GLN
1	B	734	GLN
1	B	786	GLN
1	B	789	HIS
1	B	842	GLN
1	B	848	GLN
1	B	851	ASN
1	B	852	GLN
1	B	903	HIS
1	B	986	GLN
1	C	48	GLN
1	C	182	GLN
1	C	268	HIS
1	C	281	GLN
1	C	309	ASN

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Mol	Chain	Res	Type
1	C	325	ASN
1	C	407	ASN
1	C	628	GLN
1	C	650	GLN
1	C	703	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 oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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%)	-0.21	4 (0%)	88 72	59, 104, 178, 228	0
1	B	957/1045 (91%)	-0.19	2 (0%)	91 80	61, 109, 168, 213	0
1	C	942/1045 (90%)	0.02	12 (1%)	75 50	78, 140, 198, 251	0
All	All	2876/3135 (91%)	-0.13	18 (0%)	85 66	59, 118, 187, 251	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	928	ALA	4.3
1	C	120	PRO	3.3
1	A	519	GLY	3.1
1	C	401	ALA	2.7
1	C	1013	TYR	2.7
1	C	509	ARG	2.7
1	C	452	ALA	2.7
1	B	244	VAL	2.5
1	B	15	ILE	2.5
1	C	948	GLU	2.4
1	C	929	ILE	2.2
1	C	755	VAL	2.2
1	A	483	ILE	2.2
1	C	396	ILE	2.1
1	A	426	MET	2.0
1	C	229	GLY	2.0
1	C	121	TYR	2.0
1	A	521	THR	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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
2	ZN	A	1102	1/1	0.96	0.06	138,138,138,138	0
2	ZN	C	1101	1/1	0.97	0.10	151,151,151,151	0
2	ZN	B	1101	1/1	0.98	0.04	99,99,99,99	0
2	ZN	A	1101	1/1	0.98	0.07	107,107,107,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.