



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:18 AM UTC

PDB ID : 2G63 / pdb_00002g63
Title : Crystal structure of human dipeptidyl peptidase IV (DPPIV) complexed with cyanopyrrolidine (C5-pro-pro) inhibitor 24b
Authors : Longenecker, K.L.; Fry, E.H.; Lake, M.R.; Solomon, L.R.; Pei, Z.; Li, X.
Deposited on : 2006-02-24
Resolution : 2.00 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

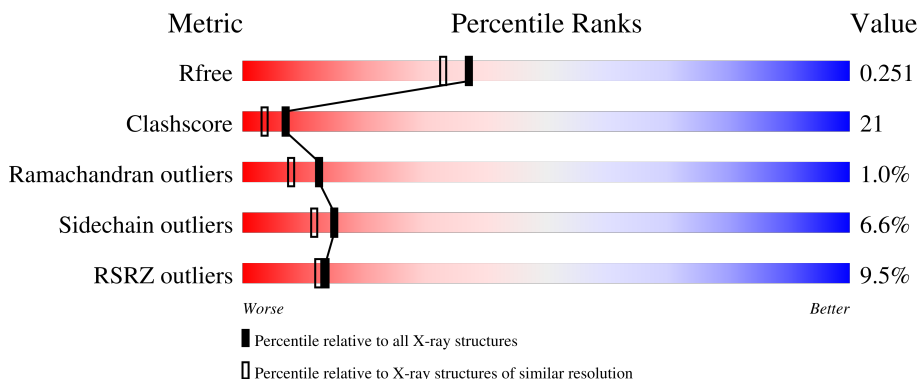
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	726	11% 66% 28% 5% •
1	B	726	14% 65% 30% 5% •
1	C	726	6% 63% 32% •
1	D	726	7% 65% 30% •

2 Entry composition [i](#)

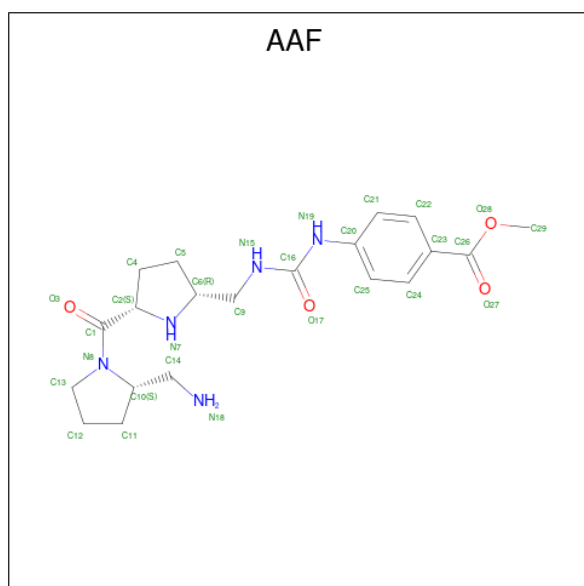
There are 3 unique types of molecules in this entry. The entry contains 28111 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5949	3816	980	1127	26			
1	B	726	Total	C	N	O	S	0	0	0
			5949	3816	980	1127	26			
1	C	726	Total	C	N	O	S	0	0	0
			5949	3816	980	1127	26			
1	D	726	Total	C	N	O	S	0	0	0
			5949	3816	980	1127	26			

- Molecule 2 is METHYL 4-{{{[(2R,5S)-5-{{[(2S)-2-(AMINOMETHYL)PYRROLIDIN-1-YL] CARBONYL}PYRROLIDIN-2-YL]METHYL}AMINO)CARBONYL]AMINO}BENZOATE (CCD ID: AAF) (formula: C₂₀H₂₉N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			29	20	5	4		

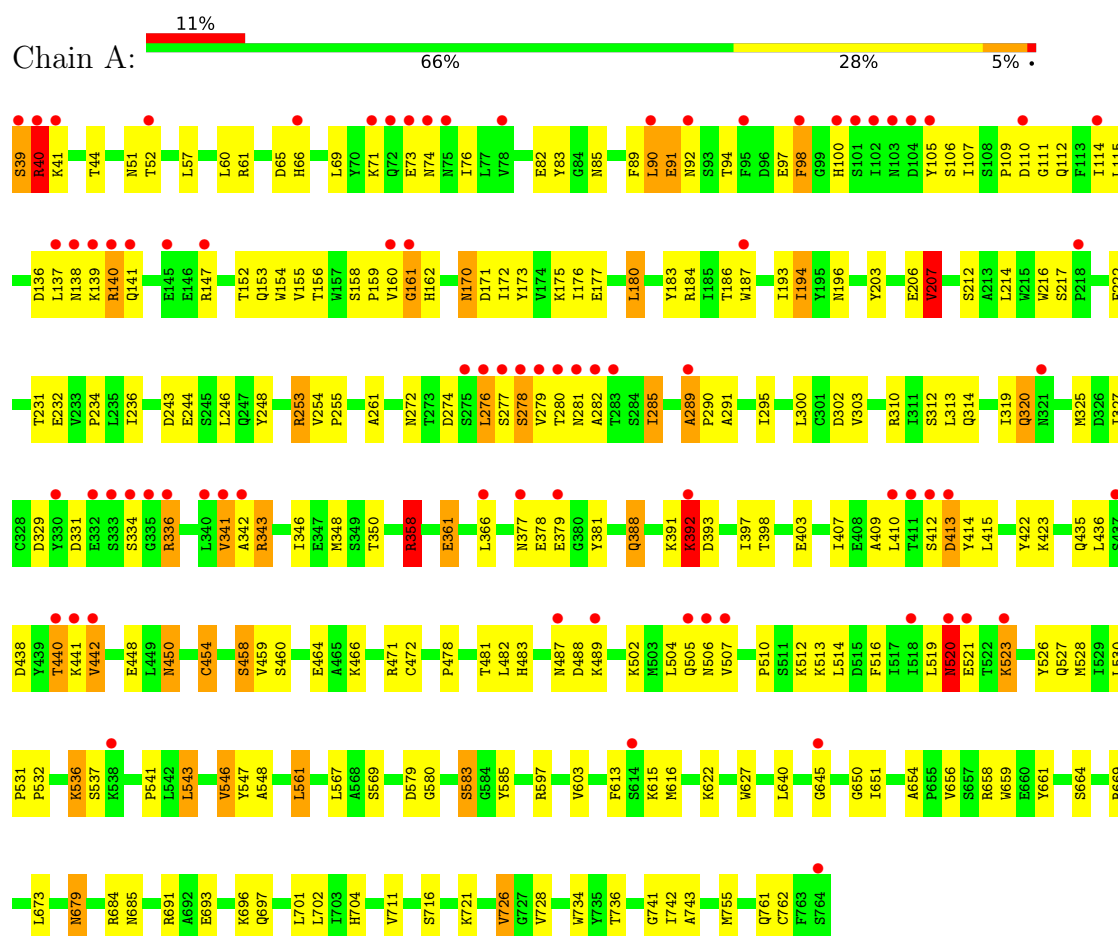
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1195	Total 1195	O 1195	0	0
3	B	1121	Total 1121	O 1121	0	0
3	C	938	Total 938	O 938	0	0
3	D	1032	Total 1032	O 1032	0	0

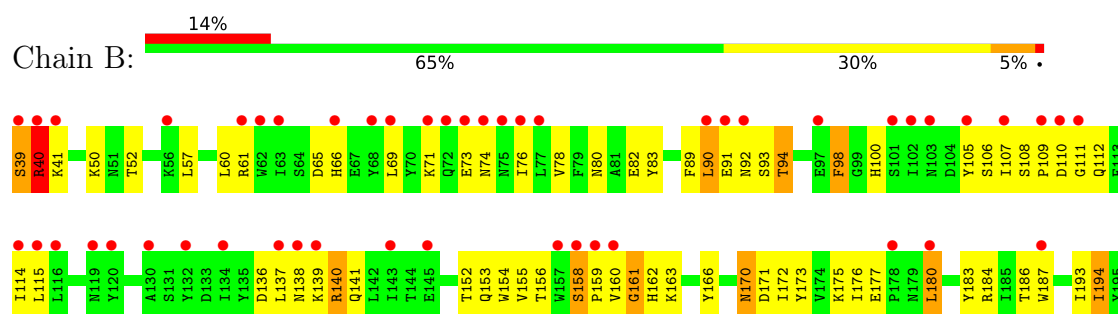
3 Residue-property plots [i](#)

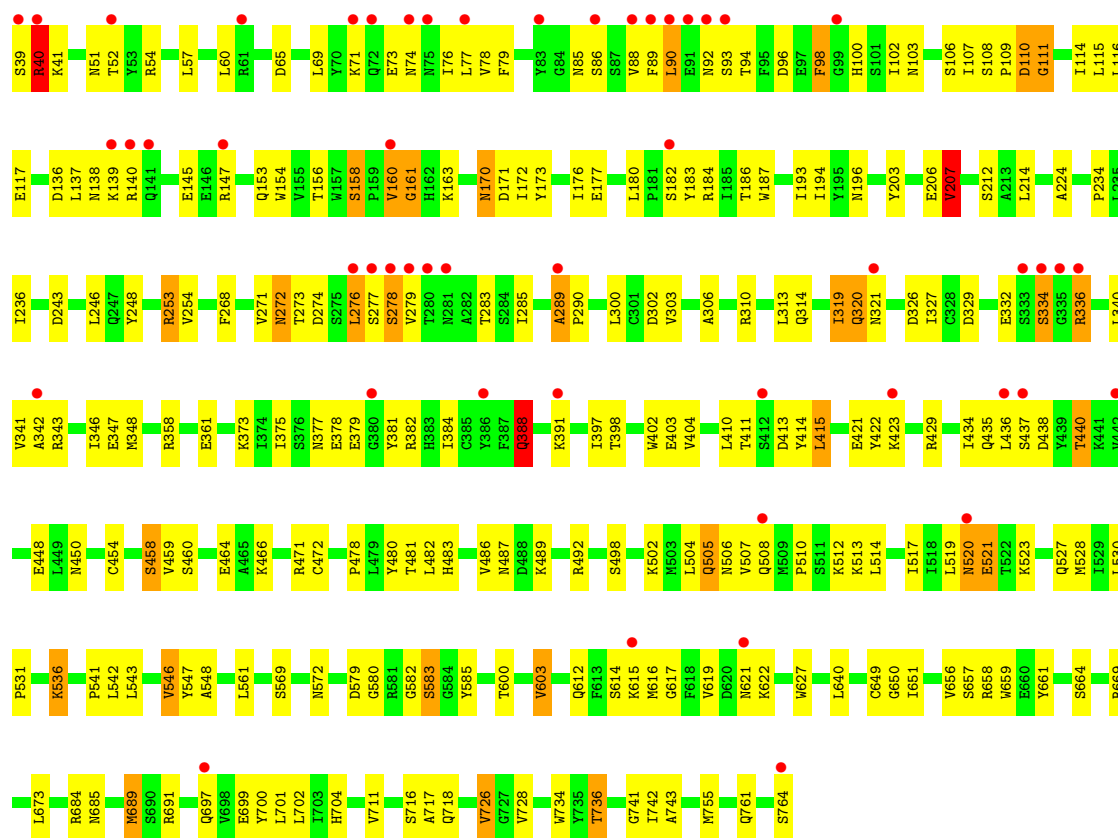
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.13Å 126.50Å 127.37Å 90.00° 96.66° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.00) 99.7 (20.00-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.251 0.214 , 0.251	Depositor DCC
R_{free} test set	12847 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 80.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28111	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: AAF

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	0.39	0/6120	0.93	29/8321 (0.3%)
1	B	0.42	1/6120 (0.0%)	0.94	31/8321 (0.4%)
1	C	0.36	0/6120	0.90	27/8321 (0.3%)
1	D	0.36	0/6120	0.90	25/8321 (0.3%)
All	All	0.38	1/24480 (0.0%)	0.92	112/33284 (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	C	0	1
1	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	630	SER	C-O	11.45	1.38	1.24

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	358	ARG	NE-CZ-NH2	11.50	129.55	119.20
1	B	358	ARG	NE-CZ-NH1	-10.03	111.47	121.50
1	A	388	GLN	N-CA-C	-8.10	96.03	109.24
1	D	656	VAL	N-CA-C	-7.85	98.54	109.21
1	B	388	GLN	N-CA-C	-7.80	96.52	109.07
1	C	656	VAL	N-CA-C	-7.74	98.69	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	378	GLU	N-CA-C	-7.72	103.31	112.89
1	B	111	GLY	N-CA-C	-7.62	105.22	115.36
1	C	378	GLU	N-CA-C	-7.55	103.52	112.89
1	A	111	GLY	N-CA-C	-7.44	105.47	115.36
1	B	656	VAL	N-CA-C	-7.28	97.80	108.87
1	B	206	GLU	N-CA-C	7.22	122.38	113.50
1	D	659	TRP	N-CA-C	7.14	119.92	111.71
1	C	206	GLU	N-CA-C	7.01	122.00	113.38
1	A	656	VAL	N-CA-C	-7.00	98.22	108.87
1	C	659	TRP	N-CA-C	6.95	119.70	111.71
1	D	388	GLN	N-CA-C	-6.91	97.15	108.41
1	D	111	GLY	N-CA-C	-6.85	106.25	115.36
1	C	388	GLN	N-CA-C	-6.80	97.43	108.52
1	A	300	LEU	N-CA-C	-6.78	97.67	108.73
1	B	300	LEU	N-CA-C	-6.72	97.78	108.73
1	D	206	GLU	N-CA-C	6.63	121.66	113.50
1	C	300	LEU	N-CA-C	-6.59	97.98	108.73
1	D	300	LEU	N-CA-C	-6.58	98.00	108.73
1	C	111	GLY	N-CA-C	-6.57	106.62	115.36
1	A	279	VAL	N-CA-C	-6.48	106.48	112.96
1	A	206	GLU	N-CA-C	6.37	122.12	113.97
1	A	458	SER	N-CA-C	-6.20	99.91	109.52
1	B	343	ARG	N-CA-C	-6.17	105.03	113.30
1	B	485	SER	N-CA-C	6.13	118.93	111.82
1	B	392	LYS	N-CA-C	6.13	118.04	111.36
1	C	319	ILE	N-CA-C	-6.11	97.70	106.55
1	D	319	ILE	N-CA-C	-6.11	97.70	106.55
1	B	458	SER	N-CA-C	-6.08	100.10	109.52
1	B	659	TRP	N-CA-C	6.07	118.69	111.71
1	A	378	GLU	N-CA-C	-6.03	105.41	112.89
1	B	378	GLU	N-CA-C	-6.02	105.42	112.89
1	B	454	CYS	N-CA-C	6.00	118.70	108.02
1	A	392	LYS	N-CA-C	6.00	117.89	111.36
1	A	454	CYS	N-CA-C	5.99	118.69	108.02
1	A	659	TRP	N-CA-C	5.99	118.60	111.71
1	B	279	VAL	N-CA-C	-5.97	106.99	112.96
1	B	664	SER	N-CA-C	5.96	117.45	111.07
1	D	458	SER	N-CA-C	-5.95	100.25	109.24
1	B	358	ARG	CD-NE-CZ	5.95	132.73	124.40
1	C	454	CYS	N-CA-C	5.91	118.03	108.41
1	C	450	ASN	CA-C-N	5.88	126.29	119.47
1	C	450	ASN	C-N-CA	5.88	126.29	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	ASN	CA-C-N	5.87	126.28	119.47
1	A	450	ASN	C-N-CA	5.87	126.28	119.47
1	C	458	SER	N-CA-C	-5.84	100.46	109.52
1	D	454	CYS	N-CA-C	5.84	117.93	108.41
1	B	546	VAL	N-CA-C	5.83	118.37	108.86
1	D	450	ASN	CA-C-N	5.83	126.24	119.47
1	D	450	ASN	C-N-CA	5.83	126.24	119.47
1	A	343	ARG	N-CA-C	-5.80	105.53	113.30
1	B	207	VAL	N-CA-C	5.78	116.98	112.12
1	A	664	SER	N-CA-C	5.78	117.25	111.07
1	D	617	GLY	N-CA-C	5.76	122.70	115.21
1	C	98	PHE	N-CA-C	-5.74	105.77	112.89
1	A	546	VAL	N-CA-C	5.71	118.17	108.86
1	D	98	PHE	N-CA-C	-5.70	105.82	112.89
1	C	206	GLU	CA-C-N	-5.70	117.12	123.16
1	C	206	GLU	C-N-CA	-5.70	117.12	123.16
1	C	548	ALA	N-CA-C	5.69	119.80	112.86
1	A	206	GLU	CA-C-N	-5.69	116.80	122.77
1	A	206	GLU	C-N-CA	-5.69	116.80	122.77
1	C	664	SER	N-CA-C	5.69	117.15	111.07
1	D	207	VAL	N-CA-C	5.68	116.11	111.62
1	A	319	ILE	N-CA-C	-5.65	98.51	107.15
1	D	206	GLU	CA-C-N	-5.65	117.17	123.16
1	D	206	GLU	C-N-CA	-5.65	117.17	123.16
1	C	236	ILE	N-CA-C	-5.64	100.30	108.87
1	C	617	GLY	N-CA-C	5.63	122.53	115.21
1	B	541	PRO	N-CA-C	-5.60	102.48	111.38
1	A	158	SER	N-CA-C	-5.58	102.17	110.20
1	A	207	VAL	N-CA-C	5.53	116.76	112.12
1	D	548	ALA	N-CA-C	5.52	119.59	112.86
1	C	582	GLY	N-CA-C	-5.51	108.13	114.69
1	A	98	PHE	N-CA-C	-5.50	105.44	111.82
1	C	207	VAL	N-CA-C	5.50	115.97	111.62
1	B	319	ILE	N-CA-C	-5.50	98.74	107.15
1	B	450	ASN	CA-C-N	5.50	125.85	119.47
1	B	450	ASN	C-N-CA	5.50	125.85	119.47
1	A	541	PRO	N-CA-C	-5.50	102.64	111.38
1	D	664	SER	N-CA-C	5.47	116.92	111.07
1	A	341	VAL	N-CA-C	-5.42	98.06	109.34
1	D	236	ILE	N-CA-C	-5.41	100.64	108.87
1	A	358	ARG	CD-NE-CZ	5.40	131.97	124.40
1	A	236	ILE	N-CA-C	-5.40	100.66	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	582	GLY	N-CA-C	-5.39	108.28	114.69
1	B	341	VAL	N-CA-C	-5.36	98.19	109.34
1	B	206	GLU	CA-C-N	-5.35	117.15	122.77
1	B	206	GLU	C-N-CA	-5.35	117.15	122.77
1	D	541	PRO	N-CA-C	-5.30	102.96	111.38
1	B	158	SER	N-CA-C	-5.26	102.62	110.20
1	B	98	PHE	N-CA-C	-5.25	105.73	111.82
1	A	743	ALA	N-CA-C	5.25	119.38	112.92
1	C	541	PRO	N-CA-C	-5.23	103.07	111.38
1	D	546	VAL	N-CA-C	5.16	117.26	108.86
1	C	546	VAL	N-CA-C	5.14	117.23	108.86
1	C	744	SER	N-CA-C	-5.13	103.76	110.53
1	D	743	ALA	N-CA-C	5.13	119.50	112.88
1	A	548	ALA	N-CA-C	5.12	119.11	112.86
1	C	158	SER	N-CA-C	-5.11	102.72	110.39
1	C	205	GLU	N-CA-C	5.11	116.66	111.14
1	A	412	SER	N-CA-C	-5.11	106.31	112.54
1	B	236	ILE	N-CA-C	-5.10	101.12	108.87
1	B	588	ASP	N-CA-C	5.07	117.70	111.82
1	B	529	ILE	N-CA-C	-5.01	99.91	107.73
1	D	158	SER	N-CA-C	-5.01	102.88	110.39
1	C	743	ALA	N-CA-C	5.00	119.33	112.88

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	700	TYR	Sidechain
1	D	700	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	5949	0	5667	243	0
1	B	5949	0	5666	243	0
1	C	5949	0	5667	254	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	5949	0	5667	247	0
2	B	29	0	27	1	0
3	A	1195	0	0	62	0
3	B	1121	0	0	63	0
3	C	938	0	0	70	0
3	D	1032	0	0	66	0
All	All	28111	0	22694	970	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 (970) 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:736:THR:HB	3:B:1870:HOH:O	1.37	1.24
1:A:289:ALA:HB1	1:A:290:PRO:HA	1.25	1.13
1:B:289:ALA:HB1	1:B:290:PRO:HA	1.28	1.12
1:A:736:THR:HG21	1:B:721:LYS:HB2	1.31	1.06
1:C:114:ILE:HD11	1:C:137:LEU:HD21	1.37	1.06
1:D:114:ILE:HD11	1:D:137:LEU:HD21	1.37	1.05
1:D:289:ALA:HB1	1:D:290:PRO:HA	1.35	1.04
1:A:721:LYS:HB2	1:B:736:THR:HG21	1.35	1.02
1:A:651:ILE:HG21	1:A:755:MET:HE3	1.40	1.02
1:B:651:ILE:HG21	1:B:755:MET:HE3	1.40	1.01
1:C:289:ALA:HB1	1:C:290:PRO:HA	1.36	1.01
1:D:651:ILE:HG21	1:D:755:MET:HE3	1.40	1.00
1:C:176:ILE:HD11	1:C:276:LEU:HD21	1.43	0.99
1:C:651:ILE:HG21	1:C:755:MET:HE3	1.41	0.99
1:D:176:ILE:HD11	1:D:276:LEU:HD21	1.43	0.98
1:C:528:MET:HE3	1:C:530:LEU:HD21	1.44	0.97
1:D:621:ASN:HB3	3:D:768:HOH:O	1.66	0.96
1:D:528:MET:HE3	1:D:530:LEU:HD21	1.44	0.94
1:A:289:ALA:HB1	1:A:290:PRO:CA	1.99	0.93
1:A:736:THR:CG2	1:B:721:LYS:HB2	2.03	0.89
1:B:289:ALA:HB1	1:B:290:PRO:CA	2.02	0.88
1:A:528:MET:HE3	1:A:530:LEU:HD21	1.56	0.88
1:B:528:MET:HE3	1:B:530:LEU:HD21	1.56	0.87
1:A:736:THR:HG22	3:B:802:HOH:O	1.75	0.87
1:D:40:ARG:HA	3:D:854:HOH:O	1.73	0.87
1:D:76:ILE:HD12	1:D:90:LEU:HD11	1.57	0.86
1:B:334:SER:HB3	1:B:336:ARG:NE	1.91	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:LYS:HE3	3:B:1586:HOH:O	1.76	0.86
1:D:361:GLU:HG2	3:D:933:HOH:O	1.74	0.85
1:A:310:ARG:HH12	1:A:343:ARG:NH1	1.75	0.85
1:A:334:SER:HB3	1:A:336:ARG:NE	1.92	0.85
1:D:89:PHE:HD1	1:D:90:LEU:HD12	1.42	0.85
1:C:76:ILE:HG22	3:C:1495:HOH:O	1.76	0.85
1:C:76:ILE:HD12	1:C:90:LEU:HD11	1.57	0.84
1:A:721:LYS:HB2	1:B:736:THR:CG2	2.06	0.84
1:B:160:VAL:HG23	1:B:161:GLY:H	1.43	0.84
1:A:334:SER:HB3	1:A:336:ARG:HE	1.43	0.83
1:A:487:ASN:HB2	3:A:788:HOH:O	1.77	0.83
1:A:762:CYS:HB2	3:A:1511:HOH:O	1.78	0.83
1:A:172:ILE:H	1:A:186:THR:HG22	1.43	0.83
1:B:172:ILE:H	1:B:186:THR:HG22	1.43	0.82
1:B:334:SER:HB3	1:B:336:ARG:HE	1.42	0.82
1:C:276:LEU:HD22	1:C:276:LEU:H	1.45	0.82
1:A:289:ALA:HB2	3:A:1489:HOH:O	1.80	0.81
1:C:627:TRP:CE3	1:C:755:MET:HE1	2.15	0.81
1:D:276:LEU:H	1:D:276:LEU:HD22	1.43	0.81
1:A:253:ARG:HH22	1:B:253:ARG:HH22	1.25	0.81
1:B:310:ARG:HH12	1:B:343:ARG:NH1	1.79	0.81
1:B:702:LEU:HD22	3:B:1886:HOH:O	1.80	0.81
1:B:627:TRP:CE3	1:B:755:MET:HE1	2.16	0.80
1:C:89:PHE:HD1	1:C:90:LEU:HD12	1.42	0.80
1:D:651:ILE:CG2	1:D:755:MET:HE3	2.12	0.80
1:C:172:ILE:H	1:C:186:THR:HG22	1.46	0.80
1:C:528:MET:CE	1:C:530:LEU:HD21	2.12	0.80
1:A:627:TRP:CE3	1:A:755:MET:HE1	2.17	0.79
1:B:140:ARG:HH11	1:B:140:ARG:HG2	1.48	0.79
1:A:140:ARG:HG2	1:A:140:ARG:HH11	1.48	0.79
1:A:160:VAL:HG23	1:A:161:GLY:H	1.45	0.79
1:D:172:ILE:H	1:D:186:THR:HG22	1.46	0.79
1:B:276:LEU:HB3	3:B:1234:HOH:O	1.82	0.79
1:C:651:ILE:CG2	1:C:755:MET:HE3	2.13	0.79
1:A:341:VAL:O	1:A:342:ALA:HB3	1.82	0.79
1:A:651:ILE:CG2	1:A:755:MET:HE3	2.14	0.78
1:D:528:MET:CE	1:D:530:LEU:HD21	2.13	0.78
1:B:207:VAL:O	1:B:358:ARG:NH2	2.16	0.78
1:D:627:TRP:CE3	1:D:755:MET:HE1	2.18	0.78
1:A:358:ARG:NH1	3:A:1447:HOH:O	2.17	0.78
1:A:281:ASN:HB2	3:A:1179:HOH:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:GLU:HG3	3:B:1613:HOH:O	1.84	0.78
1:D:726:VAL:HG12	1:D:728:VAL:HG23	1.66	0.77
1:C:334:SER:HB3	1:C:336:ARG:HE	1.48	0.77
1:D:334:SER:HB3	1:D:336:ARG:HE	1.48	0.77
1:B:176:ILE:HD11	1:B:276:LEU:HD21	1.66	0.77
1:B:651:ILE:CG2	1:B:755:MET:HE3	2.14	0.77
1:C:726:VAL:HG12	1:C:728:VAL:HG23	1.66	0.77
1:A:255:PRO:HD2	3:A:1931:HOH:O	1.83	0.77
1:A:289:ALA:CB	1:A:290:PRO:HA	2.12	0.76
1:A:282:ALA:HB3	3:A:1913:HOH:O	1.84	0.76
1:A:489:LYS:NZ	1:A:489:LYS:HB3	2.01	0.76
1:A:176:ILE:HD11	1:A:276:LEU:HD21	1.67	0.76
1:B:341:VAL:HB	3:B:887:HOH:O	1.86	0.75
1:C:717:ALA:O	1:D:736:THR:HG21	1.86	0.75
1:A:312:SER:HB2	1:A:325:MET:HE3	1.68	0.75
1:A:505:GLN:HB3	3:A:1559:HOH:O	1.85	0.75
1:A:52:THR:HG22	3:A:1873:HOH:O	1.85	0.75
1:D:289:ALA:HB1	1:D:290:PRO:CA	2.15	0.75
1:B:177:GLU:HB2	1:B:180:LEU:HD22	1.69	0.75
1:B:489:LYS:NZ	1:B:489:LYS:HB3	2.00	0.75
1:B:517:ILE:HD13	3:B:1143:HOH:O	1.87	0.75
1:B:289:ALA:CB	1:B:290:PRO:HA	2.15	0.74
1:B:723:LEU:HA	3:B:1900:HOH:O	1.86	0.74
1:A:438:ASP:OD1	1:A:440:THR:HB	1.87	0.74
1:C:90:LEU:O	1:C:90:LEU:HD22	1.86	0.74
1:C:736:THR:HG21	1:D:717:ALA:O	1.88	0.74
1:C:289:ALA:HB1	1:C:290:PRO:CA	2.16	0.74
1:D:90:LEU:HD22	1:D:90:LEU:O	1.87	0.74
1:B:528:MET:CE	1:B:530:LEU:HD21	2.18	0.74
1:C:183:TYR:HE1	1:C:277:SER:O	1.71	0.74
1:B:184:ARG:HD3	1:B:186:THR:O	1.88	0.74
1:B:327:ILE:HB	1:B:343:ARG:HG2	1.69	0.74
1:C:276:LEU:HB3	3:C:1068:HOH:O	1.88	0.73
1:D:614:SER:HB2	3:D:768:HOH:O	1.88	0.73
1:D:289:ALA:HB2	3:D:1585:HOH:O	1.88	0.73
1:A:171:ASP:OD1	1:A:186:THR:HG23	1.88	0.73
1:C:272:ASN:ND2	1:C:274:ASP:H	1.86	0.73
1:A:350:THR:HG23	3:A:1787:HOH:O	1.89	0.73
1:D:272:ASN:ND2	1:D:274:ASP:H	1.87	0.73
1:A:177:GLU:HB2	1:A:180:LEU:HD22	1.70	0.73
1:C:594:ILE:HG13	3:C:1263:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:LYS:HE3	3:A:1560:HOH:O	1.88	0.72
1:B:171:ASP:OD1	1:B:186:THR:HG23	1.90	0.72
1:A:528:MET:CE	1:A:530:LEU:HD21	2.19	0.72
1:B:312:SER:HB2	1:B:325:MET:HE3	1.70	0.72
1:A:184:ARG:HD3	1:A:186:THR:O	1.89	0.72
1:C:684:ARG:HD3	3:C:1582:HOH:O	1.89	0.72
1:A:74:ASN:C	1:A:92:ASN:HB3	2.15	0.72
1:A:207:VAL:O	1:A:358:ARG:NH2	2.23	0.71
1:B:74:ASN:C	1:B:92:ASN:HB3	2.15	0.71
1:D:320:GLN:OE1	1:D:669:ARG:HD3	1.91	0.71
1:D:684:ARG:HG3	3:D:1162:HOH:O	1.89	0.71
1:C:361:GLU:HG2	3:C:955:HOH:O	1.89	0.71
1:B:438:ASP:OD1	1:B:440:THR:HB	1.90	0.71
1:D:183:TYR:HE1	1:D:277:SER:O	1.73	0.71
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.26	0.70
1:D:673:LEU:HG	3:D:1710:HOH:O	1.89	0.70
1:B:658:ARG:HG2	1:B:661:TYR:CE2	2.26	0.70
1:C:142:LEU:HG	3:C:1702:HOH:O	1.89	0.70
1:D:334:SER:HB3	1:D:336:ARG:NE	2.07	0.70
1:C:177:GLU:HB2	1:C:180:LEU:HD22	1.72	0.70
1:C:334:SER:HB3	1:C:336:ARG:NE	2.07	0.70
1:B:341:VAL:O	1:B:342:ALA:HB3	1.90	0.70
1:A:597:ARG:HH12	1:A:679:ASN:HD21	1.40	0.70
1:D:177:GLU:HB2	1:D:180:LEU:HD22	1.72	0.70
1:C:320:GLN:OE1	1:C:669:ARG:HD3	1.92	0.70
1:C:359:PRO:HA	3:C:1500:HOH:O	1.92	0.70
1:D:600:THR:O	1:D:603:VAL:HG13	1.92	0.70
1:C:153:GLN:HE22	1:C:170:ASN:ND2	1.90	0.69
1:B:410:LEU:HD13	1:B:415:LEU:HD23	1.74	0.69
1:D:379:GLU:HB2	3:D:1305:HOH:O	1.91	0.69
1:B:597:ARG:HH12	1:B:679:ASN:HD21	1.40	0.69
1:B:704:HIS:HB2	3:B:1886:HOH:O	1.93	0.69
1:D:184:ARG:HD3	1:D:186:THR:O	1.92	0.69
1:D:153:GLN:HE22	1:D:170:ASN:ND2	1.90	0.69
1:A:392:LYS:HG3	3:A:1107:HOH:O	1.91	0.69
1:B:471:ARG:HB3	3:B:1550:HOH:O	1.92	0.69
1:A:327:ILE:HB	1:A:343:ARG:HG2	1.75	0.68
1:C:103:ASN:HB2	3:C:1205:HOH:O	1.92	0.68
1:C:600:THR:O	1:C:603:VAL:HG13	1.93	0.68
1:A:320:GLN:OE1	1:A:669:ARG:HD3	1.94	0.68
1:D:347:GLU:HG3	3:D:1766:HOH:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ASN:HB2	3:A:972:HOH:O	1.93	0.68
1:A:97:GLU:HB3	3:A:1936:HOH:O	1.93	0.68
1:B:203:TYR:HA	1:B:207:VAL:HG13	1.76	0.68
3:A:771:HOH:O	1:B:736:THR:HG22	1.92	0.68
1:C:184:ARG:HD3	1:C:186:THR:O	1.94	0.68
1:C:358:ARG:HD2	3:C:1669:HOH:O	1.93	0.68
1:A:90:LEU:O	1:A:90:LEU:HD13	1.94	0.67
1:A:253:ARG:HD3	3:A:1922:HOH:O	1.93	0.67
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.94	0.67
1:C:109:PRO:HB2	1:C:160:VAL:O	1.94	0.67
1:D:109:PRO:HB2	1:D:160:VAL:O	1.93	0.67
1:A:410:LEU:HD13	1:A:415:LEU:HD23	1.75	0.67
1:A:450:ASN:HB3	3:A:1607:HOH:O	1.94	0.67
1:B:90:LEU:HD13	1:B:90:LEU:O	1.95	0.67
1:C:98:PHE:HA	3:C:1652:HOH:O	1.93	0.67
1:A:310:ARG:NE	3:A:1515:HOH:O	2.26	0.67
1:C:203:TYR:HA	1:C:207:VAL:CG1	2.25	0.67
1:C:82:GLU:HG2	3:C:1535:HOH:O	1.94	0.66
1:D:203:TYR:HA	1:D:207:VAL:CG1	2.25	0.66
1:D:203:TYR:CD2	1:D:207:VAL:HG11	2.29	0.66
1:D:69:LEU:CD1	1:D:107:ILE:HD12	2.25	0.66
1:C:203:TYR:CD2	1:C:207:VAL:HG11	2.30	0.66
1:C:69:LEU:CD1	1:C:107:ILE:HD12	2.25	0.66
1:B:272:ASN:ND2	1:B:274:ASP:H	1.94	0.66
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.78	0.66
1:B:379:GLU:HB2	3:B:1743:HOH:O	1.94	0.66
1:A:203:TYR:HA	1:A:207:VAL:HG13	1.78	0.66
1:D:171:ASP:OD1	1:D:186:THR:HG23	1.96	0.66
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.78	0.66
1:B:52:THR:HB	3:B:1656:HOH:O	1.95	0.65
1:C:536:LYS:HG2	3:C:1268:HOH:O	1.95	0.65
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.77	0.65
1:B:109:PRO:HB2	1:B:160:VAL:O	1.96	0.65
1:B:325:MET:HE2	1:B:327:ILE:HG12	1.78	0.65
1:D:276:LEU:H	1:D:276:LEU:CD2	2.10	0.65
1:A:272:ASN:ND2	1:A:274:ASP:H	1.95	0.65
1:C:272:ASN:C	1:C:272:ASN:HD22	2.05	0.65
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.95	0.65
1:C:510:PRO:HD3	1:C:569:SER:HB2	1.78	0.64
1:D:580:GLY:O	1:D:583:SER:HB2	1.97	0.64
1:D:272:ASN:HD22	1:D:272:ASN:C	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ASP:OD1	1:C:186:THR:HG23	1.97	0.64
1:C:489:LYS:NZ	1:C:489:LYS:HB3	2.13	0.64
1:D:489:LYS:NZ	1:D:489:LYS:HB3	2.12	0.64
1:A:160:VAL:HG23	1:A:161:GLY:N	2.13	0.64
1:C:361:GLU:HG2	3:C:1108:HOH:O	1.97	0.64
1:D:279:VAL:HB	3:D:1273:HOH:O	1.97	0.64
1:B:65:ASP:OD2	1:B:466:LYS:HB2	1.98	0.64
1:D:40:ARG:HH11	1:D:40:ARG:HG2	1.63	0.64
1:A:41:LYS:HB2	3:A:1293:HOH:O	1.98	0.64
1:A:697:GLN:HG3	3:A:1278:HOH:O	1.97	0.64
1:C:51:ASN:HB2	3:C:1687:HOH:O	1.98	0.63
1:A:109:PRO:HB2	1:A:160:VAL:O	1.99	0.63
1:A:276:LEU:CD2	1:A:276:LEU:H	2.12	0.63
1:B:762:CYS:HB2	3:B:1418:HOH:O	1.98	0.63
1:C:319:ILE:HG13	3:C:1697:HOH:O	1.98	0.63
1:A:65:ASP:OD2	1:A:466:LYS:HB2	1.99	0.63
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.96	0.63
1:A:693:GLU:OE1	1:A:696:LYS:HE2	1.97	0.63
1:B:489:LYS:HB3	1:B:489:LYS:HZ3	1.64	0.63
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.34	0.63
1:A:325:MET:HE2	1:A:327:ILE:CG1	2.28	0.63
1:B:693:GLU:OE1	1:B:696:LYS:HE2	1.98	0.63
1:B:173:TYR:CE2	1:B:184:ARG:HG3	2.34	0.63
1:B:160:VAL:HG23	1:B:161:GLY:N	2.12	0.63
1:B:276:LEU:CD2	1:B:276:LEU:H	2.12	0.63
1:A:173:TYR:CE2	1:A:184:ARG:HG3	2.33	0.62
1:A:726:VAL:HG12	1:A:728:VAL:HG23	1.81	0.62
1:C:580:GLY:O	1:C:583:SER:HB2	1.99	0.62
1:C:684:ARG:HD2	3:C:1685:HOH:O	2.00	0.62
1:D:71:LYS:HB3	3:D:1461:HOH:O	1.98	0.62
1:B:243:ASP:HB3	3:B:1378:HOH:O	1.99	0.62
1:B:272:ASN:HD22	1:B:274:ASP:H	1.46	0.62
1:D:341:VAL:O	1:D:342:ALA:HB3	2.00	0.62
1:A:325:MET:HE2	1:A:327:ILE:HG12	1.81	0.62
1:A:74:ASN:HB3	1:A:92:ASN:CB	2.30	0.62
1:C:272:ASN:HD22	1:C:274:ASP:H	1.47	0.62
1:C:290:PRO:HG3	1:C:326:ASP:OD2	2.00	0.62
1:B:325:MET:HE2	1:B:327:ILE:CG1	2.30	0.61
1:D:486:VAL:HG13	1:D:487:ASN:N	2.15	0.61
1:D:54:ARG:HG2	3:D:1295:HOH:O	2.01	0.61
1:D:346:ILE:HG13	3:D:1329:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ARG:HG2	1:C:40:ARG:HH11	1.65	0.61
1:D:410:LEU:HD13	1:D:415:LEU:HD23	1.82	0.61
1:B:483:HIS:HD2	3:B:921:HOH:O	1.83	0.61
1:C:390:ASP:HB3	3:C:857:HOH:O	1.99	0.61
1:D:52:THR:HG21	3:D:1570:HOH:O	1.99	0.61
1:B:136:ASP:CG	1:B:139:LYS:HG2	2.25	0.61
1:C:114:ILE:CD1	1:C:137:LEU:HD21	2.24	0.61
1:C:486:VAL:HG13	1:C:487:ASN:N	2.16	0.61
1:B:277:SER:O	1:B:278:SER:HB3	2.00	0.61
1:C:341:VAL:O	1:C:342:ALA:HB3	2.01	0.61
1:A:277:SER:O	1:A:278:SER:HB3	2.00	0.61
1:A:272:ASN:HD22	1:A:274:ASP:H	1.49	0.60
1:B:74:ASN:HB3	1:B:92:ASN:CB	2.31	0.60
1:C:302:ASP:HB3	1:C:314:GLN:HB2	1.83	0.60
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.83	0.60
1:B:348:MET:HE3	3:B:1786:HOH:O	2.00	0.60
1:C:76:ILE:HB	1:C:90:LEU:CD1	2.30	0.60
1:C:410:LEU:HD13	1:C:415:LEU:HD23	1.83	0.60
1:D:114:ILE:CD1	1:D:137:LEU:HD21	2.23	0.60
1:A:366:LEU:HD23	3:A:1245:HOH:O	2.00	0.60
1:C:77:LEU:HD23	1:C:88:VAL:HA	1.84	0.60
1:C:276:LEU:H	1:C:276:LEU:CD2	2.11	0.60
1:D:77:LEU:HD23	1:D:88:VAL:HA	1.84	0.60
1:A:377:ASN:HB2	1:A:381:TYR:O	2.02	0.60
1:C:614:SER:HA	1:C:619:VAL:HB	1.84	0.60
1:D:614:SER:HA	1:D:619:VAL:HB	1.83	0.60
1:A:136:ASP:CG	1:A:139:LYS:HG2	2.26	0.60
1:D:290:PRO:HG3	1:D:326:ASP:OD2	2.01	0.60
1:D:76:ILE:HB	1:D:90:LEU:CD1	2.31	0.60
1:B:471:ARG:HD2	3:B:1711:HOH:O	2.02	0.60
1:D:140:ARG:HG2	1:D:140:ARG:HH11	1.66	0.60
1:C:193:ILE:HG22	1:C:194:ILE:HG13	1.84	0.60
1:C:140:ARG:HG2	1:C:140:ARG:HH11	1.67	0.59
1:B:726:VAL:HG12	1:B:728:VAL:HG23	1.83	0.59
1:C:65:ASP:OD2	1:C:466:LYS:HB2	2.02	0.59
1:D:182:SER:HB3	3:D:1765:HOH:O	2.03	0.59
1:A:261:ALA:HB2	3:B:1915:HOH:O	2.02	0.59
1:A:272:ASN:HD22	1:A:272:ASN:C	2.10	0.59
1:B:512:LYS:HD3	3:B:1081:HOH:O	2.01	0.59
1:D:93:SER:HB2	1:D:96:ASP:OD2	2.02	0.59
1:D:336:ARG:HB3	3:D:1546:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:ARG:NE	3:B:1749:HOH:O	2.18	0.59
1:B:114:ILE:CD1	1:B:137:LEU:HD21	2.32	0.59
1:B:612:GLN:HB2	3:B:1143:HOH:O	2.03	0.59
1:A:114:ILE:CD1	1:A:137:LEU:HD21	2.31	0.59
1:B:289:ALA:HB2	3:B:1085:HOH:O	2.02	0.59
1:B:377:ASN:HB2	1:B:381:TYR:O	2.02	0.59
1:B:693:GLU:HA	1:B:726:VAL:HG11	1.85	0.59
1:C:93:SER:HB2	1:C:96:ASP:OD2	2.02	0.59
1:C:721:LYS:HG2	3:C:1313:HOH:O	2.01	0.59
1:C:513:LYS:HD2	3:C:1508:HOH:O	2.03	0.59
1:D:65:ASP:OD2	1:D:466:LYS:HB2	2.02	0.59
1:A:139:LYS:HD3	3:A:1411:HOH:O	2.02	0.58
1:D:342:ALA:HA	3:D:1699:HOH:O	2.02	0.58
1:A:89:PHE:CE1	1:A:107:ILE:HD13	2.38	0.58
1:B:272:ASN:HD22	1:B:272:ASN:C	2.10	0.58
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.38	0.58
1:A:71:LYS:HG2	1:A:76:ILE:HG12	1.85	0.58
1:B:348:MET:HG3	3:B:1665:HOH:O	2.03	0.58
1:C:194:ILE:HD12	3:C:1007:HOH:O	2.02	0.58
1:C:338:ASN:HB2	3:C:1328:HOH:O	2.03	0.58
1:A:334:SER:CB	1:A:336:ARG:HE	2.15	0.58
1:D:272:ASN:HD22	1:D:274:ASP:H	1.48	0.58
1:A:506:ASN:HB2	3:A:1502:HOH:O	2.03	0.58
1:B:172:ILE:H	1:B:186:THR:CG2	2.13	0.58
1:B:248:TYR:HE1	3:B:1915:HOH:O	1.85	0.58
1:C:103:ASN:OD1	1:C:117:GLU:HG2	2.03	0.58
1:D:194:ILE:HD12	3:D:1007:HOH:O	2.03	0.58
1:D:193:ILE:HG22	1:D:194:ILE:HG13	1.85	0.58
1:B:523:LYS:HG2	3:B:1411:HOH:O	2.04	0.58
1:C:172:ILE:HB	3:C:1474:HOH:O	2.03	0.58
1:D:41:LYS:HD2	3:D:1713:HOH:O	2.02	0.58
1:A:341:VAL:O	1:A:342:ALA:CB	2.47	0.58
1:B:71:LYS:HG2	1:B:76:ILE:HG12	1.86	0.58
1:B:90:LEU:C	1:B:90:LEU:HD22	2.28	0.58
1:B:334:SER:CB	1:B:336:ARG:HE	2.14	0.58
1:B:452:GLU:HG2	3:B:1827:HOH:O	2.03	0.58
1:D:184:ARG:HD2	1:D:187:TRP:CE2	2.39	0.58
1:D:327:ILE:HB	1:D:343:ARG:HG2	1.86	0.58
1:B:74:ASN:HB3	1:B:92:ASN:HB3	1.86	0.57
1:C:422:TYR:CE2	1:C:423:LYS:HD3	2.39	0.57
1:D:621:ASN:HB3	3:D:1531:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:PHE:CE1	1:B:107:ILE:HD13	2.40	0.57
1:A:693:GLU:HA	1:A:726:VAL:HG11	1.86	0.57
1:C:203:TYR:HA	1:C:207:VAL:HG12	1.86	0.57
1:A:172:ILE:H	1:A:186:THR:CG2	2.15	0.57
1:A:90:LEU:C	1:A:90:LEU:HD22	2.30	0.57
1:D:41:LYS:HB2	3:D:1768:HOH:O	2.04	0.57
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.86	0.57
1:A:684:ARG:HD2	3:A:1478:HOH:O	2.05	0.57
1:C:106:SER:HB3	1:C:115:LEU:HB3	1.85	0.57
1:D:106:SER:HB3	1:D:115:LEU:HB3	1.85	0.57
1:A:243:ASP:HB3	3:A:1428:HOH:O	2.05	0.57
1:A:44:THR:HB	3:A:1011:HOH:O	2.04	0.57
1:B:232:GLU:HG2	3:B:1795:HOH:O	2.05	0.57
1:A:74:ASN:HB3	1:A:92:ASN:HB3	1.85	0.56
1:A:489:LYS:HB3	1:A:489:LYS:HZ3	1.70	0.56
1:D:103:ASN:OD1	1:D:117:GLU:HG2	2.04	0.56
1:A:71:LYS:HB3	3:A:1376:HOH:O	2.05	0.56
1:C:156:THR:HG21	1:C:214:LEU:HD11	1.87	0.56
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.87	0.56
1:C:40:ARG:HD3	1:C:507:VAL:C	2.30	0.56
1:C:69:LEU:HD22	3:C:1495:HOH:O	2.03	0.56
1:C:704:HIS:HD2	1:C:716:SER:OG	1.88	0.56
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.87	0.56
1:C:327:ILE:HB	1:C:343:ARG:HG2	1.86	0.56
1:D:40:ARG:HD3	1:D:507:VAL:C	2.30	0.56
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.85	0.56
1:D:277:SER:O	1:D:278:SER:HB3	2.05	0.56
1:B:538:LYS:HG2	3:B:1442:HOH:O	2.06	0.56
1:D:512:LYS:HD3	3:D:1446:HOH:O	2.06	0.56
1:D:622:LYS:HE3	3:D:1439:HOH:O	2.06	0.56
1:D:203:TYR:HA	1:D:207:VAL:HG12	1.87	0.56
1:D:156:THR:HG21	1:D:214:LEU:HD11	1.87	0.55
1:C:40:ARG:HD2	1:C:508:GLN:HG3	1.88	0.55
1:C:69:LEU:HD13	1:C:107:ILE:HD12	1.88	0.55
1:C:183:TYR:CE1	1:C:277:SER:O	2.58	0.55
1:B:65:ASP:CG	1:B:464:GLU:HB2	2.32	0.55
1:C:71:LYS:HE2	3:C:1293:HOH:O	2.06	0.55
1:A:276:LEU:HB3	3:A:1157:HOH:O	2.06	0.55
1:B:487:ASN:HB2	3:B:1750:HOH:O	2.05	0.55
1:D:69:LEU:HD13	1:D:107:ILE:HD12	1.88	0.55
1:A:407:ILE:HG23	1:A:415:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.41	0.55
1:C:340:LEU:O	1:C:343:ARG:HB3	2.07	0.55
1:D:183:TYR:CD2	1:D:276:LEU:HG	2.41	0.55
1:D:278:SER:HA	3:D:1433:HOH:O	2.06	0.55
1:D:342:ALA:HB1	3:D:1637:HOH:O	2.07	0.55
1:A:170:ASN:N	1:A:170:ASN:HD22	2.04	0.55
1:A:435:GLN:NE2	1:A:441:LYS:CD	2.70	0.55
1:C:277:SER:O	1:C:278:SER:HB3	2.06	0.55
1:A:413:ASP:HB2	3:A:1527:HOH:O	2.05	0.55
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.90	0.55
1:B:741:GLY:O	1:B:742:ILE:C	2.50	0.54
1:C:489:LYS:HB3	1:C:489:LYS:HZ3	1.72	0.54
1:B:413:ASP:HB2	3:B:1889:HOH:O	2.07	0.54
1:D:74:ASN:C	1:D:92:ASN:HB3	2.32	0.54
1:D:379:GLU:HG2	3:D:1512:HOH:O	2.06	0.54
1:D:726:VAL:CG1	1:D:728:VAL:HG23	2.37	0.54
1:D:40:ARG:HD2	1:D:508:GLN:HG3	1.88	0.54
1:D:71:LYS:HE2	3:D:1440:HOH:O	2.06	0.54
1:A:281:ASN:ND2	3:A:1642:HOH:O	2.39	0.54
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.89	0.54
1:B:114:ILE:HD12	1:B:137:LEU:HD21	1.89	0.54
1:C:183:TYR:CD2	1:C:276:LEU:HG	2.41	0.54
1:C:579:ASP:HB3	1:C:583:SER:OG	2.07	0.54
1:D:170:ASN:N	1:D:170:ASN:HD22	2.06	0.54
1:A:184:ARG:HD2	1:A:187:TRP:CD2	2.42	0.54
1:A:361:GLU:CD	3:A:1015:HOH:O	2.50	0.54
1:B:170:ASN:N	1:B:170:ASN:HD22	2.06	0.54
1:A:658:ARG:NH2	1:B:244:GLU:OE2	2.40	0.54
1:B:183:TYR:HE1	1:B:277:SER:O	1.91	0.54
1:B:704:HIS:HD2	1:B:716:SER:OG	1.91	0.54
1:C:57:LEU:HD21	3:C:1553:HOH:O	2.08	0.54
1:D:657:SER:OG	1:D:689:MET:HE1	2.07	0.54
1:A:459:VAL:HG22	1:A:460:SER:N	2.23	0.54
1:B:289:ALA:CB	1:B:290:PRO:CA	2.78	0.54
1:D:340:LEU:O	1:D:343:ARG:HB3	2.07	0.54
1:A:597:ARG:NH1	1:A:679:ASN:HD21	2.06	0.54
1:C:332:GLU:HB2	3:C:1548:HOH:O	2.07	0.54
1:C:74:ASN:C	1:C:92:ASN:HB3	2.33	0.53
1:D:289:ALA:CB	1:D:290:PRO:HA	2.24	0.53
1:A:741:GLY:O	1:A:742:ILE:C	2.51	0.53
1:B:502:LYS:O	1:B:505:GLN:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:704:HIS:HD2	1:D:716:SER:OG	1.91	0.53
1:A:114:ILE:HD12	1:A:137:LEU:HD21	1.89	0.53
1:C:341:VAL:HG12	3:C:1320:HOH:O	2.07	0.53
1:C:657:SER:OG	1:C:689:MET:HE1	2.08	0.53
1:A:379:GLU:HG3	3:A:1198:HOH:O	2.07	0.53
1:B:184:ARG:HD2	1:B:187:TRP:CD2	2.44	0.53
1:B:726:VAL:HB	3:B:1900:HOH:O	2.08	0.53
1:D:741:GLY:O	1:D:742:ILE:C	2.51	0.53
1:A:704:HIS:HD2	1:A:716:SER:OG	1.92	0.53
1:C:486:VAL:HG13	1:C:487:ASN:H	1.73	0.53
1:D:147:ARG:HB2	3:D:1010:HOH:O	2.09	0.53
1:C:243:ASP:HB3	3:C:1034:HOH:O	2.09	0.53
1:D:615:LYS:HG2	3:D:1056:HOH:O	2.08	0.53
1:D:136:ASP:CG	1:D:139:LYS:HG2	2.34	0.53
1:A:658:ARG:HG3	1:A:658:ARG:O	2.08	0.53
1:B:389:ILE:HD13	3:B:1167:HOH:O	2.08	0.53
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.89	0.53
1:B:520:ASN:O	1:B:521:GLU:HB2	2.09	0.53
1:C:333:SER:HB2	3:C:1523:HOH:O	2.09	0.53
1:D:415:LEU:HD13	1:D:415:LEU:C	2.34	0.53
1:D:60:LEU:HD12	1:D:60:LEU:C	2.34	0.53
1:B:407:ILE:HG23	1:B:415:LEU:HD21	1.91	0.52
1:C:342:ALA:HB3	3:C:1701:HOH:O	2.08	0.52
1:D:579:ASP:HB3	1:D:583:SER:OG	2.10	0.52
1:A:69:LEU:HD13	1:A:107:ILE:HD12	1.90	0.52
1:A:520:ASN:O	1:A:521:GLU:HB2	2.09	0.52
1:C:105:TYR:HB2	3:C:1293:HOH:O	2.09	0.52
1:D:486:VAL:HG13	1:D:487:ASN:H	1.73	0.52
1:A:622:LYS:HB2	1:A:622:LYS:NZ	2.25	0.52
1:A:736:THR:HG21	1:B:721:LYS:CB	2.22	0.52
1:C:736:THR:HG23	3:D:778:HOH:O	2.10	0.52
1:D:40:ARG:NH1	3:D:1185:HOH:O	2.42	0.52
1:D:377:ASN:HB3	1:D:379:GLU:H	1.73	0.52
1:A:502:LYS:O	1:A:505:GLN:HG2	2.09	0.52
1:B:471:ARG:HG3	3:B:1697:HOH:O	2.09	0.52
1:C:60:LEU:C	1:C:60:LEU:HD12	2.34	0.52
1:A:183:TYR:HE1	1:A:277:SER:O	1.92	0.52
1:B:69:LEU:HD13	1:B:107:ILE:HD12	1.91	0.52
1:C:89:PHE:CE1	1:C:107:ILE:HD13	2.45	0.52
1:C:741:GLY:O	1:C:742:ILE:C	2.52	0.52
1:D:76:ILE:HB	1:D:90:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ASP:CG	1:A:464:GLU:HB2	2.35	0.52
1:A:435:GLN:NE2	1:A:441:LYS:HD2	2.25	0.52
1:B:140:ARG:HG2	1:B:140:ARG:NH1	2.21	0.52
1:A:276:LEU:CD2	1:A:276:LEU:N	2.73	0.52
1:B:397:ILE:HG13	1:B:398:THR:HG23	1.92	0.52
1:C:422:TYR:CD2	1:C:423:LYS:HD3	2.45	0.52
1:D:422:TYR:CE2	1:D:423:LYS:HD3	2.44	0.52
1:A:342:ALA:HB3	3:A:1804:HOH:O	2.08	0.51
1:A:379:GLU:HG2	1:A:381:TYR:CD1	2.45	0.51
1:D:536:LYS:HE2	3:D:1692:HOH:O	2.10	0.51
1:D:658:ARG:HG2	1:D:661:TYR:CE2	2.45	0.51
1:A:244:GLU:HG3	1:B:689:MET:HE3	1.92	0.51
1:C:76:ILE:HB	1:C:90:LEU:HD13	1.91	0.51
1:C:99:GLY:HA3	3:C:1653:HOH:O	2.10	0.51
1:C:726:VAL:CG1	1:C:728:VAL:HG23	2.38	0.51
1:D:94:THR:HB	3:D:1445:HOH:O	2.09	0.51
1:A:74:ASN:HB3	1:A:92:ASN:CG	2.35	0.51
1:A:397:ILE:HG13	1:A:398:THR:HG23	1.92	0.51
1:D:472:CYS:O	1:D:478:PRO:HA	2.10	0.51
1:B:422:TYR:CE2	1:B:423:LYS:HD3	2.45	0.51
1:C:136:ASP:CG	1:C:139:LYS:HG2	2.35	0.51
1:C:170:ASN:N	1:C:170:ASN:HD22	2.08	0.51
1:C:377:ASN:HB2	1:C:381:TYR:O	2.11	0.51
1:B:597:ARG:NH1	1:B:679:ASN:HD21	2.06	0.51
1:C:536:LYS:HE3	3:C:1111:HOH:O	2.11	0.51
1:D:341:VAL:C	1:D:343:ARG:H	2.19	0.51
1:A:341:VAL:C	1:A:343:ARG:H	2.19	0.51
1:B:312:SER:CB	1:B:325:MET:HE3	2.38	0.51
1:B:504:LEU:HA	1:B:507:VAL:HG12	1.91	0.51
1:C:341:VAL:C	1:C:343:ARG:H	2.19	0.51
1:D:183:TYR:CE1	1:D:277:SER:O	2.60	0.51
1:A:140:ARG:HG2	1:A:140:ARG:NH1	2.21	0.51
1:A:422:TYR:CE2	1:A:423:LYS:HD3	2.46	0.51
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.75	0.51
1:C:377:ASN:HB3	1:C:379:GLU:H	1.75	0.51
1:D:89:PHE:CE1	1:D:107:ILE:HD13	2.46	0.51
1:B:74:ASN:HB3	1:B:92:ASN:CG	2.36	0.51
1:B:156:THR:HG21	1:B:214:LEU:HD11	1.93	0.51
1:B:513:LYS:HE3	1:B:530:LEU:HD11	1.93	0.51
1:C:415:LEU:C	1:C:415:LEU:HD13	2.36	0.51
1:D:277:SER:HA	3:D:1719:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ILE:N	1:A:285:ILE:CD1	2.74	0.50
1:B:516:PHE:CE2	1:B:523:LYS:HE2	2.47	0.50
1:C:39:SER:O	1:C:40:ARG:O	2.29	0.50
1:A:156:THR:HG21	1:A:214:LEU:HD11	1.93	0.50
1:A:392:LYS:HB3	3:A:1916:HOH:O	2.11	0.50
1:D:321:ASN:OD1	3:D:1754:HOH:O	2.19	0.50
1:A:504:LEU:HA	1:A:507:VAL:HG12	1.92	0.50
1:B:41:LYS:HG3	3:B:986:HOH:O	2.12	0.50
1:D:40:ARG:HH11	1:D:40:ARG:CG	2.25	0.50
1:A:139:LYS:HD2	3:A:1532:HOH:O	2.12	0.50
1:A:272:ASN:HD21	1:A:274:ASP:HB2	1.76	0.50
1:C:658:ARG:HG2	1:C:661:TYR:CE2	2.45	0.50
1:D:435:GLN:OE1	1:D:437:SER:HB2	2.11	0.50
1:A:645:GLY:HA2	3:A:1050:HOH:O	2.11	0.50
1:C:673:LEU:N	1:C:673:LEU:HD12	2.27	0.50
1:B:435:GLN:NE2	1:B:441:LYS:CD	2.74	0.50
1:B:459:VAL:HG22	1:B:460:SER:N	2.26	0.50
1:C:57:LEU:HD23	3:C:1025:HOH:O	2.11	0.50
1:C:472:CYS:O	1:C:478:PRO:HA	2.11	0.50
1:B:341:VAL:C	1:B:343:ARG:H	2.19	0.50
1:C:71:LYS:N	3:C:1251:HOH:O	2.44	0.50
1:C:158:SER:HB3	1:C:163:LYS:HB2	1.93	0.50
1:C:612:GLN:O	1:C:616:MET:HG3	2.12	0.50
1:D:673:LEU:HD12	1:D:673:LEU:N	2.27	0.50
1:B:622:LYS:NZ	3:B:1303:HOH:O	2.44	0.50
1:C:136:ASP:OD1	1:C:138:ASN:HB2	2.12	0.50
1:C:438:ASP:OD1	1:C:440:THR:HB	2.12	0.50
1:D:612:GLN:O	1:D:616:MET:HG3	2.12	0.50
1:A:415:LEU:C	1:A:415:LEU:HD13	2.36	0.49
1:D:521:GLU:HA	3:D:1395:HOH:O	2.10	0.49
1:A:285:ILE:N	1:A:285:ILE:HD13	2.27	0.49
1:A:516:PHE:CE2	1:A:523:LYS:HE2	2.47	0.49
1:B:658:ARG:O	1:B:658:ARG:HG3	2.12	0.49
1:D:306:ALA:CB	1:D:310:ARG:HD2	2.42	0.49
1:D:438:ASP:OD1	1:D:440:THR:HB	2.12	0.49
1:B:285:ILE:CD1	1:B:285:ILE:N	2.75	0.49
1:B:291:ALA:O	1:B:295:ILE:HG23	2.13	0.49
1:C:186:THR:HB	3:C:1474:HOH:O	2.12	0.49
1:C:278:SER:N	3:C:1462:HOH:O	2.45	0.49
1:D:136:ASP:OD1	1:D:138:ASN:HB2	2.11	0.49
1:A:312:SER:CB	1:A:325:MET:HE3	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:LYS:NZ	1:B:622:LYS:HB2	2.27	0.49
1:C:160:VAL:HG23	1:C:161:GLY:H	1.78	0.49
1:D:504:LEU:HA	1:D:507:VAL:HG12	1.94	0.49
1:A:379:GLU:HB2	3:A:1810:HOH:O	2.11	0.49
1:A:513:LYS:HE3	1:A:530:LEU:HD11	1.94	0.49
1:C:306:ALA:CB	1:C:310:ARG:HD2	2.43	0.49
1:B:341:VAL:O	1:B:342:ALA:CB	2.56	0.49
1:B:392:LYS:HD2	1:B:393:ASP:N	2.28	0.49
1:C:314:GLN:HG3	3:C:946:HOH:O	2.13	0.49
1:B:71:LYS:NZ	1:B:105:TYR:HB2	2.28	0.49
1:B:379:GLU:HG2	1:B:381:TYR:CD1	2.47	0.49
1:C:504:LEU:HA	1:C:507:VAL:HG12	1.95	0.49
1:D:173:TYR:HB3	1:D:182:SER:OG	2.13	0.49
1:D:481:THR:OG1	1:D:483:HIS:HE1	1.96	0.49
1:A:277:SER:O	1:A:278:SER:CB	2.61	0.49
1:D:158:SER:HB3	1:D:163:LYS:HB2	1.94	0.49
1:D:276:LEU:HD23	1:D:276:LEU:O	2.12	0.49
1:D:319:ILE:C	1:D:321:ASN:H	2.21	0.49
1:D:718:GLN:HA	1:D:718:GLN:HE21	1.78	0.49
1:A:110:ASP:OD2	1:A:162:HIS:ND1	2.45	0.49
1:C:413:ASP:HB3	1:C:414:TYR:CD1	2.48	0.49
1:C:435:GLN:OE1	1:C:437:SER:HB2	2.11	0.49
1:C:139:LYS:HD3	3:C:1349:HOH:O	2.12	0.48
1:D:39:SER:O	1:D:40:ARG:O	2.31	0.48
1:D:108:SER:C	1:D:110:ASP:N	2.71	0.48
1:D:140:ARG:HG2	1:D:140:ARG:NH1	2.27	0.48
1:D:697:GLN:HG3	3:D:1792:HOH:O	2.11	0.48
1:A:147:ARG:HG2	3:A:1675:HOH:O	2.12	0.48
1:B:276:LEU:CD2	1:B:276:LEU:N	2.74	0.48
1:B:415:LEU:HD13	1:B:415:LEU:C	2.38	0.48
1:C:108:SER:C	1:C:110:ASP:N	2.71	0.48
1:C:523:LYS:HG2	3:C:876:HOH:O	2.12	0.48
1:C:528:MET:HE2	3:C:1508:HOH:O	2.12	0.48
1:D:377:ASN:HB2	1:D:381:TYR:O	2.12	0.48
1:A:39:SER:O	1:A:40:ARG:O	2.31	0.48
1:B:98:PHE:CE2	1:B:100:HIS:HB2	2.48	0.48
1:C:102:ILE:HD13	1:C:116:LEU:HD22	1.94	0.48
1:A:704:HIS:HE1	1:A:711:VAL:O	1.96	0.48
1:C:172:ILE:H	1:C:186:THR:CG2	2.23	0.48
1:C:276:LEU:O	1:C:276:LEU:HD23	2.12	0.48
1:D:93:SER:HA	1:D:96:ASP:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ALA:HA	3:A:849:HOH:O	2.11	0.48
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.96	0.48
1:B:528:MET:HE3	1:B:530:LEU:CD2	2.38	0.48
1:C:74:ASN:HB3	1:C:92:ASN:HB3	1.96	0.48
1:C:458:SER:OG	1:C:471:ARG:HB2	2.13	0.48
1:A:71:LYS:NZ	1:A:105:TYR:HB2	2.28	0.48
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.49	0.48
1:A:140:ARG:HH11	1:A:140:ARG:CG	2.19	0.48
1:B:137:LEU:O	1:B:140:ARG:NH1	2.46	0.48
1:C:40:ARG:HH11	1:C:40:ARG:CG	2.26	0.48
1:C:481:THR:OG1	1:C:483:HIS:HE1	1.97	0.48
1:D:98:PHE:CE2	1:D:100:HIS:HB2	2.49	0.48
1:D:413:ASP:HB3	1:D:414:TYR:CD1	2.48	0.48
1:A:291:ALA:O	1:A:295:ILE:HG23	2.13	0.48
1:D:160:VAL:HG23	1:D:161:GLY:H	1.77	0.48
1:B:39:SER:O	1:B:40:ARG:O	2.31	0.48
1:B:704:HIS:HE1	1:B:711:VAL:O	1.95	0.48
1:C:140:ARG:HG2	1:C:140:ARG:NH1	2.27	0.48
1:B:61:ARG:NH1	3:B:1551:HOH:O	2.45	0.48
1:B:187:TRP:N	1:B:187:TRP:CD1	2.81	0.48
1:B:276:LEU:H	1:B:276:LEU:HD22	1.79	0.48
1:B:379:GLU:HG3	3:B:1626:HOH:O	2.12	0.48
1:B:435:GLN:NE2	1:B:441:LYS:HD2	2.29	0.48
1:C:98:PHE:CE2	1:C:100:HIS:HB2	2.49	0.48
1:D:505:GLN:HB3	3:D:1471:HOH:O	2.13	0.48
1:D:74:ASN:HB3	1:D:92:ASN:CB	2.43	0.48
1:A:137:LEU:O	1:A:140:ARG:NH1	2.46	0.47
1:C:173:TYR:HB3	1:C:182:SER:OG	2.14	0.47
1:C:520:ASN:HA	3:C:1515:HOH:O	2.13	0.47
1:D:74:ASN:HB3	1:D:92:ASN:HB3	1.95	0.47
1:D:411:THR:HG1	1:D:414:TYR:H	1.62	0.47
1:A:71:LYS:HE3	3:A:1782:HOH:O	2.14	0.47
1:B:69:LEU:CD1	1:B:107:ILE:HD12	2.44	0.47
1:B:183:TYR:HE1	1:B:277:SER:C	2.22	0.47
1:B:253:ARG:HG3	3:B:1727:HOH:O	2.14	0.47
1:D:272:ASN:HD22	1:D:273:THR:N	2.12	0.47
1:A:97:GLU:HG2	3:A:1217:HOH:O	2.14	0.47
1:C:74:ASN:HB3	1:C:92:ASN:CB	2.43	0.47
1:D:51:ASN:HA	3:D:1204:HOH:O	2.14	0.47
1:A:187:TRP:N	1:A:187:TRP:CD1	2.81	0.47
1:A:658:ARG:HG2	1:A:661:TYR:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ARG:NH2	3:B:1305:HOH:O	2.46	0.47
1:C:272:ASN:HD22	1:C:273:THR:N	2.11	0.47
1:C:272:ASN:HD21	1:C:274:ASP:HB2	1.79	0.47
1:C:343:ARG:HD2	3:C:1044:HOH:O	2.13	0.47
1:C:691:ARG:NE	3:C:1662:HOH:O	2.30	0.47
1:D:531:PRO:HB3	1:D:572:ASN:HD22	1.79	0.47
1:A:281:ASN:HB3	3:A:1866:HOH:O	2.15	0.47
1:B:764:SER:HA	3:B:1050:HOH:O	2.14	0.47
1:C:76:ILE:CD1	1:C:90:LEU:HD11	2.39	0.47
1:D:102:ILE:HD13	1:D:116:LEU:HD22	1.95	0.47
1:D:402:TRP:CD2	1:D:421:GLU:HB2	2.50	0.47
1:A:69:LEU:CD1	1:A:107:ILE:HD12	2.44	0.47
1:A:85:ASN:ND2	3:A:1859:HOH:O	2.47	0.47
1:A:580:GLY:O	1:A:583:SER:HB2	2.15	0.47
1:B:71:LYS:HZ1	1:B:105:TYR:HB2	1.79	0.47
1:B:277:SER:O	1:B:278:SER:CB	2.61	0.47
1:B:658:ARG:HG2	1:B:661:TYR:CD2	2.50	0.47
1:C:40:ARG:HB2	1:C:506:ASN:O	2.15	0.47
1:C:276:LEU:CD2	1:C:276:LEU:N	2.75	0.47
1:C:319:ILE:C	1:C:321:ASN:H	2.22	0.47
1:D:459:VAL:HG22	1:D:460:SER:N	2.29	0.47
1:A:392:LYS:HD2	1:A:393:ASP:N	2.29	0.47
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.96	0.47
1:C:40:ARG:NH1	1:C:505:GLN:O	2.47	0.47
1:C:429:ARG:NE	3:C:865:HOH:O	2.39	0.47
1:D:40:ARG:HB2	1:D:506:ASN:O	2.14	0.47
1:D:422:TYR:CD2	1:D:423:LYS:HD3	2.50	0.47
1:A:358:ARG:NH1	3:A:1346:HOH:O	2.46	0.47
1:D:272:ASN:HD21	1:D:274:ASP:HB2	1.80	0.47
1:A:407:ILE:CG2	1:A:415:LEU:HD21	2.45	0.47
1:A:276:LEU:H	1:A:276:LEU:HD22	1.78	0.47
1:C:93:SER:HA	1:C:96:ASP:OD1	2.14	0.47
1:C:531:PRO:HB3	1:C:572:ASN:HD22	1.79	0.47
1:D:483:HIS:HD2	3:D:1104:HOH:O	1.98	0.47
1:D:502:LYS:HD3	3:D:1101:HOH:O	2.15	0.47
1:A:140:ARG:NH1	1:A:140:ARG:CG	2.76	0.46
1:A:489:LYS:HB2	3:A:788:HOH:O	2.15	0.46
1:B:472:CYS:O	1:B:478:PRO:HA	2.15	0.46
1:D:726:VAL:O	1:D:726:VAL:HG13	2.15	0.46
1:D:458:SER:OG	1:D:471:ARG:HB2	2.15	0.46
1:A:366:LEU:HB3	3:A:1020:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:GLN:NE2	1:A:441:LYS:HD3	2.31	0.46
1:B:140:ARG:HH11	1:B:140:ARG:CG	2.19	0.46
1:B:310:ARG:NH1	1:B:329:ASP:OD1	2.49	0.46
1:B:726:VAL:O	1:B:726:VAL:CG1	2.63	0.46
1:C:489:LYS:HG3	3:C:821:HOH:O	2.15	0.46
1:D:65:ASP:CG	1:D:464:GLU:HB2	2.40	0.46
1:D:691:ARG:NE	3:D:1753:HOH:O	2.26	0.46
1:A:183:TYR:HE1	1:A:277:SER:C	2.23	0.46
1:A:310:ARG:CZ	3:A:1515:HOH:O	2.61	0.46
1:C:65:ASP:CG	1:C:464:GLU:HB2	2.40	0.46
1:C:354:VAL:HG12	3:C:1500:HOH:O	2.14	0.46
1:C:459:VAL:HG22	1:C:460:SER:N	2.30	0.46
1:A:342:ALA:CB	3:A:1804:HOH:O	2.62	0.46
1:B:98:PHE:CD2	1:B:100:HIS:HB2	2.51	0.46
1:B:523:LYS:HD3	3:B:1814:HOH:O	2.15	0.46
1:C:248:TYR:CZ	1:D:234:PRO:HB2	2.51	0.46
1:C:271:VAL:HG23	1:C:283:THR:O	2.16	0.46
1:D:69:LEU:HD11	1:D:107:ILE:HD12	1.96	0.46
1:B:159:PRO:HG3	3:B:1103:HOH:O	2.16	0.46
1:C:147:ARG:HD3	3:C:1473:HOH:O	2.15	0.46
1:C:538:LYS:HA	3:C:1265:HOH:O	2.15	0.46
1:C:402:TRP:CD2	1:C:421:GLU:HB2	2.50	0.46
1:C:542:LEU:C	1:C:542:LEU:HD23	2.41	0.46
1:D:358:ARG:NH2	3:D:951:HOH:O	2.48	0.46
1:D:382:ARG:NH2	3:D:802:HOH:O	2.47	0.46
1:A:74:ASN:HB2	3:A:1680:HOH:O	2.14	0.46
1:A:435:GLN:HE22	1:A:441:LYS:CD	2.27	0.46
1:A:526:TYR:OH	1:A:616:MET:HE1	2.16	0.46
1:B:41:LYS:HB2	3:B:1110:HOH:O	2.16	0.46
1:B:60:LEU:C	1:B:60:LEU:HD12	2.41	0.46
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.45	0.46
1:B:407:ILE:CG2	1:B:415:LEU:HD21	2.46	0.46
1:D:271:VAL:HG23	1:D:283:THR:O	2.15	0.46
1:D:397:ILE:HG13	1:D:398:THR:HG23	1.98	0.46
1:A:276:LEU:H	1:A:276:LEU:HD23	1.80	0.46
1:C:69:LEU:HD11	1:C:107:ILE:HD12	1.96	0.46
1:C:85:ASN:ND2	3:C:1021:HOH:O	2.49	0.46
1:C:250:LYS:HE2	3:C:1224:HOH:O	2.15	0.46
1:C:388:GLN:CB	1:C:391:LYS:HB2	2.46	0.46
1:D:160:VAL:HG21	3:D:1571:HOH:O	2.15	0.46
1:D:173:TYR:CE2	1:D:184:ARG:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:764:SER:HB2	3:D:1325:HOH:O	2.16	0.46
1:A:98:PHE:CD2	1:A:100:HIS:HB2	2.52	0.45
1:A:186:THR:HG21	1:A:196:ASN:CB	2.46	0.45
1:A:454:CYS:HB2	3:A:1607:HOH:O	2.16	0.45
1:B:140:ARG:NH1	1:B:140:ARG:CG	2.76	0.45
1:B:562:ASN:HB2	3:B:826:HOH:O	2.17	0.45
1:D:334:SER:HB3	1:D:336:ARG:CD	2.46	0.45
1:A:60:LEU:HD12	1:A:60:LEU:C	2.41	0.45
1:A:546:VAL:HG22	1:A:547:TYR:N	2.31	0.45
1:A:721:LYS:HD3	1:B:736:THR:HG23	1.98	0.45
1:B:662:TYR:CE2	2:B:800:AAF:H132	2.51	0.45
1:C:79:PHE:CD1	1:C:86:SER:HB3	2.51	0.45
1:C:310:ARG:HG3	1:C:329:ASP:OD1	2.16	0.45
1:D:40:ARG:NH1	1:D:505:GLN:O	2.50	0.45
1:D:276:LEU:CD2	1:D:276:LEU:N	2.74	0.45
1:C:154:TRP:CE2	1:C:212:SER:HB2	2.50	0.45
1:C:186:THR:HG21	1:C:196:ASN:CB	2.47	0.45
1:D:186:THR:HG21	1:D:196:ASN:CB	2.47	0.45
1:D:498:SER:O	1:D:502:LYS:HG2	2.17	0.45
1:A:71:LYS:HE2	1:A:76:ILE:CD1	2.47	0.45
1:A:161:GLY:HA3	3:A:1154:HOH:O	2.17	0.45
1:B:71:LYS:HE2	1:B:76:ILE:CD1	2.46	0.45
1:B:546:VAL:HG22	1:B:547:TYR:N	2.30	0.45
1:D:310:ARG:HG3	1:D:329:ASP:OD1	2.16	0.45
1:D:413:ASP:HB3	1:D:414:TYR:HD1	1.82	0.45
1:A:61:ARG:HG3	3:A:1672:HOH:O	2.17	0.45
1:A:114:ILE:HD11	1:A:137:LEU:HD11	1.98	0.45
1:B:80:ASN:HB2	3:B:1465:HOH:O	2.17	0.45
1:B:761:GLN:HE21	1:B:761:GLN:HB3	1.66	0.45
1:D:79:PHE:CD1	1:D:86:SER:HB3	2.51	0.45
1:D:147:ARG:HD3	3:D:1078:HOH:O	2.15	0.45
1:D:489:LYS:HB3	1:D:489:LYS:HZ3	1.79	0.45
1:C:108:SER:C	1:C:110:ASP:H	2.25	0.45
1:C:455:GLN:HA	3:C:1575:HOH:O	2.16	0.45
1:C:173:TYR:CE2	1:C:184:ARG:HG3	2.52	0.45
1:C:253:ARG:HH22	1:D:253:ARG:HH22	1.64	0.45
1:C:334:SER:HB3	1:C:336:ARG:CD	2.46	0.45
1:C:649:CYS:HB3	1:C:699:GLU:HB2	1.99	0.45
1:C:658:ARG:HD2	1:C:661:TYR:CE1	2.51	0.45
1:D:154:TRP:CE2	1:D:212:SER:HB2	2.52	0.45
1:C:512:LYS:HD3	3:C:948:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ASP:HB3	1:B:112:GLN:HB2	1.99	0.45
1:D:388:GLN:CB	1:D:391:LYS:HB2	2.47	0.45
1:A:310:ARG:NH1	1:A:329:ASP:OD1	2.50	0.45
1:B:310:ARG:CZ	3:B:1167:HOH:O	2.65	0.45
1:B:504:LEU:HA	1:B:507:VAL:CG1	2.47	0.45
1:B:579:ASP:HB3	1:B:583:SER:OG	2.17	0.45
1:D:306:ALA:HB3	1:D:310:ARG:HD2	1.98	0.45
1:B:50:LYS:HE3	3:B:1636:HOH:O	2.16	0.44
1:B:186:THR:HG21	1:B:196:ASN:CB	2.47	0.44
1:B:526:TYR:OH	1:B:616:MET:HE1	2.16	0.44
1:D:147:ARG:NH1	3:D:1473:HOH:O	2.50	0.44
1:D:542:LEU:HD23	1:D:542:LEU:C	2.42	0.44
1:B:107:ILE:HG12	1:B:114:ILE:HG12	1.99	0.44
1:B:276:LEU:H	1:B:276:LEU:HD23	1.80	0.44
1:B:697:GLN:NE2	3:B:1646:HOH:O	2.39	0.44
1:C:141:GLN:HA	3:C:1319:HOH:O	2.16	0.44
1:C:513:LYS:O	1:C:527:GLN:HA	2.17	0.44
1:A:442:VAL:HG11	3:A:1768:HOH:O	2.17	0.44
1:A:504:LEU:HA	1:A:507:VAL:CG1	2.48	0.44
1:C:528:MET:HE3	1:C:530:LEU:CD2	2.31	0.44
1:D:513:LYS:O	1:D:527:GLN:HA	2.17	0.44
1:D:704:HIS:HE1	1:D:711:VAL:O	2.00	0.44
1:A:231:THR:HG22	1:A:232:GLU:HG3	2.00	0.44
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.46	0.44
1:A:726:VAL:O	1:A:726:VAL:CG1	2.64	0.44
1:B:136:ASP:OD1	1:B:138:ASN:HB2	2.17	0.44
1:B:580:GLY:O	1:B:583:SER:HB2	2.17	0.44
1:D:492:ARG:HA	3:D:1752:HOH:O	2.17	0.44
1:A:489:LYS:HB3	1:A:489:LYS:HZ2	1.81	0.44
1:B:114:ILE:HD11	1:B:137:LEU:HD11	1.99	0.44
1:B:377:ASN:ND2	3:B:827:HOH:O	2.49	0.44
1:B:717:ALA:HA	3:B:1870:HOH:O	2.17	0.44
1:C:498:SER:O	1:C:502:LYS:HG2	2.17	0.44
1:C:397:ILE:HG13	1:C:398:THR:HG23	1.99	0.44
1:C:704:HIS:HE1	1:C:711:VAL:O	2.01	0.44
1:C:726:VAL:HG13	1:C:726:VAL:O	2.17	0.44
1:D:471:ARG:HG2	1:D:480:TYR:CD2	2.53	0.44
1:A:152:THR:HG21	1:A:155:VAL:CG2	2.48	0.44
1:A:471:ARG:HG3	3:A:1510:HOH:O	2.18	0.44
1:B:152:THR:HG21	1:B:155:VAL:CG2	2.47	0.44
1:C:471:ARG:HG2	1:C:480:TYR:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:734:TRP:CD1	1:C:736:THR:HG22	2.53	0.44
1:D:319:ILE:HD11	1:D:673:LEU:CD1	2.48	0.44
1:D:388:GLN:HG2	1:D:391:LYS:HD3	2.00	0.44
1:D:658:ARG:HD2	1:D:661:TYR:CE1	2.52	0.44
1:B:106:SER:HB3	1:B:115:LEU:HB3	2.00	0.43
1:C:306:ALA:HB3	1:C:310:ARG:HD2	1.99	0.43
1:C:321:ASN:ND2	3:C:1389:HOH:O	2.50	0.43
1:C:697:GLN:HG3	3:C:1475:HOH:O	2.18	0.43
1:D:78:VAL:HG13	1:D:78:VAL:O	2.18	0.43
1:D:172:ILE:H	1:D:186:THR:CG2	2.24	0.43
1:D:243:ASP:HB3	3:D:1071:HOH:O	2.17	0.43
1:D:343:ARG:NH2	3:D:905:HOH:O	2.49	0.43
1:D:505:GLN:HB3	3:D:822:HOH:O	2.19	0.43
1:A:107:ILE:HG12	1:A:114:ILE:HG12	2.00	0.43
1:A:377:ASN:HB3	1:A:379:GLU:H	1.82	0.43
1:B:336:ARG:H	1:B:336:ARG:HG3	1.65	0.43
1:C:184:ARG:HD2	1:C:187:TRP:CD2	2.52	0.43
1:C:516:PHE:CE2	1:C:523:LYS:HE2	2.53	0.43
1:B:110:ASP:OD2	1:B:162:HIS:ND1	2.46	0.43
1:D:52:THR:HG22	3:D:1187:HOH:O	2.18	0.43
1:D:108:SER:C	1:D:110:ASP:H	2.26	0.43
1:D:697:GLN:HG3	3:D:1488:HOH:O	2.17	0.43
1:A:184:ARG:HD2	1:A:187:TRP:CE2	2.53	0.43
1:C:388:GLN:HG2	1:C:391:LYS:HD3	2.00	0.43
1:D:546:VAL:HG22	1:D:547:TYR:N	2.33	0.43
1:A:187:TRP:NE1	3:A:1866:HOH:O	2.45	0.43
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.53	0.43
1:B:435:GLN:NE2	1:B:441:LYS:HD3	2.34	0.43
1:B:609:ALA:HA	3:B:1143:HOH:O	2.17	0.43
1:D:310:ARG:NH1	1:D:329:ASP:OD1	2.52	0.43
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.54	0.43
1:A:193:ILE:HG22	1:A:194:ILE:HG12	1.99	0.43
1:B:487:ASN:O	1:B:488:ASP:HB2	2.17	0.43
1:C:89:PHE:CD1	1:C:90:LEU:HD12	2.35	0.43
1:C:413:ASP:HB3	1:C:414:TYR:HD1	1.82	0.43
1:C:721:LYS:NZ	3:C:1313:HOH:O	2.51	0.43
1:D:98:PHE:CD2	1:D:100:HIS:HB2	2.53	0.43
1:D:147:ARG:HD2	3:D:1523:HOH:O	2.18	0.43
1:A:110:ASP:HB3	1:A:112:GLN:HB2	1.99	0.43
1:C:98:PHE:CD2	1:C:100:HIS:HB2	2.53	0.43
1:C:319:ILE:HD11	1:C:673:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:520:ASN:O	1:D:521:GLU:HB2	2.19	0.43
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.54	0.43
1:B:377:ASN:HB3	1:B:379:GLU:H	1.83	0.43
1:C:147:ARG:HB2	3:C:1018:HOH:O	2.19	0.43
1:C:310:ARG:NH1	1:C:329:ASP:OD1	2.52	0.43
1:C:546:VAL:HG22	1:C:547:TYR:N	2.34	0.43
1:C:718:GLN:HA	1:C:718:GLN:HE21	1.84	0.43
1:A:253:ARG:HG3	3:A:1821:HOH:O	2.18	0.43
1:B:177:GLU:CB	1:B:180:LEU:HD22	2.41	0.43
1:B:435:GLN:HE22	1:B:441:LYS:CD	2.32	0.43
1:D:92:ASN:HA	3:D:1633:HOH:O	2.19	0.43
1:D:415:LEU:C	1:D:415:LEU:CD1	2.92	0.43
1:A:472:CYS:O	1:A:478:PRO:HA	2.19	0.42
1:B:388:GLN:HB2	3:B:1831:HOH:O	2.18	0.42
1:B:536:LYS:NZ	1:B:536:LYS:HB3	2.34	0.42
1:B:346:ILE:HG21	1:B:348:MET:HE2	2.00	0.42
1:C:183:TYR:CE2	1:C:276:LEU:HG	2.54	0.42
1:C:237:GLU:HA	1:C:252:VAL:O	2.20	0.42
1:C:289:ALA:CB	1:C:290:PRO:HA	2.25	0.42
1:C:379:GLU:HG2	3:C:1061:HOH:O	2.19	0.42
1:C:422:TYR:CZ	1:C:423:LYS:HE3	2.54	0.42
1:D:492:ARG:HD3	3:D:889:HOH:O	2.19	0.42
1:D:528:MET:HE3	1:D:530:LEU:CD2	2.31	0.42
1:A:106:SER:HB3	1:A:115:LEU:HB3	2.00	0.42
1:A:487:ASN:O	1:A:488:ASP:HB2	2.19	0.42
1:B:654:ALA:HA	1:B:704:HIS:CD2	2.53	0.42
1:C:111:GLY:O	1:C:137:LEU:HD12	2.19	0.42
1:C:520:ASN:O	1:C:521:GLU:HB2	2.19	0.42
1:D:415:LEU:HB3	1:D:434:ILE:CG2	2.49	0.42
1:A:403:GLU:OE1	1:A:585:TYR:HA	2.20	0.42
1:A:458:SER:OG	1:A:471:ARG:HB2	2.19	0.42
1:B:630:SER:HA	1:B:654:ALA:O	2.20	0.42
1:D:184:ARG:HD2	1:D:187:TRP:CD2	2.53	0.42
1:D:403:GLU:OE1	1:D:585:TYR:HA	2.20	0.42
1:D:517:ILE:HA	3:D:1680:HOH:O	2.19	0.42
1:A:536:LYS:NZ	1:A:536:LYS:HB3	2.33	0.42
1:B:331:ASP:HB3	1:B:334:SER:HB2	2.01	0.42
1:C:334:SER:CB	1:C:336:ARG:HD2	2.49	0.42
1:C:346:ILE:HG21	1:C:348:MET:HE2	2.02	0.42
1:C:513:LYS:HE3	3:C:1577:HOH:O	2.18	0.42
1:C:660:GLU:HG3	3:C:800:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:ARG:H	1:D:336:ARG:HD2	1.85	0.42
1:A:136:ASP:OD1	1:A:138:ASN:HB2	2.19	0.42
1:B:175:LYS:NZ	3:B:1555:HOH:O	2.51	0.42
1:B:344:GLN:CD	3:B:1748:HOH:O	2.62	0.42
1:B:533:HIS:HD2	3:B:1851:HOH:O	2.00	0.42
1:B:613:PHE:C	1:B:615:LYS:H	2.27	0.42
1:B:691:ARG:NH2	3:B:1749:HOH:O	2.53	0.42
1:C:54:ARG:HE	1:C:54:ARG:HB2	1.69	0.42
1:D:40:ARG:HE	1:D:508:GLN:HG2	1.85	0.42
1:D:111:GLY:O	1:D:137:LEU:HD12	2.19	0.42
1:D:734:TRP:CD1	1:D:736:THR:HG22	2.54	0.42
1:A:334:SER:HB3	1:A:336:ARG:CD	2.50	0.42
1:A:734:TRP:NE1	3:B:1870:HOH:O	2.45	0.42
1:B:334:SER:HB3	1:B:336:ARG:CD	2.50	0.42
1:B:530:LEU:HA	1:B:531:PRO:HD3	1.95	0.42
1:B:532:PRO:HD3	1:B:569:SER:HA	2.02	0.42
1:C:268:PHE:CD2	1:C:313:LEU:HD21	2.54	0.42
1:C:536:LYS:NZ	1:C:536:LYS:CB	2.83	0.42
1:D:358:ARG:NE	3:D:1587:HOH:O	2.52	0.42
1:B:108:SER:C	1:B:110:ASP:N	2.76	0.42
1:B:247:GLN:NE2	3:B:1915:HOH:O	2.52	0.42
1:C:336:ARG:HD2	1:C:336:ARG:H	1.85	0.42
1:D:334:SER:CB	1:D:336:ARG:HD2	2.49	0.42
1:D:375:ILE:HB	3:D:1766:HOH:O	2.18	0.42
1:D:486:VAL:CG1	1:D:487:ASN:N	2.82	0.42
1:D:718:GLN:HA	1:D:718:GLN:NE2	2.35	0.42
1:A:519:LEU:O	1:A:520:ASN:C	2.62	0.42
1:A:579:ASP:HB3	1:A:583:SER:OG	2.20	0.42
1:B:231:THR:HG22	1:B:232:GLU:HG3	2.02	0.42
1:C:415:LEU:C	1:C:415:LEU:CD1	2.93	0.42
1:C:342:ALA:HA	3:C:1288:HOH:O	2.20	0.42
1:C:411:THR:HG1	1:C:414:TYR:H	1.64	0.42
1:C:415:LEU:HB3	1:C:434:ILE:CG2	2.50	0.42
1:D:57:LEU:HB3	3:D:1319:HOH:O	2.19	0.42
1:D:183:TYR:CE2	1:D:276:LEU:HG	2.54	0.42
1:D:505:GLN:HB2	3:D:1750:HOH:O	2.19	0.42
1:A:282:ALA:HB1	3:A:1288:HOH:O	2.19	0.41
1:A:346:ILE:HG21	1:A:348:MET:HE2	2.01	0.41
1:A:561:LEU:HD12	1:A:561:LEU:HA	1.92	0.41
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.20	0.41
1:C:289:ALA:HB3	3:C:1103:HOH:O	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:679:ASN:ND2	3:C:1017:HOH:O	2.53	0.41
1:D:346:ILE:HG21	1:D:348:MET:HE2	2.02	0.41
1:A:177:GLU:CB	1:A:180:LEU:HD22	2.43	0.41
1:A:512:LYS:HD3	3:A:1077:HOH:O	2.20	0.41
1:B:704:HIS:CE1	1:B:711:VAL:O	2.73	0.41
1:C:40:ARG:HE	1:C:508:GLN:HG2	1.85	0.41
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.55	0.41
1:D:54:ARG:HE	1:D:54:ARG:HB2	1.69	0.41
1:D:89:PHE:CD1	1:D:90:LEU:HD12	2.35	0.41
1:D:422:TYR:CZ	1:D:423:LYS:HE3	2.55	0.41
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.56	0.41
1:A:532:PRO:HD3	1:A:569:SER:HA	2.02	0.41
1:B:366:LEU:HD12	3:B:1691:HOH:O	2.21	0.41
1:B:543:LEU:HD12	1:B:567:LEU:HD13	2.02	0.41
1:C:615:LYS:HG2	3:C:1144:HOH:O	2.21	0.41
1:B:218:PRO:HB2	1:B:308:GLN:NE2	2.36	0.41
1:B:703:ILE:C	3:B:1886:HOH:O	2.63	0.41
1:C:388:GLN:HB2	1:C:391:LYS:HB2	2.02	0.41
1:D:283:THR:HG22	1:D:285:ILE:HD12	2.03	0.41
1:D:289:ALA:CB	1:D:290:PRO:CA	2.89	0.41
1:C:91:GLU:HB2	3:C:1085:HOH:O	2.21	0.41
1:A:175:LYS:HE3	1:A:180:LEU:O	2.21	0.41
1:B:160:VAL:CG2	1:B:161:GLY:N	2.83	0.41
1:D:519:LEU:O	1:D:520:ASN:C	2.64	0.41
1:C:392:LYS:HB3	3:C:1446:HOH:O	2.19	0.41
1:C:658:ARG:HD2	1:C:661:TYR:CZ	2.56	0.41
1:D:388:GLN:HB2	1:D:391:LYS:HB2	2.03	0.41
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.55	0.41
1:B:413:ASP:HB3	1:B:414:TYR:CD1	2.56	0.41
1:C:78:VAL:O	1:C:78:VAL:HG13	2.20	0.41
1:C:358:ARG:NH2	3:C:943:HOH:O	2.52	0.41
1:C:487:ASN:HB2	3:C:821:HOH:O	2.20	0.41
1:D:268:PHE:CD2	1:D:313:LEU:HD21	2.55	0.41
1:D:384:ILE:HG13	1:D:404:VAL:HG21	2.02	0.41
1:D:536:LYS:NZ	1:D:536:LYS:CB	2.84	0.41
1:A:40:ARG:NH1	3:A:1508:HOH:O	2.54	0.41
1:A:82:GLU:HG2	1:A:83:TYR:CZ	2.55	0.41
1:A:276:LEU:HD23	1:A:276:LEU:O	2.21	0.41
1:A:537:SER:O	1:C:350:THR:HB	2.20	0.41
1:A:691:ARG:NE	3:A:1911:HOH:O	2.21	0.41
1:B:71:LYS:HE2	1:B:76:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ILE:HB	1:B:90:LEU:HD12	2.03	0.41
1:B:82:GLU:HG2	1:B:83:TYR:CZ	2.56	0.41
1:B:93:SER:O	1:B:94:THR:C	2.64	0.41
1:B:519:LEU:O	1:B:520:ASN:C	2.63	0.41
1:B:671:MET:HE1	1:B:682:HIS:CD2	2.56	0.41
1:C:147:ARG:HH11	1:C:147:ARG:HG2	1.86	0.41
1:C:237:GLU:OE2	1:C:253:ARG:NH2	2.47	0.41
1:D:285:ILE:HD12	1:D:285:ILE:N	2.36	0.41
1:D:429:ARG:NE	3:D:876:HOH:O	2.48	0.41
1:D:649:CYS:HB3	1:D:699:GLU:HB2	2.02	0.41
1:A:331:ASP:HB3	1:A:334:SER:HB2	2.02	0.41
1:A:685:ASN:ND2	3:A:1196:HOH:O	2.51	0.41
1:B:175:LYS:HE3	1:B:180:LEU:O	2.21	0.41
1:C:384:ILE:HG13	1:C:404:VAL:HG21	2.02	0.41
1:A:409:ALA:O	1:A:415:LEU:HD22	2.21	0.40
1:A:613:PHE:C	1:A:615:LYS:H	2.27	0.40
1:A:704:HIS:CE1	1:A:711:VAL:O	2.73	0.40
1:B:369:ASN:ND2	3:B:1167:HOH:O	2.53	0.40
1:C:283:THR:HG22	1:C:285:ILE:HD12	2.02	0.40
1:D:489:LYS:HG3	3:D:1169:HOH:O	2.20	0.40
1:A:413:ASP:HB3	1:A:414:TYR:CD1	2.56	0.40
1:B:155:VAL:HG22	1:B:166:TYR:HB2	2.03	0.40
1:D:160:VAL:O	1:D:161:GLY:O	2.39	0.40
1:A:90:LEU:HD22	1:A:91:GLU:O	2.22	0.40
1:A:530:LEU:HA	1:A:531:PRO:HD3	1.96	0.40
1:B:78:VAL:O	1:B:78:VAL:HG13	2.20	0.40
1:B:158:SER:HB3	1:B:163:LYS:HB2	2.04	0.40
1:B:411:THR:HG21	3:B:1314:HOH:O	2.20	0.40
1:D:85:ASN:ND2	3:D:1371:HOH:O	2.50	0.40
1:D:507:VAL:HB	3:D:1760:HOH:O	2.21	0.40
1:A:217:SER:HB3	1:A:222:PHE:HB2	2.03	0.40
1:A:543:LEU:HD12	1:A:567:LEU:HD13	2.03	0.40
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.56	0.40
1:D:658:ARG:HD2	1:D:661:TYR:CZ	2.56	0.40
1:A:153:GLN:HE22	1:A:170:ASN:HD21	1.70	0.40
1:A:156:THR:CG2	1:A:214:LEU:HD11	2.52	0.40
1:A:513:LYS:O	1:A:527:GLN:HA	2.22	0.40
1:A:693:GLU:HB2	3:A:965:HOH:O	2.22	0.40
1:C:81:ALA:O	1:C:492:ARG:NH2	2.54	0.40
1:C:630:SER:HA	1:C:654:ALA:O	2.21	0.40
1:C:696:LYS:NZ	3:C:1402:HOH:O	2.54	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	724/726 (100%)	678 (94%)	39 (5%)	7 (1%)	12	8
1	B	724/726 (100%)	678 (94%)	39 (5%)	7 (1%)	12	8
1	C	724/726 (100%)	677 (94%)	40 (6%)	7 (1%)	12	8
1	D	724/726 (100%)	676 (93%)	41 (6%)	7 (1%)	12	8
All	All	2896/2904 (100%)	2709 (94%)	159 (6%)	28 (1%)	12	8

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	278	SER
1	B	40	ARG
1	B	278	SER
1	C	40	ARG
1	C	278	SER
1	D	40	ARG
1	D	278	SER
1	A	161	GLY
1	A	289	ALA
1	B	161	GLY
1	B	289	ALA
1	C	161	GLY
1	C	289	ALA
1	C	320	GLN
1	D	161	GLY
1	D	289	ALA
1	D	320	GLN
1	A	520	ASN
1	B	520	ASN

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Mol	Chain	Res	Type
1	A	320	GLN
1	B	320	GLN
1	C	520	ASN
1	D	520	ASN
1	C	334	SER
1	D	334	SER
1	A	94	THR
1	B	94	THR

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	651/651 (100%)	604 (93%)	47 (7%)	13	10
1	B	651/651 (100%)	604 (93%)	47 (7%)	13	10
1	C	651/651 (100%)	612 (94%)	39 (6%)	17	14
1	D	651/651 (100%)	612 (94%)	39 (6%)	17	14
All	All	2604/2604 (100%)	2432 (93%)	172 (7%)	15	12

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	40	ARG
1	A	57	LEU
1	A	66	HIS
1	A	73	GLU
1	A	90	LEU
1	A	91	GLU
1	A	140	ARG
1	A	141	GLN
1	A	170	ASN
1	A	180	LEU
1	A	194	ILE
1	A	207	VAL

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Mol	Chain	Res	Type
1	A	246	LEU
1	A	253	ARG
1	A	254	VAL
1	A	276	LEU
1	A	280	THR
1	A	285	ILE
1	A	303	VAL
1	A	313	LEU
1	A	336	ARG
1	A	358	ARG
1	A	361	GLU
1	A	388	GLN
1	A	391	LYS
1	A	392	LYS
1	A	413	ASP
1	A	436	LEU
1	A	440	THR
1	A	442	VAL
1	A	448	GLU
1	A	482	LEU
1	A	514	LEU
1	A	520	ASN
1	A	523	LYS
1	A	536	LYS
1	A	543	LEU
1	A	561	LEU
1	A	583	SER
1	A	603	VAL
1	A	673	LEU
1	A	679	ASN
1	A	701	LEU
1	A	702	LEU
1	A	726	VAL
1	A	761	GLN
1	B	39	SER
1	B	40	ARG
1	B	57	LEU
1	B	66	HIS
1	B	73	GLU
1	B	90	LEU
1	B	91	GLU
1	B	140	ARG

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Mol	Chain	Res	Type
1	B	141	GLN
1	B	170	ASN
1	B	180	LEU
1	B	194	ILE
1	B	207	VAL
1	B	246	LEU
1	B	253	ARG
1	B	254	VAL
1	B	276	LEU
1	B	280	THR
1	B	285	ILE
1	B	303	VAL
1	B	313	LEU
1	B	336	ARG
1	B	361	GLU
1	B	388	GLN
1	B	391	LYS
1	B	392	LYS
1	B	413	ASP
1	B	436	LEU
1	B	440	THR
1	B	442	VAL
1	B	448	GLU
1	B	482	LEU
1	B	514	LEU
1	B	520	ASN
1	B	523	LYS
1	B	536	LYS
1	B	543	LEU
1	B	561	LEU
1	B	583	SER
1	B	603	VAL
1	B	611	ARG
1	B	658	ARG
1	B	673	LEU
1	B	701	LEU
1	B	702	LEU
1	B	726	VAL
1	B	761	GLN
1	C	40	ARG
1	C	73	GLU
1	C	90	LEU

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Mol	Chain	Res	Type
1	C	110	ASP
1	C	145	GLU
1	C	160	VAL
1	C	170	ASN
1	C	207	VAL
1	C	246	LEU
1	C	253	ARG
1	C	254	VAL
1	C	272	ASN
1	C	276	LEU
1	C	303	VAL
1	C	332	GLU
1	C	336	ARG
1	C	373	LYS
1	C	388	GLN
1	C	415	LEU
1	C	436	LEU
1	C	440	THR
1	C	448	GLU
1	C	482	LEU
1	C	505	GLN
1	C	514	LEU
1	C	521	GLU
1	C	523	LYS
1	C	536	LYS
1	C	543	LEU
1	C	561	LEU
1	C	583	SER
1	C	603	VAL
1	C	685	ASN
1	C	689	MET
1	C	701	LEU
1	C	702	LEU
1	C	726	VAL
1	C	736	THR
1	C	761	GLN
1	D	40	ARG
1	D	73	GLU
1	D	90	LEU
1	D	110	ASP
1	D	145	GLU
1	D	160	VAL

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Mol	Chain	Res	Type
1	D	170	ASN
1	D	207	VAL
1	D	246	LEU
1	D	253	ARG
1	D	254	VAL
1	D	272	ASN
1	D	276	LEU
1	D	303	VAL
1	D	332	GLU
1	D	336	ARG
1	D	373	LYS
1	D	388	GLN
1	D	415	LEU
1	D	436	LEU
1	D	440	THR
1	D	448	GLU
1	D	482	LEU
1	D	505	GLN
1	D	514	LEU
1	D	521	GLU
1	D	523	LYS
1	D	536	LYS
1	D	543	LEU
1	D	561	LEU
1	D	583	SER
1	D	603	VAL
1	D	685	ASN
1	D	689	MET
1	D	701	LEU
1	D	702	LEU
1	D	726	VAL
1	D	736	THR
1	D	761	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	72	GLN
1	A	75	ASN
1	A	92	ASN
1	A	112	GLN

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Mol	Chain	Res	Type
1	A	169	ASN
1	A	170	ASN
1	A	247	GLN
1	A	272	ASN
1	A	314	GLN
1	A	369	ASN
1	A	435	GLN
1	A	483	HIS
1	A	487	ASN
1	A	533	HIS
1	A	572	ASN
1	A	612	GLN
1	A	679	ASN
1	A	685	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	A	761	GLN
1	B	51	ASN
1	B	72	GLN
1	B	75	ASN
1	B	92	ASN
1	B	169	ASN
1	B	170	ASN
1	B	272	ASN
1	B	314	GLN
1	B	369	ASN
1	B	435	GLN
1	B	483	HIS
1	B	487	ASN
1	B	533	HIS
1	B	572	ASN
1	B	612	GLN
1	B	679	ASN
1	B	685	ASN
1	B	694	ASN
1	B	704	HIS
1	B	718	GLN
1	B	731	GLN
1	B	761	GLN
1	C	51	ASN
1	C	72	GLN

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Mol	Chain	Res	Type
1	C	100	HIS
1	C	169	ASN
1	C	170	ASN
1	C	227	GLN
1	C	272	ASN
1	C	314	GLN
1	C	369	ASN
1	C	377	ASN
1	C	388	GLN
1	C	483	HIS
1	C	487	ASN
1	C	505	GLN
1	C	520	ASN
1	C	533	HIS
1	C	572	ASN
1	C	612	GLN
1	C	679	ASN
1	C	694	ASN
1	C	704	HIS
1	C	718	GLN
1	C	761	GLN
1	D	51	ASN
1	D	72	GLN
1	D	100	HIS
1	D	169	ASN
1	D	170	ASN
1	D	227	GLN
1	D	272	ASN
1	D	314	GLN
1	D	369	ASN
1	D	377	ASN
1	D	388	GLN
1	D	483	HIS
1	D	487	ASN
1	D	520	ASN
1	D	533	HIS
1	D	572	ASN
1	D	612	GLN
1	D	679	ASN
1	D	694	ASN
1	D	704	HIS
1	D	718	GLN

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Mol	Chain	Res	Type
1	D	761	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	AAF	B	800	1	31,31,31	1.48	7 (22%)	37,42,42	1.08	4 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AAF	B	800	1	-	2/25/44/44	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	AAF	C1-N8	3.05	1.41	1.34
2	B	800	AAF	C14-C10	2.85	1.56	1.53
2	B	800	AAF	C25-C20	2.83	1.44	1.39
2	B	800	AAF	C14-N18	-2.78	1.34	1.48
2	B	800	AAF	C22-C23	2.58	1.43	1.39
2	B	800	AAF	C24-C23	2.43	1.43	1.39
2	B	800	AAF	C22-C21	2.28	1.42	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	AAF	C12-C13-N8	2.40	107.36	103.24
2	B	800	AAF	C29-O28-C26	2.39	120.40	115.81
2	B	800	AAF	C11-C10-C14	-2.29	103.61	112.17
2	B	800	AAF	C14-C10-N8	2.25	118.39	110.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

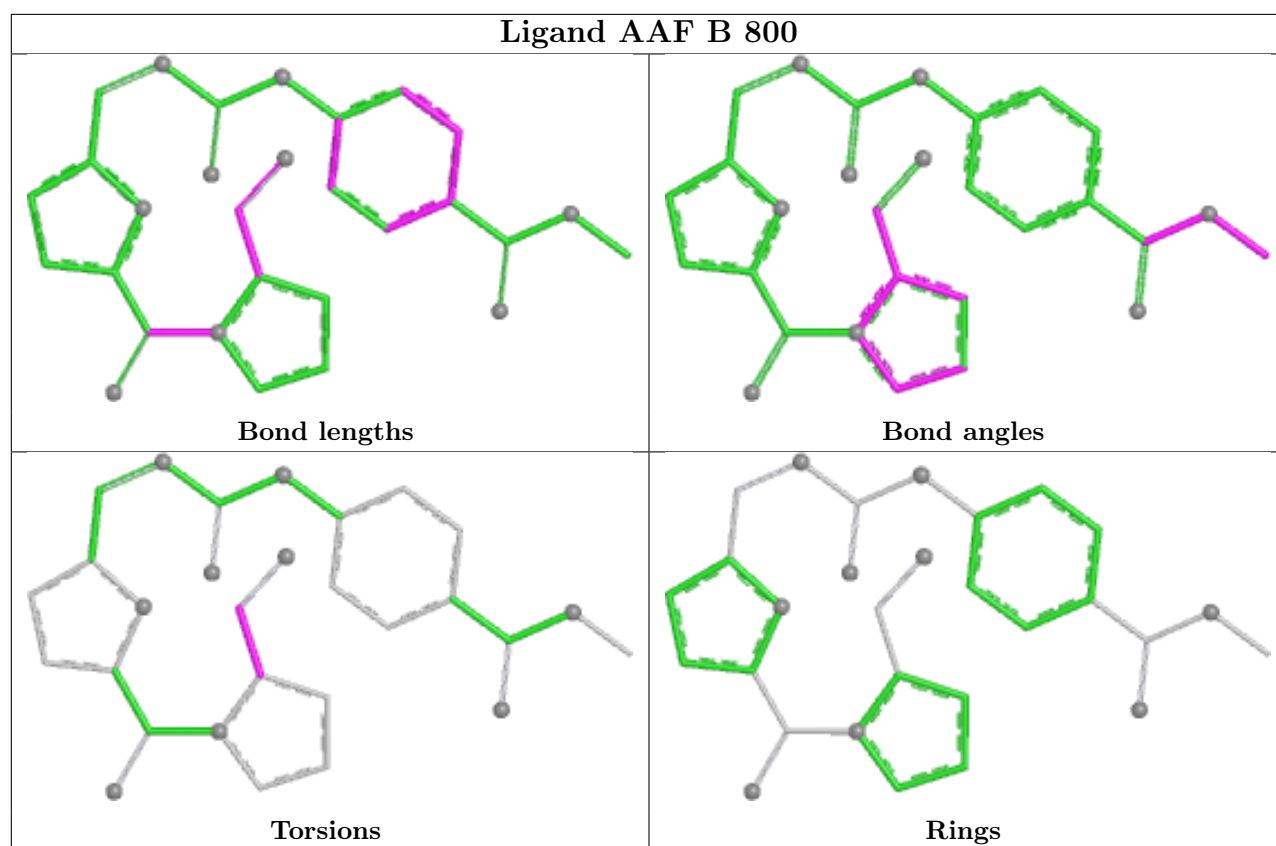
Mol	Chain	Res	Type	Atoms
2	B	800	AAF	N8-C10-C14-N18
2	B	800	AAF	C11-C10-C14-N18

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	AAF	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	726/726 (100%)	0.55	79 (10%) 10 9	16, 27, 56, 88	0
1	B	726/726 (100%)	0.64	100 (13%) 6 6	15, 28, 63, 85	0
1	C	726/726 (100%)	0.44	46 (6%) 26 24	18, 34, 61, 79	0
1	D	726/726 (100%)	0.41	51 (7%) 22 21	18, 32, 60, 79	0
All	All	2904/2904 (100%)	0.51	276 (9%) 14 12	15, 30, 60, 88	0

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	VAL	12.3
1	A	282	ALA	8.3
1	A	280	THR	8.0
1	D	289	ALA	6.7
1	A	342	ALA	6.6
1	A	281	ASN	6.6
1	B	111	GLY	6.6
1	B	341	VAL	6.2
1	A	278	SER	5.8
1	B	277	SER	5.4
1	A	277	SER	5.1
1	A	289	ALA	5.1
1	D	342	ALA	4.9
1	B	39	SER	4.8
1	B	160	VAL	4.7
1	C	277	SER	4.7
1	A	276	LEU	4.7
1	A	333	SER	4.6
1	C	333	SER	4.6
1	B	342	ALA	4.4
1	C	39	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	71	LYS	4.2
1	C	105	TYR	4.2
1	D	39	SER	4.2
1	D	90	LEU	4.2
1	D	621	ASN	4.2
1	B	114	ILE	4.1
1	A	412	SER	4.1
1	C	71	LYS	4.1
1	B	289	ALA	4.0
1	C	289	ALA	4.0
1	B	278	SER	4.0
1	A	114	ILE	3.9
1	B	103	ASN	3.9
1	C	138	ASN	3.7
1	B	66	HIS	3.7
1	A	283	THR	3.7
1	D	276	LEU	3.7
1	A	377	ASN	3.7
1	C	520	ASN	3.7
1	A	645	GLY	3.6
1	B	90	LEU	3.6
1	D	520	ASN	3.6
1	A	366	LEU	3.6
1	B	105	TYR	3.6
1	A	72	GLN	3.6
1	A	74	ASN	3.5
1	B	137	LEU	3.5
1	A	90	LEU	3.5
1	B	72	GLN	3.5
1	B	143	ILE	3.4
1	B	413	ASP	3.4
1	D	160	VAL	3.4
1	A	392	LYS	3.4
1	B	321	ASN	3.4
1	B	73	GLU	3.4
1	A	538	LYS	3.4
1	A	103	ASN	3.3
1	A	413	ASP	3.3
1	B	109	PRO	3.3
1	B	764	SER	3.3
1	C	98	PHE	3.3
1	A	161	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	88	VAL	3.3
1	A	71	LYS	3.3
1	D	71	LYS	3.3
1	C	390	ASP	3.3
1	D	277	SER	3.2
1	D	279	VAL	3.2
1	B	330	TYR	3.2
1	B	76	ILE	3.2
1	B	366	LEU	3.2
1	D	92	ASN	3.2
1	A	139	LYS	3.2
1	D	334	SER	3.2
1	A	341	VAL	3.2
1	C	389	ILE	3.2
1	A	73	GLU	3.2
1	A	187	TRP	3.1
1	B	282	ALA	3.1
1	A	39	SER	3.1
1	B	61	ARG	3.1
1	B	276	LEU	3.1
1	B	63	ILE	3.1
1	B	134	ILE	3.1
1	B	377	ASN	3.1
1	B	97	GLU	3.1
1	B	40	ARG	3.0
1	B	340	LEU	3.0
1	B	412	SER	3.0
1	A	140	ARG	3.0
1	B	333	SER	3.0
1	C	276	LEU	3.0
1	D	72	GLN	3.0
1	D	333	SER	3.0
1	B	180	LEU	3.0
1	A	487	ASN	3.0
1	B	440	THR	3.0
1	B	159	PRO	3.0
1	B	442	VAL	2.9
1	D	40	ARG	2.9
1	D	61	ARG	2.9
1	B	334	SER	2.9
1	B	367	ASP	2.9
1	B	336	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	307	THR	2.8
1	A	334	SER	2.8
1	B	487	ASN	2.8
1	D	391	LYS	2.8
1	C	182	SER	2.8
1	D	74	ASN	2.8
1	A	110	ASP	2.8
1	B	411	THR	2.8
1	C	341	VAL	2.8
1	B	466	LYS	2.8
1	A	92	ASN	2.8
1	C	72	GLN	2.8
1	B	443	THR	2.8
1	D	280	THR	2.8
1	A	518	ILE	2.8
1	C	536	LYS	2.7
1	B	120	TYR	2.7
1	B	343	ARG	2.7
1	A	160	VAL	2.7
1	A	102	ILE	2.7
1	B	138	ASN	2.7
1	C	114	ILE	2.7
1	B	62	TRP	2.7
1	C	110	ASP	2.7
1	B	414	TYR	2.7
1	C	764	SER	2.7
1	C	391	LYS	2.7
1	D	380	GLY	2.7
1	A	440	THR	2.7
1	B	280	THR	2.7
1	A	105	TYR	2.7
1	B	107	ILE	2.7
1	D	88	VAL	2.7
1	D	615	LYS	2.7
1	A	520	ASN	2.6
1	B	69	LEU	2.6
1	D	412	SER	2.6
1	B	337	TRP	2.6
1	B	102	ILE	2.6
1	B	74	ASN	2.6
1	D	423	LYS	2.6
1	A	321	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	336	ARG	2.6
1	A	614	SER	2.6
1	A	764	SER	2.6
1	B	217	SER	2.6
1	D	77	LEU	2.6
1	C	160	VAL	2.5
1	B	281	ASN	2.5
1	C	102	ILE	2.5
1	C	40	ARG	2.5
1	B	505	GLN	2.5
1	C	275	SER	2.5
1	D	86	SER	2.5
1	D	697	GLN	2.5
1	A	507	VAL	2.5
1	B	132	TYR	2.5
1	B	462	SER	2.5
1	A	41	LYS	2.5
1	A	489	LYS	2.5
1	D	89	PHE	2.5
1	B	75	ASN	2.5
1	D	442	VAL	2.4
1	D	764	SER	2.4
1	A	340	LEU	2.4
1	B	116	LEU	2.4
1	C	340	LEU	2.4
1	A	335	GLY	2.4
1	C	321	ASN	2.4
1	C	377	ASN	2.4
1	B	187	TRP	2.4
1	A	218	PRO	2.4
1	B	178	PRO	2.4
1	A	138	ASN	2.4
1	B	68	TYR	2.3
1	A	137	LEU	2.3
1	C	74	ASN	2.3
1	B	101	SER	2.3
1	B	486	VAL	2.3
1	D	91	GLU	2.3
1	C	75	ASN	2.3
1	D	321	ASN	2.3
1	B	275	SER	2.3
1	B	327	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	435	GLN	2.3
1	B	467	TYR	2.3
1	A	40	ARG	2.3
1	B	482	LEU	2.3
1	D	336	ARG	2.3
1	B	139	LYS	2.3
1	B	392	LYS	2.3
1	A	95	PHE	2.3
1	B	339	CYS	2.3
1	B	615	LYS	2.3
1	C	187	TRP	2.3
1	B	145	GLU	2.2
1	C	73	GLU	2.2
1	A	505	GLN	2.2
1	C	334	SER	2.2
1	D	83	TYR	2.2
1	A	523	LYS	2.2
1	B	389	ILE	2.2
1	D	52	THR	2.2
1	D	281	ASN	2.2
1	C	507	VAL	2.2
1	B	465	ALA	2.2
1	D	436	LEU	2.2
1	A	66	HIS	2.2
1	C	141	GLN	2.2
1	A	437	SER	2.2
1	B	370	SER	2.2
1	A	147	ARG	2.2
1	D	140	ARG	2.2
1	C	92	ASN	2.2
1	A	332	GLU	2.2
1	C	482	LEU	2.2
1	C	614	SER	2.2
1	D	93	SER	2.2
1	D	147	ARG	2.2
1	D	386	TYR	2.2
1	C	506	ASN	2.2
1	B	110	ASP	2.2
1	A	98	PHE	2.1
1	B	222	PHE	2.1
1	A	442	VAL	2.1
1	B	115	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	275	SER	2.1
1	D	278	SER	2.1
1	A	441	LYS	2.1
1	A	330	TYR	2.1
1	A	506	ASN	2.1
1	A	52	THR	2.1
1	A	141	GLN	2.1
1	D	508	GLN	2.1
1	B	220	GLY	2.1
1	B	279	VAL	2.1
1	B	56	LYS	2.1
1	B	158	SER	2.1
1	D	437	SER	2.1
1	A	75	ASN	2.1
1	A	521	GLU	2.1
1	B	119	ASN	2.1
1	A	104	ASP	2.1
1	A	336	ARG	2.1
1	C	76	ILE	2.1
1	D	99	GLY	2.1
1	C	442	VAL	2.1
1	C	538	LYS	2.1
1	B	130	ALA	2.1
1	B	291	ALA	2.1
1	A	101	SER	2.1
1	B	77	LEU	2.1
1	B	519	LEU	2.1
1	C	77	LEU	2.1
1	C	90	LEU	2.1
1	A	145	GLU	2.1
1	B	92	ASN	2.1
1	D	141	GLN	2.1
1	A	100	HIS	2.1
1	B	157	TRP	2.1
1	D	75	ASN	2.0
1	C	61	ARG	2.0
1	A	411	THR	2.0
1	B	41	LYS	2.0
1	D	139	LYS	2.0
1	A	78	VAL	2.0
1	A	379	GLU	2.0
1	B	91	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	182	SER	2.0
1	A	410	LEU	2.0
1	D	335	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

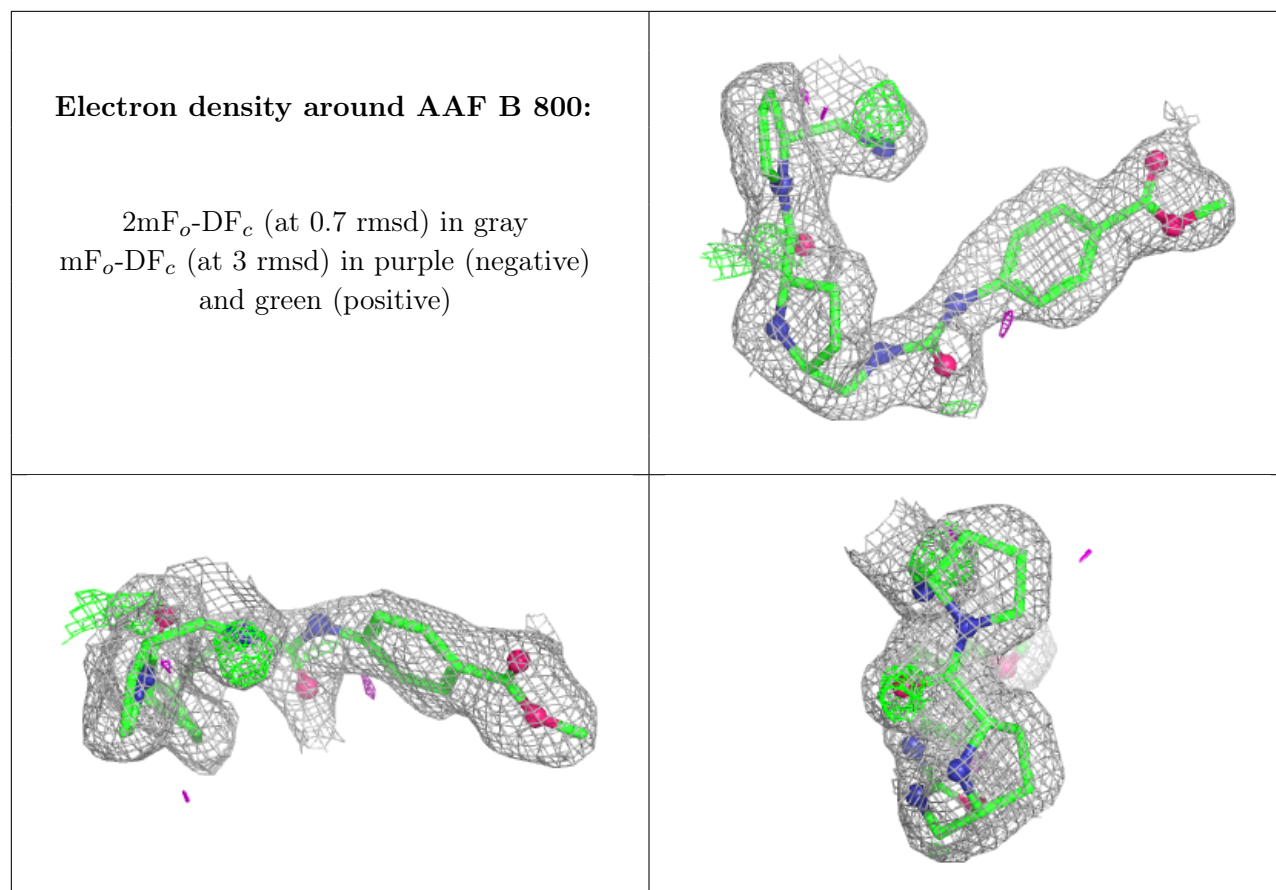
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AAF	B	800	29/29	0.91	0.10	26,31,48,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.