



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:15 PM EDT

PDB ID : 2ZAG / pdb_00002zag
Title : Crystal structure of the SeMet-substituted soluble domain of STT3 from P. furiosus
Authors : Maita, N.
Deposited on : 2007-10-05
Resolution : 3.00 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
Mogul : 2022.3.0, CSD as543be (2022)
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

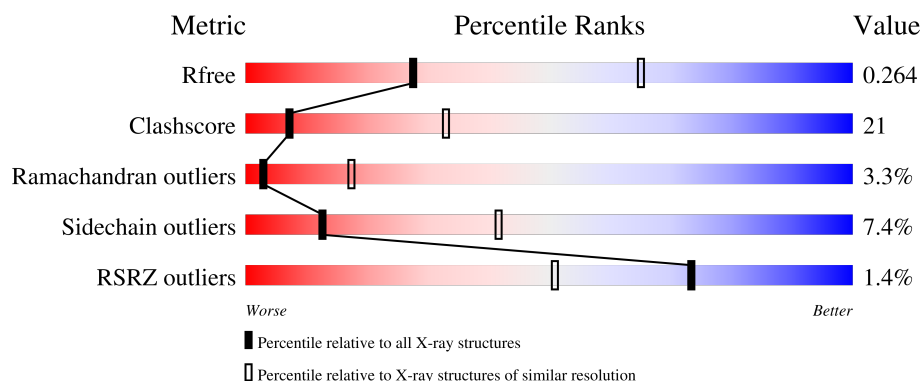
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	2% 50% 39% 7% • •
1	B	497	% 54% 36% 5% •
1	C	497	% 50% 38% 7% •
1	D	497	% 53% 36% 7% •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15179 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
1	A	478	Total	C	N	O	S	Se	0	0	0
			3790	2444	615	725	2	4			
1	B	477	Total	C	N	O	S	Se	0	0	0
			3786	2441	617	722	2	4			
1	C	478	Total	C	N	O	S	Se	0	0	0
			3792	2445	618	723	2	4			
1	D	480	Total	C	N	O	S	Se	0	0	0
			3803	2452	621	724	2	4			

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

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

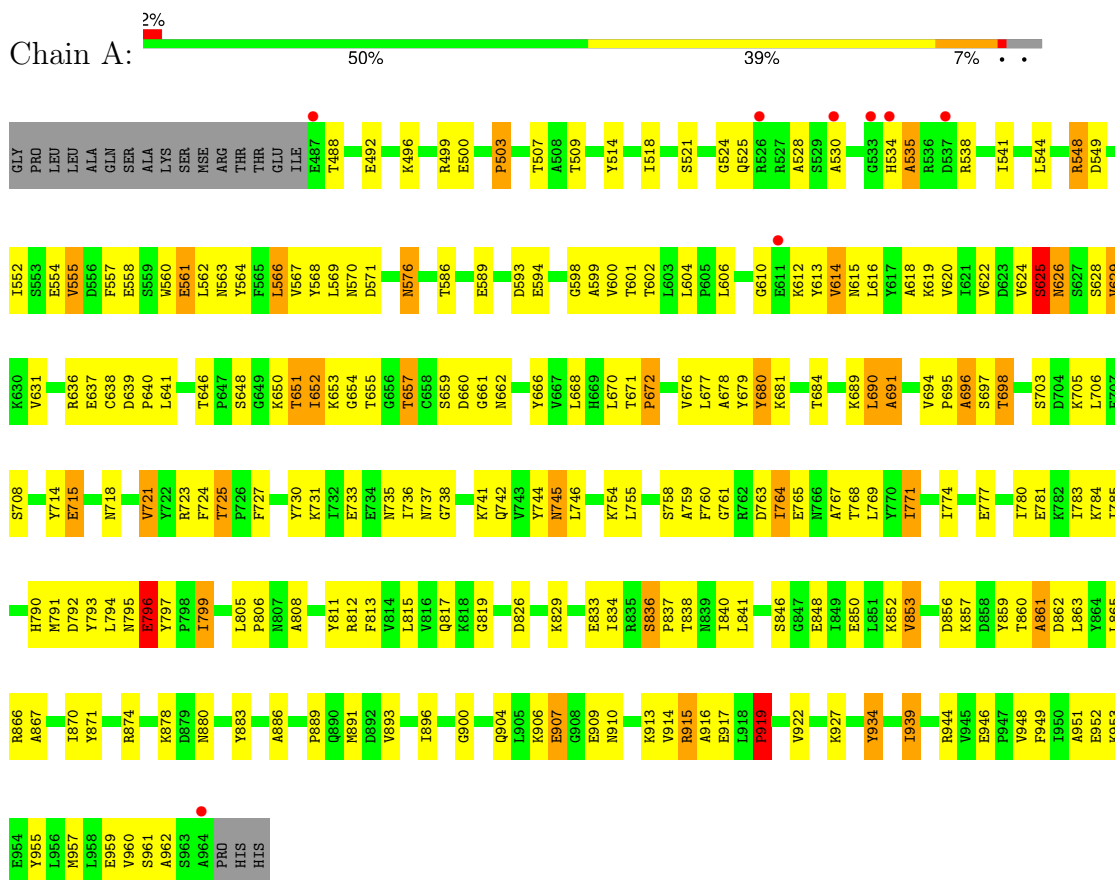
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

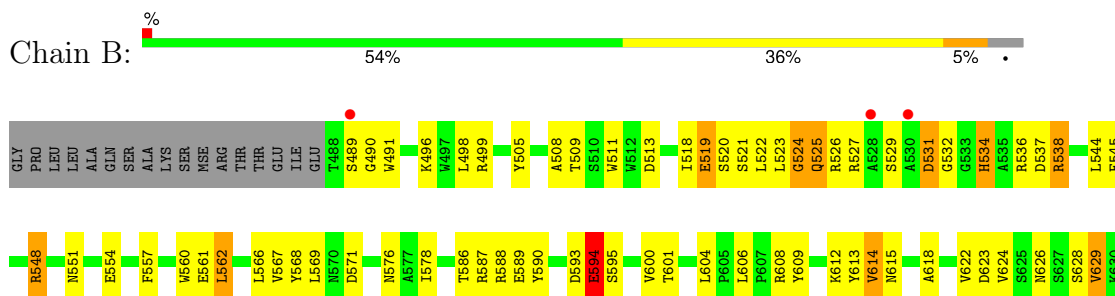
3 Residue-property plots

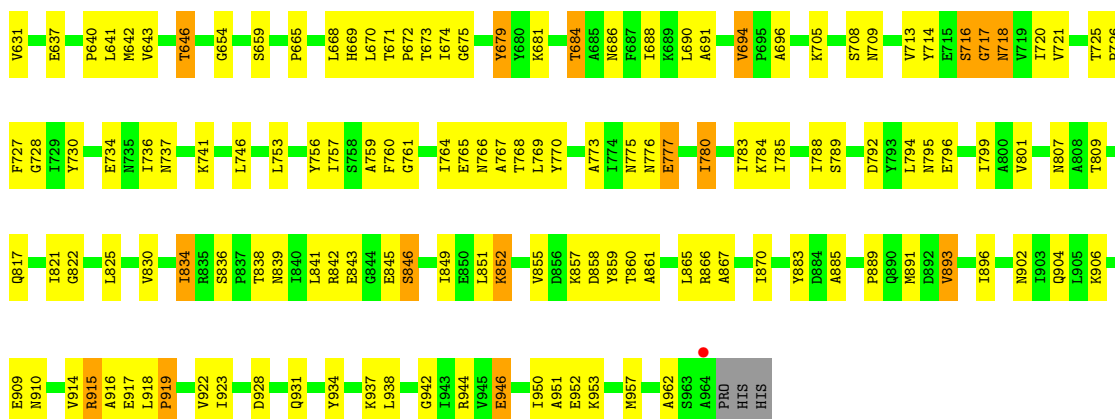
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

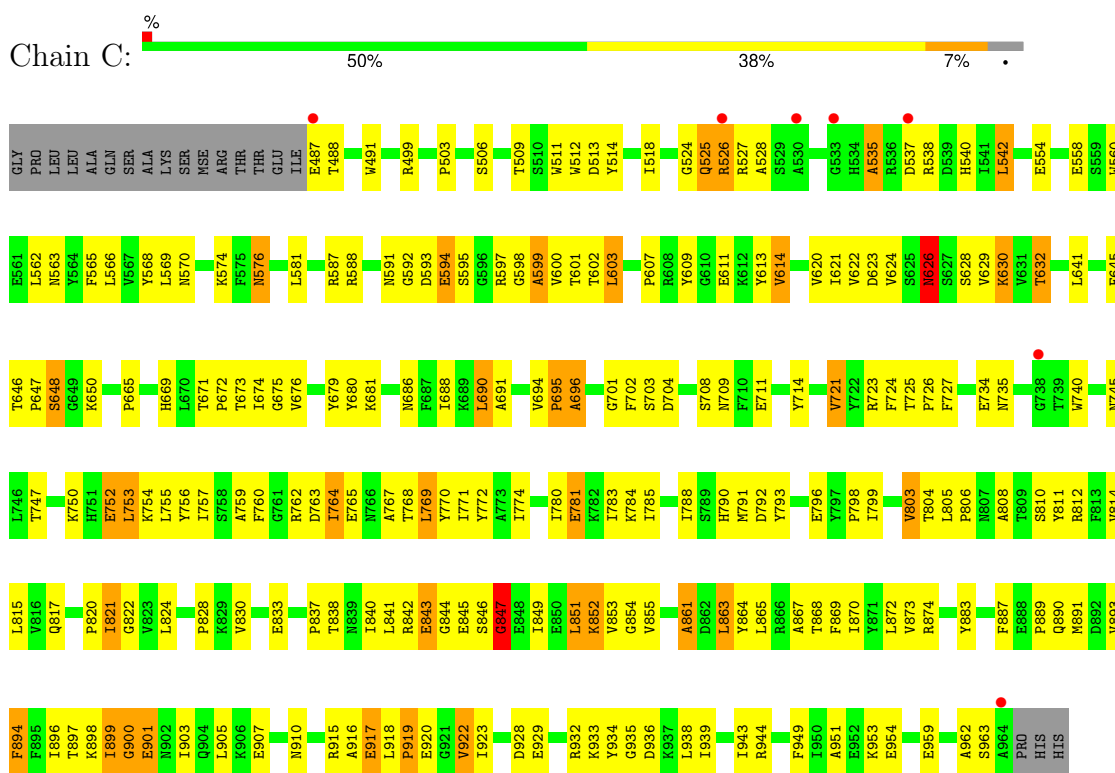


- Molecule 1: Oligosaccharyl transferase stt3 subunit related protein

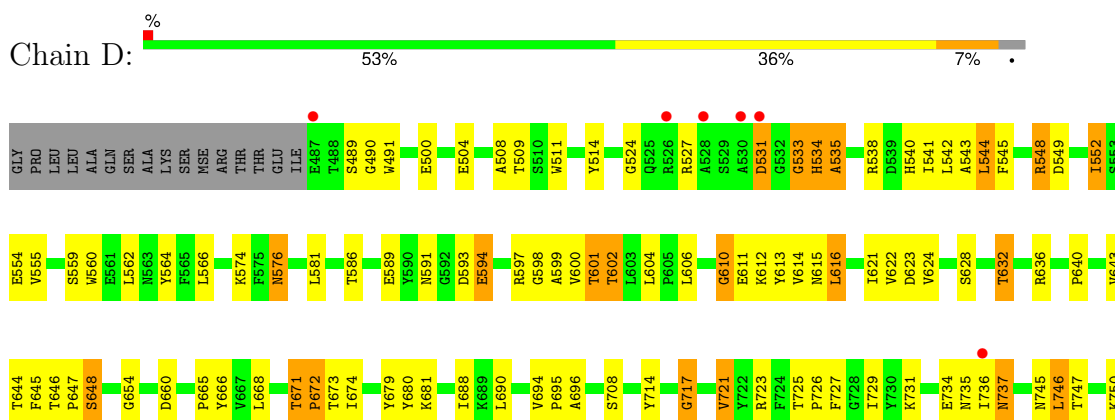


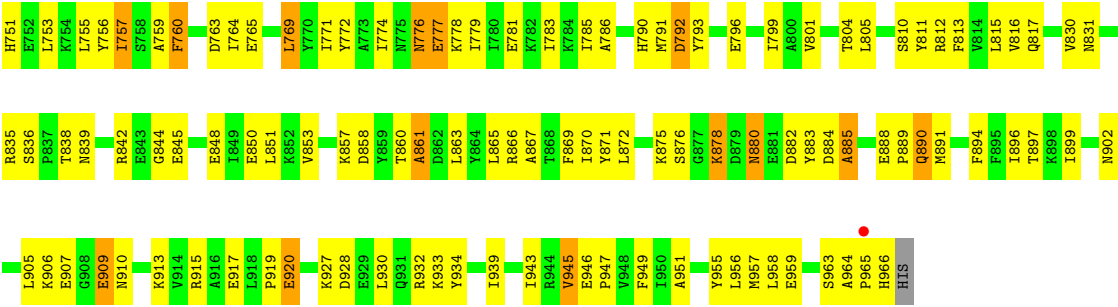


• Molecule 1: Oligosaccharyl transferase stt3 subunit related protein



• 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	137.40Å 266.40Å 73.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.00) 99.5 (20.00-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.15 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.272 0.216 , 0.264	Depositor DCC
R_{free} test set	3928 reflections (7.11%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15179	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: 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	0.56	0/3876	1.07	25/5261 (0.5%)
1	B	0.51	0/3872	1.03	15/5255 (0.3%)
1	C	0.46	0/3878	0.98	13/5263 (0.2%)
1	D	0.56	0/3891	1.02	13/5283 (0.2%)
All	All	0.52	0/15517	1.02	66/21062 (0.3%)

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	D	0	1

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	641	LEU	N-CA-C	-10.29	100.46	113.23
1	C	611	GLU	N-CA-C	-8.02	102.81	112.59
1	A	614	VAL	N-CA-C	7.64	118.73	108.27
1	D	860	THR	N-CA-C	-7.63	96.09	108.52
1	D	878	LYS	N-CA-C	-7.38	104.42	113.50
1	C	526	ARG	N-CA-C	7.10	118.99	110.19
1	A	771	ILE	N-CA-C	-7.04	98.25	108.11
1	B	679	TYR	N-CA-C	-6.99	101.31	110.53
1	A	660	ASP	N-CA-C	-6.96	104.05	112.54
1	B	614	VAL	N-CA-C	6.94	118.72	108.45
1	B	694	VAL	CA-C-N	6.60	126.28	119.82
1	B	694	VAL	C-N-CA	6.60	126.28	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	521	SER	N-CA-C	6.56	118.43	111.28
1	D	602	THR	N-CA-C	6.42	118.35	111.36
1	A	659	SER	N-CA-C	-6.37	105.36	113.01
1	C	753	LEU	N-CA-C	6.37	118.75	109.07
1	D	885	ALA	N-CA-C	6.37	119.59	110.10
1	A	934	TYR	N-CA-C	6.25	121.67	113.30
1	C	614	VAL	N-CA-C	6.18	117.19	108.17
1	D	861	ALA	N-CA-C	6.18	119.26	109.50
1	A	862	ASP	N-CA-C	-6.12	100.88	110.36
1	A	952	GLU	N-CA-C	-5.98	99.53	109.46
1	B	629	VAL	N-CA-C	5.98	117.09	108.48
1	D	708	SER	N-CA-C	-5.88	106.11	113.28
1	A	697	SER	N-CA-C	5.83	117.94	108.26
1	A	861	ALA	N-CA-C	5.83	118.55	109.52
1	C	847	GLY	N-CA-C	5.82	126.97	113.18
1	D	865	LEU	N-CA-C	-5.75	99.36	108.73
1	A	680	TYR	N-CA-C	5.74	117.54	111.28
1	B	764	ILE	N-CA-C	-5.70	99.52	108.23
1	B	885	ALA	N-CA-C	5.67	118.67	110.28
1	A	561	GLU	N-CA-C	-5.64	103.62	111.52
1	C	680	TYR	N-CA-C	5.61	118.12	111.33
1	B	860	THR	N-CA-C	-5.58	97.36	107.75
1	C	929	GLU	N-CA-C	-5.58	105.59	112.90
1	A	886	ALA	N-CA-C	-5.55	99.97	109.24
1	D	680	TYR	N-CA-C	5.55	118.05	111.33
1	B	809	THR	N-CA-C	-5.53	106.66	113.41
1	B	708	SER	N-CA-C	-5.51	106.06	112.89
1	C	861	ALA	N-CA-C	5.51	117.35	109.14
1	B	718	ASN	N-CA-C	-5.49	106.47	112.72
1	A	761	GLY	N-CA-C	5.46	121.34	114.25
1	A	661	GLY	N-CA-C	-5.45	107.17	114.25
1	D	783	ILE	N-CA-C	5.36	116.43	108.23
1	B	761	GLY	N-CA-C	5.33	122.14	115.21
1	C	708	SER	N-CA-C	-5.32	106.84	113.38
1	A	691	ALA	N-CA-C	5.30	117.87	111.40
1	A	865	LEU	N-CA-C	-5.30	98.61	107.99
1	A	636	ARG	N-CA-C	5.28	117.34	110.43
1	B	561	GLU	N-CA-C	-5.27	105.50	112.24
1	C	542	LEU	N-CA-C	-5.27	105.62	111.36
1	A	708	SER	N-CA-C	-5.25	107.05	113.50
1	D	880	ASN	N-CA-C	5.24	118.78	112.38
1	A	853	VAL	N-CA-C	5.21	115.36	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	764	ILE	N-CA-C	-5.18	100.43	107.99
1	A	764	ILE	N-CA-C	-5.17	100.32	108.23
1	D	930	LEU	N-CA-C	-5.17	105.54	111.07
1	B	536	ARG	N-CA-C	5.10	121.66	110.80
1	D	888	GLU	N-CA-C	5.10	116.33	109.24
1	C	936	ASP	N-CA-C	-5.09	107.02	113.18
1	C	803	VAL	N-CA-C	5.07	115.00	108.82
1	D	760	PHE	N-CA-C	5.07	117.18	107.75
1	A	760	PHE	N-CA-C	5.05	116.87	107.99
1	A	651	THR	N-CA-C	5.04	115.64	107.32
1	B	937	LYS	N-CA-C	-5.03	107.11	113.20
1	A	678	ALA	N-CA-C	5.02	117.24	108.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	955	TYR	Sidechain

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	3790	0	3721	157	0
1	B	3786	0	3724	133	0
1	C	3792	0	3728	184	0
1	D	3803	0	3726	164	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	1	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	1	0
All	All	15179	0	14899	623	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (623) 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:C:560:TRP:HE1	1:C:891:MSE:HE1	1.25	0.98
1:B:537:ASP:HB3	1:B:870:ILE:HD12	1.46	0.97
1:B:834:ILE:HD13	1:B:834:ILE:H	1.32	0.95
1:B:560:TRP:HE1	1:B:891:MSE:HE1	1.36	0.89
1:A:846:SER:HB3	1:A:917:GLU:HG3	1.57	0.87
1:A:863:LEU:HB3	1:A:900:GLY:HA3	1.54	0.87
1:C:487:GLU:CG	1:C:488:THR:H	1.87	0.86
1:D:757:ILE:HD13	1:D:757:ILE:H	1.40	0.85
1:C:841:LEU:HD11	1:C:916:ALA:HB1	1.59	0.85
1:D:535:ALA:HB3	1:D:538:ARG:HB2	1.60	0.84
1:D:755:LEU:HB2	1:D:799:ILE:HG22	1.61	0.81
1:D:906:LYS:H	1:D:910:ASN:HD21	1.30	0.78
1:A:541:ILE:HG23	1:A:555:VAL:HG21	1.64	0.78
1:A:606:LEU:HD23	1:A:615:ASN:HB2	1.66	0.77
1:B:569:LEU:HD12	1:B:718:ASN:HA	1.66	0.77
1:B:852:LYS:H	1:B:852:LYS:HZ2	1.30	0.77
1:B:861:ALA:HB2	1:B:951:ALA:HB2	1.64	0.77
1:B:867:ALA:HB2	1:B:896:ILE:HD11	1.66	0.76
1:A:813:PHE:HB3	1:A:957:MSE:HE3	1.67	0.75
1:C:861:ALA:HB2	1:C:951:ALA:HB2	1.69	0.75
1:B:490:GLY:HA3	1:B:717:GLY:H	1.51	0.75
1:A:745:ASN:HB2	1:A:961:SER:O	1.87	0.74
1:C:771:ILE:HG13	1:C:785:ILE:HD13	1.69	0.73
1:A:569:LEU:HB2	1:A:718:ASN:HB3	1.70	0.73
1:D:747:THR:HG21	1:D:965:PRO:HB3	1.72	0.72
1:D:491:TRP:HZ3	1:D:566:LEU:HD23	1.54	0.72
1:D:747:THR:HG22	1:D:963:SER:HB2	1.72	0.72
1:D:791:MSE:O	1:D:792:ASP:HB3	1.89	0.72
1:D:600:VAL:HG12	1:D:601:THR:N	2.04	0.71
1:B:560:TRP:NE1	1:B:891:MSE:HE1	2.05	0.71
1:B:709:ASN:ND2	1:B:760:PHE:HB2	2.06	0.70
1:D:560:TRP:HE1	1:D:891:MSE:HE1	1.56	0.70
1:D:863:LEU:HD23	1:D:899:ILE:HG13	1.73	0.70
1:A:625:SER:O	1:A:626:ASN:HB3	1.92	0.70
1:B:569:LEU:HD23	1:B:691:ALA:HB1	1.73	0.69
1:B:834:ILE:H	1:B:834:ILE:CD1	2.03	0.69
1:C:621:ILE:HB	1:C:632:THR:HG23	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:767:ALA:HB2	1:C:817:GLN:HE21	1.57	0.68
1:C:624:VAL:HG22	1:C:629:VAL:HG12	1.75	0.68
1:C:623:ASP:HB3	1:C:630:LYS:HB3	1.74	0.68
1:C:671:THR:HG22	1:C:673:THR:H	1.59	0.68
1:A:600:VAL:HG11	1:A:679:TYR:CD1	2.28	0.67
1:D:839:ASN:HA	1:D:945:VAL:HG23	1.75	0.67
1:B:593:ASP:HB2	1:B:594:GLU:OE2	1.93	0.67
1:A:934:TYR:CE2	1:D:897:THR:HG22	2.29	0.67
1:D:896:ILE:HG22	1:D:897:THR:HG23	1.76	0.67
1:C:767:ALA:HB2	1:C:817:GLN:HB3	1.75	0.66
1:B:834:ILE:HD13	1:B:834:ILE:N	2.07	0.66
1:C:560:TRP:NE1	1:C:891:MSE:HE1	2.07	0.66
1:C:867:ALA:HA	1:C:944:ARG:O	1.95	0.66
1:D:540:HIS:ND1	1:D:872:LEU:HD21	2.11	0.66
1:D:765:GLU:H	1:D:817:GLN:NE2	1.94	0.66
1:C:781:GLU:HG3	1:C:783:ILE:HG23	1.78	0.65
1:B:688:ILE:HG22	1:B:694:VAL:HB	1.79	0.65
1:C:863:LEU:HG	1:C:899:ILE:HD12	1.76	0.65
1:B:785:ILE:HB	1:B:801:VAL:HG21	1.79	0.65
1:C:735:ASN:HB3	1:C:752:GLU:HB3	1.79	0.65
1:A:767:ALA:HB2	1:A:817:GLN:HE21	1.61	0.65
1:A:765:GLU:H	1:A:817:GLN:HE22	1.43	0.65
1:C:641:LEU:HD11	1:C:665:PRO:HA	1.79	0.65
1:A:544:LEU:HD13	1:A:889:PRO:HG2	1.79	0.64
1:A:652:ILE:HD12	1:A:653:LYS:N	2.12	0.64
1:A:560:TRP:HE1	1:A:891:MSE:HE1	1.61	0.64
1:A:755:LEU:HB2	1:A:799:ILE:HG22	1.78	0.64
1:A:541:ILE:HG23	1:A:555:VAL:CG2	2.28	0.64
1:A:745:ASN:C	1:A:745:ASN:HD22	2.05	0.64
1:B:846:SER:OG	1:B:917:GLU:HG3	1.98	0.64
1:B:505:TYR:HE2	1:B:825:LEU:HD21	1.64	0.63
1:B:838:THR:HA	1:B:946:GLU:HG2	1.80	0.63
1:C:922:VAL:HG23	1:C:923:ILE:H	1.63	0.63
1:A:684:THR:HG21	1:A:698:THR:HG22	1.81	0.62
1:B:865:LEU:HD13	1:B:918:LEU:HD13	1.81	0.62
1:D:850:GLU:HG3	1:D:913:LYS:HG2	1.81	0.62
1:A:774:ILE:O	1:A:808:ALA:HB1	1.99	0.62
1:D:763:ASP:OD2	1:D:792:ASP:HA	2.00	0.61
1:D:870:ILE:HD11	1:D:891:MSE:HE3	1.81	0.61
1:B:767:ALA:HB2	1:B:817:GLN:HB3	1.82	0.61
1:B:637:GLU:H	1:B:659:SER:HB2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:714:TYR:HB3	1:B:721:VAL:CG1	2.31	0.61
1:C:671:THR:HB	1:C:674:ILE:O	2.00	0.61
1:A:600:VAL:HG12	1:A:601:THR:N	2.14	0.61
1:A:735:ASN:C	1:A:735:ASN:HD22	2.08	0.61
1:D:679:TYR:HE2	1:D:681:LYS:HD2	1.65	0.61
1:D:774:ILE:HB	1:D:810:SER:OG	2.01	0.61
1:A:846:SER:HB3	1:A:917:GLU:CG	2.30	0.61
1:A:586:THR:OG1	1:A:589:GLU:HG3	2.01	0.61
1:C:851:LEU:O	1:C:851:LEU:HD12	2.01	0.61
1:D:600:VAL:CG1	1:D:601:THR:N	2.64	0.61
1:C:830:VAL:O	1:C:833:GLU:HG2	2.00	0.60
1:C:518:ILE:HD11	1:D:616:LEU:HD11	1.83	0.60
1:C:613:TYR:HB2	1:C:622:VAL:HB	1.82	0.60
1:D:714:TYR:HB3	1:D:721:VAL:CG1	2.31	0.60
1:A:919:PRO:HB2	1:A:922:VAL:HG13	1.82	0.59
1:A:934:TYR:HE2	1:D:897:THR:HG22	1.66	0.59
1:C:593:ASP:HA	1:C:883:TYR:CE2	2.37	0.59
1:A:698:THR:HG21	1:D:932:ARG:HE	1.68	0.59
1:A:746:LEU:O	1:A:962:ALA:HA	2.01	0.59
1:A:771:ILE:HG13	1:A:785:ILE:HD13	1.84	0.59
1:B:508:ALA:O	1:B:532:GLY:HA2	2.02	0.59
1:C:540:HIS:HD2	1:C:872:LEU:HD21	1.65	0.59
1:C:592:GLY:N	1:C:599:ALA:HB2	2.18	0.59
1:C:646:THR:O	1:C:672:PRO:HD3	2.02	0.59
1:D:842:ARG:HB2	1:D:842:ARG:HH11	1.67	0.59
1:C:491:TRP:HZ3	1:C:566:LEU:HD23	1.67	0.59
1:C:844:GLY:HA2	1:C:918:LEU:O	2.03	0.59
1:D:759:ALA:HB3	1:D:793:TYR:HA	1.85	0.58
1:D:764:ILE:HA	1:D:817:GLN:HE22	1.68	0.58
1:D:765:GLU:H	1:D:817:GLN:HE22	1.51	0.58
1:A:765:GLU:H	1:A:817:GLN:NE2	2.01	0.58
1:D:870:ILE:HD11	1:D:891:MSE:CE	2.33	0.58
1:D:671:THR:HG22	1:D:673:THR:H	1.69	0.58
1:B:569:LEU:HB2	1:B:718:ASN:HB3	1.85	0.58
1:C:750:LYS:HD2	1:C:804:THR:HG23	1.84	0.58
1:B:757:ILE:HD12	1:B:957:MSE:HE1	1.85	0.58
1:B:612:LYS:HE2	1:B:623:ASP:OD2	2.04	0.58
1:C:846:SER:O	1:C:916:ALA:HB3	2.04	0.58
1:C:918:LEU:HD12	1:C:919:PRO:HD2	1.86	0.58
1:B:792:ASP:HB3	1:B:795:ASN:HB2	1.86	0.58
1:D:600:VAL:HG11	1:D:679:TYR:CD1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:LEU:HD12	1:A:960:VAL:HG21	1.86	0.57
1:B:526:ARG:O	1:B:527:ARG:HG2	2.03	0.57
1:B:857:LYS:HG2	1:B:858:ASP:H	1.69	0.57
1:C:852:LYS:HB2	1:C:852:LYS:NZ	2.19	0.57
1:D:964:ALA:HB1	1:D:966:HIS:ND1	2.19	0.57
1:B:852:LYS:H	1:B:852:LYS:NZ	2.02	0.57
1:C:626:ASN:ND2	1:C:628:SER:H	2.02	0.57
1:C:838:THR:HG23	1:C:944:ARG:HG2	1.86	0.57
1:D:964:ALA:HB1	1:D:966:HIS:CE1	2.39	0.57
1:D:560:TRP:NE1	1:D:891:MSE:HE1	2.20	0.57
1:D:769:LEU:N	1:D:769:LEU:HD23	2.20	0.57
1:B:746:LEU:O	1:B:962:ALA:HA	2.04	0.57
1:B:788:ILE:HD11	1:B:799:ILE:HD13	1.86	0.57
1:A:679:TYR:HE2	1:A:681:LYS:HD2	1.69	0.57
1:B:560:TRP:HE1	1:B:891:MSE:CE	2.13	0.57
1:A:694:VAL:C	1:A:696:ALA:H	2.13	0.57
1:C:774:ILE:O	1:C:808:ALA:HB1	2.05	0.57
1:D:511:TRP:HH2	1:D:581:LEU:HD12	1.68	0.57
1:A:499:ARG:HG3	1:A:500:GLU:HG3	1.86	0.56
1:B:544:LEU:HD12	1:B:548:ARG:HG3	1.85	0.56
1:C:540:HIS:CD2	1:C:872:LEU:HD21	2.40	0.56
1:A:528:ALA:HB3	1:A:530:ALA:O	2.06	0.56
1:A:705:LYS:HB3	1:A:758:SER:OG	2.05	0.56
1:C:840:ILE:HG23	1:C:841:LEU:HG	1.87	0.56
1:A:731:LYS:HG3	1:A:742:GLN:NE2	2.21	0.56
1:B:643:VAL:HG13	1:B:668:LEU:HD23	1.87	0.56
1:A:840:ILE:O	1:A:841:LEU:HD12	2.06	0.56
1:D:597:ARG:HB3	1:D:597:ARG:NH1	2.21	0.56
1:D:772:TYR:HB2	1:D:812:ARG:HB2	1.88	0.56
1:C:701:GLY:O	1:C:703:SER:N	2.39	0.55
1:C:772:TYR:HB2	1:C:812:ARG:HB2	1.88	0.55
1:B:671:THR:HG22	1:B:673:THR:HG22	1.86	0.55
1:A:614:VAL:HG23	1:A:620:VAL:O	2.06	0.55
1:D:640:PRO:O	1:D:654:GLY:HA3	2.06	0.55
1:A:909:GLU:C	1:A:910:ASN:HD22	2.14	0.55
1:C:714:TYR:HB3	1:C:721:VAL:HG13	1.87	0.55
1:C:726:PRO:HB2	1:C:727:PHE:CE1	2.42	0.55
1:D:858:ASP:OD2	1:D:906:LYS:HA	2.06	0.55
1:D:490:GLY:HA3	1:D:717:GLY:H	1.71	0.55
1:A:791:MSE:HG3	1:A:797:TYR:CE2	2.40	0.55
1:D:906:LYS:N	1:D:910:ASN:HD21	2.02	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:586:THR:OG1	1:D:589:GLU:HG3	2.06	0.55
1:D:750:LYS:HB3	1:D:804:THR:HA	1.89	0.55
1:B:606:LEU:HD23	1:B:615:ASN:HB2	1.89	0.54
1:C:535:ALA:HB3	1:C:538:ARG:HB2	1.89	0.54
1:C:740:TRP:CZ3	1:C:754:LYS:HG3	2.42	0.54
1:A:680:TYR:CE1	1:D:933:LYS:HB2	2.42	0.54
1:A:765:GLU:N	1:A:817:GLN:HE22	2.05	0.54
1:A:880:ASN:ND2	1:A:939:ILE:HD11	2.23	0.54
1:B:775:ASN:O	1:B:777:GLU:N	2.40	0.54
1:C:601:THR:HG22	1:C:601:THR:O	2.07	0.54
1:D:805:LEU:HB3	1:D:811:TYR:CE2	2.42	0.54
1:C:727:PHE:CD2	1:C:764:ILE:HG12	2.43	0.54
1:B:821:ILE:HG23	1:B:953:LYS:HD2	1.90	0.54
1:D:905:LEU:HA	1:D:910:ASN:ND2	2.23	0.54
1:A:604:LEU:HG	1:A:615:ASN:HD22	1.72	0.53
1:B:505:TYR:CE2	1:B:825:LEU:HD21	2.42	0.53
1:B:714:TYR:O	1:B:721:VAL:HG12	2.08	0.53
1:C:558:GLU:OE2	1:C:558:GLU:HA	2.07	0.53
1:D:757:ILE:HD13	1:D:757:ILE:N	2.16	0.53
1:D:811:TYR:O	1:D:959:GLU:HA	2.08	0.53
1:C:537:ASP:HB2	1:C:870:ILE:HG21	1.90	0.53
1:C:780:ILE:O	1:C:781:GLU:HG2	2.08	0.53
1:C:874:ARG:HD3	1:C:887:PHE:HE1	1.72	0.53
1:B:568:TYR:HB3	1:B:571:ASP:OD2	2.08	0.53
1:D:548:ARG:HH21	1:D:875:LYS:NZ	2.06	0.53
1:D:769:LEU:HD22	1:D:815:LEU:CD2	2.38	0.53
1:A:488:THR:HG21	1:A:492:GLU:HG2	1.90	0.53
1:C:814:VAL:HG11	1:C:954:GLU:HG2	1.89	0.53
1:B:534:HIS:O	1:B:538:ARG:HG3	2.08	0.53
1:C:511:TRP:HH2	1:C:581:LEU:HD12	1.74	0.53
1:C:609:TYR:HB2	1:C:614:VAL:HG12	1.91	0.53
1:C:861:ALA:HB2	1:C:951:ALA:CB	2.37	0.53
1:D:610:GLY:C	1:D:612:LYS:H	2.16	0.53
1:A:768:THR:HG23	1:A:784:LYS:HE2	1.91	0.53
1:B:825:LEU:HD13	1:B:909:GLU:HG2	1.90	0.53
1:C:554:GLU:HG2	1:C:760:PHE:CE1	2.44	0.53
1:C:603:LEU:HD21	1:C:688:ILE:HD11	1.91	0.53
1:D:576:ASN:ND2	1:D:602:THR:H	2.07	0.53
1:B:734:GLU:HG3	1:B:753:LEU:HD23	1.90	0.53
1:C:688:ILE:HG22	1:C:694:VAL:HB	1.90	0.53
1:D:688:ILE:HG22	1:D:694:VAL:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:776:ASN:O	1:D:777:GLU:HB2	2.09	0.53
1:D:844:GLY:HA2	1:D:920:GLU:HG3	1.90	0.53
1:D:928:ASP:HB3	1:D:932:ARG:NH2	2.24	0.53
1:A:819:GLY:HA3	1:A:953:LYS:HD3	1.90	0.53
1:B:861:ALA:HB1	1:B:950:ILE:O	2.08	0.53
1:A:616:LEU:HD11	1:B:518:ILE:HD11	1.92	0.52
1:B:836:SER:C	1:B:838:THR:H	2.16	0.52
1:C:745:ASN:ND2	1:C:963:SER:HB2	2.24	0.52
1:C:626:ASN:N	1:C:626:ASN:HD22	2.06	0.52
1:C:781:GLU:OE1	1:C:806:PRO:HG3	2.10	0.52
1:A:861:ALA:HB2	1:A:951:ALA:HB2	1.90	0.52
1:D:791:MSE:O	1:D:792:ASP:CB	2.57	0.52
1:A:560:TRP:NE1	1:A:891:MSE:HE1	2.24	0.52
1:A:576:ASN:HD21	1:A:602:THR:H	1.58	0.52
1:A:860:THR:HG23	1:A:904:GLN:NE2	2.24	0.52
1:C:763:ASP:OD2	1:C:792:ASP:HA	2.09	0.52
1:D:836:SER:C	1:D:838:THR:H	2.17	0.52
1:D:853:VAL:HG21	1:D:949:PHE:CE1	2.45	0.52
1:B:604:LEU:HD21	1:B:618:ALA:CB	2.39	0.52
1:B:725:THR:HG23	1:B:725:THR:O	2.09	0.52
1:C:874:ARG:HH11	1:C:874:ARG:HG2	1.75	0.52
1:C:785:ILE:HG22	1:C:803:VAL:HG11	1.91	0.52
1:D:489:SER:O	1:D:717:GLY:HA3	2.09	0.52
1:D:613:TYR:HB2	1:D:622:VAL:HB	1.91	0.52
1:D:876:SER:O	1:D:885:ALA:HA	2.10	0.52
1:A:640:PRO:O	1:A:654:GLY:HA3	2.10	0.52
1:C:558:GLU:HB3	1:C:762:ARG:NE	2.25	0.52
1:A:715:GLU:OE1	1:A:715:GLU:N	2.43	0.51
1:D:746:LEU:HD21	1:D:753:LEU:HD21	1.92	0.51
1:A:857:LYS:HE2	1:A:859:TYR:CZ	2.46	0.51
1:C:499:ARG:HG2	1:C:527:ARG:NH1	2.25	0.51
1:A:650:LYS:HD3	1:A:651:THR:H	1.75	0.51
1:B:684:THR:HG22	1:B:696:ALA:O	2.11	0.51
1:B:859:TYR:O	1:B:904:GLN:HA	2.10	0.51
1:D:757:ILE:HD11	1:D:791:MSE:HE1	1.92	0.51
1:D:871:TYR:N	1:D:871:TYR:CD2	2.77	0.51
1:A:680:TYR:CD1	1:D:933:LYS:HB2	2.46	0.51
1:B:788:ILE:HD12	1:B:788:ILE:N	2.25	0.51
1:C:769:LEU:HD11	1:C:815:LEU:HD12	1.91	0.51
1:D:671:THR:HB	1:D:674:ILE:O	2.11	0.51
1:D:714:TYR:HB3	1:D:721:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:731:LYS:HD2	1:D:756:TYR:CE1	2.45	0.51
1:A:836:SER:C	1:A:838:THR:H	2.19	0.51
1:C:841:LEU:HD21	1:C:849:ILE:HD11	1.92	0.51
1:A:863:LEU:HD13	1:A:949:PHE:CE2	2.46	0.51
1:B:730:TYR:CZ	1:B:756:TYR:HB3	2.46	0.51
1:C:671:THR:HG23	1:C:672:PRO:HD2	1.93	0.51
1:A:852:LYS:HD3	1:A:909:GLU:OE1	2.11	0.50
1:D:857:LYS:HA	1:D:907:GLU:HG2	1.93	0.50
1:A:705:LYS:HG2	1:A:730:TYR:CE2	2.46	0.50
1:B:604:LEU:HD21	1:B:618:ALA:HB3	1.93	0.50
1:A:913:LYS:O	1:A:914:VAL:HG23	2.11	0.50
1:B:588:ARG:HB2	1:B:883:TYR:HB3	1.93	0.50
1:C:811:TYR:O	1:C:959:GLU:HA	2.11	0.50
1:A:668:LEU:HD21	1:A:670:LEU:HD21	1.93	0.50
1:D:866:ARG:NH1	3:D:8:CL:CL	2.78	0.50
1:D:905:LEU:HD23	1:D:910:ASN:HD22	1.76	0.50
1:B:557:PHE:HB3	1:B:562:LEU:HD12	1.92	0.50
1:C:487:GLU:CG	1:C:488:THR:N	2.56	0.50
1:D:576:ASN:ND2	1:D:602:THR:OG1	2.42	0.50
1:D:813:PHE:HB3	1:D:957:MSE:HE3	1.93	0.50
1:A:764:ILE:O	1:A:790:HIS:HA	2.10	0.50
1:D:560:TRP:HE1	1:D:891:MSE:CE	2.24	0.50
1:D:830:VAL:HB	1:D:835:ARG:HG3	1.92	0.50
1:B:519:GLU:HG2	1:B:525:GLN:NE2	2.26	0.50
1:D:541:ILE:HG13	1:D:891:MSE:HE3	1.93	0.50
1:A:499:ARG:HB3	1:A:499:ARG:NH1	2.27	0.50
1:B:531:ASP:OD1	1:B:531:ASP:N	2.41	0.50
1:C:846:SER:O	1:C:847:GLY:O	2.29	0.50
1:C:849:ILE:HG12	1:C:916:ALA:HB2	1.94	0.50
1:B:775:ASN:O	1:B:776:ASN:HB3	2.11	0.50
1:B:624:VAL:HG13	1:B:629:VAL:HG12	1.93	0.49
1:B:914:VAL:HG12	1:B:915:ARG:O	2.12	0.49
1:A:568:TYR:HB3	1:A:571:ASP:OD2	2.11	0.49
1:A:600:VAL:HG12	1:A:601:THR:H	1.77	0.49
1:A:680:TYR:O	1:D:932:ARG:HD2	2.12	0.49
1:C:568:TYR:CZ	1:C:570:ASN:HB2	2.47	0.49
1:C:828:PRO:HD3	1:C:837:PRO:HG3	1.94	0.49
1:C:853:VAL:HG21	1:C:949:PHE:CE2	2.47	0.49
1:B:537:ASP:CB	1:B:870:ILE:HD12	2.32	0.49
1:B:613:TYR:CE1	1:B:670:LEU:HD22	2.47	0.49
1:C:842:ARG:O	1:C:918:LEU:HD23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:880:ASN:ND2	1:D:939:ILE:HD11	2.27	0.49
1:A:909:GLU:C	1:A:910:ASN:ND2	2.71	0.49
1:C:799:ILE:O	1:C:799:ILE:HG23	2.12	0.49
1:A:631:VAL:HB	1:A:638:CYS:O	2.12	0.49
1:B:769:LEU:HD12	1:B:785:ILE:CG1	2.42	0.49
1:C:781:GLU:CD	1:C:806:PRO:HG3	2.36	0.49
1:D:838:THR:HA	1:D:946:GLU:HG2	1.93	0.49
1:B:593:ASP:C	1:B:595:SER:H	2.21	0.49
1:A:610:GLY:C	1:A:612:LYS:H	2.18	0.49
1:A:780:ILE:O	1:A:781:GLU:HB2	2.12	0.49
1:C:745:ASN:HD21	1:C:963:SER:HB2	1.77	0.49
1:A:534:HIS:O	1:A:538:ARG:HB2	2.13	0.49
1:A:724:PHE:CG	1:A:725:THR:N	2.80	0.49
1:A:853:VAL:HG21	1:A:949:PHE:CE1	2.47	0.49
1:C:709:ASN:OD1	1:C:760:PHE:HB2	2.12	0.49
1:C:568:TYR:CE2	1:C:570:ASN:HB2	2.48	0.49
1:C:811:TYR:HE1	1:C:962:ALA:HB2	1.78	0.49
1:D:508:ALA:HA	1:D:564:TYR:O	2.13	0.49
1:D:871:TYR:CE2	1:D:890:GLN:HB3	2.47	0.49
1:A:600:VAL:HG13	1:A:666:TYR:OH	2.13	0.49
1:A:866:ARG:NH1	3:A:5:CL:CL	2.81	0.49
1:B:496:LYS:HA	1:B:499:ARG:CZ	2.43	0.49
1:B:849:ILE:HG22	1:B:851:LEU:HD23	1.94	0.49
1:C:509:THR:OG1	1:C:562:LEU:HD13	2.13	0.49
1:C:626:ASN:ND2	1:C:626:ASN:N	2.59	0.48
1:C:853:VAL:HG12	1:C:854:GLY:N	2.28	0.48
1:D:491:TRP:CZ3	1:D:566:LEU:HD23	2.41	0.48
1:D:548:ARG:NH2	1:D:875:LYS:NZ	2.61	0.48
1:B:537:ASP:OD1	1:B:942:GLY:HA3	2.12	0.48
1:B:922:VAL:O	1:B:923:ILE:HB	2.14	0.48
1:C:747:THR:HB	1:C:963:SER:O	2.13	0.48
1:C:764:ILE:O	1:C:790:HIS:HA	2.13	0.48
1:A:557:PHE:HB3	1:A:562:LEU:HD23	1.96	0.48
1:C:669:HIS:HB2	1:C:676:VAL:HG13	1.94	0.48
1:D:867:ALA:HB3	1:D:894:PHE:CE2	2.48	0.48
1:D:745:ASN:O	1:D:746:LEU:HB2	2.11	0.48
1:C:647:PRO:O	1:C:648:SER:HB3	2.14	0.48
1:A:594:GLU:O	1:B:587:ARG:NH2	2.47	0.48
1:B:830:VAL:HG22	1:B:849:ILE:HG12	1.95	0.48
1:C:898:LYS:HG2	1:C:901:GLU:OE2	2.13	0.48
1:D:726:PRO:HG2	1:D:727:PHE:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:734:GLU:HG2	1:D:735:ASN:N	2.29	0.48
1:A:813:PHE:HB3	1:A:957:MSE:CE	2.42	0.48
1:C:790:HIS:HE1	1:C:792:ASP:HB2	1.77	0.48
1:C:558:GLU:HB2	1:C:726:PRO:HG3	1.96	0.48
1:C:765:GLU:H	1:C:817:GLN:NE2	2.12	0.48
1:C:770:TYR:HB2	1:C:772:TYR:HE1	1.79	0.48
1:C:855:VAL:HG23	1:C:907:GLU:HA	1.96	0.48
1:A:666:TYR:HB3	1:A:677:LEU:HD11	1.95	0.48
1:B:554:GLU:HA	1:B:760:PHE:CZ	2.49	0.48
1:C:852:LYS:HB2	1:C:852:LYS:HZ2	1.77	0.48
1:D:514:TYR:OH	1:D:574:LYS:HE2	2.13	0.47
1:D:544:LEU:HD12	1:D:548:ARG:HG3	1.95	0.47
1:D:729:ILE:HG12	1:D:757:ILE:HG22	1.96	0.47
1:B:736:ILE:HD12	1:B:741:LYS:HD3	1.95	0.47
1:C:754:LYS:NZ	1:C:754:LYS:HB3	2.29	0.47
1:A:805:LEU:HB3	1:A:811:TYR:CE2	2.49	0.47
1:D:848:GLU:OE1	1:D:913:LYS:HD3	2.14	0.47
1:A:689:LYS:HE3	1:A:696:ALA:O	2.13	0.47
1:A:714:TYR:HB3	1:A:721:VAL:CG1	2.44	0.47
1:A:736:ILE:O	1:A:737:ASN:HB2	2.14	0.47
1:B:526:ARG:C	1:B:527:ARG:HG2	2.38	0.47
1:D:593:ASP:HB2	1:D:594:GLU:OE1	2.14	0.47
1:A:566:LEU:HD12	1:A:721:VAL:HB	1.95	0.47
1:C:853:VAL:HG21	1:C:949:PHE:HE2	1.79	0.47
1:C:869:PHE:CE1	1:C:943:ILE:HG23	2.50	0.47
1:A:694:VAL:O	1:A:696:ALA:N	2.40	0.47
1:B:857:LYS:HG2	1:B:858:ASP:N	2.28	0.47
1:C:759:ALA:HB3	1:C:793:TYR:HA	1.96	0.47
1:D:533:GLY:O	1:D:534:HIS:C	2.57	0.47
1:D:548:ARG:HH21	1:D:875:LYS:HZ1	1.63	0.47
1:D:723:ARG:NH2	1:D:956:LEU:O	2.48	0.47
1:A:826:ASP:OD1	1:A:852:LYS:HD2	2.14	0.47
1:A:867:ALA:HB2	1:A:896:ILE:HD11	1.97	0.47
1:B:609:TYR:HB2	1:B:614:VAL:HG12	1.96	0.47
1:B:641:LEU:HD11	1:B:665:PRO:HA	1.96	0.47
1:C:774:ILE:HB	1:C:810:SER:OG	2.15	0.47
1:C:903:ILE:N	1:C:903:ILE:HD12	2.30	0.47
1:A:548:ARG:NH1	1:A:552:ILE:HG21	2.30	0.47
1:B:511:TRP:CE2	1:B:578:ILE:HG12	2.50	0.47
1:D:734:GLU:HA	1:D:753:LEU:HD23	1.97	0.47
1:A:759:ALA:HB3	1:A:793:TYR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:771:ILE:HG13	1:C:785:ILE:HG21	1.96	0.47
1:D:917:GLU:O	1:D:919:PRO:HD3	2.15	0.47
1:B:498:LEU:HD21	1:B:721:VAL:HG21	1.97	0.46
1:C:674:ILE:HG13	1:C:675:GLY:N	2.29	0.46
1:B:674:ILE:HG12	1:B:675:GLY:N	2.29	0.46
1:C:740:TRP:HZ3	1:C:753:LEU:HA	1.79	0.46
1:C:756:TYR:CD2	1:C:798:PRO:HB3	2.50	0.46
1:A:657:THR:HG22	1:A:662:ASN:O	2.15	0.46
1:C:838:THR:CG2	1:C:944:ARG:HG2	2.45	0.46
1:D:540:HIS:CE1	1:D:872:LEU:HD11	2.50	0.46
1:A:625:SER:O	1:A:626:ASN:CB	2.62	0.46
1:A:706:LEU:HD23	1:A:706:LEU:C	2.41	0.46
1:D:636:ARG:HE	1:D:660:ASP:CG	2.23	0.46
1:B:688:ILE:CG2	1:B:694:VAL:HB	2.44	0.46
1:B:842:ARG:O	1:B:918:LEU:HD23	2.16	0.46
1:C:701:GLY:O	1:C:704:ASP:N	2.48	0.46
1:C:734:GLU:HG3	1:C:735:ASN:N	2.30	0.46
1:C:894:PHE:HD2	1:C:894:PHE:O	1.98	0.46
1:D:731:LYS:HD2	1:D:756:TYR:CD1	2.50	0.46
1:A:514:TYR:O	1:A:518:ILE:HG12	2.15	0.46
1:B:626:ASN:C	1:B:628:SER:H	2.24	0.46
1:C:853:VAL:HG12	1:C:854:GLY:H	1.81	0.46
1:A:604:LEU:HG	1:A:615:ASN:ND2	2.30	0.46
1:A:624:VAL:HG22	1:A:629:VAL:HG22	1.98	0.46
1:B:544:LEU:HD22	1:B:889:PRO:HG2	1.97	0.46
1:C:514:TYR:HE2	1:D:616:LEU:O	1.99	0.46
1:A:736:ILE:HD12	1:A:741:LYS:HD3	1.97	0.46
1:B:919:PRO:O	1:B:922:VAL:HG22	2.16	0.46
1:D:757:ILE:O	1:D:796:GLU:HG2	2.14	0.46
1:D:815:LEU:HD13	1:D:816:VAL:N	2.31	0.46
1:A:805:LEU:HB3	1:A:811:TYR:HE2	1.81	0.46
1:B:713:VAL:HG22	1:B:721:VAL:O	2.16	0.46
1:D:621:ILE:HB	1:D:632:THR:HG23	1.97	0.46
1:B:538:ARG:HH11	1:B:944:ARG:NH2	2.13	0.46
1:B:757:ILE:O	1:B:796:GLU:HG2	2.16	0.46
1:D:812:ARG:HG3	1:D:959:GLU:HG3	1.98	0.45
1:C:727:PHE:CE2	1:C:764:ILE:HG12	2.51	0.45
1:B:569:LEU:HD21	1:B:691:ALA:O	2.16	0.45
1:C:933:LYS:HG2	1:C:934:TYR:CE2	2.51	0.45
1:D:543:ALA:O	1:D:545:PHE:N	2.50	0.45
1:D:612:LYS:HE2	1:D:623:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:747:THR:HG22	1:D:963:SER:CB	2.44	0.45
1:C:587:ARG:NH2	1:D:594:GLU:O	2.49	0.45
1:C:768:THR:HG21	1:C:784:LYS:HE2	1.98	0.45
1:C:815:LEU:HD23	1:C:815:LEU:C	2.41	0.45
1:C:905:LEU:HA	1:C:910:ASN:ND2	2.30	0.45
1:D:861:ALA:HB2	1:D:951:ALA:HB2	1.98	0.45
1:B:765:GLU:O	1:B:766:ASN:C	2.58	0.45
1:D:576:ASN:HD21	1:D:602:THR:H	1.63	0.45
1:D:958:LEU:HD12	1:D:959:GLU:H	1.81	0.45
1:A:562:LEU:HD11	1:A:564:TYR:O	2.16	0.45
1:A:618:ALA:O	1:A:619:LYS:HB2	2.15	0.45
1:A:626:ASN:HD21	1:A:628:SER:CB	2.30	0.45
1:A:735:ASN:HD22	1:A:736:ILE:N	2.14	0.45
1:C:669:HIS:HB2	1:C:676:VAL:CG1	2.47	0.45
1:C:769:LEU:HD21	1:C:788:ILE:CD1	2.47	0.45
1:D:643:VAL:HG22	1:D:668:LEU:HB3	1.99	0.45
1:C:845:GLU:HG2	1:C:846:SER:H	1.82	0.45
1:A:953:LYS:HE2	1:A:955:TYR:CE2	2.52	0.45
1:C:791:MSE:O	1:C:792:ASP:HB3	2.16	0.45
1:C:868:THR:HA	1:C:893:VAL:HG12	1.98	0.45
1:A:815:LEU:C	1:A:815:LEU:HD23	2.42	0.45
1:B:551:ASN:OD1	1:B:794:LEU:HD22	2.17	0.45
1:B:709:ASN:HD22	1:B:760:PHE:HB2	1.78	0.45
1:C:814:VAL:HG12	1:C:815:LEU:N	2.32	0.45
1:D:540:HIS:HE1	1:D:872:LEU:HD11	1.82	0.45
1:D:665:PRO:C	1:D:666:TYR:CD1	2.95	0.45
1:D:872:LEU:HD23	1:D:889:PRO:HA	1.98	0.45
1:A:548:ARG:HH11	1:A:548:ARG:HB3	1.81	0.45
1:B:726:PRO:O	1:B:759:ALA:HA	2.16	0.45
1:C:686:ASN:O	1:C:690:LEU:HB2	2.16	0.45
1:A:601:THR:HG22	1:A:601:THR:O	2.17	0.44
1:A:735:ASN:HD21	1:A:738:GLY:N	2.15	0.44
1:B:841:LEU:HD23	1:B:845:GLU:OE2	2.17	0.44
1:D:909:GLU:H	1:D:909:GLU:HG2	1.51	0.44
1:A:567:VAL:HG11	1:A:690:LEU:HB3	1.99	0.44
1:B:768:THR:HG23	1:B:784:LYS:HE2	1.98	0.44
1:C:576:ASN:ND2	1:C:602:THR:OG1	2.48	0.44
1:C:595:SER:HB3	1:C:597:ARG:NH2	2.32	0.44
1:D:600:VAL:CG1	1:D:601:THR:H	2.30	0.44
1:A:812:ARG:HE	1:A:959:GLU:CD	2.24	0.44
1:B:852:LYS:HA	1:B:910:ASN:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:606:LEU:HD23	1:D:615:ASN:HB2	1.98	0.44
1:D:830:VAL:O	1:D:831:ASN:HB2	2.18	0.44
1:A:613:TYR:HB2	1:A:622:VAL:HB	1.98	0.44
1:B:524:GLY:O	1:B:525:GLN:HB3	2.18	0.44
1:B:934:TYR:HB2	1:B:938:LEU:HB2	2.00	0.44
1:C:499:ARG:CD	1:C:525:GLN:HE22	2.31	0.44
1:A:796:GLU:CD	1:A:796:GLU:H	2.25	0.44
1:C:873:VAL:HG23	1:C:890:GLN:HG3	2.00	0.44
1:B:727:PHE:HB3	1:B:957:MSE:HE3	2.00	0.44
1:C:928:ASP:O	1:C:932:ARG:HG2	2.18	0.44
1:D:842:ARG:HB2	1:D:842:ARG:NH1	2.31	0.44
1:A:733:GLU:OE2	1:A:754:LYS:HD2	2.17	0.44
1:A:742:GLN:HG2	1:A:744:TYR:CZ	2.53	0.44
1:A:783:ILE:O	1:A:785:ILE:HG23	2.18	0.44
1:A:863:LEU:HB3	1:A:900:GLY:CA	2.38	0.44
1:C:714:TYR:HB3	1:C:721:VAL:CG1	2.47	0.44
1:B:511:TRP:CZ2	1:B:578:ILE:HG12	2.53	0.44
1:C:805:LEU:HB3	1:C:811:TYR:CE2	2.53	0.44
1:B:646:THR:O	1:B:672:PRO:HD3	2.18	0.43
1:C:569:LEU:HD23	1:C:691:ALA:HB1	2.00	0.43
1:C:765:GLU:H	1:C:817:GLN:HE22	1.64	0.43
1:C:506:SER:HA	1:C:563:ASN:OD1	2.18	0.43
1:C:594:GLU:HA	1:D:883:TYR:OH	2.18	0.43
1:C:695:PRO:O	1:C:696:ALA:C	2.61	0.43
1:A:569:LEU:HD12	1:A:691:ALA:HB1	1.99	0.43
1:C:820:PRO:O	1:C:953:LYS:HD2	2.18	0.43
1:C:842:ARG:HB2	1:C:845:GLU:HB2	2.00	0.43
1:D:836:SER:C	1:D:838:THR:N	2.76	0.43
1:D:882:ASP:OD2	1:D:884:ASP:HB2	2.18	0.43
1:A:568:TYR:CE2	1:A:570:ASN:HB2	2.54	0.43
1:A:593:ASP:HA	1:A:883:TYR:CE2	2.53	0.43
1:A:610:GLY:C	1:A:612:LYS:N	2.77	0.43
1:A:763:ASP:OD1	1:A:792:ASP:HA	2.18	0.43
1:B:586:THR:HG23	1:B:589:GLU:OE1	2.17	0.43
1:C:558:GLU:HB2	1:C:726:PRO:CG	2.49	0.43
1:D:645:PHE:HB3	1:D:648:SER:HB3	2.00	0.43
1:B:600:VAL:CG1	1:B:601:THR:N	2.80	0.43
1:D:543:ALA:O	1:D:544:LEU:C	2.60	0.43
1:B:513:ASP:CG	1:B:534:HIS:HB3	2.44	0.43
1:B:669:HIS:CG	1:B:694:VAL:HG11	2.54	0.43
1:B:866:ARG:HD2	1:B:893:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:711:GLU:OE2	1:C:723:ARG:NH1	2.52	0.43
1:A:735:ASN:C	1:A:735:ASN:ND2	2.77	0.43
1:B:640:PRO:C	1:B:642:MSE:N	2.77	0.43
1:C:898:LYS:O	1:C:899:ILE:HG23	2.17	0.43
1:D:878:LYS:HG2	1:D:882:ASP:OD1	2.18	0.43
1:A:639:ASP:OD1	1:A:655:THR:HG23	2.19	0.43
1:A:727:PHE:CE2	1:A:764:ILE:HG12	2.53	0.43
1:B:640:PRO:O	1:B:654:GLY:HA3	2.18	0.43
1:B:671:THR:HB	1:B:674:ILE:O	2.19	0.43
1:C:591:ASN:HD21	1:D:591:ASN:ND2	2.16	0.43
1:D:624:VAL:HA	1:D:628:SER:O	2.18	0.43
1:D:771:ILE:C	1:D:772:TYR:HD1	2.26	0.43
1:D:597:ARG:HB3	1:D:597:ARG:HH11	1.82	0.42
1:A:600:VAL:CG1	1:A:601:THR:N	2.81	0.42
1:A:715:GLU:N	1:A:715:GLU:CD	2.77	0.42
1:A:867:ALA:HA	1:A:944:ARG:O	2.19	0.42
1:C:512:TRP:HE3	1:C:514:TYR:CE1	2.36	0.42
1:C:865:LEU:HD23	1:C:865:LEU:HA	1.93	0.42
1:D:771:ILE:HG13	1:D:785:ILE:HD13	2.01	0.42
1:A:850:GLU:HG3	1:A:913:LYS:HG2	2.00	0.42
1:C:872:LEU:HD23	1:C:889:PRO:HA	2.01	0.42
1:D:785:ILE:HB	1:D:801:VAL:CG2	2.49	0.42
1:A:848:GLU:OE1	1:A:913:LYS:HD3	2.19	0.42
1:B:769:LEU:CD1	1:B:785:ILE:HD11	2.49	0.42
1:B:915:ARG:HG3	1:B:916:ALA:N	2.32	0.42
1:C:537:ASP:HB2	1:C:870:ILE:HG13	2.02	0.42
1:C:811:TYR:CE1	1:C:962:ALA:HB2	2.54	0.42
1:D:842:ARG:HH12	1:D:845:GLU:CD	2.27	0.42
1:A:558:GLU:OE2	1:A:558:GLU:HA	2.20	0.42
1:A:684:THR:HG21	1:A:698:THR:N	2.35	0.42
1:A:705:LYS:HG2	1:A:730:TYR:CD2	2.54	0.42
1:C:607:PRO:HA	1:C:674:ILE:HD12	2.01	0.42
1:C:641:LEU:CD1	1:C:665:PRO:HA	2.49	0.42
1:A:745:ASN:C	1:A:745:ASN:ND2	2.74	0.42
1:B:705:LYS:HG2	1:B:730:TYR:CE2	2.55	0.42
1:C:754:LYS:HB3	1:C:754:LYS:HZ3	1.83	0.42
1:C:896:ILE:HG22	1:C:897:THR:HG23	2.01	0.42
1:C:915:ARG:HG2	1:C:915:ARG:HH11	1.84	0.42
1:D:500:GLU:O	1:D:500:GLU:HG2	2.19	0.42
1:D:777:GLU:C	1:D:778:LYS:HD2	2.45	0.42
1:A:767:ALA:HB2	1:A:817:GLN:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:LYS:HA	1:A:833:GLU:O	2.20	0.42
1:B:489:SER:O	1:B:717:GLY:HA3	2.19	0.42
1:B:538:ARG:HD2	1:B:560:TRP:CZ2	2.54	0.42
1:C:828:PRO:CD	1:C:837:PRO:HG3	2.50	0.42
1:D:812:ARG:CG	1:D:959:GLU:HG3	2.50	0.42
1:A:871:TYR:N	1:A:871:TYR:CD2	2.86	0.42
1:A:878:LYS:HE2	1:D:765:GLU:OE1	2.20	0.42
1:A:769:LEU:HD21	1:A:815:LEU:HD12	2.02	0.42
1:A:857:LYS:HB3	1:A:859:TYR:CE1	2.55	0.42
1:A:874:ARG:HH11	1:A:874:ARG:HG2	1.85	0.42
1:B:728:GLY:HA2	1:B:957:MSE:HB3	2.02	0.42
1:C:614:VAL:HG23	1:C:620:VAL:O	2.19	0.42
1:D:769:LEU:HD22	1:D:815:LEU:HD23	2.01	0.42
1:A:576:ASN:ND2	1:A:602:THR:HG23	2.35	0.41
1:A:648:SER:OG	1:A:650:LYS:HB2	2.20	0.41
1:C:588:ARG:HB2	1:C:883:TYR:HB3	2.02	0.41
1:C:755:LEU:O	1:C:798:PRO:HA	2.19	0.41
1:C:769:LEU:N	1:C:769:LEU:HD22	2.35	0.41
1:D:554:GLU:HG2	1:D:760:PHE:CE1	2.55	0.41
1:C:645:PHE:HB2	1:C:650:LYS:HB3	2.01	0.41
1:C:796:GLU:CD	1:C:796:GLU:H	2.28	0.41
1:D:688:ILE:CG2	1:D:694:VAL:HB	2.50	0.41
1:D:764:ILE:O	1:D:790:HIS:HA	2.21	0.41
1:D:869:PHE:CE1	1:D:943:ILE:HD13	2.55	0.41
1:A:666:TYR:HB3	1:A:677:LEU:CD1	2.50	0.41
1:C:868:THR:CB	1:C:893:VAL:HG12	2.50	0.41
1:D:562:LEU:HD11	1:D:564:TYR:O	2.20	0.41
1:D:646:THR:O	1:D:672:PRO:HD3	2.20	0.41
1:A:548:ARG:HH12	1:A:552:ILE:HG21	1.86	0.41
1:A:671:THR:O	1:A:672:PRO:C	2.63	0.41
1:C:863:LEU:HD12	1:C:864:TYR:N	2.35	0.41
1:D:598:GLY:O	1:D:599:ALA:C	2.64	0.41
1:D:947:PRO:O	1:D:947:PRO:HG2	2.20	0.41
1:B:714:TYR:HB3	1:B:721:VAL:HG11	2.02	0.41
1:B:768:THR:CG2	1:B:784:LYS:HE2	2.51	0.41
1:B:773:ALA:HB3	1:B:780:ILE:HB	2.03	0.41
1:C:679:TYR:HE2	1:C:681:LYS:HD2	1.86	0.41
1:C:938:LEU:HD12	1:C:939:ILE:H	1.85	0.41
1:A:552:ILE:HG12	1:A:552:ILE:O	2.19	0.41
1:A:598:GLY:O	1:A:599:ALA:C	2.63	0.41
1:C:822:GLY:HA2	1:C:854:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:846:SER:HA	1:C:917:GLU:HA	2.03	0.41
1:D:933:LYS:HD3	1:D:934:TYR:CZ	2.56	0.41
1:A:534:HIS:HB3	1:A:535:ALA:H	1.72	0.41
1:A:906:LYS:O	1:A:907:GLU:C	2.64	0.41
1:C:695:PRO:HG2	1:C:696:ALA:H	1.85	0.41
1:C:849:ILE:CG1	1:C:916:ALA:HB2	2.50	0.41
1:D:735:ASN:C	1:D:737:ASN:H	2.27	0.41
1:B:587:ARG:O	1:B:590:TYR:HB3	2.21	0.41
1:B:671:THR:CG2	1:B:673:THR:HG22	2.51	0.41
1:C:526:ARG:C	1:C:527:ARG:HG2	2.46	0.41
1:C:598:GLY:O	1:C:599:ALA:C	2.63	0.41
1:C:602:THR:HA	1:C:679:TYR:HB2	2.03	0.41
1:C:759:ALA:O	1:C:793:TYR:HB2	2.20	0.41
1:C:764:ILE:HA	1:C:817:GLN:HE22	1.85	0.41
1:C:872:LEU:HB2	1:C:939:ILE:HB	2.02	0.41
1:A:496:LYS:HE2	1:A:500:GLU:OE1	2.21	0.41
1:A:503:PRO:HB3	1:A:856:ASP:CG	2.46	0.41
1:A:915:ARG:HG3	1:A:916:ALA:N	2.35	0.41
1:B:622:VAL:HG13	1:B:631:VAL:HG22	2.02	0.41
1:C:514:TYR:HE1	1:C:574:LYS:HE3	1.85	0.41
1:C:565:PHE:C	1:C:565:PHE:CD2	2.99	0.41
1:C:724:PHE:CG	1:C:725:THR:N	2.89	0.41
1:C:725:THR:HA	1:C:726:PRO:HD3	1.92	0.41
1:C:863:LEU:HB3	1:C:900:GLY:HA3	2.03	0.41
1:C:889:PRO:C	1:C:890:GLN:HG2	2.45	0.41
1:D:527:ARG:HB2	1:D:531:ASP:OD2	2.21	0.41
1:D:544:LEU:HD22	1:D:889:PRO:HB2	2.03	0.41
1:D:647:PRO:O	1:D:648:SER:C	2.64	0.41
1:A:554:GLU:OE1	1:A:794:LEU:HD23	2.21	0.41
1:B:567:VAL:CG2	1:B:720:ILE:HB	2.50	0.41
1:B:671:THR:C	1:B:673:THR:N	2.79	0.41
1:B:727:PHE:O	1:B:957:MSE:HG2	2.21	0.41
1:D:542:LEU:HD23	1:D:542:LEU:HA	1.85	0.41
1:A:870:ILE:HD11	1:A:891:MSE:CE	2.51	0.40
1:A:562:LEU:HD12	1:A:563:ASN:H	1.86	0.40
1:B:491:TRP:HZ3	1:B:566:LEU:HD13	1.86	0.40
1:B:545:PHE:O	1:B:686:ASN:HB2	2.21	0.40
1:B:679:TYR:HE2	1:B:681:LYS:HD2	1.86	0.40
1:C:843:GLU:O	1:C:920:GLU:HA	2.20	0.40
1:D:543:ALA:C	1:D:545:PHE:N	2.78	0.40
1:D:544:LEU:HD11	1:D:552:ILE:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:TYR:CE1	1:D:933:LYS:HG3	2.56	0.40
1:B:705:LYS:HG2	1:B:730:TYR:CD2	2.57	0.40
1:C:821:ILE:HG22	1:C:953:LYS:HE3	2.02	0.40
1:D:736:ILE:HG22	1:D:736:ILE:O	2.20	0.40
1:B:521:SER:O	1:B:523:LEU:N	2.53	0.40
1:B:822:GLY:HA2	1:B:855:VAL:HG12	2.02	0.40
1:B:914:VAL:HG12	1:B:915:ARG:N	2.37	0.40
1:C:757:ILE:HD13	1:C:791:MSE:HE1	2.04	0.40
1:C:896:ILE:HG21	1:C:918:LEU:CD1	2.51	0.40
1:D:769:LEU:HG	1:D:786:ALA:HB3	2.02	0.40
1:D:610:GLY:O	1:D:611:GLU:HB2	2.21	0.40
1:D:746:LEU:HD13	1:D:805:LEU:HD11	2.03	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	476/497 (96%)	414 (87%)	49 (10%)	13 (3%)	4	22
1	B	475/497 (96%)	408 (86%)	54 (11%)	13 (3%)	4	22
1	C	476/497 (96%)	398 (84%)	59 (12%)	19 (4%)	2	14
1	D	478/497 (96%)	410 (86%)	50 (10%)	18 (4%)	2	15
All	All	1905/1988 (96%)	1630 (86%)	212 (11%)	63 (3%)	3	17

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	535	ALA
1	A	626	ASN
1	A	696	ALA

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Mol	Chain	Res	Type
1	B	529	SER
1	B	777	GLU
1	B	843	GLU
1	C	626	ASN
1	C	648	SER
1	C	696	ALA
1	C	702	PHE
1	C	847	GLY
1	D	695	PRO
1	A	524	GLY
1	A	796	GLU
1	B	520	SER
1	B	522	LEU
1	B	594	GLU
1	B	716	SER
1	C	901	GLU
1	C	922	VAL
1	D	534	HIS
1	D	535	ALA
1	D	610	GLY
1	D	776	ASN
1	A	625	SER
1	A	695	PRO
1	A	806	PRO
1	A	907	GLU
1	B	525	GLN
1	B	737	ASN
1	C	524	GLY
1	C	528	ALA
1	C	535	ALA
1	C	781	GLU
1	C	900	GLY
1	D	544	LEU
1	D	717	GLY
1	D	737	ASN
1	D	746	LEU
1	A	919	PRO
1	B	717	GLY
1	C	917	GLU
1	C	935	GLY
1	D	524	GLY
1	D	696	ALA

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Mol	Chain	Res	Type
1	D	902	ASN
1	A	629	VAL
1	D	781	GLU
1	D	792	ASP
1	B	524	GLY
1	C	503	PRO
1	C	599	ALA
1	D	648	SER
1	A	939	ILE
1	C	899	ILE
1	C	919	PRO
1	D	533	GLY
1	A	837	PRO
1	C	695	PRO
1	D	552	ILE
1	D	672	PRO
1	B	780	ILE
1	B	919	PRO

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	404/419 (96%)	367 (91%)	37 (9%)	8	33
1	B	404/419 (96%)	374 (93%)	30 (7%)	13	42
1	C	404/419 (96%)	383 (95%)	21 (5%)	21	55
1	D	404/419 (96%)	373 (92%)	31 (8%)	12	40
All	All	1616/1676 (96%)	1497 (93%)	119 (7%)	13	42

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	503	PRO
1	A	507	THR
1	A	509	THR

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Mol	Chain	Res	Type
1	A	525	GLN
1	A	548	ARG
1	A	549	ASP
1	A	555	VAL
1	A	561	GLU
1	A	566	LEU
1	A	576	ASN
1	A	625	SER
1	A	637	GLU
1	A	646	THR
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	715	GLU
1	A	721	VAL
1	A	723	ARG
1	A	725	THR
1	A	745	ASN
1	A	777	GLU
1	A	795	ASN
1	A	796	GLU
1	A	799	ILE
1	A	834	ILE
1	A	836	SER
1	A	893	VAL
1	A	915	ARG
1	A	919	PRO
1	A	927	LYS
1	A	946	GLU
1	A	948	VAL
1	B	509	THR
1	B	519	GLU
1	B	531	ASP
1	B	534	HIS
1	B	538	ARG
1	B	548	ARG
1	B	562	LEU
1	B	576	ASN

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Mol	Chain	Res	Type
1	B	594	GLU
1	B	608	ARG
1	B	646	THR
1	B	684	THR
1	B	690	LEU
1	B	716	SER
1	B	770	TYR
1	B	783	ILE
1	B	789	SER
1	B	807	ASN
1	B	834	ILE
1	B	839	ASN
1	B	846	SER
1	B	852	LYS
1	B	893	VAL
1	B	902	ASN
1	B	906	LYS
1	B	915	ARG
1	B	928	ASP
1	B	931	GLN
1	B	946	GLU
1	B	952	GLU
1	C	513	ASP
1	C	525	GLN
1	C	542	LEU
1	C	576	ASN
1	C	594	GLU
1	C	600	VAL
1	C	603	LEU
1	C	626	ASN
1	C	630	LYS
1	C	632	THR
1	C	690	LEU
1	C	721	VAL
1	C	752	GLU
1	C	769	LEU
1	C	821	ILE
1	C	824	LEU
1	C	843	GLU
1	C	851	LEU
1	C	852	LYS
1	C	863	LEU

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Mol	Chain	Res	Type
1	C	894	PHE
1	D	504	GLU
1	D	509	THR
1	D	531	ASP
1	D	548	ARG
1	D	549	ASP
1	D	555	VAL
1	D	559	SER
1	D	576	ASN
1	D	594	GLU
1	D	601	THR
1	D	604	LEU
1	D	614	VAL
1	D	616	LEU
1	D	632	THR
1	D	644	THR
1	D	671	THR
1	D	690	LEU
1	D	721	VAL
1	D	725	THR
1	D	751	HIS
1	D	757	ILE
1	D	769	LEU
1	D	777	GLU
1	D	779	ILE
1	D	851	LEU
1	D	890	GLN
1	D	909	GLU
1	D	915	ARG
1	D	920	GLU
1	D	927	LYS
1	D	945	VAL

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	501	ASN
1	A	576	ASN
1	A	615	ASN
1	A	626	ASN
1	A	662	ASN
1	A	735	ASN

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Mol	Chain	Res	Type
1	A	745	ASN
1	A	776	ASN
1	A	807	ASN
1	A	817	GLN
1	A	839	ASN
1	A	902	ASN
1	A	904	GLN
1	B	807	ASN
1	B	890	GLN
1	B	904	GLN
1	B	931	GLN
1	C	525	GLN
1	C	540	HIS
1	C	570	ASN
1	C	576	ASN
1	C	626	ASN
1	C	662	ASN
1	C	718	ASN
1	C	735	ASN
1	C	737	ASN
1	C	742	GLN
1	C	745	ASN
1	C	790	HIS
1	C	807	ASN
1	C	817	GLN
1	C	839	ASN
1	C	904	GLN
1	D	570	ASN
1	D	576	ASN
1	D	591	ASN
1	D	709	ASN
1	D	735	ASN
1	D	742	GLN
1	D	802	ASN
1	D	817	GLN
1	D	890	GLN
1	D	902	ASN
1	D	910	ASN

5.3.3 RNA ⓘ

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	474/497 (95%)	-0.37	8 (1%) 69 45	12, 41, 67, 82	0
1	B	473/497 (95%)	-0.28	4 (0%) 82 64	14, 49, 71, 85	0
1	C	474/497 (95%)	-0.05	7 (1%) 72 49	25, 61, 86, 97	0
1	D	476/497 (95%)	-0.34	7 (1%) 72 49	13, 41, 81, 99	0
All	All	1897/1988 (95%)	-0.26	26 (1%) 73 51	12, 47, 79, 99	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	964	ALA	3.5
1	C	487	GLU	3.5
1	C	964	ALA	3.3
1	D	736	ILE	3.2
1	A	530	ALA	3.0
1	D	531	ASP	3.0
1	A	533	GLY	2.9
1	D	528	ALA	2.9
1	C	526	ARG	2.8
1	B	964	ALA	2.7
1	A	534	HIS	2.5
1	B	530	ALA	2.5
1	D	526	ARG	2.5
1	D	530	ALA	2.4
1	D	965	PRO	2.4
1	D	487	GLU	2.4
1	A	487	GLU	2.3
1	C	533	GLY	2.3
1	C	537	ASP	2.3
1	B	528	ALA	2.2
1	A	611	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	738	GLY	2.2
1	A	537	ASP	2.2
1	A	526	ARG	2.2
1	B	489	SER	2.1
1	C	530	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
3	CL	C	7	1/1	0.88	0.09	79,79,79,79	0
3	CL	B	6	1/1	0.93	0.13	69,69,69,69	0
2	CA	D	4	1/1	0.95	0.10	30,30,30,30	0
3	CL	A	5	1/1	0.95	0.08	48,48,48,48	0
2	CA	A	1	1/1	0.96	0.12	32,32,32,32	0
2	CA	B	2	1/1	0.97	0.09	34,34,34,34	0
2	CA	C	3	1/1	0.98	0.13	57,57,57,57	0
3	CL	D	8	1/1	0.98	0.07	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.