



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 10:27 AM EDT

PDB ID : 4ZLJ / pdb_00004zlj
Title : Crystal structure of transporter AcrB
Authors : Ababou, A.; Koronakis, V.
Deposited on : 2015-05-01
Resolution : 3.26 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

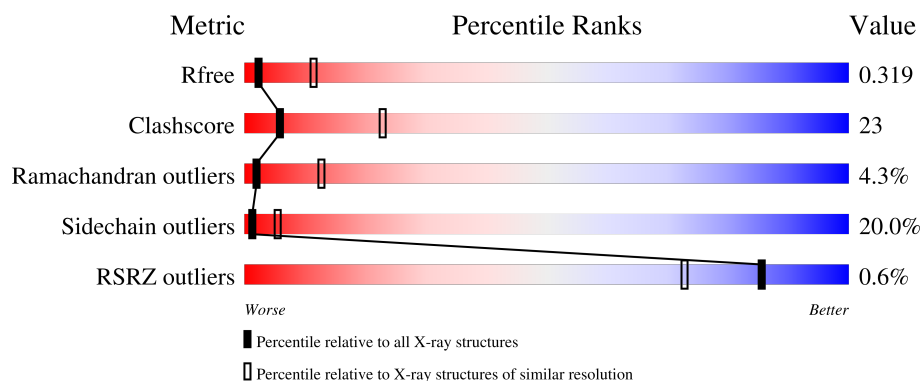
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	1049	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7855 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.

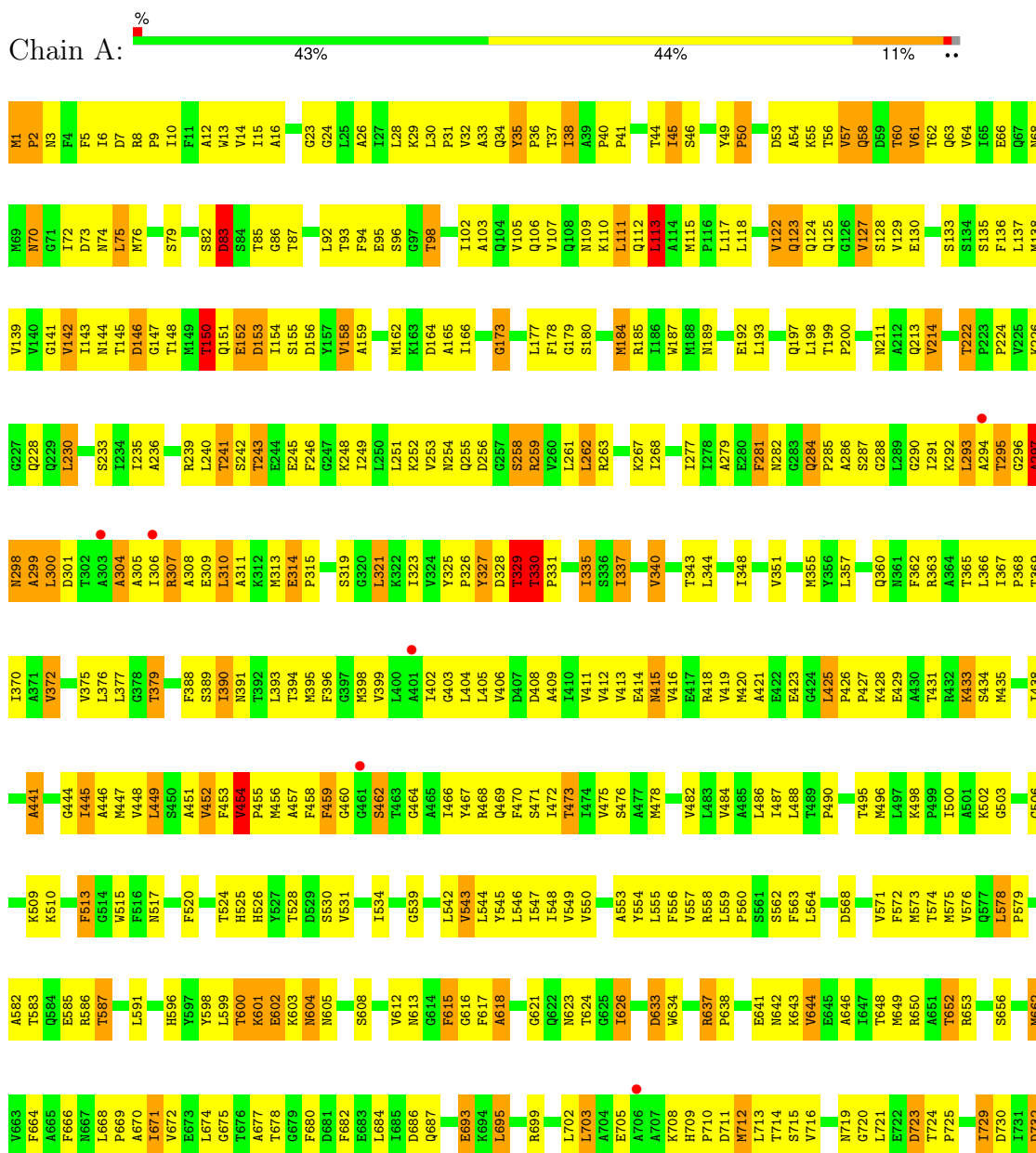
- Molecule 1 is a protein called Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1034	7855	5055	1296	1460	44	0	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: Multidrug efflux pump subunit AcrB



ASP	A981	M902	M825	K735
HIS	F982	L903	E826	
HIS	L983	V904	Q830	V741
	L984		A831	S742
	G985	L907	A832	D745
	V986		P833	I746
	N987	L913	G834	
	P988		K835	
	L989	R919	A840	T749
	V990	G920	M841	L750
	I991	T921	E842	S757
		N923	L843	Y758
	S997	D924	M844	V759
	G998	Y925	E845	N760
	A999	Y926	Q846	
	Q1000	F927	L847	D764
	N1001	Q928		
	A1002		L851	K769
	V1003	L931		K770
	G1004	L932	Y857	V771
	T1005	T933	D858	Y772
	G1006	T934	W859	V773
	V1007	I935		
	M1008	G936	M862	E776
		L937	Q865	A777
	M1011	S938	E866	K778
	V1012	A939	R867	
	T1013	K940	L868	M781
	A1014	N941	S869	
	T1015	A942		D785
	V1016	I943	P874	
	L1017	L944	S875	D788
	A1018	T945	W876	Y789
	I1019	V946	L877	Y790
	F1020		Y877	V791
	F1021	K950	A878	
	V1022		I879	P800
	P1023	M953	S880	F801
	V1024		L881	
	F1025	E956	I882	F804
	F1026	G957	V883	S805
	V1027	K958	W884	S806
	V1028	G959	F885	S807
	V1029	L960	L886	R808
	R1030		C887	
	R1031	L965	L888	
				Y811
	S1034	V968	G812	
ARG	LYS	R969	S813	
	ASN	M970	P814	
	GLU	R971	R815	
	ASP	L972	L816	
	ILE	R973	E817	
	GLU	P974	R818	
	HIS	I975		
	SER	L976	G821	
	HIS	S979	L822	
	THR		P823	
	VAL	L980	S824	

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	144.99Å 144.99Å 521.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 3.26 19.97 – 3.26	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.97-3.26) 97.0 (19.97-3.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.248 , 0.318 0.254 , 0.319	Depositor DCC
R_{free} test set	1670 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	93.2	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7855	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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

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	0.73	2/8005 (0.0%)	1.13	44/10871 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	ILE	CA-CB	-6.26	1.47	1.54
1	A	454	VAL	CA-CB	5.62	1.56	1.54

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	832	ALA	CA-C-N	8.06	129.92	119.84
1	A	832	ALA	C-N-CA	8.06	129.92	119.84
1	A	680	PHE	N-CA-C	7.54	117.95	108.45
1	A	40	PRO	CA-C-N	7.22	127.21	119.78
1	A	40	PRO	C-N-CA	7.22	127.21	119.78
1	A	83	ASP	N-CA-C	7.16	121.16	109.85
1	A	297	ALA	N-CA-C	-7.12	99.91	110.23
1	A	460	GLY	N-CA-C	7.11	124.29	112.85
1	A	462	SER	N-CA-C	-7.09	104.50	113.72
1	A	282	ASN	N-CA-C	-7.06	101.75	111.28
1	A	314	GLU	CA-C-N	7.03	126.55	119.24
1	A	314	GLU	C-N-CA	7.03	126.55	119.24
1	A	777	ALA	N-CA-C	7.00	118.56	111.07
1	A	284	GLN	CA-C-N	-6.93	112.79	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	GLN	C-N-CA	-6.93	112.79	120.14
1	A	867	ARG	N-CA-C	6.76	125.21	110.80
1	A	573	MET	N-CA-C	6.51	118.66	108.96
1	A	297	ALA	CA-C-N	6.45	133.31	121.70
1	A	297	ALA	C-N-CA	6.45	133.31	121.70
1	A	576	VAL	CB-CA-C	-6.31	100.78	110.50
1	A	173	GLY	N-CA-C	6.28	123.10	115.31
1	A	103	ALA	N-CA-C	-6.15	104.58	111.28
1	A	102	ILE	CB-CA-C	-6.01	104.27	111.97
1	A	960	LEU	N-CA-C	5.88	118.17	111.11
1	A	113	LEU	N-CA-C	-5.75	98.56	110.80
1	A	255	GLN	N-CA-C	-5.70	105.05	112.23
1	A	49	TYR	CA-C-N	5.69	127.23	120.23
1	A	49	TYR	C-N-CA	5.69	127.23	120.23
1	A	426	PRO	CA-C-N	5.69	126.95	119.84
1	A	426	PRO	C-N-CA	5.69	126.95	119.84
1	A	300	LEU	N-CA-C	-5.62	106.27	113.01
1	A	304	ALA	N-CA-C	-5.55	105.38	111.82
1	A	714	THR	N-CA-C	5.54	117.60	109.24
1	A	96	SER	N-CA-C	-5.53	103.23	110.53
1	A	578	LEU	CA-C-N	5.37	126.56	119.84
1	A	578	LEU	C-N-CA	5.37	126.56	119.84
1	A	291	ILE	N-CA-C	5.36	115.49	107.51
1	A	367	ILE	CA-C-N	-5.21	114.41	120.04
1	A	367	ILE	C-N-CA	-5.21	114.41	120.04
1	A	40	PRO	N-CA-C	-5.20	104.36	110.70
1	A	749	THR	N-CA-C	-5.15	105.74	112.23
1	A	781	MET	N-CA-C	-5.15	108.02	114.56
1	A	50	PRO	N-CA-C	5.10	118.51	110.50
1	A	281	PHE	CB-CA-C	-5.07	102.72	111.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	ALA	Peptide
1	A	459	PHE	Peptide

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	7855	0	8006	364	0
All	All	7855	0	8006	364	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 23.

All (364) 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:242:SER:HB3	1:A:245:GLU:HG3	1.55	0.86
1:A:254:ASN:HB2	1:A:258:SER:HB2	1.57	0.84
1:A:653:ARG:O	1:A:656:SER:OG	1.95	0.82
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.60	0.81
1:A:418:ARG:HD3	1:A:970:MET:HG3	1.61	0.81
1:A:146:ASP:HB3	1:A:148:THR:HG23	1.64	0.80
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.63	0.80
1:A:469:GLN:O	1:A:473:THR:OG1	2.00	0.78
1:A:445:ILE:HG21	1:A:940:LYS:HZ3	1.48	0.78
1:A:75:LEU:HD12	1:A:92:LEU:HD23	1.67	0.77
1:A:403:GLY:HA3	1:A:982:PHE:HE1	1.50	0.77
1:A:419:VAL:HG21	1:A:434:SER:HB2	1.67	0.76
1:A:713:LEU:HD13	1:A:843:LEU:HD23	1.67	0.76
1:A:423:GLU:HB3	1:A:425:LEU:HD13	1.66	0.76
1:A:545:TYR:HB2	1:A:1021:PHE:HE1	1.52	0.75
1:A:554:TYR:OH	1:A:558:ARG:NH1	2.20	0.74
1:A:678:THR:O	1:A:830:GLN:NE2	2.21	0.73
1:A:41:PRO:HG2	1:A:98:THR:HG22	1.70	0.73
1:A:398:MET:HE3	1:A:473:THR:HG22	1.69	0.73
1:A:907:LEU:HD22	1:A:1017:LEU:HB3	1.71	0.73
1:A:945:ILE:HD13	1:A:968:VAL:HG22	1.70	0.73
1:A:403:GLY:HA3	1:A:982:PHE:CE1	2.25	0.71
1:A:35:TYR:HD2	1:A:671:ILE:HD12	1.56	0.71
1:A:712:MET:SD	1:A:835:LYS:NZ	2.57	0.70
1:A:420:MET:HB3	1:A:500:ILE:HB	1.73	0.70
1:A:571:VAL:HG23	1:A:668:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:ARG:HB3	1:A:642:ASN:HB3	1.75	0.69
1:A:421:ALA:O	1:A:503:GLY:N	2.21	0.68
1:A:466:ILE:HD12	1:A:466:ILE:H	1.58	0.68
1:A:187:TRP:HB2	1:A:267:LYS:HB2	1.75	0.67
1:A:307:ARG:HH21	1:A:311:ALA:HA	1.60	0.66
1:A:189:ASN:HD22	1:A:192:GLU:H	1.41	0.66
1:A:26:ALA:O	1:A:30:LEU:HB2	1.95	0.66
1:A:953:MET:HE1	1:A:1030:ARG:HH11	1.61	0.66
1:A:568:ASP:OD2	1:A:637:ARG:NH2	2.29	0.66
1:A:451:ALA:HB1	1:A:883:VAL:HG12	1.78	0.65
1:A:983:ILE:HG23	1:A:1008:MET:HG3	1.77	0.65
1:A:612:VAL:HG23	1:A:626:ILE:HG23	1.79	0.65
1:A:404:LEU:HD23	1:A:940:LYS:HD2	1.79	0.65
1:A:604:ASN:OD1	1:A:604:ASN:N	2.23	0.65
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.80	0.64
1:A:524:THR:HG22	1:A:972:LEU:HD12	1.80	0.64
1:A:539:GLY:HA2	1:A:542:LEU:HD22	1.78	0.63
1:A:877:TYR:O	1:A:880:SER:N	2.31	0.63
1:A:57:VAL:HG21	1:A:86:GLY:HA2	1.79	0.63
1:A:431:THR:HA	1:A:434:SER:HB3	1.80	0.63
1:A:1022:VAL:HA	1:A:1025:PHE:HB2	1.79	0.63
1:A:112:GLN:HA	1:A:115:MET:HB2	1.79	0.63
1:A:764:ASP:HB3	1:A:769:LYS:HD2	1.79	0.63
1:A:894:SER:HB3	1:A:897:ILE:HB	1.80	0.63
1:A:960:LEU:HD11	1:A:1031:ARG:HG3	1.81	0.63
1:A:429:GLU:O	1:A:433:LYS:HG2	1.99	0.62
1:A:363:ARG:NE	1:A:496:MET:O	2.28	0.62
1:A:94:PHE:HB3	1:A:98:THR:HG21	1.81	0.62
1:A:329:THR:O	1:A:329:THR:OG1	2.12	0.62
1:A:372:VAL:HG22	1:A:405:LEU:HD13	1.81	0.62
1:A:960:LEU:HD13	1:A:1030:ARG:HB3	1.82	0.62
1:A:1:MET:H2	1:A:2:PRO:HD3	1.64	0.62
1:A:228:GLN:NE2	1:A:230:LEU:HD23	2.14	0.62
1:A:563:PHE:HB2	1:A:867:ARG:NH2	2.15	0.62
1:A:668:LEU:O	1:A:670:ALA:N	2.32	0.62
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.81	0.61
1:A:402:ILE:O	1:A:406:VAL:HG13	2.00	0.61
1:A:662:MET:HG3	1:A:664:PHE:CE1	2.35	0.61
1:A:641:GLU:O	1:A:650:ARG:NH2	2.34	0.60
1:A:111:LEU:HD22	1:A:115:MET:HG2	1.83	0.60
1:A:638:PRO:O	1:A:642:ASN:ND2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:GLU:OE2	1:A:859:TRP:NE1	2.32	0.60
1:A:58:GLN:O	1:A:63:GLN:HG3	2.03	0.59
1:A:281:PHE:HE1	1:A:608:SER:HB2	1.67	0.59
1:A:293:LEU:HG	1:A:297:ALA:HB3	1.85	0.59
1:A:545:TYR:HB2	1:A:1021:PHE:CE1	2.35	0.59
1:A:677:ALA:HB2	1:A:867:ARG:NH1	2.18	0.59
1:A:246:PHE:O	1:A:249:ILE:HG13	2.03	0.58
1:A:709:HIS:O	1:A:711:ASP:N	2.35	0.58
1:A:395:MET:O	1:A:399:VAL:HG23	2.03	0.58
1:A:695:LEU:HB3	1:A:825:MET:HE3	1.84	0.58
1:A:154:ILE:HG22	1:A:287:SER:HB3	1.86	0.58
1:A:758:TYR:CE1	1:A:770:LYS:HD3	2.38	0.58
1:A:150:THR:OG1	1:A:151:GLN:N	2.33	0.58
1:A:473:THR:O	1:A:476:SER:OG	2.22	0.58
1:A:139:VAL:HG22	1:A:290:GLY:HA2	1.86	0.58
1:A:719:ASN:ND2	1:A:826:GLU:OE1	2.37	0.57
1:A:83:ASP:OD2	1:A:83:ASP:N	2.37	0.57
1:A:297:ALA:HA	1:A:298:ASN:HB2	1.85	0.57
1:A:841:MET:O	1:A:845:GLU:HG3	2.03	0.57
1:A:328:ASP:C	1:A:330:THR:H	2.12	0.57
1:A:467:TYR:HE2	1:A:868:LEU:HD21	1.70	0.56
1:A:305:ALA:O	1:A:308:ALA:HB3	2.06	0.56
1:A:602:GLU:OE2	1:A:605:ASN:ND2	2.36	0.56
1:A:366:LEU:O	1:A:370:ILE:HG13	2.05	0.56
1:A:686:ASP:HB3	1:A:823:PRO:HB2	1.88	0.56
1:A:455:PRO:HB3	1:A:879:ILE:HD11	1.87	0.56
1:A:979:SER:HA	1:A:1011:MET:HE2	1.86	0.56
1:A:705:GLU:HB3	1:A:847:LEU:HD22	1.87	0.55
1:A:919:ARG:HD2	1:A:921:LEU:HD13	1.89	0.55
1:A:393:LEU:HD22	1:A:470:PHE:HE2	1.71	0.55
1:A:249:ILE:HD12	1:A:262:LEU:HD12	1.88	0.55
1:A:615:PHE:H	1:A:624:THR:HG23	1.71	0.55
1:A:897:ILE:O	1:A:900:SER:OG	2.22	0.55
1:A:375:VAL:HG22	1:A:484:VAL:HG21	1.89	0.55
1:A:675:GLY:C	1:A:677:ALA:H	2.15	0.55
1:A:281:PHE:CE1	1:A:608:SER:HB2	2.42	0.55
1:A:61:VAL:HG13	1:A:118:LEU:HD22	1.88	0.55
1:A:16:ALA:HB2	1:A:488:LEU:HD13	1.89	0.55
1:A:897:ILE:HD13	1:A:950:LYS:HD2	1.88	0.55
1:A:259:ARG:HD2	1:A:261:LEU:HD21	1.89	0.54
1:A:467:TYR:CE2	1:A:868:LEU:HD21	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:VAL:HG21	1:A:942:ALA:HB2	1.88	0.54
1:A:600:THR:OG1	1:A:601:LYS:N	2.41	0.54
1:A:35:TYR:CD2	1:A:671:ILE:HD12	2.39	0.54
1:A:53:ASP:O	1:A:55:LYS:N	2.40	0.54
1:A:458:PHE:O	1:A:876:LEU:HD13	2.07	0.54
1:A:637:ARG:CB	1:A:642:ASN:HB3	2.37	0.54
1:A:712:MET:HA	1:A:835:LYS:HD2	1.90	0.54
1:A:454:VAL:HG23	1:A:475:VAL:HG21	1.89	0.54
1:A:572:PHE:HZ	1:A:598:TYR:HE1	1.56	0.54
1:A:144:ASN:OD1	1:A:147:GLY:N	2.41	0.53
1:A:393:LEU:HD22	1:A:470:PHE:CE2	2.42	0.53
1:A:699:ARG:HD2	1:A:703:LEU:HG	1.91	0.53
1:A:56:THR:O	1:A:60:THR:HB	2.08	0.53
1:A:118:LEU:HB3	1:A:122:VAL:CG1	2.39	0.53
1:A:453:PHE:O	1:A:471:SER:OG	2.26	0.53
1:A:556:PHE:CD1	1:A:913:LEU:HD21	2.44	0.53
1:A:596:HIS:CE1	1:A:600:THR:HG21	2.43	0.53
1:A:677:ALA:HB2	1:A:867:ARG:HH12	1.73	0.53
1:A:582:ALA:HB3	1:A:623:ASN:HD22	1.74	0.53
1:A:396:PHE:HE1	1:A:999:ALA:HB1	1.74	0.53
1:A:214:VAL:HG13	1:A:236:ALA:HB3	1.91	0.53
1:A:404:LEU:HD22	1:A:478:MET:HE1	1.90	0.53
1:A:418:ARG:HD3	1:A:970:MET:CG	2.36	0.52
1:A:869:SER:HB2	1:A:928:GLN:HE22	1.73	0.52
1:A:466:ILE:HG21	1:A:925:VAL:HG11	1.92	0.52
1:A:38:ILE:HG21	1:A:674:LEU:HD22	1.90	0.52
1:A:709:HIS:C	1:A:711:ASP:H	2.16	0.52
1:A:582:ALA:HA	1:A:586:ARG:CZ	2.39	0.52
1:A:416:VAL:HG12	1:A:420:MET:HE2	1.91	0.52
1:A:633:ASP:O	1:A:637:ARG:HD3	2.09	0.52
1:A:5:PHE:CE2	1:A:487:ILE:HG23	2.45	0.52
1:A:979:SER:O	1:A:983:ILE:HG13	2.10	0.52
1:A:435:MET:HG3	1:A:490:PRO:HB3	1.91	0.52
1:A:979:SER:HB2	1:A:1015:THR:HG21	1.92	0.52
1:A:110:LYS:O	1:A:113:LEU:HB3	2.10	0.51
1:A:530:SER:O	1:A:534:ILE:HG23	2.10	0.51
1:A:475:VAL:O	1:A:478:MET:HB2	2.11	0.51
1:A:173:GLY:HA3	1:A:294:ALA:HB2	1.90	0.51
1:A:448:VAL:HG12	1:A:887:CYS:HB2	1.91	0.51
1:A:729:ILE:HD12	1:A:750:LEU:HD21	1.93	0.51
1:A:10:ILE:HA	1:A:13:TRP:HD1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ILE:HG23	1:A:106:GLN:HB2	1.93	0.51
1:A:213:GLN:OE1	1:A:239:ARG:N	2.43	0.51
1:A:874:PRO:O	1:A:877:TYR:HB2	2.11	0.51
1:A:899:PHE:HA	1:A:902:MET:HB2	1.93	0.51
1:A:506:GLY:HA3	1:A:517:ASN:HD22	1.76	0.51
1:A:403:GLY:HA2	1:A:406:VAL:HG22	1.92	0.50
1:A:23:GLY:HA3	1:A:377:LEU:O	2.11	0.50
1:A:60:THR:HG22	1:A:61:VAL:CG2	2.42	0.50
1:A:241:THR:OG1	1:A:245:GLU:OE1	2.27	0.50
1:A:438:ILE:O	1:A:441:ALA:HB3	2.10	0.50
1:A:458:PHE:HA	1:A:459:PHE:HB3	1.94	0.50
1:A:64:VAL:HG21	1:A:117:LEU:HB3	1.94	0.50
1:A:252:LYS:NZ	1:A:254:ASN:OD1	2.44	0.50
1:A:732:ASP:OD2	1:A:735:LYS:HB2	2.12	0.50
1:A:553:ALA:O	1:A:557:VAL:HG22	2.12	0.50
1:A:151:GLN:HB3	1:A:285:PRO:HB3	1.94	0.50
1:A:388:PHE:HE2	1:A:472:ILE:HB	1.76	0.50
1:A:36:PRO:HG3	1:A:469:GLN:HG3	1.94	0.49
1:A:150:THR:O	1:A:154:ILE:HG13	2.12	0.49
1:A:394:THR:O	1:A:398:MET:HG2	2.12	0.49
1:A:445:ILE:HD13	1:A:940:LYS:HG2	1.93	0.49
1:A:562:SER:HB3	1:A:924:ASP:HB3	1.94	0.49
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.47	0.49
1:A:545:TYR:HA	1:A:548:ILE:HD12	1.94	0.49
1:A:790:TYR:CE1	1:A:800:PRO:HB3	2.47	0.49
1:A:907:LEU:HD11	1:A:1025:PHE:HE2	1.76	0.49
1:A:142:VAL:HG21	1:A:158:VAL:HG11	1.94	0.49
1:A:177:LEU:HG	1:A:178:PHE:N	2.27	0.49
1:A:419:VAL:O	1:A:423:GLU:HB2	2.11	0.49
1:A:544:LEU:O	1:A:547:ILE:HB	2.13	0.49
1:A:562:SER:O	1:A:924:ASP:HA	2.12	0.49
1:A:30:LEU:HD23	1:A:390:ILE:HG13	1.94	0.49
1:A:328:ASP:C	1:A:330:THR:N	2.70	0.49
1:A:524:THR:O	1:A:528:THR:HG23	2.13	0.49
1:A:832:ALA:O	1:A:834:GLY:N	2.46	0.49
1:A:50:PRO:HG3	1:A:125:GLN:NE2	2.28	0.49
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.95	0.49
1:A:531:VAL:O	1:A:534:ILE:HG12	2.13	0.49
1:A:545:TYR:O	1:A:549:VAL:HG23	2.13	0.49
1:A:960:LEU:H	1:A:960:LEU:HD23	1.78	0.48
1:A:987:MET:O	1:A:991:ILE:HD13	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TYR:HB3	1:A:36:PRO:HD2	1.95	0.48
1:A:137:LEU:HD12	1:A:293:LEU:HB2	1.96	0.48
1:A:616:GLY:O	1:A:618:ALA:N	2.46	0.48
1:A:466:ILE:O	1:A:469:GLN:HB2	2.13	0.48
1:A:578:LEU:HD13	1:A:587:THR:HG23	1.94	0.48
1:A:184:MET:HB3	1:A:771:VAL:HG22	1.95	0.48
1:A:10:ILE:O	1:A:14:VAL:HG23	2.13	0.48
1:A:403:GLY:O	1:A:406:VAL:HG22	2.14	0.48
1:A:412:VAL:O	1:A:416:VAL:HG23	2.12	0.48
1:A:449:LEU:HD23	1:A:478:MET:HE1	1.95	0.48
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.68	0.48
1:A:677:ALA:HB2	1:A:867:ARG:NH2	2.28	0.48
1:A:118:LEU:HB3	1:A:122:VAL:HG11	1.95	0.48
1:A:723:ASP:OD1	1:A:723:ASP:N	2.46	0.48
1:A:841:MET:HG2	1:A:859:TRP:CH2	2.48	0.48
1:A:441:ALA:HB1	1:A:944:LEU:HD21	1.96	0.47
1:A:575:MET:HG2	1:A:666:PHE:HE1	1.79	0.47
1:A:831:ALA:HA	1:A:840:ALA:HB2	1.96	0.47
1:A:76:MET:HG3	1:A:95:GLU:OE2	2.14	0.47
1:A:556:PHE:HD1	1:A:913:LEU:HD21	1.78	0.47
1:A:956:GLU:HB3	1:A:958:LYS:HG3	1.96	0.47
1:A:418:ARG:NH1	1:A:970:MET:HA	2.30	0.47
1:A:568:ASP:OD1	1:A:644:VAL:HG13	2.13	0.47
1:A:677:ALA:HB2	1:A:867:ARG:CZ	2.44	0.47
1:A:189:ASN:ND2	1:A:192:GLU:H	2.11	0.47
1:A:360:GLN:HB3	1:A:513:PHE:CE2	2.49	0.47
1:A:708:LYS:O	1:A:709:HIS:ND1	2.48	0.47
1:A:58:GLN:OE1	1:A:818:ARG:HD2	2.14	0.47
1:A:444:GLY:HA3	1:A:891:LEU:HD22	1.95	0.47
1:A:459:PHE:O	1:A:464:GLY:HA3	2.14	0.47
1:A:391:ASN:O	1:A:395:MET:HG2	2.15	0.47
1:A:145:THR:OG1	1:A:146:ASP:N	2.47	0.46
1:A:662:MET:HG3	1:A:664:PHE:HE1	1.77	0.46
1:A:60:THR:HG22	1:A:61:VAL:HG22	1.97	0.46
1:A:458:PHE:HB3	1:A:459:PHE:HD1	1.81	0.46
1:A:34:GLN:O	1:A:391:ASN:HB2	2.16	0.46
1:A:448:VAL:O	1:A:451:ALA:HB3	2.16	0.46
1:A:457:ALA:HB1	1:A:468:ARG:HG3	1.98	0.46
1:A:587:THR:HB	1:A:613:ASN:HD21	1.80	0.46
1:A:35:TYR:HE2	1:A:671:ILE:HB	1.80	0.46
1:A:10:ILE:HA	1:A:13:TRP:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:LEU:HB3	1:A:913:LEU:HB3	1.97	0.46
1:A:599:LEU:O	1:A:603:LYS:HG2	2.16	0.46
1:A:142:VAL:HG12	1:A:321:LEU:HD22	1.97	0.45
1:A:513:PHE:HD1	1:A:513:PHE:HA	1.69	0.45
1:A:38:ILE:HG23	1:A:462:SER:HB2	1.98	0.45
1:A:546:LEU:O	1:A:550:VAL:HG23	2.17	0.45
1:A:695:LEU:O	1:A:699:ARG:HB2	2.16	0.45
1:A:58:GLN:O	1:A:62:THR:HB	2.16	0.45
1:A:985:GLY:O	1:A:988:PRO:HD2	2.16	0.45
1:A:73:ASP:O	1:A:74:ASN:HB2	2.15	0.45
1:A:254:ASN:HD22	1:A:258:SER:HB3	1.81	0.45
1:A:300:LEU:HD23	1:A:304:ALA:HB2	1.98	0.45
1:A:965:LEU:HA	1:A:968:VAL:HB	1.98	0.45
1:A:94:PHE:CB	1:A:98:THR:HG21	2.47	0.45
1:A:199:THR:HG22	1:A:791:VAL:HA	1.99	0.45
1:A:33:ALA:HB2	1:A:299:ALA:HB2	1.99	0.44
1:A:445:ILE:O	1:A:449:LEU:HD13	2.17	0.44
1:A:637:ARG:O	1:A:643:LYS:NZ	2.38	0.44
1:A:885:PHE:HA	1:A:888:LEU:HD12	1.99	0.44
1:A:211:ASN:HA	1:A:240:LEU:HD13	1.99	0.44
1:A:393:LEU:HD13	1:A:466:ILE:HG23	2.00	0.44
1:A:972:LEU:HD23	1:A:1019:ILE:HD11	1.99	0.44
1:A:574:THR:O	1:A:626:ILE:HA	2.18	0.44
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.80	0.44
1:A:702:LEU:HA	1:A:702:LEU:HD12	1.68	0.44
1:A:165:ALA:HB1	1:A:309:GLU:OE1	2.18	0.44
1:A:953:MET:HE1	1:A:1030:ARG:NH1	2.30	0.44
1:A:314:GLU:N	1:A:315:PRO:HD2	2.33	0.44
1:A:520:PHE:O	1:A:524:THR:HG23	2.17	0.44
1:A:582:ALA:HB3	1:A:623:ASN:HB3	2.00	0.44
1:A:649:MET:O	1:A:652:THR:HG22	2.17	0.44
1:A:674:LEU:HD12	1:A:674:LEU:HA	1.86	0.44
1:A:693:GLU:H	1:A:693:GLU:CD	2.24	0.44
1:A:162:MET:HG2	1:A:313:MET:SD	2.58	0.44
1:A:987:MET:N	1:A:988:PRO:HD2	2.33	0.44
1:A:1021:PHE:HB3	1:A:1025:PHE:CE2	2.53	0.44
1:A:70:ASN:O	1:A:110:LYS:HE2	2.18	0.43
1:A:924:ASP:OD2	1:A:926:TYR:HB2	2.17	0.43
1:A:62:THR:O	1:A:66:GLU:HG3	2.18	0.43
1:A:544:LEU:O	1:A:548:ILE:HG13	2.18	0.43
1:A:997:SER:O	1:A:1000:GLN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ALA:CA	1:A:298:ASN:HB2	2.47	0.43
1:A:448:VAL:HG23	1:A:449:LEU:HD13	1.99	0.43
1:A:892:TYR:CD1	1:A:897:ILE:HG22	2.53	0.43
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.74	0.43
1:A:411:VAL:O	1:A:415:ASN:HB2	2.18	0.43
1:A:415:ASN:OD1	1:A:971:ARG:NH2	2.52	0.43
1:A:868:LEU:HB3	1:A:869:SER:H	1.60	0.43
1:A:162:MET:HA	1:A:313:MET:SD	2.58	0.43
1:A:1024:VAL:HA	1:A:1027:VAL:HG22	2.00	0.43
1:A:287:SER:OG	1:A:288:GLY:N	2.50	0.43
1:A:389:SER:O	1:A:391:ASN:N	2.49	0.43
1:A:393:LEU:HD12	1:A:469:GLN:HG3	1.99	0.43
1:A:866:GLU:O	1:A:867:ARG:HB2	2.18	0.43
1:A:10:ILE:O	1:A:13:TRP:HB2	2.19	0.43
1:A:111:LEU:HD12	1:A:129:VAL:CG2	2.49	0.43
1:A:262:LEU:HB3	1:A:268:ILE:HD11	1.99	0.43
1:A:310:LEU:HD21	1:A:323:ILE:HD12	2.01	0.43
1:A:877:TYR:OH	1:A:928:GLN:HG2	2.19	0.43
1:A:572:PHE:HB2	1:A:666:PHE:O	2.18	0.43
1:A:633:ASP:OD2	1:A:634:TRP:N	2.52	0.43
1:A:641:GLU:HA	1:A:646:ALA:HB3	2.00	0.43
1:A:742:SER:HB3	1:A:745:ASP:CG	2.44	0.43
1:A:355:MET:SD	1:A:368:PRO:HG3	2.59	0.43
1:A:559:LEU:HD12	1:A:560:PRO:HD2	2.00	0.43
1:A:575:MET:HG2	1:A:666:PHE:CE1	2.53	0.43
1:A:144:ASN:O	1:A:284:GLN:NE2	2.52	0.42
1:A:152:GLU:H	1:A:152:GLU:HG2	1.44	0.42
1:A:409:ALA:O	1:A:413:VAL:HG23	2.18	0.42
1:A:165:ALA:HB3	1:A:313:MET:HE2	2.00	0.42
1:A:712:MET:O	1:A:713:LEU:HD12	2.19	0.42
1:A:922:THR:OG1	1:A:923:ASN:N	2.52	0.42
1:A:150:THR:HG23	1:A:153:ASP:OD2	2.20	0.42
1:A:300:LEU:HD23	1:A:300:LEU:O	2.19	0.42
1:A:325:TYR:O	1:A:327:TYR:N	2.47	0.42
1:A:138:MET:HE2	1:A:328:ASP:OD1	2.19	0.42
1:A:141:GLY:HA2	1:A:288:GLY:HA3	2.01	0.42
1:A:211:ASN:O	1:A:760:ASN:ND2	2.53	0.42
1:A:785:ASP:O	1:A:788:ASP:HB2	2.19	0.42
1:A:1020:PHE:O	1:A:1023:PRO:HD2	2.18	0.42
1:A:711:ASP:C	1:A:712:MET:HG2	2.44	0.42
1:A:5:PHE:HD2	1:A:12:ALA:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ILE:O	1:A:428:LYS:HE3	2.20	0.42
1:A:30:LEU:HA	1:A:31:PRO:HD3	1.86	0.42
1:A:337:ILE:HD12	1:A:337:ILE:HA	1.91	0.42
1:A:720:GLY:O	1:A:721:LEU:HD23	2.20	0.42
1:A:1001:ASN:O	1:A:1005:THR:HG23	2.20	0.42
1:A:110:LYS:HA	1:A:110:LYS:HD2	1.89	0.42
1:A:297:ALA:HA	1:A:298:ASN:CB	2.50	0.42
1:A:813:SER:HA	1:A:814:PRO:HD3	1.76	0.42
1:A:68:ASN:O	1:A:110:LYS:HB3	2.20	0.42
1:A:971:ARG:HG2	1:A:975:ILE:HD11	2.02	0.41
1:A:1019:ILE:HD12	1:A:1019:ILE:HA	1.89	0.41
1:A:725:PRO:HG3	1:A:811:TYR:CE1	2.55	0.41
1:A:931:LEU:O	1:A:935:ILE:HG23	2.20	0.41
1:A:24:GLY:O	1:A:28:LEU:HG	2.21	0.41
1:A:133:SER:O	1:A:292:LYS:HD3	2.21	0.41
1:A:177:LEU:HD23	1:A:179:GLY:O	2.20	0.41
1:A:360:GLN:HG2	1:A:513:PHE:CE1	2.55	0.41
1:A:621:GLY:O	1:A:624:THR:HG22	2.20	0.41
1:A:1:MET:N	1:A:2:PRO:HD3	2.31	0.41
1:A:279:ALA:HB3	1:A:286:ALA:O	2.20	0.41
1:A:423:GLU:N	1:A:502:LYS:HG3	2.36	0.41
1:A:105:VAL:O	1:A:106:GLN:C	2.63	0.41
1:A:155:SER:OG	1:A:179:GLY:HA3	2.21	0.41
1:A:449:LEU:HA	1:A:452:VAL:HG13	2.01	0.41
1:A:10:ILE:HA	1:A:13:TRP:HB2	2.02	0.41
1:A:222:THR:HA	1:A:224:PRO:HD3	2.02	0.41
1:A:366:LEU:O	1:A:369:THR:HB	2.20	0.41
1:A:801:PHE:HA	1:A:804:PHE:CE2	2.56	0.41
1:A:123:GLN:H	1:A:123:GLN:HG3	1.69	0.41
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.20	0.41
1:A:34:GLN:C	1:A:391:ASN:HB2	2.46	0.41
1:A:294:ALA:O	1:A:296:GLY:N	2.53	0.41
1:A:644:VAL:O	1:A:648:THR:HG23	2.21	0.41
1:A:703:LEU:HD23	1:A:703:LEU:HA	1.78	0.41
1:A:818:ARG:NH2	1:A:821:GLY:O	2.43	0.41
1:A:111:LEU:HD11	1:A:127:VAL:HG21	2.03	0.41
1:A:156:ASP:O	1:A:159:ALA:N	2.54	0.41
1:A:251:LEU:HA	1:A:251:LEU:HD23	1.64	0.41
1:A:745:ASP:O	1:A:749:THR:HG23	2.20	0.41
1:A:896:SER:O	1:A:899:PHE:N	2.54	0.41
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:PRO:O	1:A:335:ILE:HG13	2.22	0.40
1:A:408:ASP:O	1:A:412:VAL:HG23	2.21	0.40
1:A:933:THR:O	1:A:937:LEU:HB2	2.21	0.40
1:A:242:SER:OG	1:A:243:THR:N	2.54	0.40
1:A:677:ALA:HB2	1:A:867:ARG:HH22	1.86	0.40
1:A:72:ILE:HG23	1:A:106:GLN:CB	2.51	0.40
1:A:45:ILE:HD11	1:A:107:VAL:HG12	2.04	0.40
1:A:379:THR:HG21	1:A:398:MET:HE1	2.04	0.40
1:A:456:MET:C	1:A:458:PHE:N	2.80	0.40
1:A:543:VAL:O	1:A:547:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1032/1049 (98%)	865 (84%)	123 (12%)	44 (4%)	2 13

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	113	LEU
1	A	146	ASP
1	A	295	THR
1	A	299	ALA
1	A	510	LYS
1	A	579	PRO
1	A	617	PHE
1	A	833	PRO
1	A	866	GLU
1	A	867	ARG

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Mol	Chain	Res	Type
1	A	919	ARG
1	A	921	LEU
1	A	150	THR
1	A	298	ASN
1	A	319	SER
1	A	327	TYR
1	A	390	ILE
1	A	601	LYS
1	A	618	ALA
1	A	672	VAL
1	A	865	GLN
1	A	136	PHE
1	A	301	ASP
1	A	330	THR
1	A	600	THR
1	A	615	PHE
1	A	633	ASP
1	A	669	PRO
1	A	9	PRO
1	A	54	ALA
1	A	877	TYR
1	A	329	THR
1	A	441	ALA
1	A	602	GLU
1	A	710	PRO
1	A	862	MET
1	A	997	SER
1	A	326	PRO
1	A	427	PRO
1	A	776	GLU
1	A	815	ARG
1	A	35	TYR
1	A	746	ILE

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	840/855 (98%)	672 (80%)	168 (20%)	1 5

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	ASN
1	A	7	ASP
1	A	8	ARG
1	A	15	ILE
1	A	29	LYS
1	A	32	VAL
1	A	37	THR
1	A	38	ILE
1	A	44	THR
1	A	45	ILE
1	A	46	SER
1	A	57	VAL
1	A	58	GLN
1	A	60	THR
1	A	61	VAL
1	A	70	ASN
1	A	75	LEU
1	A	79	SER
1	A	82	SER
1	A	83	ASP
1	A	85	THR
1	A	87	THR
1	A	93	THR
1	A	98	THR
1	A	109	ASN
1	A	111	LEU
1	A	113	LEU
1	A	122	VAL
1	A	123	GLN
1	A	124	GLN
1	A	127	VAL
1	A	128	SER
1	A	130	GLU
1	A	135	SER
1	A	142	VAL
1	A	150	THR
1	A	152	GLU

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Mol	Chain	Res	Type
1	A	153	ASP
1	A	158	VAL
1	A	164	ASP
1	A	166	ILE
1	A	180	SER
1	A	184	MET
1	A	185	ARG
1	A	197	GLN
1	A	198	LEU
1	A	200	PRO
1	A	214	VAL
1	A	222	THR
1	A	226	LYS
1	A	230	LEU
1	A	233	SER
1	A	241	THR
1	A	243	THR
1	A	248	LYS
1	A	253	VAL
1	A	256	ASP
1	A	258	SER
1	A	259	ARG
1	A	262	LEU
1	A	263	ARG
1	A	277	ILE
1	A	293	LEU
1	A	295	THR
1	A	306	ILE
1	A	307	ARG
1	A	310	LEU
1	A	321	LEU
1	A	329	THR
1	A	330	THR
1	A	335	ILE
1	A	337	ILE
1	A	340	VAL
1	A	343	THR
1	A	348	ILE
1	A	357	LEU
1	A	362	PHE
1	A	365	THR
1	A	372	VAL

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Mol	Chain	Res	Type
1	A	376	LEU
1	A	379	THR
1	A	414	GLU
1	A	415	ASN
1	A	425	LEU
1	A	433	LYS
1	A	445	ILE
1	A	447	MET
1	A	449	LEU
1	A	452	VAL
1	A	454	VAL
1	A	473	THR
1	A	486	LEU
1	A	495	THR
1	A	498	LYS
1	A	509	LYS
1	A	513	PHE
1	A	515	TRP
1	A	525	HIS
1	A	526	HIS
1	A	543	VAL
1	A	564	LEU
1	A	583	THR
1	A	585	GLU
1	A	587	THR
1	A	591	LEU
1	A	604	ASN
1	A	626	ILE
1	A	637	ARG
1	A	644	VAL
1	A	652	THR
1	A	662	MET
1	A	671	ILE
1	A	684	LEU
1	A	687	GLN
1	A	693	GLU
1	A	695	LEU
1	A	703	LEU
1	A	712	MET
1	A	715	SER
1	A	716	VAL
1	A	723	ASP

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Mol	Chain	Res	Type
1	A	724	THR
1	A	729	ILE
1	A	730	ASP
1	A	732	ASP
1	A	741	VAL
1	A	757	SER
1	A	771	VAL
1	A	773	VAL
1	A	776	GLU
1	A	778	LYS
1	A	791	VAL
1	A	806	SER
1	A	808	ARG
1	A	817	GLU
1	A	833	PRO
1	A	846	GLN
1	A	851	LEU
1	A	858	ASP
1	A	865	GLN
1	A	868	LEU
1	A	879	ILE
1	A	881	LEU
1	A	886	LEU
1	A	902	MET
1	A	903	LEU
1	A	904	VAL
1	A	922	THR
1	A	928	GLN
1	A	937	LEU
1	A	938	SER
1	A	945	ILE
1	A	946	VAL
1	A	969	ARG
1	A	971	ARG
1	A	973	ARG
1	A	976	LEU
1	A	989	LEU
1	A	990	VAL
1	A	1003	VAL
1	A	1005	THR
1	A	1007	VAL
1	A	1015	THR

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Mol	Chain	Res	Type
1	A	1016	VAL
1	A	1022	VAL
1	A	1029	VAL
1	A	1030	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	120	GLN
1	A	123	GLN
1	A	189	ASN
1	A	194	ASN
1	A	588	GLN
1	A	623	ASN
1	A	719	ASN
1	A	928	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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 [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	1034/1049 (98%)	-0.36	6 (0%) 85 73	14, 69, 128, 143	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	461	GLY	3.5
1	A	401	ALA	3.1
1	A	306	ILE	2.7
1	A	294	ALA	2.5
1	A	303	ALA	2.5
1	A	706	ALA	2.4

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.