



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:20 PM UTC

PDB ID : 2ZAI / pdb_00002zai
Title : Crystal structure of the soluble domain of STT3 from *P. furiosus*
Authors : Maita, N.
Deposited on : 2007-10-05
Resolution : 2.70 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

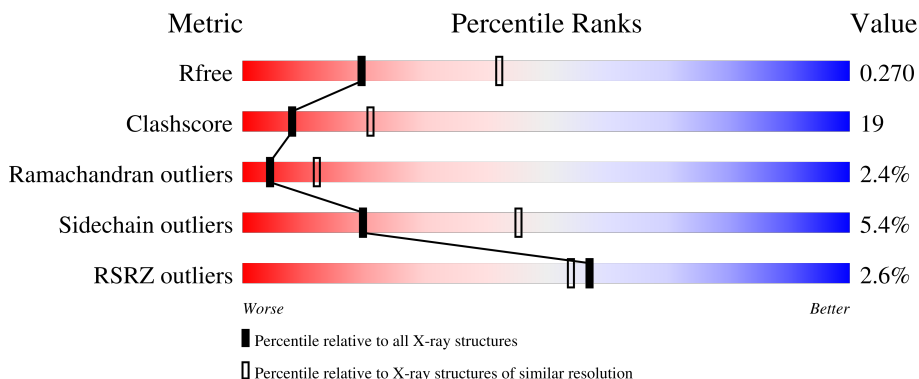
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	497	
1	B	497	
1	C	497	
1	D	497	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15005 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 Oligosaccharyl transferase stt3 subunit related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	472	Total 3756	C 2427	N 607	O 716	S 6	0	0	0
1	B	468	Total 3724	C 2407	N 602	O 709	S 6	0	0	0
1	C	470	Total 3737	C 2416	N 604	O 711	S 6	0	0	0
1	D	471	Total 3746	C 2421	N 608	O 711	S 6	0	0	0

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Cl 1	0	0
3	B	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0
3	D	1	Total 1	Cl 1	0	0

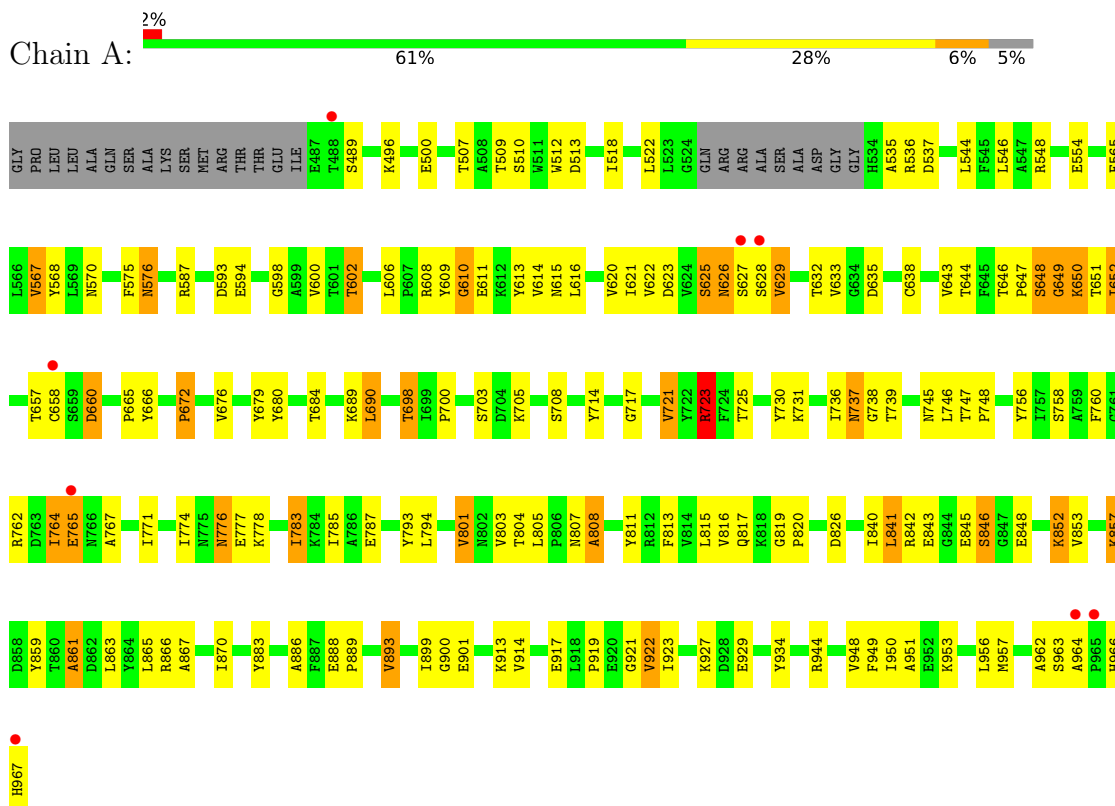
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	B	11	Total O 11 11	0	0
4	D	11	Total O 11 11	0	0

3 Residue-property plots i

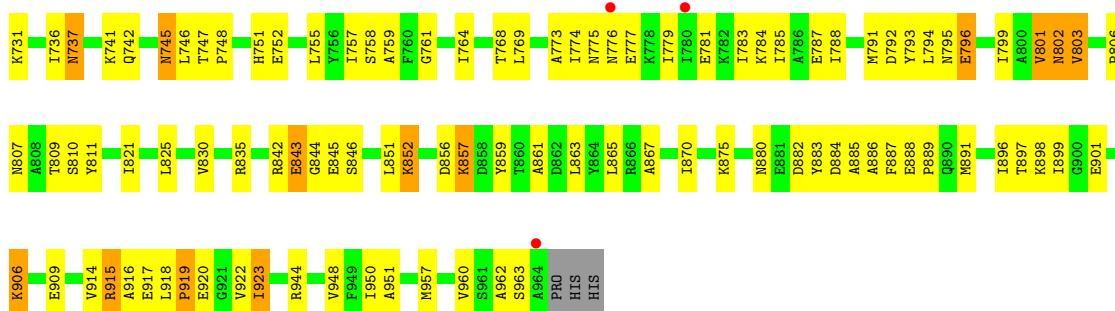
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Oligosaccharyl transferase stt3 subunit related protein

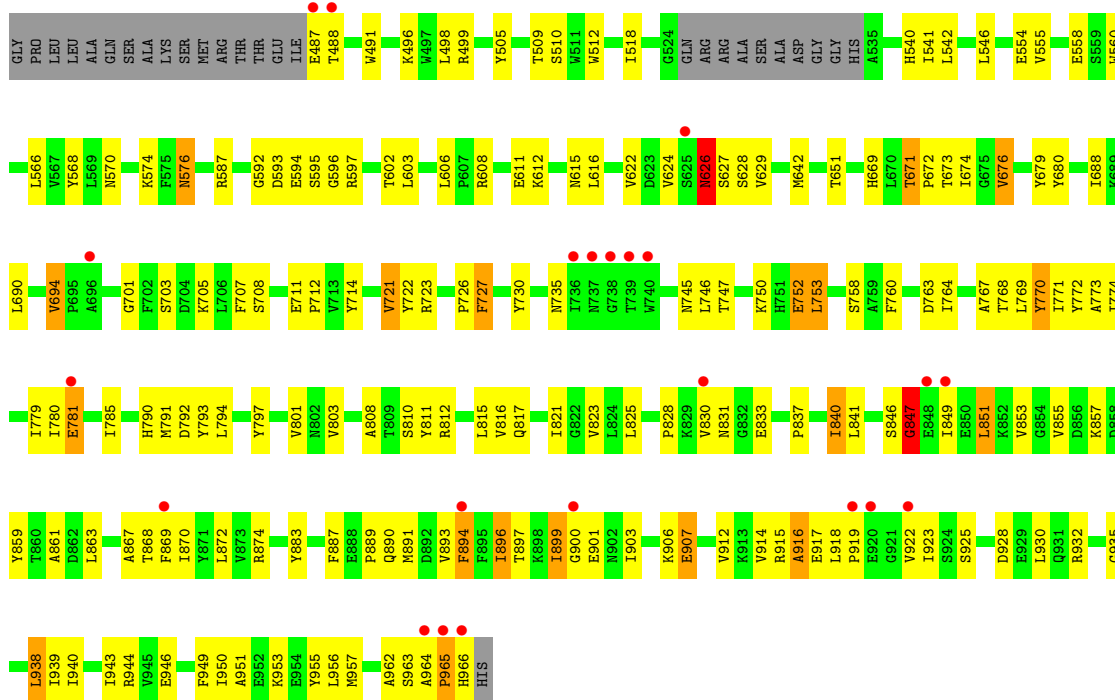


- Molecule 1: Oligosaccharyl transferase stt3 subunit related protein

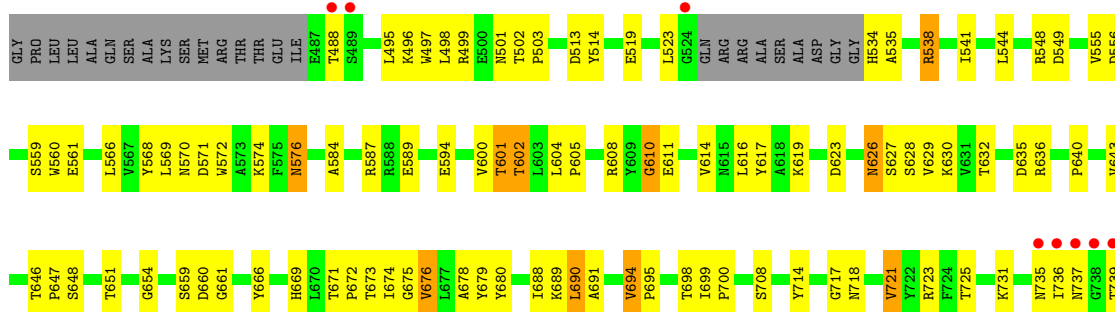


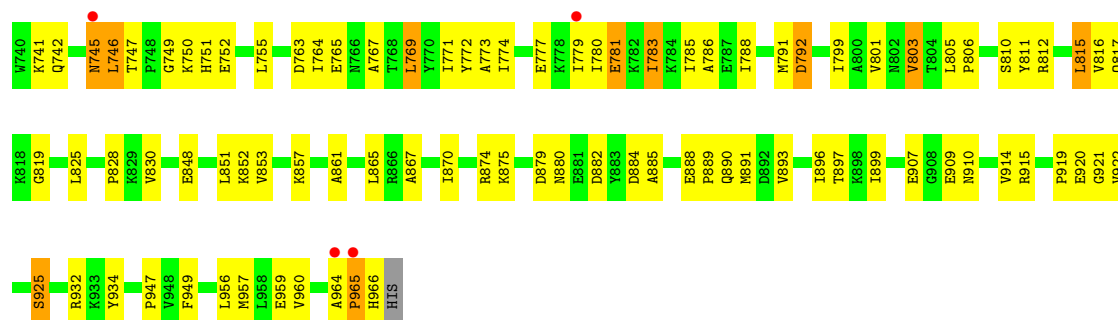


• Molecule 1: Oligosaccharyl transferase stt3 subunit related protein



• Molecule 1: Oligosaccharyl transferase stt3 subunit related protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	136.94Å 265.30Å 74.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.70) 99.6 (20.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.68Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.273 0.225 , 0.270	Depositor DCC
R_{free} test set	3805 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtrriage
Anisotropy	0.625	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15005	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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 i

5.1 Standard geometry i

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

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	0.48	0/3847	0.99	17/5228 (0.3%)
1	B	0.46	0/3812	0.95	15/5180 (0.3%)
1	C	0.40	0/3826	0.93	11/5200 (0.2%)
1	D	0.48	0/3837	0.97	19/5216 (0.4%)
All	All	0.46	0/15322	0.96	62/20824 (0.3%)

There are no bond length outliers.

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	694	VAL	CA-C-N	8.14	128.23	119.28
1	B	694	VAL	C-N-CA	8.14	128.23	119.28
1	B	546	LEU	N-CA-C	8.06	120.98	111.71
1	A	635	ASP	N-CA-C	-7.69	104.03	113.41
1	D	694	VAL	CA-C-N	7.13	127.29	119.87
1	D	694	VAL	C-N-CA	7.13	127.29	119.87
1	A	764	ILE	N-CA-C	-6.96	98.55	108.58
1	D	786	ALA	N-CA-C	6.66	117.27	107.88
1	A	865	LEU	N-CA-C	-6.62	97.72	108.52
1	C	694	VAL	CA-C-N	6.62	126.31	119.56
1	C	694	VAL	C-N-CA	6.62	126.31	119.56
1	A	546	LEU	N-CA-C	6.55	118.42	111.28
1	B	708	SER	N-CA-C	-6.45	104.45	112.90
1	D	690	LEU	N-CA-C	6.39	119.24	111.82
1	A	708	SER	N-CA-C	-6.32	105.40	113.23
1	A	783	ILE	N-CA-C	6.29	116.44	106.88
1	C	597	ARG	N-CA-C	6.26	117.68	108.86
1	A	886	ALA	N-CA-C	-6.17	99.67	109.23
1	D	602	THR	N-CA-C	6.15	117.65	111.07
1	D	783	ILE	N-CA-C	6.03	117.46	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	PHE	N-CA-C	6.00	118.61	111.71
1	B	629	VAL	N-CA-C	5.95	117.33	108.46
1	B	513	ASP	N-CA-C	5.87	119.52	111.54
1	D	865	LEU	N-CA-C	-5.83	99.02	108.52
1	A	922	VAL	N-CA-C	5.83	116.48	110.36
1	C	680	TYR	N-CA-C	5.78	118.33	111.33
1	A	861	ALA	N-CA-C	5.76	117.73	109.14
1	B	880	ASN	N-CA-C	5.74	119.09	111.75
1	B	803	VAL	N-CA-C	5.73	117.61	108.89
1	C	611	GLU	N-CA-C	-5.71	104.72	112.26
1	A	966	HIS	N-CA-C	5.68	120.35	112.90
1	C	938	LEU	N-CA-C	5.67	119.15	110.20
1	B	761	GLY	N-CA-C	5.63	121.79	115.08
1	C	708	SER	N-CA-C	-5.60	106.49	113.38
1	B	764	ILE	N-CA-C	-5.58	100.54	108.58
1	D	764	ILE	N-CA-C	-5.51	100.50	108.87
1	A	602	THR	N-CA-C	5.51	116.96	111.07
1	A	660	ASP	N-CA-C	-5.50	106.53	113.18
1	B	886	ALA	N-CA-C	-5.50	100.71	109.23
1	A	723	ARG	N-CA-C	-5.49	100.73	109.96
1	B	576	ASN	N-CA-C	-5.43	105.52	111.82
1	D	880	ASN	N-CA-C	5.43	119.00	112.38
1	B	679	TYR	N-CA-C	-5.41	102.38	110.23
1	A	513	ASP	N-CA-C	5.40	119.03	111.74
1	C	847	GLY	N-CA-C	5.37	125.92	113.18
1	C	679	TYR	N-CA-C	-5.26	102.60	110.23
1	C	546	LEU	N-CA-C	5.21	116.96	111.28
1	D	803	VAL	N-CA-C	5.21	117.35	108.86
1	D	695	PRO	N-CA-C	5.16	120.37	114.03
1	D	947	PRO	N-CA-C	-5.16	101.85	112.47
1	D	708	SER	N-CA-C	-5.15	106.85	113.23
1	A	598	GLY	N-CA-C	5.14	121.20	115.08
1	B	773	ALA	N-CA-C	-5.14	102.25	109.96
1	D	819	GLY	CA-C-N	-5.13	114.70	120.14
1	D	819	GLY	C-N-CA	-5.13	114.70	120.14
1	B	885	ALA	N-CA-C	5.12	117.72	110.50
1	D	680	TYR	N-CA-C	5.12	118.31	111.75
1	D	934	TYR	N-CA-C	5.11	120.36	113.72
1	D	861	ALA	N-CA-C	5.09	117.89	109.85
1	D	885	ALA	N-CA-C	5.06	118.19	110.20
1	A	690	LEU	N-CA-C	5.03	117.66	111.82
1	C	753	LEU	N-CA-C	5.01	116.85	108.99

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	3756	0	3688	123	0
1	B	3724	0	3670	157	0
1	C	3737	0	3681	163	0
1	D	3746	0	3677	146	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	0	3	0
4	B	11	0	0	1	0
4	D	11	0	0	1	0
All	All	15005	0	14716	577	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 19.

All (577) 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:650:LYS:HD3	1:A:651:THR:H	1.13	1.13
1:D:560:TRP:HE1	1:D:891:MET:HE1	1.23	1.03
1:A:650:LYS:HD3	1:A:651:THR:N	1.76	0.99
1:C:841:LEU:HD11	1:C:916:ALA:HB1	1.41	0.98
1:C:861:ALA:HB2	1:C:951:ALA:HB2	1.45	0.98
1:C:626:ASN:HD22	1:C:628:SER:H	1.13	0.96
1:B:560:TRP:HE1	1:B:891:MET:HE1	1.32	0.94
1:C:560:TRP:HE1	1:C:891:MET:HE1	1.31	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:495:LEU:HD13	1:D:519:GLU:HG3	1.48	0.92
1:C:487:GLU:CG	1:C:488:THR:H	1.83	0.91
1:C:828:PRO:HB2	1:C:840:ILE:HD11	1.51	0.91
1:D:870:ILE:HD11	1:D:891:MET:HE3	1.53	0.89
1:D:815:LEU:HB2	1:D:957:MET:HE2	1.57	0.86
1:B:867:ALA:HB2	1:B:896:ILE:HD11	1.57	0.86
1:C:747:THR:HG22	1:C:963:SER:O	1.76	0.86
1:D:714:TYR:HB3	1:D:721:VAL:HG13	1.59	0.85
1:B:899:ILE:O	1:B:914:VAL:HG11	1.77	0.84
1:D:560:TRP:NE1	1:D:891:MET:HE1	1.92	0.84
1:A:764:ILE:HA	1:A:817:GLN:HE22	1.43	0.83
1:B:560:TRP:NE1	1:B:891:MET:HE1	1.93	0.83
1:B:870:ILE:HD11	1:B:891:MET:HE3	1.58	0.83
1:C:593:ASP:HA	1:C:883:TYR:CE2	2.14	0.82
1:C:764:ILE:HA	1:C:817:GLN:HE22	1.43	0.82
1:B:757:ILE:HD12	1:B:957:MET:HE1	1.64	0.78
1:D:805:LEU:HB3	1:D:811:TYR:HE2	1.48	0.78
1:D:791:MET:O	1:D:792:ASP:HB3	1.84	0.77
1:A:861:ALA:HB2	1:A:951:ALA:HB2	1.65	0.76
1:C:671:THR:HB	1:C:674:ILE:O	1.85	0.76
1:B:791:MET:SD	1:B:796:GLU:HA	2.26	0.75
1:C:938:LEU:C	1:C:939:ILE:HD12	2.11	0.75
1:C:853:VAL:HG21	1:C:949:PHE:CE2	2.21	0.75
1:C:671:THR:HG22	1:C:673:THR:H	1.52	0.75
1:B:565:PHE:HE1	1:B:567:VAL:HG12	1.51	0.74
1:C:918:LEU:HD12	1:C:919:PRO:HD2	1.69	0.74
1:C:560:TRP:NE1	1:C:891:MET:HE1	2.03	0.74
1:D:853:VAL:HG21	1:D:949:PHE:CE1	2.23	0.74
1:D:514:TYR:OH	1:D:574:LYS:HE2	1.87	0.74
1:B:569:LEU:HB2	1:B:718:ASN:HB3	1.70	0.73
1:C:576:ASN:HD21	1:C:602:THR:H	1.36	0.73
1:D:671:THR:HG22	1:D:673:THR:H	1.53	0.73
1:C:870:ILE:HD11	1:C:891:MET:HE3	1.69	0.73
1:C:487:GLU:CG	1:C:488:THR:N	2.51	0.73
1:C:505:TYR:CE2	1:C:825:LEU:HD21	2.24	0.72
1:D:569:LEU:HB2	1:D:718:ASN:HB3	1.72	0.72
1:A:593:ASP:HA	1:A:883:TYR:CE2	2.25	0.72
1:D:714:TYR:HB3	1:D:721:VAL:CG1	2.19	0.72
1:C:746:LEU:O	1:C:962:ALA:HA	1.89	0.71
1:A:616:LEU:HD11	1:B:518:ILE:HD11	1.71	0.71
1:B:671:THR:HG22	1:B:673:THR:H	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:723:ARG:NH2	1:C:956:LEU:O	2.24	0.71
1:A:544:LEU:HD13	1:A:889:PRO:HG2	1.71	0.70
1:D:785:ILE:HB	1:D:801:VAL:HG21	1.73	0.70
1:A:747:THR:HG22	1:A:963:SER:O	1.92	0.70
1:C:498:LEU:HD11	1:C:566:LEU:HD11	1.74	0.70
1:C:841:LEU:CD1	1:C:916:ALA:HB1	2.21	0.70
1:C:922:VAL:HG23	1:C:923:ILE:H	1.55	0.69
1:B:671:THR:HB	1:B:674:ILE:O	1.91	0.69
1:D:779:ILE:HD12	1:D:779:ILE:O	1.93	0.69
1:D:805:LEU:HB3	1:D:811:TYR:CE2	2.27	0.69
1:B:714:TYR:HB3	1:B:721:VAL:CG1	2.23	0.69
1:C:846:SER:HA	1:C:917:GLU:HA	1.75	0.69
1:D:496:LYS:O	1:D:499:ARG:HG2	1.93	0.68
1:B:785:ILE:HB	1:B:801:VAL:HG21	1.76	0.68
1:C:671:THR:HG23	1:C:672:PRO:HD2	1.73	0.68
1:C:868:THR:HG22	1:C:893:VAL:HG12	1.75	0.68
1:C:540:HIS:CD2	1:C:872:LEU:HD21	2.29	0.68
1:D:600:VAL:HG21	1:D:679:TYR:CD1	2.28	0.68
1:C:896:ILE:HG22	1:C:897:THR:HG23	1.75	0.68
1:D:538:ARG:HD2	1:D:560:TRP:CZ2	2.28	0.67
1:D:576:ASN:HD21	1:D:602:THR:H	1.43	0.67
1:D:769:LEU:HD13	1:D:957:MET:HE1	1.77	0.67
1:D:538:ARG:HD2	1:D:560:TRP:CE2	2.30	0.67
1:D:765:GLU:H	1:D:817:GLN:NE2	1.92	0.67
1:D:780:ILE:O	1:D:781:GLU:HB3	1.95	0.67
1:C:669:HIS:HB2	1:C:676:VAL:HG13	1.76	0.67
1:C:785:ILE:HB	1:C:801:VAL:HG21	1.77	0.67
1:A:737:ASN:C	1:A:739:THR:H	2.03	0.67
1:B:711:GLU:OE2	1:B:723:ARG:NH1	2.28	0.66
1:C:855:VAL:HG23	1:C:907:GLU:HA	1.76	0.66
1:D:626:ASN:HD22	1:D:626:ASN:N	1.91	0.66
1:B:560:TRP:HE1	1:B:891:MET:CE	2.07	0.66
1:D:496:LYS:HA	1:D:499:ARG:NE	2.11	0.66
1:A:512:TRP:N	4:A:16:HOH:O	2.29	0.65
1:A:813:PHE:HB3	1:A:957:MET:HE3	1.79	0.65
1:C:714:TYR:HB3	1:C:721:VAL:HG13	1.77	0.65
1:D:896:ILE:HG22	1:D:897:THR:HG23	1.77	0.65
1:D:636:ARG:HD2	1:D:660:ASP:HB3	1.80	0.64
1:A:964:ALA:HB3	1:A:967:HIS:CD2	2.32	0.64
1:A:610:GLY:O	1:A:611:GLU:HB2	1.97	0.64
1:A:643:VAL:HB	1:A:652:ILE:HG23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:560:TRP:HE1	1:D:891:MET:CE	2.05	0.64
1:C:745:ASN:ND2	1:C:963:SER:HB2	2.13	0.64
1:A:934:TYR:CE2	1:D:897:THR:HG22	2.34	0.63
1:B:613:TYR:HB2	1:B:622:VAL:HB	1.80	0.63
1:B:600:VAL:HG11	1:B:679:TYR:CD1	2.34	0.63
1:B:776:ASN:H	1:B:809:THR:HG21	1.63	0.63
1:C:541:ILE:CG2	1:C:555:VAL:HG11	2.29	0.63
1:A:771:ILE:HG13	1:A:785:ILE:HD13	1.80	0.63
1:B:505:TYR:HE2	1:B:825:LEU:HD21	1.64	0.63
1:B:612:LYS:HE2	1:B:623:ASP:OD2	1.99	0.62
1:C:849:ILE:HG12	1:C:916:ALA:HB2	1.81	0.62
1:D:548:ARG:NH2	1:D:875:LYS:NZ	2.47	0.62
1:B:688:ILE:HG22	1:B:694:VAL:HB	1.82	0.62
1:D:769:LEU:N	1:D:769:LEU:HD23	2.14	0.62
1:A:783:ILE:O	1:A:785:ILE:HG23	2.00	0.61
1:C:869:PHE:CE1	1:C:943:ILE:HG23	2.36	0.61
1:D:610:GLY:O	1:D:611:GLU:HB2	1.99	0.61
1:D:765:GLU:H	1:D:817:GLN:HE22	1.45	0.61
1:C:603:LEU:HD21	1:C:688:ILE:HD11	1.81	0.61
1:C:624:VAL:HG12	1:C:629:VAL:HG22	1.81	0.61
1:C:846:SER:O	1:C:847:GLY:O	2.18	0.61
1:C:849:ILE:CG1	1:C:916:ALA:HB2	2.30	0.61
1:D:608:ARG:HH21	1:D:611:GLU:HA	1.66	0.61
1:C:560:TRP:HE1	1:C:891:MET:CE	2.09	0.61
1:A:815:LEU:HD23	1:A:816:VAL:N	2.15	0.61
1:D:921:GLY:O	1:D:925:SER:HB2	2.00	0.61
1:A:565:PHE:CE2	1:A:567:VAL:HG12	2.36	0.60
1:A:801:VAL:HG13	1:A:803:VAL:HG23	1.83	0.60
1:C:841:LEU:HD11	1:C:916:ALA:CB	2.24	0.60
1:B:565:PHE:CE1	1:B:567:VAL:HG12	2.34	0.60
1:C:558:GLU:HB2	1:C:726:PRO:HG3	1.83	0.60
1:C:840:ILE:CG2	1:C:841:LEU:HG	2.31	0.60
1:D:671:THR:HB	1:D:674:ILE:O	2.01	0.60
1:B:906:LYS:H	1:B:906:LYS:HD3	1.66	0.60
1:C:964:ALA:C	1:C:966:HIS:H	2.09	0.60
1:B:784:LYS:HE2	1:B:787:GLU:OE2	2.01	0.60
1:B:505:TYR:CE2	1:B:825:LEU:HD21	2.36	0.60
1:C:894:PHE:HD2	1:C:894:PHE:O	1.85	0.60
1:A:819:GLY:HA3	1:A:953:LYS:HD3	1.83	0.59
1:B:752:GLU:HG3	1:B:802:ASN:HD21	1.67	0.59
1:D:736:ILE:HD11	1:D:741:LYS:HE2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:LEU:HD12	1:B:548:ARG:HG3	1.84	0.59
1:B:714:TYR:HB3	1:B:721:VAL:HG13	1.84	0.59
1:C:853:VAL:HG21	1:C:949:PHE:HE2	1.66	0.59
1:D:825:LEU:CD1	1:D:909:GLU:HG2	2.32	0.59
1:B:861:ALA:HB2	1:B:951:ALA:HB2	1.85	0.59
1:B:825:LEU:CD1	1:B:909:GLU:HG2	2.33	0.59
1:B:843:GLU:O	1:B:918:LEU:HB3	2.03	0.59
1:C:771:ILE:HD12	1:C:785:ILE:HG21	1.84	0.59
1:A:613:TYR:HB2	1:A:622:VAL:HB	1.85	0.59
1:D:781:GLU:OE1	1:D:806:PRO:HG3	2.03	0.59
1:B:511:TRP:HB3	4:B:975:HOH:O	2.03	0.58
1:B:513:ASP:OD2	1:B:516:TYR:HB3	2.03	0.58
1:B:560:TRP:CE2	1:B:891:MET:HE1	2.38	0.58
1:C:863:LEU:H	1:C:900:GLY:HA3	1.69	0.58
1:A:863:LEU:HB3	1:A:900:GLY:HA3	1.85	0.58
1:C:791:MET:O	1:C:792:ASP:HB3	2.03	0.58
1:C:815:LEU:HD23	1:C:816:VAL:N	2.18	0.58
1:D:541:ILE:HG22	1:D:555:VAL:HG11	1.86	0.58
1:B:613:TYR:CE1	1:B:670:LEU:HD22	2.39	0.58
1:C:568:TYR:CE2	1:C:570:ASN:HB2	2.39	0.58
1:C:938:LEU:HD12	1:C:939:ILE:H	1.68	0.58
1:A:648:SER:O	1:A:650:LYS:N	2.36	0.57
1:C:771:ILE:HG13	1:C:785:ILE:HD13	1.85	0.57
1:C:779:ILE:O	1:C:780:ILE:HD13	2.04	0.57
1:C:576:ASN:ND2	1:C:602:THR:HG23	2.19	0.57
1:A:861:ALA:HB1	1:A:950:ILE:O	2.03	0.57
1:B:784:LYS:NZ	1:B:787:GLU:HG2	2.19	0.57
1:C:840:ILE:HG22	1:C:841:LEU:HG	1.86	0.57
1:C:861:ALA:HB2	1:C:951:ALA:CB	2.29	0.57
1:A:714:TYR:HB3	1:A:721:VAL:HG13	1.87	0.57
1:C:626:ASN:HD22	1:C:628:SER:N	1.92	0.57
1:A:565:PHE:HE2	1:A:567:VAL:HG12	1.70	0.57
1:B:736:ILE:HD12	1:B:741:LYS:HD3	1.87	0.57
1:D:774:ILE:HB	1:D:810:SER:OG	2.04	0.57
1:D:867:ALA:HB2	1:D:896:ILE:HD11	1.87	0.57
1:C:712:PRO:HG3	1:C:722:TYR:CE2	2.40	0.57
1:B:569:LEU:HD13	1:B:691:ALA:HB1	1.87	0.56
1:B:795:ASN:O	1:B:796:GLU:O	2.23	0.56
1:C:669:HIS:HB2	1:C:676:VAL:CG1	2.34	0.56
1:A:646:THR:HG23	4:A:10:HOH:O	2.06	0.56
1:C:771:ILE:HD11	1:C:785:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:874:ARG:HB2	1:C:887:PHE:CE1	2.40	0.56
1:C:938:LEU:HD12	1:C:939:ILE:N	2.19	0.56
1:D:556:ASP:OD2	1:D:559:SER:HB2	2.05	0.56
1:D:623:ASP:HB3	1:D:630:LYS:HB3	1.87	0.56
1:B:725:THR:HG23	1:B:725:THR:O	2.04	0.56
1:D:763:ASP:OD2	1:D:792:ASP:HA	2.06	0.56
1:D:749:GLY:O	1:D:805:LEU:N	2.39	0.56
1:A:736:ILE:O	1:A:737:ASN:HB2	2.05	0.56
1:A:576:ASN:HD21	1:A:602:THR:H	1.54	0.56
1:C:914:VAL:HG12	1:C:915:ARG:N	2.21	0.56
1:D:688:ILE:HG22	1:D:694:VAL:HB	1.86	0.56
1:A:554:GLU:HG2	1:A:760:PHE:CE1	2.41	0.55
1:C:626:ASN:HD22	1:C:627:SER:H	1.54	0.55
1:C:938:LEU:HD11	1:C:940:ILE:HD12	1.87	0.55
1:C:541:ILE:HG22	1:C:555:VAL:HG11	1.88	0.55
1:C:906:LYS:O	1:C:907:GLU:C	2.50	0.55
1:B:915:ARG:HG3	1:B:916:ALA:N	2.21	0.55
1:D:750:LYS:HA	1:D:803:VAL:O	2.06	0.55
1:B:898:LYS:HE2	1:B:901:GLU:HG2	1.88	0.55
1:D:616:LEU:HD22	1:D:616:LEU:O	2.06	0.55
1:D:671:THR:HG23	1:D:672:PRO:HD2	1.89	0.55
1:D:791:MET:O	1:D:792:ASP:CB	2.55	0.55
1:A:815:LEU:HD23	1:A:815:LEU:C	2.31	0.55
1:D:568:TYR:HB3	1:D:571:ASP:OD2	2.06	0.55
1:A:776:ASN:O	1:A:778:LYS:HG3	2.06	0.55
1:A:853:VAL:HG21	1:A:949:PHE:CE1	2.42	0.55
1:B:496:LYS:HA	1:B:499:ARG:CZ	2.36	0.55
1:B:593:ASP:HB2	1:B:594:GLU:OE2	2.07	0.55
1:B:626:ASN:O	1:B:627:SER:HB3	2.06	0.55
1:D:626:ASN:N	1:D:626:ASN:ND2	2.55	0.55
1:B:488:THR:HG21	1:B:492:GLU:HB2	1.89	0.55
1:B:746:LEU:O	1:B:962:ALA:HA	2.05	0.55
1:B:768:THR:HG23	1:B:787:GLU:OE2	2.06	0.55
1:B:768:THR:HG23	1:B:784:LYS:HE2	1.88	0.55
1:C:780:ILE:O	1:C:781:GLU:CB	2.54	0.55
1:A:723:ARG:NH2	1:A:956:LEU:O	2.40	0.54
1:B:640:PRO:O	1:B:654:GLY:HA3	2.07	0.54
1:C:711:GLU:OE2	1:C:723:ARG:NH1	2.38	0.54
1:C:771:ILE:CD1	1:C:785:ILE:HD13	2.37	0.54
1:C:899:ILE:O	1:C:914:VAL:HG11	2.05	0.54
1:C:518:ILE:HD11	1:D:616:LEU:HD21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:ILE:HB	1:A:632:THR:OG1	2.08	0.54
1:C:857:LYS:HG3	1:C:859:TYR:CE1	2.41	0.54
1:C:774:ILE:HB	1:C:810:SER:OG	2.07	0.54
1:B:701:GLY:O	1:B:705:LYS:HG3	2.08	0.54
1:D:569:LEU:HD23	1:D:691:ALA:HB1	1.89	0.54
1:B:593:ASP:HA	1:B:883:TYR:CE2	2.43	0.54
1:C:774:ILE:O	1:C:808:ALA:HB1	2.07	0.54
1:D:659:SER:C	1:D:661:GLY:H	2.15	0.54
1:A:518:ILE:HD11	1:B:616:LEU:HD21	1.89	0.53
1:A:857:LYS:NZ	1:A:857:LYS:HB3	2.23	0.53
1:C:764:ILE:O	1:C:790:HIS:HA	2.07	0.53
1:B:851:LEU:HD12	1:B:851:LEU:O	2.08	0.53
1:C:791:MET:HE2	1:C:797:TYR:H	1.73	0.53
1:D:488:THR:HG23	1:D:488:THR:O	2.08	0.53
1:B:825:LEU:HD13	1:B:909:GLU:HG2	1.90	0.53
1:C:626:ASN:ND2	1:C:628:SER:H	1.95	0.53
1:C:771:ILE:CG1	1:C:785:ILE:HD13	2.38	0.53
1:D:773:ALA:HB3	1:D:780:ILE:O	2.07	0.53
1:A:606:LEU:HD23	1:A:615:ASN:HB2	1.90	0.53
1:B:821:ILE:HD12	1:B:821:ILE:C	2.34	0.53
1:C:712:PRO:HG3	1:C:722:TYR:HE2	1.71	0.53
1:B:757:ILE:HG23	1:B:957:MET:CE	2.39	0.53
1:B:922:VAL:O	1:B:923:ILE:HB	2.08	0.53
1:C:830:VAL:O	1:C:833:GLU:HG2	2.09	0.53
1:A:626:ASN:HD21	1:A:629:VAL:H	1.55	0.53
1:A:714:TYR:HB3	1:A:721:VAL:CG1	2.38	0.53
1:A:684:THR:HG21	1:A:698:THR:HG22	1.91	0.52
1:A:745:ASN:ND2	1:A:963:SER:HB3	2.24	0.52
1:C:815:LEU:HB2	1:C:957:MET:SD	2.49	0.52
1:A:647:PRO:O	1:A:649:GLY:N	2.42	0.52
1:B:548:ARG:NH2	1:B:888:GLU:OE2	2.42	0.52
1:B:540:HIS:CE1	1:B:581:LEU:HD22	2.44	0.52
1:D:747:THR:HG21	1:D:965:PRO:HB3	1.90	0.52
1:A:846:SER:OG	1:A:917:GLU:HG2	2.10	0.52
1:D:772:TYR:HB2	1:D:812:ARG:HB2	1.90	0.52
1:A:919:PRO:HB2	1:A:922:VAL:HG13	1.91	0.52
1:B:699:ILE:HB	1:B:702:PHE:HB2	1.92	0.52
1:D:723:ARG:NH2	1:D:956:LEU:O	2.42	0.52
1:B:562:LEU:C	1:B:562:LEU:HD23	2.35	0.52
1:C:815:LEU:HD23	1:C:815:LEU:C	2.35	0.52
1:C:846:SER:O	1:C:916:ALA:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:922:VAL:HG23	1:C:923:ILE:N	2.23	0.52
1:B:600:VAL:HG12	1:B:601:THR:N	2.25	0.52
1:C:840:ILE:HG22	1:C:841:LEU:N	2.24	0.52
1:C:868:THR:OG1	1:C:944:ARG:HB2	2.10	0.52
1:D:857:LYS:HA	1:D:907:GLU:HG2	1.91	0.52
1:C:671:THR:HG23	1:C:672:PRO:CD	2.39	0.51
1:C:953:LYS:HD3	1:C:955:TYR:CZ	2.45	0.51
1:A:964:ALA:HB3	1:A:967:HIS:NE2	2.26	0.51
1:B:842:ARG:O	1:B:918:LEU:HD23	2.10	0.51
1:C:608:ARG:HG2	1:C:608:ARG:HH11	1.73	0.51
1:D:496:LYS:HA	1:D:499:ARG:HE	1.73	0.51
1:A:774:ILE:O	1:A:808:ALA:HB1	2.09	0.51
1:C:701:GLY:O	1:C:705:LYS:HG3	2.09	0.51
1:A:620:VAL:HG22	1:A:633:VAL:HG22	1.93	0.51
1:B:490:GLY:HA3	1:B:716:SER:HB3	1.92	0.51
1:B:600:VAL:HG13	1:B:666:TYR:OH	2.11	0.51
1:D:636:ARG:CD	1:D:660:ASP:HB3	2.41	0.51
1:D:769:LEU:HD22	1:D:815:LEU:CD2	2.41	0.51
1:D:626:ASN:O	1:D:627:SER:HB3	2.10	0.51
1:C:594:GLU:HG2	1:C:595:SER:N	2.24	0.51
1:A:764:ILE:CA	1:A:817:GLN:HE22	2.20	0.51
1:C:763:ASP:OD2	1:C:792:ASP:HA	2.10	0.51
1:D:815:LEU:HD13	1:D:816:VAL:N	2.25	0.51
1:D:769:LEU:HD21	1:D:788:ILE:HG13	1.92	0.51
1:A:731:LYS:HD2	1:A:756:TYR:CD1	2.45	0.50
1:B:562:LEU:HD23	1:B:563:ASN:N	2.26	0.50
1:D:626:ASN:C	1:D:628:SER:H	2.18	0.50
1:A:746:LEU:O	1:A:962:ALA:HA	2.12	0.50
1:B:493:ASP:HB2	1:B:716:SER:OG	2.11	0.50
1:B:793:TYR:CE1	1:B:794:LEU:HG	2.47	0.50
1:A:866:ARG:HD2	1:A:893:VAL:CG2	2.41	0.50
1:B:737:ASN:OD1	1:B:737:ASN:O	2.30	0.50
1:B:751:HIS:N	1:B:803:VAL:O	2.44	0.50
1:B:731:LYS:HG3	1:B:742:GLN:NE2	2.27	0.50
1:A:913:LYS:O	1:A:914:VAL:HG23	2.11	0.50
1:B:775:ASN:HA	1:B:809:THR:HG23	1.92	0.50
1:C:505:TYR:HE2	1:C:825:LEU:HD21	1.76	0.50
1:C:853:VAL:CG2	1:C:949:PHE:HE2	2.24	0.50
1:D:805:LEU:HD13	1:D:811:TYR:CE2	2.46	0.50
1:A:509:THR:HG22	1:A:510:SER:N	2.27	0.50
1:A:626:ASN:C	1:A:626:ASN:HD22	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:828:PRO:CD	1:C:837:PRO:HG3	2.41	0.50
1:B:560:TRP:CZ2	1:B:891:MET:HE1	2.47	0.49
1:B:593:ASP:C	1:B:595:SER:H	2.20	0.49
1:C:896:ILE:HG21	1:C:918:LEU:CD1	2.42	0.49
1:A:496:LYS:O	1:A:500:GLU:HG3	2.12	0.49
1:B:713:VAL:O	1:B:714:TYR:HB2	2.12	0.49
1:B:784:LYS:HZ3	1:B:787:GLU:HG2	1.76	0.49
1:B:843:GLU:C	1:B:845:GLU:H	2.21	0.49
1:C:769:LEU:HG	1:C:785:ILE:HD11	1.94	0.49
1:B:568:TYR:HB3	1:B:571:ASP:OD2	2.11	0.49
1:B:801:VAL:HG13	1:B:803:VAL:HG13	1.94	0.49
1:C:853:VAL:HG21	1:C:949:PHE:CZ	2.47	0.49
1:D:830:VAL:HA	1:D:848:GLU:O	2.12	0.49
1:A:616:LEU:HD21	1:B:491:TRP:CD1	2.48	0.49
1:A:680:TYR:O	1:D:932:ARG:HD2	2.13	0.49
1:A:848:GLU:OE1	1:A:913:LYS:HD3	2.12	0.49
1:D:771:ILE:CD1	1:D:785:ILE:HG21	2.42	0.49
1:A:803:VAL:HG12	1:A:804:THR:N	2.26	0.49
1:A:600:VAL:HG11	1:A:679:TYR:CD1	2.48	0.49
1:B:875:LYS:HD3	1:B:888:GLU:HB2	1.95	0.49
1:C:780:ILE:O	1:C:781:GLU:HB3	2.12	0.49
1:D:646:THR:HG23	1:D:647:PRO:HA	1.94	0.49
1:A:820:PRO:HA	1:A:950:ILE:HD13	1.95	0.48
1:B:636:ARG:HG2	1:B:660:ASP:OD2	2.13	0.48
1:C:746:LEU:O	1:C:811:TYR:HE1	1.96	0.48
1:D:736:ILE:O	1:D:737:ASN:HB2	2.13	0.48
1:A:665:PRO:HB2	1:A:680:TYR:CD2	2.48	0.48
1:B:684:THR:O	1:B:689:LYS:NZ	2.46	0.48
1:B:752:GLU:HG3	1:B:802:ASN:ND2	2.29	0.48
1:A:628:SER:O	1:A:629:VAL:HB	2.12	0.48
1:B:882:ASP:CG	1:B:884:ASP:HB2	2.38	0.48
1:D:568:TYR:CZ	1:D:570:ASN:HB2	2.48	0.48
1:B:688:ILE:CG2	1:B:694:VAL:HB	2.42	0.48
1:B:755:LEU:CD1	1:B:769:LEU:HD21	2.44	0.48
1:C:830:VAL:O	1:C:831:ASN:HB2	2.14	0.48
1:D:636:ARG:HE	1:D:660:ASP:HB3	1.78	0.48
1:A:609:TYR:HB2	1:A:614:VAL:HG12	1.95	0.48
1:B:843:GLU:O	1:B:845:GLU:N	2.45	0.48
1:C:608:ARG:HG2	1:C:608:ARG:NH1	2.29	0.48
1:C:771:ILE:CD1	1:C:785:ILE:HG21	2.43	0.48
1:D:828:PRO:HB3	1:D:851:LEU:CD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:624:VAL:CG1	1:C:629:VAL:HG22	2.43	0.48
1:C:726:PRO:HB2	1:C:727:PHE:CE1	2.48	0.48
1:A:600:VAL:HG11	1:A:679:TYR:CG	2.49	0.48
1:A:610:GLY:O	1:A:611:GLU:CB	2.61	0.48
1:A:748:PRO:CG	1:A:807:ASN:HA	2.44	0.48
1:C:745:ASN:HD22	1:C:963:SER:HB2	1.77	0.48
1:A:600:VAL:HG13	1:A:666:TYR:OH	2.14	0.48
1:B:736:ILE:O	1:B:736:ILE:HG22	2.13	0.48
1:A:861:ALA:CB	1:A:951:ALA:HB2	2.41	0.47
1:C:491:TRP:CZ3	1:C:566:LEU:HD23	2.49	0.47
1:C:554:GLU:HG2	1:C:760:PHE:CE1	2.49	0.47
1:D:589:GLU:O	1:D:600:VAL:HG12	2.14	0.47
1:A:648:SER:C	1:A:650:LYS:H	2.22	0.47
1:B:919:PRO:O	1:B:922:VAL:HG22	2.14	0.47
1:B:716:SER:HB3	1:B:717:GLY:H	1.56	0.47
1:C:861:ALA:HB1	1:C:950:ILE:C	2.39	0.47
1:B:757:ILE:HD12	1:B:957:MET:CE	2.41	0.47
1:D:746:LEU:HD12	1:D:960:VAL:HG21	1.96	0.47
1:A:548:ARG:HH21	1:A:888:GLU:CD	2.23	0.47
1:A:626:ASN:O	1:A:627:SER:HB3	2.14	0.47
1:A:745:ASN:ND2	1:A:963:SER:CB	2.78	0.47
1:A:922:VAL:HG23	1:A:923:ILE:N	2.29	0.47
1:C:594:GLU:C	1:C:596:GLY:N	2.71	0.47
1:C:841:LEU:HD21	1:C:849:ILE:HD11	1.95	0.47
1:D:745:ASN:O	1:D:746:LEU:HB2	2.14	0.47
1:A:568:TYR:CZ	1:A:570:ASN:HB2	2.50	0.47
1:A:853:VAL:HG21	1:A:949:PHE:CZ	2.50	0.47
1:A:866:ARG:HD2	1:A:893:VAL:HG21	1.97	0.47
1:A:901:GLU:OE1	1:A:901:GLU:HA	2.14	0.47
1:B:867:ALA:HA	1:B:944:ARG:O	2.15	0.47
1:C:928:ASP:O	1:C:932:ARG:HG2	2.14	0.47
1:D:541:ILE:CG2	1:D:555:VAL:HG11	2.44	0.47
1:C:750:LYS:HA	1:C:803:VAL:O	2.15	0.47
1:C:874:ARG:HB2	1:C:887:PHE:HE1	1.77	0.47
1:D:736:ILE:HB	1:D:739:THR:HB	1.97	0.47
1:A:616:LEU:HD11	1:B:518:ILE:CD1	2.43	0.46
1:C:574:LYS:HG3	1:D:617:TYR:OH	2.15	0.46
1:B:489:SER:O	1:B:717:GLY:HA3	2.15	0.46
1:B:551:ASN:CG	1:B:794:LEU:HD22	2.40	0.46
1:C:870:ILE:CD1	1:C:891:MET:HE3	2.42	0.46
1:B:569:LEU:HD23	1:B:718:ASN:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:616:LEU:HD13	1:D:616:LEU:C	2.40	0.46
1:D:688:ILE:CG2	1:D:694:VAL:HB	2.45	0.46
1:D:736:ILE:O	1:D:736:ILE:HG22	2.14	0.46
1:C:768:THR:HB	1:C:770:TYR:HE1	1.79	0.46
1:D:852:LYS:HA	1:D:910:ASN:O	2.15	0.46
1:B:593:ASP:O	1:B:595:SER:N	2.48	0.46
1:A:594:GLU:O	1:B:587:ARG:NH2	2.49	0.46
1:C:903:ILE:N	1:C:903:ILE:HD12	2.30	0.46
1:C:915:ARG:HG2	1:C:915:ARG:HH11	1.81	0.46
1:D:560:TRP:CE2	1:D:891:MET:HE1	2.50	0.46
1:A:665:PRO:HB2	1:A:680:TYR:HD2	1.80	0.46
1:B:852:LYS:HE3	1:B:852:LYS:N	2.30	0.46
1:C:703:SER:O	1:C:707:PHE:HD1	1.99	0.46
1:B:845:GLU:HG2	1:B:846:SER:N	2.31	0.46
1:A:843:GLU:OE2	1:A:921:GLY:HA2	2.15	0.46
1:B:887:PHE:O	1:B:889:PRO:HD3	2.15	0.46
1:D:636:ARG:NE	1:D:660:ASP:HB3	2.31	0.46
1:D:853:VAL:HG21	1:D:949:PHE:HE1	1.79	0.46
1:B:781:GLU:OE1	1:B:806:PRO:HG3	2.16	0.45
1:D:600:VAL:HG21	1:D:679:TYR:CE1	2.51	0.45
1:A:867:ALA:HA	1:A:944:ARG:O	2.16	0.45
1:D:888:GLU:HA	1:D:889:PRO:HD3	1.83	0.45
1:A:725:THR:O	1:A:725:THR:HG23	2.16	0.45
1:B:588:ARG:HG3	1:B:598:GLY:HA3	1.98	0.45
1:B:917:GLU:O	1:B:919:PRO:HD3	2.17	0.45
1:D:669:HIS:HB2	1:D:676:VAL:HG13	1.98	0.45
1:D:698:THR:C	1:D:699:ILE:HD12	2.41	0.45
1:A:919:PRO:HB2	1:A:922:VAL:CG1	2.46	0.45
1:B:882:ASP:OD2	1:B:884:ASP:HB2	2.16	0.45
1:D:771:ILE:HG13	1:D:785:ILE:HD13	1.99	0.45
1:B:594:GLU:HG3	1:B:883:TYR:CE1	2.52	0.45
1:B:788:ILE:CG1	1:B:799:ILE:HD11	2.46	0.45
1:C:767:ALA:HB2	1:C:817:GLN:HB3	1.99	0.45
1:A:660:ASP:OD1	1:A:660:ASP:O	2.35	0.45
1:D:569:LEU:CD2	1:D:691:ALA:HB1	2.47	0.45
1:D:767:ALA:HB2	1:D:817:GLN:HE21	1.82	0.45
1:D:828:PRO:HB3	1:D:851:LEU:HD23	1.99	0.45
1:D:919:PRO:HB2	1:D:922:VAL:CG2	2.47	0.45
1:A:626:ASN:ND2	1:A:629:VAL:H	2.14	0.45
1:A:764:ILE:C	1:A:765:GLU:HG2	2.42	0.45
1:A:805:LEU:HB3	1:A:811:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:SER:OG	1:B:650:LYS:NZ	2.50	0.45
1:B:792:ASP:OD2	1:B:795:ASN:ND2	2.50	0.45
1:B:810:SER:HB2	1:B:960:VAL:O	2.17	0.45
1:A:626:ASN:HD21	1:A:629:VAL:N	2.14	0.45
1:B:500:GLU:O	1:B:501:ASN:ND2	2.50	0.45
1:C:863:LEU:HD13	1:C:949:PHE:CE1	2.52	0.45
1:C:964:ALA:O	1:C:966:HIS:N	2.49	0.45
1:D:600:VAL:HG23	1:D:666:TYR:OH	2.17	0.45
1:A:518:ILE:O	1:A:522:LEU:HB3	2.16	0.44
1:B:600:VAL:HG11	1:B:679:TYR:CG	2.51	0.44
1:C:606:LEU:HD23	1:C:615:ASN:HB2	1.99	0.44
1:C:867:ALA:HB3	1:C:894:PHE:CE2	2.52	0.44
1:C:870:ILE:HD11	1:C:891:MET:CE	2.43	0.44
1:C:688:ILE:HG22	1:C:694:VAL:HB	1.98	0.44
1:C:914:VAL:CG1	1:C:915:ARG:N	2.80	0.44
1:B:624:VAL:HG13	1:B:629:VAL:HG12	1.99	0.44
1:C:764:ILE:HG23	1:C:817:GLN:NE2	2.32	0.44
1:D:771:ILE:HG13	1:D:785:ILE:HG21	2.00	0.44
1:A:646:THR:O	1:A:672:PRO:HD3	2.18	0.44
1:C:512:TRP:CH2	1:D:619:LYS:HD2	2.53	0.44
1:D:635:ASP:HB2	1:D:636:ARG:NH1	2.33	0.44
1:D:674:ILE:HG12	1:D:675:GLY:N	2.32	0.44
1:A:705:LYS:HB3	1:A:758:SER:OG	2.17	0.44
1:A:899:ILE:O	1:A:914:VAL:HG11	2.17	0.44
1:B:495:LEU:HD13	1:B:519:GLU:HG3	1.98	0.44
1:B:569:LEU:HD23	1:B:718:ASN:C	2.41	0.44
1:B:914:VAL:HG12	1:B:915:ARG:N	2.31	0.44
1:B:922:VAL:HG23	1:B:923:ILE:HG12	2.00	0.44
1:C:793:TYR:CD1	1:C:794:LEU:HG	2.52	0.44
1:D:755:LEU:HB2	1:D:799:ILE:HG22	1.98	0.44
1:D:812:ARG:HG3	1:D:959:GLU:HG3	1.99	0.44
1:B:695:PRO:O	1:B:696:ALA:C	2.60	0.44
1:B:759:ALA:HB3	1:B:793:TYR:HA	2.00	0.44
1:B:863:LEU:HD12	1:B:948:VAL:O	2.17	0.44
1:B:630:LYS:HD2	1:B:637:GLU:OE2	2.17	0.44
1:B:724:PHE:CE2	1:B:726:PRO:HD3	2.52	0.44
1:B:857:LYS:HG2	1:B:859:TYR:CE1	2.53	0.44
1:D:587:ARG:HD3	4:D:34:HOH:O	2.16	0.44
1:A:625:SER:C	1:A:627:SER:H	2.26	0.44
1:B:830:VAL:CG2	1:B:835:ARG:HG3	2.48	0.44
1:D:640:PRO:O	1:D:654:GLY:HA3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:806:PRO:O	1:B:807:ASN:C	2.60	0.43
1:D:731:LYS:HG3	1:D:742:GLN:OE1	2.18	0.43
1:A:568:TYR:CE2	1:A:570:ASN:HB2	2.53	0.43
1:A:762:ARG:O	1:A:793:TYR:HB3	2.18	0.43
1:C:705:LYS:HB3	1:C:758:SER:OG	2.18	0.43
1:C:714:TYR:HB3	1:C:721:VAL:CG1	2.47	0.43
1:D:549:ASP:OD2	1:D:689:LYS:NZ	2.47	0.43
1:D:815:LEU:CB	1:D:957:MET:HE2	2.39	0.43
1:B:723:ARG:NH1	1:B:723:ARG:HB3	2.34	0.43
1:A:537:ASP:O	1:A:870:ILE:HG21	2.18	0.43
1:B:632:THR:HG22	1:B:637:GLU:HG3	2.00	0.43
1:D:568:TYR:CE2	1:D:570:ASN:HB2	2.53	0.43
1:B:755:LEU:HD12	1:B:769:LEU:HD21	2.01	0.43
1:C:594:GLU:C	1:C:596:GLY:H	2.26	0.43
1:C:791:MET:O	1:C:792:ASP:CB	2.67	0.43
1:C:793:TYR:CE1	1:C:794:LEU:HG	2.54	0.43
1:A:857:LYS:HG2	1:A:859:TYR:CE1	2.54	0.43
1:B:802:ASN:HD22	1:B:802:ASN:HA	1.67	0.43
1:B:851:LEU:C	1:B:852:LYS:HE3	2.44	0.43
1:C:872:LEU:HB2	1:C:939:ILE:HB	2.00	0.43
1:A:626:ASN:C	1:A:626:ASN:ND2	2.76	0.43
1:A:700:PRO:HA	4:A:20:HOH:O	2.19	0.43
1:A:840:ILE:O	1:A:841:LEU:HD12	2.18	0.43
1:B:747:THR:O	1:B:751:HIS:NE2	2.48	0.43
1:B:788:ILE:HD12	1:B:788:ILE:N	2.34	0.43
1:D:600:VAL:HG22	1:D:601:THR:H	1.84	0.43
1:D:779:ILE:O	1:D:780:ILE:HD13	2.19	0.43
1:A:489:SER:HB3	1:A:568:TYR:HE1	1.83	0.43
1:A:611:GLU:HA	1:A:611:GLU:OE1	2.19	0.42
1:C:770:TYR:N	1:C:770:TYR:CD1	2.87	0.42
1:D:799:ILE:O	1:D:799:ILE:HG23	2.19	0.42
1:A:866:ARG:CZ	1:A:948:VAL:HG21	2.49	0.42
1:B:788:ILE:HD12	1:B:788:ILE:H	1.85	0.42
1:A:731:LYS:HD2	1:A:756:TYR:CE1	2.53	0.42
1:B:588:ARG:HB2	1:B:883:TYR:HB3	2.02	0.42
1:B:788:ILE:HG13	1:B:799:ILE:HD11	2.00	0.42
1:C:576:ASN:ND2	1:C:602:THR:H	2.12	0.42
1:C:828:PRO:HD2	1:C:837:PRO:HG3	2.01	0.42
1:A:737:ASN:O	1:A:739:THR:N	2.52	0.42
1:B:865:LEU:HD13	1:B:918:LEU:HD13	2.00	0.42
1:C:773:ALA:HB3	1:C:780:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:CYS:HA	1:A:658:CYS:HA	2.01	0.42
1:B:490:GLY:CA	1:B:716:SER:HB3	2.50	0.42
1:B:774:ILE:HD13	1:B:779:ILE:HA	2.01	0.42
1:C:823:VAL:O	1:C:825:LEU:HD23	2.19	0.42
1:D:602:THR:O	1:D:678:ALA:HA	2.19	0.42
1:D:735:ASN:HB3	1:D:752:GLU:HB2	2.02	0.42
1:D:779:ILE:H	1:D:779:ILE:HG13	1.69	0.42
1:A:826:ASP:OD1	1:A:852:LYS:HD2	2.19	0.42
1:D:699:ILE:HA	1:D:700:PRO:HD2	1.91	0.42
1:A:737:ASN:C	1:A:739:THR:N	2.67	0.42
1:B:712:PRO:HB3	1:B:722:TYR:CE2	2.55	0.42
1:B:729:ILE:HG12	1:B:757:ILE:HD13	2.01	0.42
1:B:745:ASN:OD1	1:B:963:SER:HB2	2.20	0.42
1:B:748:PRO:HG3	1:B:811:TYR:OH	2.20	0.42
1:C:849:ILE:HD11	1:C:916:ALA:HB2	2.01	0.42
1:B:861:ALA:HB1	1:B:950:ILE:O	2.20	0.42
1:C:705:LYS:HG2	1:C:730:TYR:CE2	2.55	0.42
1:A:537:ASP:OD1	1:A:537:ASP:N	2.51	0.42
1:A:647:PRO:C	1:A:649:GLY:H	2.28	0.42
1:C:735:ASN:HB3	1:C:752:GLU:HB3	2.02	0.42
1:D:498:LEU:HD11	1:D:566:LEU:HD11	2.02	0.42
1:C:587:ARG:NH2	1:D:594:GLU:O	2.54	0.41
1:C:889:PRO:C	1:C:890:GLN:HG2	2.45	0.41
1:C:939:ILE:HD12	1:C:939:ILE:N	2.34	0.41
1:D:497:TRP:O	1:D:501:ASN:ND2	2.53	0.41
1:A:684:THR:O	1:A:689:LYS:NZ	2.53	0.41
1:B:725:THR:O	1:B:725:THR:CG2	2.68	0.41
1:A:489:SER:HB3	1:A:568:TYR:CE1	2.56	0.41
1:A:648:SER:C	1:A:650:LYS:N	2.78	0.41
1:C:642:MET:SD	1:C:651:THR:HG23	2.60	0.41
1:A:803:VAL:CG1	1:A:804:THR:N	2.83	0.41
1:B:919:PRO:O	1:B:920:GLU:C	2.63	0.41
1:D:544:LEU:HD12	1:D:548:ARG:HG3	2.02	0.41
1:D:750:LYS:C	1:D:751:HIS:ND1	2.78	0.41
1:D:882:ASP:OD2	1:D:884:ASP:HB2	2.20	0.41
1:A:842:ARG:HB2	1:A:845:GLU:OE2	2.20	0.41
1:B:488:THR:C	1:B:490:GLY:H	2.29	0.41
1:B:906:LYS:HD3	1:B:906:LYS:N	2.33	0.41
1:D:572:TRP:CE2	1:D:605:PRO:HG3	2.56	0.41
1:D:600:VAL:HG22	1:D:601:THR:N	2.35	0.41
1:D:725:THR:O	1:D:725:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:VAL:HG22	1:A:615:ASN:N	2.36	0.41
1:B:503:PRO:HB3	1:B:856:ASP:CG	2.46	0.41
1:A:767:ALA:HA	1:A:816:VAL:O	2.20	0.41
1:B:811:TYR:CE1	1:B:962:ALA:HB2	2.56	0.41
1:C:849:ILE:CD1	1:C:916:ALA:HB2	2.51	0.41
1:C:930:LEU:HB3	1:C:938:LEU:HD22	2.02	0.41
1:D:502:THR:HA	1:D:503:PRO:HD3	1.91	0.41
1:D:899:ILE:O	1:D:914:VAL:HG21	2.21	0.41
1:B:857:LYS:HB3	1:B:857:LYS:NZ	2.36	0.41
1:C:851:LEU:HD12	1:C:912:VAL:HB	2.03	0.41
1:C:887:PHE:O	1:C:889:PRO:HD3	2.21	0.41
1:D:534:HIS:O	1:D:535:ALA:HB2	2.21	0.41
1:D:569:LEU:O	1:D:572:TRP:HD1	2.04	0.41
1:D:769:LEU:HD21	1:D:788:ILE:CD1	2.50	0.41
1:A:730:TYR:CZ	1:A:756:TYR:HB3	2.55	0.40
1:D:643:VAL:O	1:D:651:THR:HA	2.21	0.40
1:D:659:SER:C	1:D:661:GLY:N	2.75	0.40
1:A:794:LEU:HD11	1:D:920:GLU:HB3	2.03	0.40
1:C:496:LYS:HA	1:C:499:ARG:NH2	2.36	0.40
1:D:548:ARG:NH2	1:D:875:LYS:HZ1	2.19	0.40
1:D:608:ARG:HD2	1:D:672:PRO:O	2.21	0.40
1:D:874:ARG:CZ	1:D:879:ASP:HA	2.51	0.40
1:D:964:ALA:HB1	1:D:966:HIS:ND1	2.36	0.40
1:B:567:VAL:HG22	1:B:720:ILE:HB	2.04	0.40
1:C:509:THR:HG22	1:C:510:SER:N	2.36	0.40
1:C:965:PRO:O	1:C:966:HIS:C	2.64	0.40
1:D:548:ARG:HD3	1:D:584:ALA:HB2	2.02	0.40
1:B:490:GLY:HA3	1:B:717:GLY:H	1.86	0.40
1:B:705:LYS:HB3	1:B:758:SER:OG	2.21	0.40
1:B:725:THR:HA	1:B:726:PRO:HD2	1.90	0.40
1:C:612:LYS:HB2	1:C:622:VAL:O	2.22	0.40
1:D:811:TYR:O	1:D:959:GLU:HA	2.21	0.40
1:D:812:ARG:CG	1:D:959:GLU:HG3	2.51	0.40
1:D:964:ALA:HB1	1:D:966:HIS:CE1	2.56	0.40
1:C:558:GLU:HB2	1:C:726:PRO:CG	2.51	0.40
1:C:772:TYR:HB2	1:C:812:ARG:HB2	2.03	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	468/497 (94%)	430 (92%)	26 (6%)	12 (3%)	4	11
1	B	464/497 (93%)	419 (90%)	31 (7%)	14 (3%)	3	8
1	C	466/497 (94%)	404 (87%)	50 (11%)	12 (3%)	4	11
1	D	467/497 (94%)	425 (91%)	35 (8%)	7 (2%)	8	22
All	All	1865/1988 (94%)	1678 (90%)	142 (8%)	45 (2%)	4	12

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	536	ARG
1	B	796	GLU
1	B	843	GLU
1	C	847	GLY
1	A	610	GLY
1	A	648	SER
1	A	649	GLY
1	A	776	ASN
1	A	808	ALA
1	B	594	GLU
1	B	844	GLY
1	C	901	GLU
1	C	935	GLY
1	A	717	GLY
1	A	737	ASN
1	B	716	SER
1	B	737	ASN
1	C	626	ASN
1	C	781	GLU
1	C	907	GLU
1	D	523	LEU
1	D	746	LEU

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Mol	Chain	Res	Type
1	A	625	SER
1	A	629	VAL
1	B	522	LEU
1	B	696	ALA
1	B	777	GLU
1	C	916	ALA
1	C	925	SER
1	D	648	SER
1	A	535	ALA
1	B	501	ASN
1	B	923	ILE
1	C	899	ILE
1	C	965	PRO
1	D	792	ASP
1	B	714	TYR
1	D	781	GLU
1	B	919	PRO
1	C	592	GLY
1	D	610	GLY
1	A	738	GLY
1	B	717	GLY
1	C	896	ILE
1	D	717	GLY

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	402/424 (95%)	373 (93%)	29 (7%)	13	32
1	B	399/424 (94%)	381 (96%)	18 (4%)	24	52
1	C	400/424 (94%)	383 (96%)	17 (4%)	26	54
1	D	400/424 (94%)	377 (94%)	23 (6%)	18	42
All	All	1601/1696 (94%)	1514 (95%)	87 (5%)	20	45

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	507	THR
1	A	567	VAL
1	A	576	ASN
1	A	587	ARG
1	A	608	ARG
1	A	623	ASP
1	A	626	ASN
1	A	644	THR
1	A	650	LYS
1	A	652	ILE
1	A	657	THR
1	A	672	PRO
1	A	676	VAL
1	A	690	LEU
1	A	698	THR
1	A	703	SER
1	A	721	VAL
1	A	723	ARG
1	A	765	GLU
1	A	777	GLU
1	A	787	GLU
1	A	801	VAL
1	A	841	LEU
1	A	846	SER
1	A	852	LYS
1	A	857	LYS
1	A	893	VAL
1	A	927	LYS
1	A	929	GLU
1	B	513	ASP
1	B	538	ARG
1	B	548	ARG
1	B	594	GLU
1	B	616	LEU
1	B	635	ASP
1	B	646	THR
1	B	716	SER
1	B	721	VAL
1	B	745	ASN
1	B	783	ILE
1	B	801	VAL
1	B	802	ASN
1	B	852	LYS

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Mol	Chain	Res	Type
1	B	857	LYS
1	B	897	THR
1	B	906	LYS
1	B	915	ARG
1	C	542	LEU
1	C	576	ASN
1	C	616	LEU
1	C	626	ASN
1	C	671	THR
1	C	676	VAL
1	C	690	LEU
1	C	721	VAL
1	C	727	PHE
1	C	752	GLU
1	C	753	LEU
1	C	770	TYR
1	C	821	ILE
1	C	840	ILE
1	C	851	LEU
1	C	894	PHE
1	C	946	GLU
1	D	513	ASP
1	D	538	ARG
1	D	561	GLU
1	D	576	ASN
1	D	601	THR
1	D	604	LEU
1	D	614	VAL
1	D	626	ASN
1	D	629	VAL
1	D	632	THR
1	D	676	VAL
1	D	690	LEU
1	D	721	VAL
1	D	745	ASN
1	D	769	LEU
1	D	777	GLU
1	D	783	ILE
1	D	815	LEU
1	D	890	GLN
1	D	893	VAL
1	D	915	ARG

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Mol	Chain	Res	Type
1	D	925	SER
1	D	965	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	576	ASN
1	A	626	ASN
1	A	662	ASN
1	A	709	ASN
1	A	718	ASN
1	A	742	GLN
1	A	745	ASN
1	A	802	ASN
1	A	817	GLN
1	A	839	ASN
1	A	890	GLN
1	A	902	ASN
1	B	501	ASN
1	B	540	HIS
1	B	709	ASN
1	B	718	ASN
1	B	742	GLN
1	B	775	ASN
1	B	795	ASN
1	B	802	ASN
1	B	839	ASN
1	C	540	HIS
1	C	576	ASN
1	C	626	ASN
1	C	709	ASN
1	C	718	ASN
1	C	742	GLN
1	C	745	ASN
1	C	775	ASN
1	C	776	ASN
1	C	817	GLN
1	D	501	ASN
1	D	570	ASN
1	D	576	ASN
1	D	626	ASN
1	D	709	ASN

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Mol	Chain	Res	Type
1	D	718	ASN
1	D	742	GLN
1	D	745	ASN
1	D	790	HIS
1	D	802	ASN
1	D	807	ASN
1	D	817	GLN
1	D	931	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 8 ligands modelled in this entry, 8 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

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, 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	472/497 (94%)	-0.17	8 (1%) 69 67	10, 37, 59, 89	0
1	B	468/497 (94%)	0.08	7 (1%) 72 70	17, 46, 64, 81	0
1	C	470/497 (94%)	0.43	22 (4%) 36 33	25, 57, 81, 94	0
1	D	471/497 (94%)	-0.11	12 (2%) 58 55	13, 36, 75, 97	0
All	All	1881/1988 (94%)	0.06	49 (2%) 57 54	10, 43, 75, 97	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	736	ILE	5.1
1	C	966	HIS	4.9
1	D	738	GLY	4.4
1	B	964	ALA	4.4
1	C	487	GLU	4.3
1	B	488	THR	3.7
1	C	964	ALA	3.3
1	D	488	THR	3.2
1	B	489	SER	3.0
1	C	965	PRO	3.0
1	A	628	SER	3.0
1	C	625	SER	3.0
1	D	739	THR	2.8
1	C	781	GLU	2.8
1	D	737	ASN	2.7
1	C	739	THR	2.5
1	A	967	HIS	2.5
1	C	488	THR	2.5
1	C	830	VAL	2.5
1	C	922	VAL	2.5
1	B	780	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	488	THR	2.4
1	C	920	GLU	2.4
1	D	524	GLY	2.4
1	D	964	ALA	2.4
1	C	736	ILE	2.4
1	C	737	ASN	2.4
1	A	765	GLU	2.3
1	D	779	ILE	2.3
1	C	919	PRO	2.3
1	B	661	GLY	2.3
1	A	658	CYS	2.2
1	B	776	ASN	2.2
1	D	965	PRO	2.2
1	A	627	SER	2.2
1	C	740	TRP	2.2
1	C	900	GLY	2.2
1	C	849	ILE	2.2
1	D	745	ASN	2.2
1	C	848	GLU	2.2
1	C	869	PHE	2.2
1	C	696	ALA	2.1
1	D	489	SER	2.1
1	C	894	PHE	2.1
1	A	965	PRO	2.1
1	C	738	GLY	2.1
1	D	735	ASN	2.1
1	B	635	ASP	2.0
1	A	964	ALA	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(Å ²)	Q<0.9
2	CA	B	2	1/1	0.91	0.09	37,37,37,37	0
3	CL	C	7	1/1	0.91	0.12	55,55,55,55	0
3	CL	B	6	1/1	0.92	0.08	44,44,44,44	0
2	CA	C	3	1/1	0.94	0.13	53,53,53,53	0
2	CA	D	4	1/1	0.94	0.14	38,38,38,38	0
3	CL	A	5	1/1	0.97	0.07	31,31,31,31	0
2	CA	A	1	1/1	0.98	0.09	26,26,26,26	0
3	CL	D	8	1/1	0.98	0.04	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.