



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:39 PM UTC

PDB ID : 2OAG / pdb_00002oag
Title : Crystal structure of human dipeptidyl peptidase IV (DPPIV) with pyrrolidin
e-constrained phenethylamine 29g
Authors : Backes, B.J.; Longenecker, K.L.; Hamilton, G.L.; Stewart, K.D.; Lai, C.;
Kopecka, H.
Deposited on : 2006-12-15
Resolution : 2.30 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

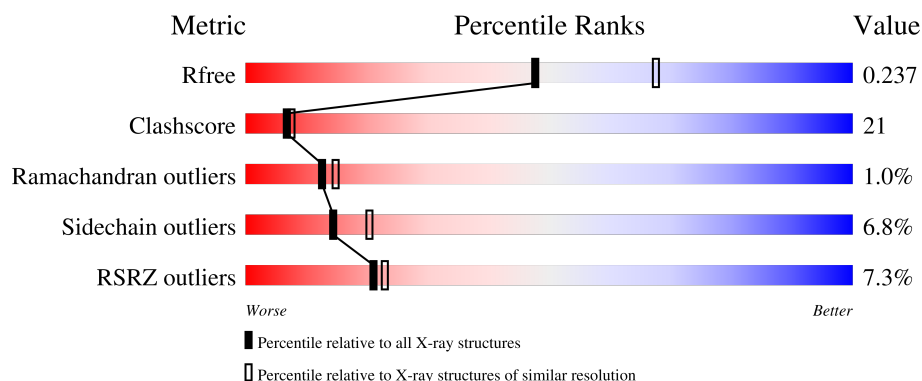
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	7% 63% 31% 5%
1	B	726	11% 65% 30% 5%
1	C	726	5% 61% 33% 5%
1	D	726	7% 61% 33% 5%

2 Entry composition [i](#)

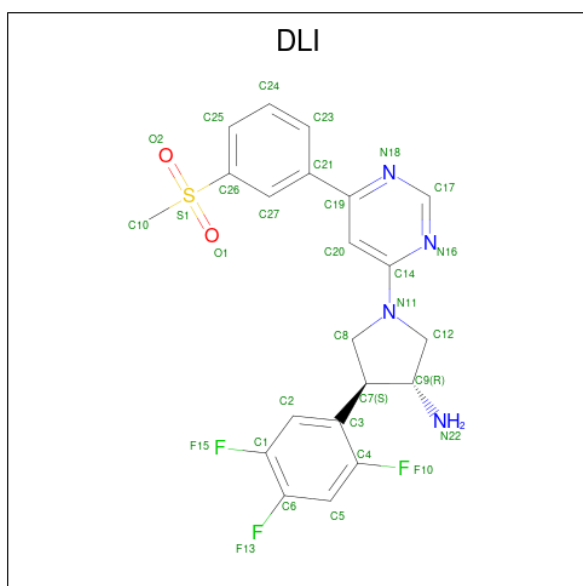
There are 3 unique types of molecules in this entry. The entry contains 27142 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (3R,4S)-1-{6-[3-(METHYLSULFONYL)PHENYL]PYRIMIDIN-4-YL}-4-(2,4,5-TRIFLUOROPHENYL)PYRROLIDIN-3-AMINE (CCD ID: DLI) (formula: $C_{21}H_{19}F_3N_4O_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	S	0	0
			31	21	3	4	2	1		

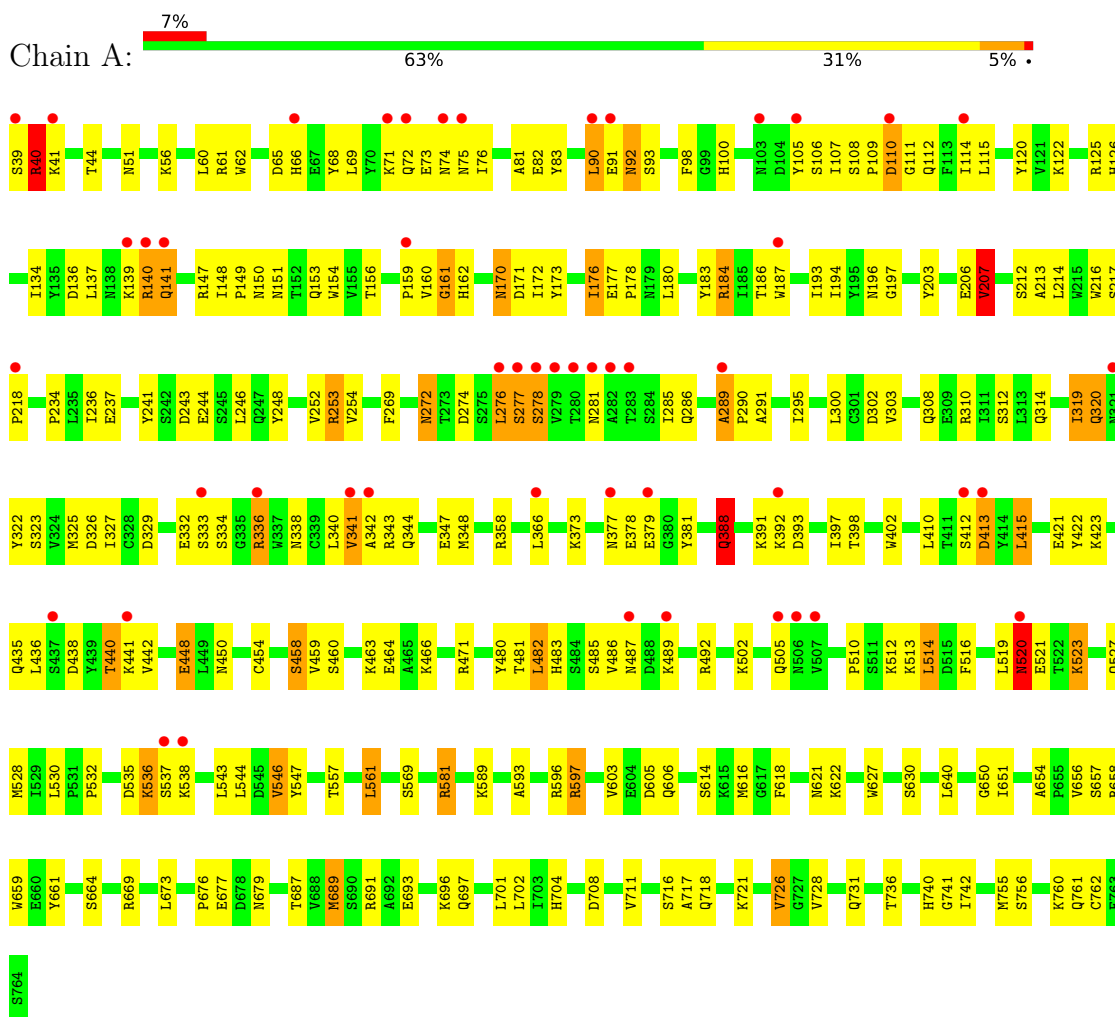
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	946	Total 946	O 946	0	0
3	B	844	Total 844	O 844	0	0
3	C	768	Total 768	O 768	0	0
3	D	757	Total 757	O 757	0	0

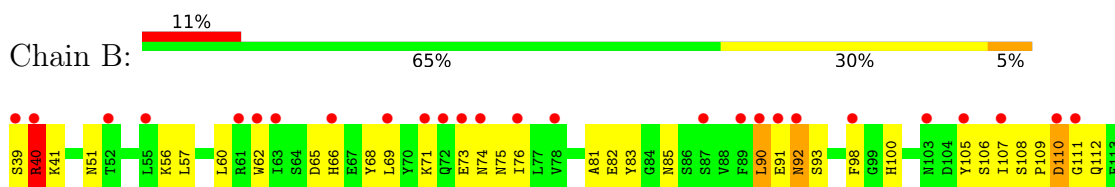
3 Residue-property plots

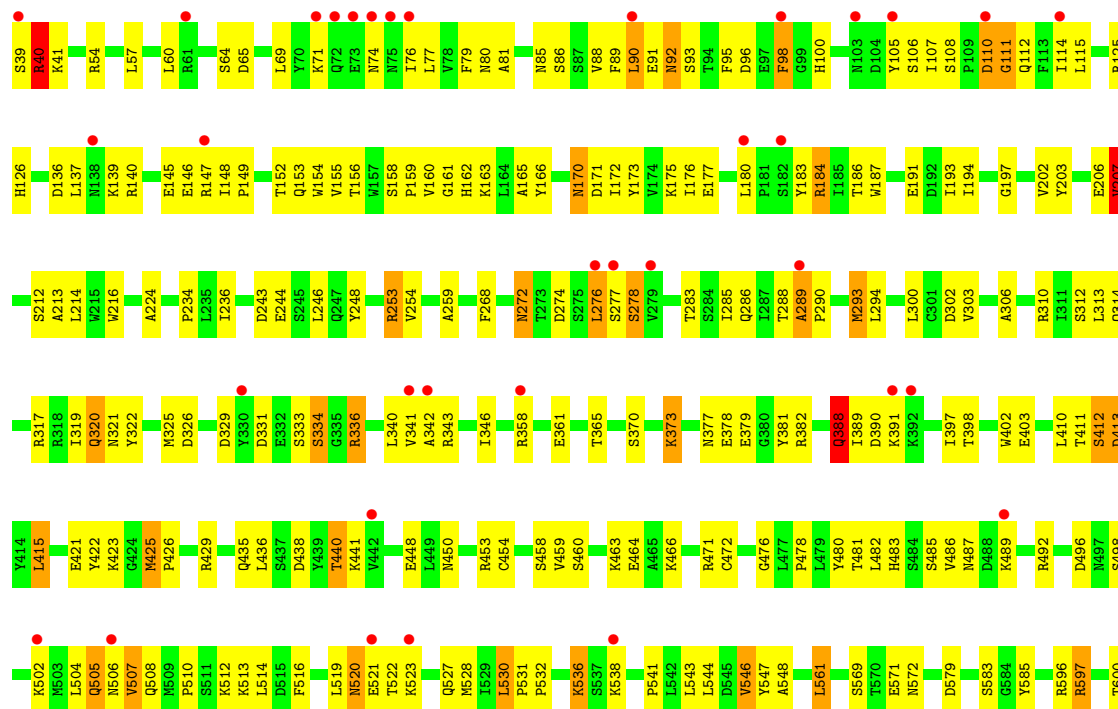
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

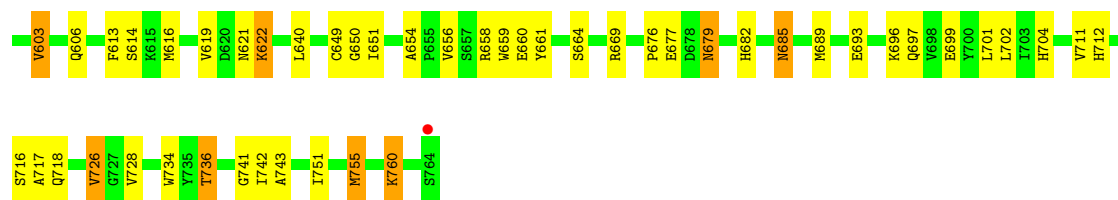
• Molecule 1: Dipeptidyl peptidase 4



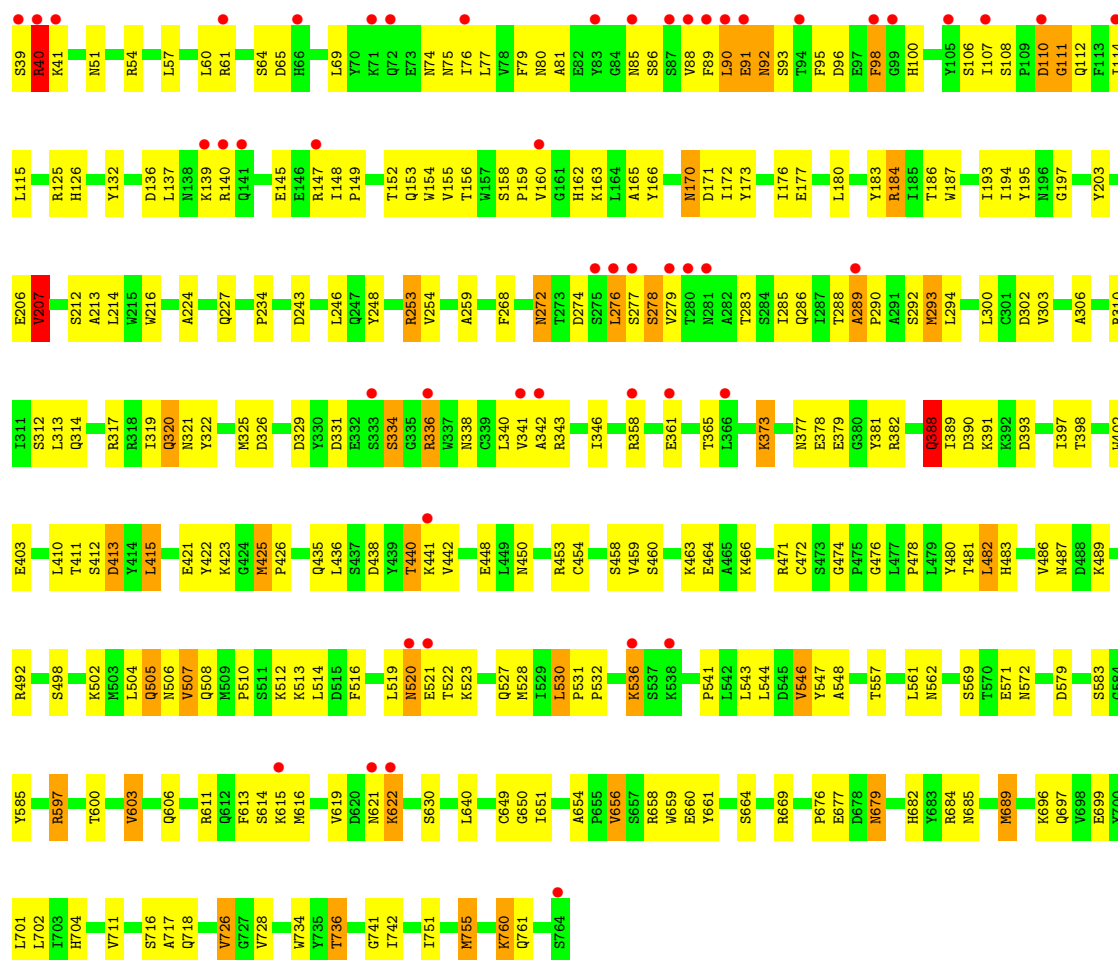
• Molecule 1: Dipeptidyl peptidase 4







• 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	120.01Å 126.22Å 127.56Å 90.00° 96.51° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.30) 97.4 (50.00-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.197 , 0.240 0.196 , 0.237	Depositor DCC
R_{free} test set	8153 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 72.3	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	0.94	EDS
Total number of atoms	27142	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: DLI

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	0.38	0/6120	0.93	22/8321 (0.3%)
1	B	0.37	0/6120	0.93	20/8321 (0.2%)
1	C	0.35	1/6120 (0.0%)	0.93	27/8321 (0.3%)
1	D	0.35	1/6120 (0.0%)	0.93	28/8321 (0.3%)
All	All	0.36	2/24480 (0.0%)	0.93	97/33284 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	755	MET	SD-CE	-7.08	1.61	1.79
1	C	755	MET	SD-CE	-7.04	1.61	1.79

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	160	VAL	N-CA-C	10.79	120.14	111.62
1	C	160	VAL	N-CA-C	10.71	120.08	111.62
1	D	378	GLU	N-CA-C	-8.88	101.88	112.89
1	C	378	GLU	N-CA-C	-8.77	102.02	112.89
1	D	207	VAL	N-CA-C	8.63	118.44	111.62
1	B	378	GLU	N-CA-C	-8.62	102.75	113.18
1	A	378	GLU	N-CA-C	-8.42	103.00	113.18
1	C	207	VAL	N-CA-C	8.36	118.22	111.62
1	B	207	VAL	N-CA-C	8.08	118.45	111.90
1	B	111	GLY	N-CA-C	-7.85	105.01	115.21
1	A	111	GLY	N-CA-C	-7.81	105.06	115.21
1	D	111	GLY	N-CA-C	-7.81	104.98	115.36
1	A	207	VAL	N-CA-C	7.78	118.20	111.90
1	C	111	GLY	N-CA-C	-7.65	105.18	115.36
1	D	425	MET	CA-C-N	7.55	127.26	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	425	MET	C-N-CA	7.55	127.26	119.56
1	B	656	VAL	N-CA-C	-7.50	99.01	109.21
1	A	656	VAL	N-CA-C	-7.36	99.21	109.21
1	C	206	GLU	N-CA-C	7.16	122.28	112.90
1	A	388	GLN	N-CA-C	-7.12	96.92	108.52
1	D	656	VAL	N-CA-C	-7.11	99.54	109.21
1	D	206	GLU	N-CA-C	6.94	121.99	112.90
1	B	388	GLN	N-CA-C	-6.85	97.35	108.52
1	C	425	MET	CA-C-N	6.83	126.52	119.56
1	C	425	MET	C-N-CA	6.83	126.52	119.56
1	C	656	VAL	N-CA-C	-6.77	100.00	109.21
1	A	630	SER	CB-CA-C	-6.70	108.12	117.23
1	A	206	GLU	N-CA-C	6.68	121.66	112.90
1	B	206	GLU	N-CA-C	6.64	121.59	112.90
1	A	458	SER	N-CA-C	-6.49	99.47	109.52
1	C	664	SER	N-CA-C	6.45	117.97	111.07
1	D	664	SER	N-CA-C	6.44	117.96	111.07
1	A	341	VAL	N-CA-C	-6.38	96.08	109.34
1	D	388	GLN	N-CA-C	-6.35	98.06	108.41
1	C	388	GLN	N-CA-C	-6.32	98.11	108.41
1	B	630	SER	CB-CA-C	-6.30	108.67	117.23
1	A	546	VAL	N-CA-C	6.22	119.00	108.86
1	B	546	VAL	N-CA-C	6.19	118.94	108.86
1	B	341	VAL	N-CA-C	-6.18	96.49	109.34
1	A	300	LEU	N-CA-C	-6.17	98.68	108.73
1	B	300	LEU	N-CA-C	-6.13	98.74	108.73
1	B	659	TRP	N-CA-C	6.13	118.75	111.71
1	C	458	SER	N-CA-C	-6.09	100.04	109.24
1	C	300	LEU	N-CA-C	-6.09	98.80	108.73
1	A	659	TRP	N-CA-C	6.03	118.65	111.71
1	A	450	ASN	CA-C-N	5.99	127.33	119.84
1	A	450	ASN	C-N-CA	5.99	127.33	119.84
1	B	450	ASN	CA-C-N	5.99	127.33	119.84
1	B	450	ASN	C-N-CA	5.99	127.33	119.84
1	D	458	SER	N-CA-C	-5.98	100.21	109.24
1	D	300	LEU	N-CA-C	-5.94	99.05	108.73
1	B	454	CYS	N-CA-C	5.92	118.57	108.02
1	B	458	SER	N-CA-C	-5.92	100.34	109.52
1	C	454	CYS	N-CA-C	5.87	118.30	108.02
1	D	546	VAL	N-CA-C	5.87	117.89	108.85
1	C	365	THR	N-CA-C	-5.84	102.82	110.53
1	C	546	VAL	N-CA-C	5.83	117.82	108.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	541	PRO	N-CA-C	-5.82	102.12	111.38
1	D	541	PRO	N-CA-C	-5.79	102.17	111.38
1	D	454	CYS	N-CA-C	5.73	118.05	108.02
1	A	454	CYS	N-CA-C	5.72	118.19	108.02
1	D	530	LEU	CA-C-N	5.64	123.78	119.66
1	D	530	LEU	C-N-CA	5.64	123.78	119.66
1	D	365	THR	N-CA-C	-5.64	103.08	110.53
1	A	664	SER	N-CA-C	5.64	117.10	111.07
1	B	485	SER	N-CA-C	5.59	118.14	111.71
1	B	412	SER	N-CA-C	-5.56	105.76	112.54
1	A	319	ILE	N-CA-C	-5.53	98.69	107.15
1	C	530	LEU	CA-C-N	5.52	123.69	119.66
1	C	530	LEU	C-N-CA	5.52	123.69	119.66
1	C	659	TRP	N-CA-C	5.51	119.10	112.38
1	C	450	ASN	CA-C-N	5.45	125.79	119.47
1	C	450	ASN	C-N-CA	5.45	125.79	119.47
1	A	412	SER	N-CA-C	-5.41	105.94	112.54
1	B	319	ILE	N-CA-C	-5.38	98.75	106.55
1	C	98	PHE	N-CA-C	-5.36	106.25	112.89
1	D	450	ASN	CA-C-N	5.35	125.68	119.47
1	D	450	ASN	C-N-CA	5.35	125.68	119.47
1	C	202	VAL	N-CA-C	5.31	116.03	110.62
1	A	448	GLU	N-CA-C	5.30	119.74	113.16
1	A	485	SER	N-CA-C	5.30	117.80	111.71
1	D	98	PHE	N-CA-C	-5.30	106.32	112.89
1	B	548	ALA	N-CA-C	5.28	119.67	113.23
1	D	548	ALA	N-CA-C	5.28	119.30	112.86
1	C	548	ALA	N-CA-C	5.27	119.29	112.86
1	A	236	ILE	N-CA-C	-5.18	100.96	108.36
1	B	664	SER	N-CA-C	5.16	116.59	111.07
1	C	412	SER	N-CA-C	-5.14	106.70	112.87
1	D	412	SER	N-CA-C	-5.12	106.73	112.87
1	A	44	THR	N-CA-C	5.12	117.13	110.53
1	C	92	ASN	N-CA-C	-5.07	105.83	111.36
1	D	206	GLU	CA-C-N	-5.05	117.81	123.16
1	D	206	GLU	C-N-CA	-5.05	117.81	123.16
1	D	659	TRP	N-CA-C	5.03	118.51	112.38
1	C	743	ALA	N-CA-C	5.02	119.36	112.88
1	D	92	ASN	N-CA-C	-5.01	105.90	111.36
1	D	630	SER	CB-CA-C	-5.00	110.42	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5949	0	5667	263	0
1	B	5949	0	5667	238	0
1	C	5949	0	5667	259	0
1	D	5949	0	5667	258	0
2	B	31	0	19	1	0
3	A	946	0	0	54	0
3	B	844	0	0	31	0
3	C	768	0	0	44	0
3	D	757	0	0	42	0
All	All	27142	0	22687	997	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 (997) 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:289:ALA:HB1	1:C:290:PRO:HA	1.36	1.06
1:B:334:SER:HB3	1:B:336:ARG:HE	1.16	1.06
1:D:289:ALA:HB1	1:D:290:PRO:HA	1.35	1.04
1:A:334:SER:HB3	1:A:336:ARG:HE	1.18	1.03
1:A:289:ALA:HB1	1:A:290:PRO:HA	1.42	1.01
1:D:621:ASN:HB3	3:D:843:HOH:O	1.62	0.99
1:B:651:ILE:HG21	1:B:755:MET:HE3	1.45	0.97
1:B:289:ALA:HB1	1:B:290:PRO:HA	1.42	0.96
1:A:736:THR:HG22	3:B:4007:HOH:O	1.67	0.94
1:A:651:ILE:HG21	1:A:755:MET:HE3	1.45	0.94
1:A:289:ALA:HB1	1:A:290:PRO:CA	1.99	0.92
1:D:293:MET:HE2	1:D:317:ARG:HG3	1.53	0.91
1:A:334:SER:HB3	1:A:336:ARG:NE	1.87	0.90
1:B:334:SER:HB3	1:B:336:ARG:NE	1.85	0.90
1:B:289:ALA:HB1	1:B:290:PRO:CA	2.01	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ILE:H	1:B:186:THR:HG22	1.38	0.88
1:D:176:ILE:HD11	1:D:276:LEU:HD21	1.54	0.88
1:C:176:ILE:HD11	1:C:276:LEU:HD21	1.54	0.88
1:C:76:ILE:HD12	1:C:90:LEU:HD11	1.56	0.88
1:C:253:ARG:HH22	1:D:253:ARG:HH22	1.20	0.87
1:D:76:ILE:HD12	1:D:90:LEU:HD11	1.57	0.87
1:A:172:ILE:H	1:A:186:THR:HG22	1.39	0.87
1:C:172:ILE:H	1:C:186:THR:HG22	1.38	0.86
1:D:614:SER:HB2	3:D:843:HOH:O	1.76	0.85
1:C:293:MET:HE2	1:C:317:ARG:HG3	1.56	0.85
1:D:334:SER:HB3	1:D:336:ARG:HE	1.41	0.84
1:A:338:ASN:HB3	3:A:1471:HOH:O	1.76	0.84
1:C:621:ASN:HB3	3:C:1173:HOH:O	1.77	0.84
1:D:289:ALA:HB1	1:D:290:PRO:CA	2.07	0.84
1:C:726:VAL:HG12	1:C:728:VAL:HG23	1.60	0.84
1:A:253:ARG:HH22	1:B:253:ARG:HH22	1.24	0.83
1:A:276:LEU:HB3	3:A:1446:HOH:O	1.79	0.83
1:A:281:ASN:HB2	3:A:1217:HOH:O	1.78	0.83
1:D:276:LEU:H	1:D:276:LEU:HD22	1.41	0.83
1:C:276:LEU:HD22	1:C:276:LEU:H	1.42	0.83
1:D:172:ILE:H	1:D:186:THR:HG22	1.40	0.83
1:C:334:SER:HB3	1:C:336:ARG:HE	1.41	0.83
1:A:487:ASN:HB2	3:A:907:HOH:O	1.79	0.82
3:A:776:HOH:O	1:B:736:THR:HG22	1.78	0.82
1:C:289:ALA:HB1	1:C:290:PRO:CA	2.08	0.82
1:D:726:VAL:HG12	1:D:728:VAL:HG23	1.59	0.82
1:A:76:ILE:HD12	1:A:90:LEU:HD11	1.61	0.82
1:C:528:MET:HE3	1:C:530:LEU:HD21	1.62	0.81
1:B:76:ILE:HD12	1:B:90:LEU:HD11	1.62	0.81
1:A:341:VAL:O	1:A:342:ALA:HB3	1.80	0.80
1:A:140:ARG:HG2	1:A:140:ARG:HH11	1.45	0.80
1:B:140:ARG:HH11	1:B:140:ARG:HG2	1.46	0.80
1:A:691:ARG:NH1	3:A:1584:HOH:O	2.14	0.80
1:A:762:CYS:HB2	3:A:1267:HOH:O	1.83	0.79
1:C:272:ASN:HD22	1:C:274:ASP:H	1.31	0.79
1:D:334:SER:HB3	1:D:336:ARG:NE	1.98	0.78
1:A:726:VAL:HG12	1:A:728:VAL:HG23	1.66	0.78
1:B:489:LYS:NZ	1:B:489:LYS:HB3	1.99	0.78
1:C:334:SER:HB3	1:C:336:ARG:NE	1.99	0.78
1:A:489:LYS:NZ	1:A:489:LYS:HB3	1.99	0.78
1:A:51:ASN:HB2	3:A:1110:HOH:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:SER:HB2	1:A:40:ARG:HE	1.50	0.77
1:B:341:VAL:O	1:B:342:ALA:HB3	1.86	0.76
1:A:627:TRP:CE3	1:A:755:MET:HE1	2.21	0.76
1:B:138:ASN:HA	3:B:4664:HOH:O	1.85	0.76
1:C:272:ASN:ND2	1:C:274:ASP:H	1.83	0.76
1:D:528:MET:HE3	1:D:530:LEU:HD21	1.66	0.76
1:D:106:SER:HB3	1:D:115:LEU:HB3	1.67	0.76
1:B:39:SER:HB2	1:B:40:ARG:HE	1.50	0.76
1:C:276:LEU:H	1:C:276:LEU:CD2	1.99	0.76
1:D:276:LEU:H	1:D:276:LEU:CD2	1.98	0.76
1:D:272:ASN:ND2	1:D:274:ASP:H	1.84	0.76
1:C:717:ALA:O	1:D:736:THR:HG21	1.86	0.75
1:D:272:ASN:HD22	1:D:274:ASP:H	1.33	0.75
1:B:160:VAL:HG23	1:B:161:GLY:H	1.51	0.75
1:B:272:ASN:HD22	1:B:274:ASP:H	1.33	0.75
1:B:627:TRP:CE3	1:B:755:MET:HE1	2.22	0.75
1:C:736:THR:HG21	1:D:717:ALA:O	1.86	0.75
1:C:358:ARG:NH1	3:C:1424:HOH:O	2.20	0.75
1:C:106:SER:HB3	1:C:115:LEU:HB3	1.67	0.74
1:B:726:VAL:HG12	1:B:728:VAL:HG23	1.67	0.74
1:D:40:ARG:HA	3:D:1013:HOH:O	1.87	0.74
1:A:171:ASP:OD1	1:A:186:THR:HG23	1.87	0.74
1:B:243:ASP:HB3	3:B:4287:HOH:O	1.87	0.74
1:B:171:ASP:OD1	1:B:186:THR:HG23	1.86	0.74
1:D:651:ILE:HG21	1:D:755:MET:HE2	1.69	0.73
1:D:184:ARG:NH1	1:D:187:TRP:HA	2.03	0.73
1:C:184:ARG:NH1	1:C:187:TRP:HA	2.03	0.73
1:A:160:VAL:HG23	1:A:161:GLY:H	1.54	0.73
1:C:538:LYS:HG2	3:C:1456:HOH:O	1.90	0.72
1:A:736:THR:CG2	1:B:721:LYS:HB2	2.19	0.72
1:D:54:ARG:HG2	3:D:1051:HOH:O	1.89	0.72
1:C:41:LYS:HB2	3:C:1002:HOH:O	1.91	0.71
1:A:651:ILE:CG2	1:A:755:MET:HE3	2.20	0.71
1:D:114:ILE:CD1	1:D:137:LEU:HD21	2.21	0.71
1:D:361:GLU:HG2	3:D:789:HOH:O	1.90	0.71
1:A:721:LYS:HB2	1:B:736:THR:HG21	1.71	0.71
1:B:693:GLU:OE1	1:B:696:LYS:HE2	1.91	0.71
1:A:693:GLU:OE1	1:A:696:LYS:HE2	1.91	0.70
1:A:721:LYS:HB2	1:B:736:THR:CG2	2.20	0.70
1:C:114:ILE:CD1	1:C:137:LEU:HD21	2.22	0.70
1:D:614:SER:HA	1:D:619:VAL:HB	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ALA:HB2	3:A:1302:HOH:O	1.90	0.70
1:B:74:ASN:C	1:B:92:ASN:HB3	2.17	0.70
1:C:676:PRO:HG2	1:C:677:GLU:OE2	1.91	0.70
1:A:697:GLN:HG3	3:A:1370:HOH:O	1.90	0.70
1:B:272:ASN:ND2	1:B:274:ASP:H	1.90	0.70
1:C:528:MET:CE	1:C:530:LEU:HD21	2.21	0.70
1:D:528:MET:CE	1:D:530:LEU:HD21	2.21	0.70
1:A:193:ILE:HG22	1:A:194:ILE:HG13	1.74	0.69
1:A:392:LYS:HB3	3:A:992:HOH:O	1.91	0.69
1:B:410:LEU:HD13	1:B:415:LEU:HD23	1.73	0.69
1:C:614:SER:HA	1:C:619:VAL:HB	1.74	0.69
1:B:193:ILE:HG22	1:B:194:ILE:HG13	1.74	0.69
1:D:171:ASP:OD1	1:D:186:THR:HG23	1.93	0.69
1:A:272:ASN:HD22	1:A:274:ASP:H	1.39	0.69
1:C:171:ASP:OD1	1:C:186:THR:HG23	1.92	0.69
1:D:676:PRO:HG2	1:D:677:GLU:OE2	1.91	0.69
1:A:341:VAL:O	1:A:342:ALA:CB	2.42	0.68
1:A:410:LEU:HD13	1:A:415:LEU:HD23	1.75	0.68
1:A:74:ASN:C	1:A:92:ASN:HB3	2.17	0.68
1:A:366:LEU:HD23	3:A:1437:HOH:O	1.94	0.68
1:A:736:THR:HG21	1:B:721:LYS:HB2	1.75	0.68
1:C:105:TYR:HB2	3:C:1041:HOH:O	1.93	0.68
1:B:651:ILE:CG2	1:B:755:MET:HE3	2.21	0.68
1:D:651:ILE:HG21	1:D:755:MET:CE	2.24	0.67
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.29	0.67
1:A:272:ASN:ND2	1:A:274:ASP:H	1.93	0.67
1:C:69:LEU:CD1	1:C:107:ILE:HD12	2.25	0.67
1:A:289:ALA:CB	1:A:290:PRO:HA	2.21	0.67
1:C:651:ILE:HG21	1:C:755:MET:HE2	1.77	0.67
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.78	0.67
1:B:160:VAL:HG23	1:B:161:GLY:N	2.10	0.67
1:C:429:ARG:NE	3:C:1421:HOH:O	2.28	0.67
1:B:289:ALA:CB	1:B:290:PRO:HA	2.21	0.66
1:D:320:GLN:OE1	1:D:669:ARG:HD3	1.95	0.66
1:C:651:ILE:HG21	1:C:755:MET:CE	2.26	0.66
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.94	0.66
1:A:489:LYS:HB3	1:A:489:LYS:HZ3	1.60	0.66
1:B:105:TYR:HB2	3:B:4361:HOH:O	1.96	0.66
1:D:177:GLU:HB2	1:D:180:LEU:HD22	1.77	0.66
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.77	0.66
1:A:289:ALA:CB	1:A:290:PRO:CA	2.74	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LYS:HD3	3:C:1223:HOH:O	1.94	0.66
1:D:69:LEU:CD1	1:D:107:ILE:HD12	2.25	0.66
1:D:334:SER:HB3	1:D:336:ARG:HD2	1.78	0.66
1:D:334:SER:HB3	1:D:336:ARG:CD	2.25	0.65
1:B:596:ARG:O	1:B:597:ARG:HD3	1.97	0.65
1:D:90:LEU:HD22	1:D:90:LEU:O	1.95	0.65
1:D:140:ARG:HG2	1:D:140:ARG:HH11	1.61	0.65
1:C:90:LEU:O	1:C:90:LEU:HD22	1.96	0.65
1:D:153:GLN:HE22	1:D:170:ASN:ND2	1.94	0.65
1:D:272:ASN:HD22	1:D:272:ASN:C	2.04	0.65
1:C:140:ARG:HG2	1:C:140:ARG:HH11	1.62	0.65
1:C:361:GLU:HG2	3:C:839:HOH:O	1.97	0.65
1:A:320:GLN:OE1	1:A:669:ARG:HD3	1.95	0.65
1:A:561:LEU:HB3	3:A:1680:HOH:O	1.95	0.65
1:C:302:ASP:HB3	1:C:314:GLN:HB2	1.76	0.65
1:C:334:SER:HB3	1:C:336:ARG:CD	2.26	0.65
1:D:358:ARG:NH2	3:D:1416:HOH:O	2.30	0.65
1:A:596:ARG:O	1:A:597:ARG:HD3	1.97	0.64
1:A:438:ASP:OD1	1:A:440:THR:HB	1.97	0.64
1:B:312:SER:HB2	1:B:325:MET:HE3	1.79	0.64
1:C:153:GLN:HE22	1:C:170:ASN:ND2	1.94	0.64
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.96	0.64
1:B:272:ASN:HD22	1:B:272:ASN:C	2.06	0.64
1:C:184:ARG:HH11	1:C:187:TRP:HA	1.62	0.64
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.79	0.64
1:A:312:SER:HB2	1:A:325:MET:HE3	1.79	0.64
1:B:502:LYS:O	1:B:505:GLN:HG2	1.98	0.64
1:C:272:ASN:HD22	1:C:272:ASN:C	2.05	0.64
1:C:320:GLN:OE1	1:C:669:ARG:HD3	1.97	0.64
1:C:57:LEU:HD21	3:C:1136:HOH:O	1.98	0.64
1:A:502:LYS:O	1:A:505:GLN:HG2	1.97	0.64
1:B:76:ILE:HB	1:B:90:LEU:CD1	2.28	0.64
1:C:277:SER:O	1:C:278:SER:HB3	1.96	0.64
1:A:39:SER:O	1:A:40:ARG:O	2.16	0.64
1:B:39:SER:O	1:B:40:ARG:O	2.15	0.64
1:C:290:PRO:HG3	1:C:326:ASP:OD2	1.98	0.64
1:C:334:SER:HB3	1:C:336:ARG:HD2	1.78	0.63
1:D:93:SER:HA	1:D:96:ASP:OD1	1.97	0.63
1:A:160:VAL:HG23	1:A:161:GLY:N	2.12	0.63
1:A:76:ILE:HB	1:A:90:LEU:CD1	2.29	0.63
1:B:442:VAL:HG13	3:B:4689:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:SER:HA	1:C:96:ASP:OD1	1.98	0.63
1:A:366:LEU:HB3	3:A:1261:HOH:O	1.98	0.63
1:C:76:ILE:HB	1:C:90:LEU:CD1	2.29	0.63
1:C:289:ALA:CB	1:C:290:PRO:HA	2.21	0.63
1:D:173:TYR:CE2	1:D:184:ARG:HG2	2.33	0.63
1:B:438:ASP:OD1	1:B:440:THR:HB	1.99	0.63
1:C:331:ASP:HB3	1:C:334:SER:HB2	1.81	0.63
1:D:147:ARG:HD3	3:D:948:HOH:O	1.99	0.63
1:D:341:VAL:O	1:D:342:ALA:HB3	1.98	0.63
1:A:114:ILE:CD1	1:A:137:LEU:HD21	2.29	0.63
1:C:510:PRO:HD3	1:C:569:SER:HB2	1.79	0.63
1:C:760:LYS:HB3	3:C:1519:HOH:O	1.98	0.62
1:D:340:LEU:O	1:D:343:ARG:HB3	1.98	0.62
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.82	0.62
1:C:177:GLU:HB2	1:C:180:LEU:HD22	1.79	0.62
1:D:40:ARG:HH11	1:D:40:ARG:HG2	1.64	0.62
1:C:340:LEU:O	1:C:343:ARG:HB3	1.99	0.62
1:D:277:SER:O	1:D:278:SER:HB3	1.98	0.62
1:A:377:ASN:HB3	1:A:379:GLU:H	1.64	0.62
1:D:74:ASN:C	1:D:92:ASN:HB3	2.24	0.62
1:D:184:ARG:HH11	1:D:187:TRP:HA	1.63	0.62
1:C:65:ASP:OD2	1:C:466:LYS:HB2	1.99	0.62
1:C:183:TYR:HE1	1:C:277:SER:O	1.83	0.62
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.96	0.62
1:A:272:ASN:HD22	1:A:272:ASN:C	2.06	0.62
1:B:114:ILE:CD1	1:B:137:LEU:HD21	2.29	0.62
1:D:65:ASP:OD2	1:D:466:LYS:HB2	1.99	0.62
1:C:173:TYR:CE2	1:C:184:ARG:HG2	2.35	0.62
1:A:39:SER:HB2	1:A:40:ARG:NE	2.15	0.62
1:C:74:ASN:C	1:C:92:ASN:HB3	2.24	0.62
1:A:159:PRO:HG2	1:A:217:SER:O	2.00	0.61
1:C:410:LEU:HD13	1:C:415:LEU:HD23	1.82	0.61
1:A:170:ASN:N	1:A:170:ASN:HD22	1.97	0.61
1:B:377:ASN:HB3	1:B:379:GLU:H	1.65	0.61
1:A:56:LYS:HE3	3:A:1393:HOH:O	2.01	0.61
1:C:341:VAL:O	1:C:342:ALA:HB3	1.99	0.61
1:D:290:PRO:HG3	1:D:326:ASP:OD2	2.00	0.61
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.82	0.61
1:A:184:ARG:HH11	1:A:187:TRP:HA	1.66	0.61
1:C:390:ASP:HB3	3:C:1086:HOH:O	1.99	0.61
1:C:158:SER:HB3	1:C:163:LYS:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:ASP:HB3	1:D:334:SER:HB2	1.81	0.61
1:D:489:LYS:NZ	1:D:489:LYS:HB3	2.16	0.61
1:A:289:ALA:HB1	1:A:290:PRO:C	2.25	0.60
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.65	0.60
1:B:616:MET:HE2	1:B:618:PHE:CZ	2.35	0.60
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.83	0.60
1:C:191:GLU:HG3	3:C:1215:HOH:O	2.00	0.60
1:D:76:ILE:HB	1:D:90:LEU:CD1	2.30	0.60
1:A:616:MET:HE2	1:A:618:PHE:CZ	2.36	0.60
1:A:616:MET:HE2	1:A:618:PHE:HZ	1.67	0.60
1:B:184:ARG:HH11	1:B:187:TRP:HA	1.65	0.60
1:C:40:ARG:HG2	1:C:40:ARG:HH11	1.65	0.60
1:B:289:ALA:CB	1:B:290:PRO:CA	2.76	0.60
1:C:412:SER:HB3	3:C:1512:HOH:O	2.02	0.60
1:D:158:SER:HB3	1:D:163:LYS:HB2	1.82	0.60
1:C:333:SER:HB2	3:C:1046:HOH:O	2.00	0.60
1:D:183:TYR:HE1	1:D:277:SER:O	1.85	0.60
1:D:410:LEU:HD13	1:D:415:LEU:HD23	1.82	0.60
1:A:72:GLN:HB3	3:A:1335:HOH:O	2.01	0.60
1:A:528:MET:CE	1:A:530:LEU:HD21	2.31	0.60
1:A:61:ARG:HG3	3:A:1599:HOH:O	2.02	0.60
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.84	0.60
1:B:290:PRO:HG3	1:B:326:ASP:OD2	2.02	0.60
1:B:528:MET:CE	1:B:530:LEU:HD21	2.31	0.60
1:B:616:MET:HE2	1:B:618:PHE:HZ	1.66	0.60
1:A:253:ARG:HH22	1:B:253:ARG:NH2	1.98	0.60
1:B:159:PRO:HG2	1:B:217:SER:O	2.01	0.60
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.37	0.60
1:B:39:SER:HB2	1:B:40:ARG:NE	2.15	0.59
1:B:512:LYS:HD3	3:B:4204:HOH:O	2.02	0.59
1:A:177:GLU:HB2	1:A:180:LEU:HD22	1.84	0.59
1:C:422:TYR:CE2	1:C:423:LYS:HD3	2.37	0.59
1:A:310:ARG:HH12	1:A:343:ARG:NH1	2.00	0.59
1:B:184:ARG:HD3	1:B:186:THR:O	2.02	0.59
1:A:272:ASN:HD21	1:A:274:ASP:HB2	1.68	0.59
1:A:290:PRO:HG3	1:A:326:ASP:OD2	2.01	0.59
1:C:489:LYS:NZ	1:C:489:LYS:HB3	2.18	0.59
1:D:154:TRP:CE2	1:D:212:SER:HB2	2.37	0.59
1:A:310:ARG:NE	3:A:1082:HOH:O	2.35	0.59
1:B:56:LYS:HE3	3:B:4521:HOH:O	2.01	0.59
1:D:40:ARG:NH1	3:D:1417:HOH:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:SER:HB2	1:D:325:MET:HE3	1.84	0.59
1:C:154:TRP:CE2	1:C:212:SER:HB2	2.37	0.58
1:D:77:LEU:HD23	1:D:88:VAL:HA	1.85	0.58
1:D:61:ARG:HG2	3:D:1448:HOH:O	2.03	0.58
1:D:139:LYS:HD3	3:D:1345:HOH:O	2.03	0.58
1:A:184:ARG:HD3	1:A:186:THR:O	2.04	0.58
1:B:289:ALA:HB1	1:B:290:PRO:C	2.28	0.58
1:B:184:ARG:NH1	1:B:187:TRP:HA	2.18	0.58
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.37	0.58
1:C:147:ARG:HD3	3:C:1283:HOH:O	2.04	0.58
1:D:289:ALA:CB	1:D:290:PRO:HA	2.21	0.58
1:A:597:ARG:HH12	1:A:679:ASN:HD21	1.52	0.58
1:B:177:GLU:HB2	1:B:180:LEU:HD22	1.86	0.58
1:A:338:ASN:HB2	3:A:914:HOH:O	2.04	0.58
1:A:341:VAL:HG11	3:A:1407:HOH:O	2.04	0.58
1:A:184:ARG:NH1	1:A:187:TRP:HA	2.19	0.57
1:D:613:PHE:O	1:D:616:MET:HB2	2.03	0.57
1:A:140:ARG:HG2	1:A:140:ARG:NH1	2.15	0.57
1:D:697:GLN:HG3	3:D:1264:HOH:O	2.05	0.57
1:A:276:LEU:H	1:A:276:LEU:HD23	1.69	0.57
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.85	0.57
1:C:172:ILE:H	1:C:186:THR:CG2	2.13	0.57
1:B:310:ARG:HG3	1:B:329:ASP:OD1	2.05	0.57
1:B:341:VAL:O	1:B:342:ALA:CB	2.49	0.57
1:C:613:PHE:O	1:C:616:MET:HB2	2.03	0.57
1:A:622:LYS:HB2	1:A:622:LYS:NZ	2.20	0.57
1:B:90:LEU:HD22	1:B:90:LEU:O	2.05	0.57
1:D:170:ASN:N	1:D:170:ASN:HD22	2.03	0.57
1:D:293:MET:HE2	1:D:317:ARG:CG	2.31	0.57
1:B:658:ARG:HG2	1:B:661:TYR:CE2	2.39	0.57
1:C:77:LEU:HD23	1:C:88:VAL:HA	1.86	0.57
1:A:464:GLU:HG3	3:A:1683:HOH:O	2.05	0.57
1:B:581:ARG:HB2	1:B:605:ASP:OD2	2.04	0.57
1:B:392:LYS:HG3	1:B:393:ASP:H	1.70	0.57
1:C:293:MET:CE	1:C:317:ARG:HG3	2.32	0.57
1:D:39:SER:O	1:D:40:ARG:O	2.23	0.57
1:B:340:LEU:C	1:B:341:VAL:O	2.44	0.56
1:B:597:ARG:HH12	1:B:679:ASN:HD21	1.53	0.56
1:A:71:LYS:NZ	1:A:105:TYR:HB2	2.19	0.56
1:A:581:ARG:HB2	1:A:605:ASP:OD2	2.05	0.56
1:B:74:ASN:HB2	3:B:4264:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ARG:HG2	1:B:140:ARG:NH1	2.16	0.56
1:C:60:LEU:C	1:C:60:LEU:HD12	2.30	0.56
1:C:161:GLY:HA3	3:C:1435:HOH:O	2.05	0.56
1:C:341:VAL:HG12	3:C:1265:HOH:O	2.06	0.56
1:D:341:VAL:C	1:D:343:ARG:H	2.12	0.56
1:D:654:ALA:HA	1:D:704:HIS:CD2	2.40	0.56
1:B:170:ASN:N	1:B:170:ASN:HD22	2.01	0.56
1:B:310:ARG:HH12	1:B:343:ARG:NH1	2.03	0.56
1:A:156:THR:HG21	1:A:214:LEU:HD11	1.88	0.56
1:B:71:LYS:NZ	1:B:105:TYR:HB2	2.20	0.56
1:D:279:VAL:HB	3:D:1256:HOH:O	2.04	0.56
1:A:90:LEU:O	1:A:90:LEU:HD22	2.05	0.56
1:C:312:SER:HB2	1:C:325:MET:HE3	1.86	0.56
1:C:697:GLN:HG3	3:C:1134:HOH:O	2.06	0.56
1:C:341:VAL:C	1:C:343:ARG:H	2.12	0.56
1:D:293:MET:CE	1:D:317:ARG:HG3	2.31	0.56
1:A:218:PRO:HB2	1:A:308:GLN:NE2	2.21	0.56
1:B:276:LEU:HD23	1:B:276:LEU:H	1.70	0.56
1:D:243:ASP:HB3	3:D:1167:HOH:O	2.05	0.56
1:B:147:ARG:HD3	3:B:4493:HOH:O	2.05	0.56
1:B:654:ALA:HA	1:B:704:HIS:CD2	2.40	0.56
1:C:39:SER:O	1:C:40:ARG:O	2.24	0.56
1:A:139:LYS:HD3	3:A:1198:HOH:O	2.06	0.56
1:B:156:THR:HG21	1:B:214:LEU:HD11	1.88	0.56
1:B:756:SER:O	1:B:760:LYS:HG3	2.06	0.56
1:D:338:ASN:HB2	3:D:1218:HOH:O	2.06	0.56
1:D:377:ASN:HB3	1:D:379:GLU:H	1.71	0.56
1:D:422:TYR:CE2	1:D:423:LYS:HD3	2.41	0.56
1:D:489:LYS:HB3	1:D:489:LYS:HZ3	1.71	0.56
1:B:218:PRO:HB2	1:B:308:GLN:NE2	2.20	0.55
1:B:276:LEU:H	1:B:276:LEU:CD2	2.19	0.55
1:C:654:ALA:HA	1:C:704:HIS:CD2	2.41	0.55
1:D:60:LEU:HD12	1:D:60:LEU:C	2.30	0.55
1:A:310:ARG:HG3	1:A:329:ASP:OD1	2.06	0.55
1:A:253:ARG:NH2	1:B:253:ARG:HH22	1.99	0.55
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.41	0.55
1:B:161:GLY:HA3	3:B:4359:HOH:O	2.05	0.55
1:C:170:ASN:N	1:C:170:ASN:HD22	2.04	0.55
1:A:736:THR:HG23	1:B:721:LYS:HB2	1.89	0.55
1:D:438:ASP:OD2	1:D:441:LYS:HG3	2.06	0.55
1:D:481:THR:OG1	1:D:483:HIS:HE1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:ALA:O	1:B:736:THR:HG21	2.07	0.55
1:C:536:LYS:HE3	3:C:1107:HOH:O	2.06	0.55
1:D:415:LEU:HD13	1:D:415:LEU:C	2.32	0.55
1:C:108:SER:C	1:C:110:ASP:H	2.14	0.55
1:A:276:LEU:H	1:A:276:LEU:CD2	2.19	0.55
1:C:741:GLY:O	1:C:742:ILE:C	2.50	0.55
1:A:310:ARG:CZ	3:A:1082:HOH:O	2.53	0.55
1:C:388:GLN:CB	1:C:391:LYS:HD3	2.37	0.55
1:C:438:ASP:OD2	1:C:441:LYS:HG3	2.07	0.55
1:D:741:GLY:O	1:D:742:ILE:C	2.50	0.55
1:B:321:ASN:ND2	3:B:4147:HOH:O	2.40	0.55
1:A:741:GLY:O	1:A:742:ILE:C	2.50	0.54
1:A:736:THR:HG21	1:B:717:ALA:O	2.08	0.54
1:B:520:ASN:O	1:B:521:GLU:HB2	2.07	0.54
1:C:377:ASN:HB2	1:C:381:TYR:O	2.06	0.54
1:A:520:ASN:O	1:A:521:GLU:HB2	2.07	0.54
1:C:481:THR:OG1	1:C:483:HIS:HE1	1.89	0.54
1:D:172:ILE:H	1:D:186:THR:CG2	2.15	0.54
1:B:441:LYS:HE3	3:B:4309:HOH:O	2.07	0.54
1:D:512:LYS:HD3	3:D:1439:HOH:O	2.07	0.54
1:A:392:LYS:HG3	1:A:393:ASP:H	1.71	0.54
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.89	0.54
1:D:125:ARG:HG2	1:D:126:HIS:NE2	2.22	0.54
1:A:161:GLY:HA3	3:A:994:HOH:O	2.08	0.54
1:A:513:LYS:HG3	3:A:1695:HOH:O	2.07	0.54
1:B:622:LYS:HB2	1:B:622:LYS:NZ	2.23	0.54
1:D:622:LYS:HB2	1:D:622:LYS:NZ	2.23	0.54
1:B:57:LEU:HB3	3:B:4313:HOH:O	2.07	0.54
1:C:377:ASN:HB3	1:C:379:GLU:H	1.72	0.54
1:C:622:LYS:HB2	1:C:622:LYS:NZ	2.23	0.54
1:A:285:ILE:N	1:A:285:ILE:HD12	2.23	0.54
1:A:415:LEU:C	1:A:415:LEU:HD13	2.32	0.54
1:A:538:LYS:HG2	3:A:1668:HOH:O	2.08	0.54
1:A:676:PRO:HG2	1:A:677:GLU:OE2	2.08	0.54
1:D:388:GLN:CB	1:D:391:LYS:HD3	2.38	0.54
1:A:388:GLN:HG3	3:A:1249:HOH:O	2.08	0.54
1:A:392:LYS:HG3	1:A:393:ASP:N	2.23	0.53
1:B:764:SER:HA	3:B:4322:HOH:O	2.08	0.53
1:C:125:ARG:HG2	1:C:126:HIS:NE2	2.24	0.53
1:D:377:ASN:HB2	1:D:381:TYR:O	2.08	0.53
1:A:277:SER:O	1:A:278:SER:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:SER:O	1:A:760:LYS:HG3	2.08	0.53
3:C:791:HOH:O	1:D:736:THR:HG23	2.08	0.53
1:D:93:SER:HA	1:D:96:ASP:CG	2.34	0.53
1:B:535:ASP:OD1	1:B:537:SER:HB3	2.08	0.53
1:C:80:ASN:HB3	1:C:85:ASN:OD1	2.09	0.53
1:D:61:ARG:HG3	3:D:1513:HOH:O	2.06	0.53
1:B:85:ASN:ND2	3:B:4474:HOH:O	2.42	0.53
1:B:278:SER:HB3	3:B:4698:HOH:O	2.09	0.53
1:C:41:LYS:H	1:C:41:LYS:HD3	1.73	0.53
1:C:140:ARG:HG2	1:C:140:ARG:NH1	2.24	0.53
1:B:392:LYS:HG3	1:B:393:ASP:N	2.23	0.53
1:D:600:THR:O	1:D:603:VAL:HG13	2.09	0.53
1:C:658:ARG:HG2	1:C:661:TYR:CE2	2.44	0.53
1:A:244:GLU:CD	1:B:689:MET:HG3	2.33	0.53
1:A:487:ASN:ND2	3:A:890:HOH:O	2.41	0.53
1:C:422:TYR:CD2	1:C:423:LYS:HD3	2.44	0.53
1:D:194:ILE:HD12	3:D:1095:HOH:O	2.09	0.53
1:D:520:ASN:O	1:D:521:GLU:HB2	2.08	0.53
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.91	0.53
1:B:377:ASN:HB2	1:B:381:TYR:O	2.09	0.53
1:B:415:LEU:HD13	1:B:415:LEU:C	2.34	0.53
1:C:415:LEU:C	1:C:415:LEU:HD13	2.34	0.53
1:C:512:LYS:HD3	3:C:888:HOH:O	2.09	0.53
1:B:718:GLN:HA	1:B:718:GLN:HE21	1.74	0.52
1:C:293:MET:HE2	1:C:317:ARG:CG	2.33	0.52
1:C:502:LYS:O	1:C:505:GLN:HG2	2.09	0.52
1:D:41:LYS:H	1:D:41:LYS:HD3	1.73	0.52
1:D:108:SER:C	1:D:110:ASP:H	2.15	0.52
1:D:390:ASP:HB3	3:D:1443:HOH:O	2.10	0.52
1:B:489:LYS:HB3	1:B:489:LYS:HZ3	1.71	0.52
1:D:684:ARG:HG3	3:D:1350:HOH:O	2.08	0.52
1:A:147:ARG:HD3	3:A:1214:HOH:O	2.10	0.52
1:A:535:ASP:OD1	1:A:537:SER:HB3	2.10	0.52
1:A:718:GLN:HE21	1:A:718:GLN:HA	1.75	0.52
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.44	0.52
1:B:334:SER:HB3	1:B:336:ARG:CD	2.39	0.52
1:B:487:ASN:HB2	3:B:4104:HOH:O	2.09	0.52
1:B:513:LYS:O	1:B:527:GLN:HA	2.09	0.52
1:D:183:TYR:CD2	1:D:276:LEU:HG	2.43	0.52
1:D:197:GLY:C	1:D:213:ALA:HB3	2.34	0.52
1:D:751:ILE:O	1:D:755:MET:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:GLY:O	1:B:742:ILE:C	2.51	0.52
1:A:704:HIS:HE1	1:A:711:VAL:O	1.92	0.52
1:C:57:LEU:HD23	3:C:917:HOH:O	2.09	0.52
1:A:334:SER:HB3	1:A:336:ARG:CD	2.39	0.52
1:A:459:VAL:HG22	1:A:460:SER:N	2.24	0.52
1:B:277:SER:O	1:B:278:SER:HB3	2.09	0.52
1:B:676:PRO:HG2	1:B:677:GLU:OE2	2.10	0.52
1:C:486:VAL:HG13	1:C:487:ASN:N	2.25	0.52
1:D:136:ASP:CG	1:D:139:LYS:HG2	2.35	0.52
1:D:658:ARG:HG2	1:D:661:TYR:CE2	2.45	0.52
1:A:340:LEU:C	1:A:341:VAL:O	2.45	0.52
1:A:513:LYS:O	1:A:527:GLN:HA	2.10	0.52
1:C:93:SER:HA	1:C:96:ASP:CG	2.34	0.52
1:A:56:LYS:HD2	3:A:1079:HOH:O	2.10	0.52
1:A:397:ILE:HG13	1:A:398:THR:HG23	1.92	0.52
1:C:277:SER:O	1:C:278:SER:CB	2.58	0.52
1:D:140:ARG:HG2	1:D:140:ARG:NH1	2.23	0.52
1:D:486:VAL:HG13	1:D:487:ASN:N	2.25	0.52
1:A:276:LEU:HD23	3:A:1365:HOH:O	2.09	0.51
1:B:183:TYR:HE1	1:B:277:SER:O	1.93	0.51
1:B:397:ILE:HG13	1:B:398:THR:HG23	1.91	0.51
1:B:459:VAL:HG22	1:B:460:SER:N	2.24	0.51
1:C:203:TYR:HA	1:C:207:VAL:HG13	1.92	0.51
1:A:377:ASN:HB2	1:A:381:TYR:O	2.10	0.51
1:B:90:LEU:HD22	1:B:90:LEU:C	2.36	0.51
1:C:136:ASP:CG	1:C:139:LYS:HG2	2.35	0.51
1:D:203:TYR:HA	1:D:207:VAL:HG13	1.93	0.51
1:B:285:ILE:HD12	1:B:285:ILE:N	2.25	0.51
1:B:402:TRP:CD2	1:B:421:GLU:HB2	2.46	0.51
1:C:314:GLN:HE22	1:C:373:LYS:HZ1	1.59	0.51
1:C:520:ASN:O	1:C:521:GLU:HB2	2.09	0.51
1:A:90:LEU:HD22	1:A:90:LEU:C	2.35	0.51
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.93	0.51
1:C:197:GLY:C	1:C:213:ALA:HB3	2.35	0.51
1:C:751:ILE:O	1:C:755:MET:HG3	2.10	0.51
1:D:523:LYS:HG2	3:D:978:HOH:O	2.11	0.51
1:A:71:LYS:HZ3	1:A:105:TYR:HB2	1.75	0.51
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.45	0.51
1:C:81:ALA:O	1:C:492:ARG:NH2	2.44	0.51
1:C:156:THR:HG21	1:C:214:LEU:HD11	1.93	0.51
1:D:341:VAL:HG22	1:D:342:ALA:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ASP:OD2	1:A:162:HIS:ND1	2.44	0.51
1:C:243:ASP:HB3	3:C:1080:HOH:O	2.11	0.51
1:C:272:ASN:HD21	1:C:274:ASP:HB2	1.75	0.51
1:C:341:VAL:HG22	1:C:342:ALA:N	2.26	0.51
1:C:397:ILE:HG13	1:C:398:THR:HG23	1.92	0.51
1:C:606:GLN:NE2	3:C:774:HOH:O	2.40	0.50
1:A:392:LYS:HG3	3:A:1330:HOH:O	2.11	0.50
1:A:422:TYR:CE2	1:A:423:LYS:HD3	2.46	0.50
1:C:321:ASN:ND2	3:C:1514:HOH:O	2.45	0.50
1:D:272:ASN:HD21	1:D:274:ASP:HB2	1.77	0.50
1:D:277:SER:O	1:D:278:SER:CB	2.59	0.50
1:D:502:LYS:O	1:D:505:GLN:HG2	2.10	0.50
1:C:85:ASN:ND2	3:C:911:HOH:O	2.44	0.50
1:C:183:TYR:CD2	1:C:276:LEU:HG	2.45	0.50
1:B:110:ASP:OD2	1:B:162:HIS:ND1	2.45	0.50
1:C:600:THR:O	1:C:603:VAL:HG13	2.10	0.50
1:C:760:LYS:HE2	3:C:1519:HOH:O	2.10	0.50
1:A:183:TYR:HE1	1:A:277:SER:O	1.94	0.50
1:D:472:CYS:O	1:D:478:PRO:HA	2.11	0.50
1:A:108:SER:C	1:A:110:ASP:N	2.69	0.50
1:A:597:ARG:NH1	1:A:679:ASN:HD21	2.09	0.50
1:B:71:LYS:HZ3	1:B:105:TYR:HB2	1.75	0.50
1:C:276:LEU:CD2	1:C:276:LEU:N	2.68	0.50
1:D:322:TYR:OH	1:D:346:ILE:HD13	2.12	0.50
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.92	0.50
1:B:489:LYS:HB3	1:B:489:LYS:HZ2	1.76	0.50
1:C:472:CYS:O	1:C:478:PRO:HA	2.11	0.50
1:C:487:ASN:HB2	3:C:812:HOH:O	2.11	0.50
1:D:397:ILE:HG13	1:D:398:THR:HG23	1.93	0.50
1:D:597:ARG:NH1	1:D:682:HIS:HB2	2.26	0.50
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.93	0.50
1:A:658:ARG:HG3	1:A:658:ARG:O	2.11	0.50
1:B:516:PHE:CE2	1:B:523:LYS:HE2	2.47	0.50
1:C:193:ILE:HG22	1:C:194:ILE:HG13	1.94	0.50
1:C:489:LYS:HB3	1:C:489:LYS:HZ3	1.77	0.50
1:D:80:ASN:HB3	1:D:85:ASN:OD1	2.11	0.50
1:D:114:ILE:HD11	1:D:137:LEU:HD21	1.92	0.50
1:A:147:ARG:HB2	3:A:888:HOH:O	2.11	0.50
1:A:310:ARG:NH2	3:A:1082:HOH:O	2.43	0.50
1:B:109:PRO:HG2	1:B:160:VAL:O	2.12	0.50
1:B:622:LYS:HB2	1:B:622:LYS:HZ2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:GLN:NE2	3:B:4265:HOH:O	2.44	0.50
1:B:108:SER:C	1:B:110:ASP:N	2.68	0.49
1:B:704:HIS:HE1	1:B:711:VAL:O	1.93	0.49
1:B:276:LEU:CD2	1:B:276:LEU:N	2.76	0.49
1:B:606:GLN:NE2	3:B:4001:HOH:O	2.34	0.49
1:B:106:SER:HB3	1:B:115:LEU:HB3	1.93	0.49
1:B:203:TYR:HA	1:B:207:VAL:HG13	1.94	0.49
1:B:289:ALA:HB3	3:B:4250:HOH:O	2.13	0.49
1:B:483:HIS:HD2	3:B:4452:HOH:O	1.94	0.49
1:C:89:PHE:HD1	1:C:90:LEU:HD12	1.76	0.49
1:D:276:LEU:CD2	1:D:276:LEU:N	2.67	0.49
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.47	0.49
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.42	0.49
1:A:471:ARG:HG2	1:A:480:TYR:CD2	2.46	0.49
1:D:422:TYR:CD2	1:D:423:LYS:HD3	2.47	0.49
1:B:422:TYR:CE2	1:B:423:LYS:HD3	2.48	0.49
1:C:40:ARG:HB2	1:C:506:ASN:O	2.13	0.49
1:C:597:ARG:NH1	1:C:682:HIS:HB2	2.27	0.49
1:A:276:LEU:CD2	1:A:276:LEU:N	2.75	0.49
1:A:392:LYS:HG2	3:A:1399:HOH:O	2.11	0.49
1:B:81:ALA:O	1:B:492:ARG:NH2	2.45	0.49
1:C:486:VAL:HG13	3:C:812:HOH:O	2.13	0.49
1:C:736:THR:HG23	3:D:804:HOH:O	2.13	0.49
1:D:388:GLN:HG2	1:D:391:LYS:HD3	1.94	0.49
1:A:81:ALA:O	1:A:492:ARG:NH2	2.44	0.49
1:A:186:THR:HG21	1:A:196:ASN:CB	2.42	0.49
1:B:528:MET:HE3	1:B:530:LEU:HD21	1.95	0.49
1:D:508:GLN:HG2	3:D:1465:HOH:O	2.12	0.49
1:C:107:ILE:HG12	1:C:114:ILE:HG12	1.95	0.49
1:C:388:GLN:HG2	1:C:391:LYS:HD3	1.94	0.49
1:D:89:PHE:HD1	1:D:90:LEU:HD12	1.77	0.49
1:A:471:ARG:HD3	3:A:1265:HOH:O	2.12	0.49
1:B:171:ASP:HB2	3:B:4055:HOH:O	2.13	0.49
1:D:679:ASN:ND2	3:D:920:HOH:O	2.44	0.49
1:D:704:HIS:HD2	1:D:716:SER:OG	1.96	0.49
1:A:106:SER:HB3	1:A:115:LEU:HB3	1.95	0.49
1:C:289:ALA:CB	1:C:290:PRO:CA	2.83	0.49
1:D:69:LEU:HD11	1:D:107:ILE:HD12	1.94	0.49
1:A:358:ARG:HA	3:A:864:HOH:O	2.12	0.48
1:A:458:SER:OG	1:A:471:ARG:HB2	2.13	0.48
1:B:65:ASP:OD2	1:B:466:LYS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:GLU:HG2	3:B:4837:HOH:O	2.12	0.48
1:D:704:HIS:HE1	1:D:711:VAL:O	1.96	0.48
1:C:322:TYR:OH	1:C:346:ILE:HD13	2.13	0.48
1:C:597:ARG:HG3	1:C:600:THR:HG21	1.95	0.48
1:D:81:ALA:O	1:D:492:ARG:NH2	2.45	0.48
1:B:60:LEU:C	1:B:60:LEU:HD12	2.38	0.48
1:B:597:ARG:NH1	1:B:679:ASN:HD21	2.10	0.48
1:C:285:ILE:N	1:C:285:ILE:HD12	2.29	0.48
1:B:658:ARG:O	1:B:658:ARG:HG3	2.12	0.48
1:D:156:THR:HG21	1:D:214:LEU:HD11	1.95	0.48
1:D:289:ALA:HA	1:D:294:LEU:HD11	1.96	0.48
1:A:109:PRO:HG2	1:A:160:VAL:O	2.13	0.48
1:A:516:PHE:CE2	1:A:523:LYS:HE2	2.48	0.48
1:B:51:ASN:HB2	3:B:4582:HOH:O	2.12	0.48
1:D:172:ILE:N	1:D:186:THR:HG22	2.20	0.48
1:D:193:ILE:HG22	1:D:194:ILE:HG13	1.96	0.48
1:B:322:TYR:CE2	1:B:348:MET:HE2	2.48	0.48
1:C:54:ARG:HG2	3:C:1152:HOH:O	2.13	0.48
1:D:40:ARG:HB2	1:D:506:ASN:O	2.13	0.48
1:A:489:LYS:HD3	3:A:1259:HOH:O	2.13	0.48
1:D:285:ILE:N	1:D:285:ILE:HD12	2.29	0.48
1:A:514:LEU:HD12	1:A:557:THR:HG22	1.96	0.48
1:B:411:THR:HG1	1:B:414:TYR:H	1.58	0.48
1:D:314:GLN:HE22	1:D:373:LYS:HZ1	1.60	0.48
1:B:458:SER:OG	1:B:471:ARG:HB2	2.13	0.48
1:C:114:ILE:HD11	1:C:137:LEU:HD21	1.95	0.48
1:C:382:ARG:NH2	3:C:769:HOH:O	2.46	0.48
1:D:402:TRP:CD2	1:D:421:GLU:HB2	2.49	0.48
1:A:704:HIS:HD2	1:A:716:SER:OG	1.96	0.48
1:B:74:ASN:HB3	1:B:92:ASN:HB3	1.94	0.48
1:B:140:ARG:NH1	1:B:140:ARG:CG	2.77	0.48
1:D:51:ASN:HA	3:D:1304:HOH:O	2.13	0.48
1:B:186:THR:HG21	1:B:196:ASN:CB	2.44	0.47
1:D:40:ARG:HH11	1:D:40:ARG:CG	2.27	0.47
1:A:60:LEU:HD12	1:A:60:LEU:C	2.40	0.47
1:B:108:SER:C	1:B:110:ASP:H	2.22	0.47
1:C:165:ALA:HB2	1:C:216:TRP:CZ2	2.50	0.47
1:A:74:ASN:HB3	1:A:92:ASN:OD1	2.14	0.47
1:A:203:TYR:HA	1:A:207:VAL:HG13	1.95	0.47
1:B:69:LEU:HD13	1:B:107:ILE:HD12	1.97	0.47
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:HIS:HD2	1:B:716:SER:OG	1.97	0.47
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.50	0.47
1:A:74:ASN:HB3	1:A:92:ASN:HB3	1.95	0.47
1:A:544:LEU:HD21	1:A:606:GLN:HG3	1.97	0.47
1:A:657:SER:OG	1:A:689:MET:HE1	2.14	0.47
1:D:107:ILE:HG12	1:D:114:ILE:HG12	1.96	0.47
1:D:165:ALA:HB2	1:D:216:TRP:CZ2	2.50	0.47
1:D:289:ALA:CB	1:D:290:PRO:CA	2.82	0.47
1:D:726:VAL:CG1	1:D:728:VAL:HG23	2.39	0.47
1:A:171:ASP:HA	1:A:186:THR:CG2	2.44	0.47
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.97	0.47
1:A:721:LYS:HB2	1:B:736:THR:HG23	1.97	0.47
1:B:197:GLY:C	1:B:213:ALA:HB3	2.40	0.47
1:B:471:ARG:HG2	1:B:480:TYR:CD2	2.49	0.47
1:C:69:LEU:HD13	1:C:107:ILE:HD12	1.96	0.47
1:D:471:ARG:HG2	1:D:480:TYR:CD2	2.49	0.47
1:B:658:ARG:HB2	1:B:687:THR:HG22	1.97	0.47
1:C:89:PHE:CE1	1:C:107:ILE:HD13	2.49	0.47
1:C:402:TRP:CD2	1:C:421:GLU:HB2	2.50	0.47
1:C:704:HIS:HE1	1:C:711:VAL:O	1.96	0.47
1:D:536:LYS:HG2	3:D:996:HOH:O	2.14	0.47
1:A:197:GLY:C	1:A:213:ALA:HB3	2.40	0.47
1:A:435:GLN:NE2	1:A:441:LYS:HD2	2.29	0.47
1:B:528:MET:HE1	1:B:618:PHE:CE1	2.49	0.47
1:C:310:ARG:HG3	1:C:329:ASP:OD1	2.15	0.47
1:C:435:GLN:HG2	1:C:438:ASP:H	1.80	0.47
1:D:108:SER:C	1:D:110:ASP:N	2.73	0.47
1:D:597:ARG:HG3	1:D:600:THR:HG21	1.96	0.47
1:A:125:ARG:HG2	1:A:126:HIS:CD2	2.50	0.47
1:A:140:ARG:NH1	1:A:140:ARG:CG	2.77	0.47
1:C:108:SER:C	1:C:110:ASP:N	2.72	0.47
1:C:194:ILE:HD12	3:C:1047:HOH:O	2.15	0.47
1:B:125:ARG:HB3	3:B:4009:HOH:O	2.14	0.47
1:B:544:LEU:HD21	1:B:606:GLN:HG3	1.96	0.47
1:A:325:MET:HE2	1:A:327:ILE:HD11	1.97	0.47
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.50	0.47
1:A:718:GLN:HE22	1:A:721:LYS:NZ	2.13	0.46
1:B:98:PHE:CE2	1:B:100:HIS:HB2	2.50	0.46
1:B:514:LEU:HD12	1:B:557:THR:HG22	1.96	0.46
1:D:310:ARG:HG3	1:D:329:ASP:OD1	2.14	0.46
1:A:341:VAL:C	1:A:343:ARG:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:LYS:HB2	3:A:1645:HOH:O	2.15	0.46
1:B:159:PRO:HD3	1:B:216:TRP:HB3	1.95	0.46
1:C:40:ARG:HD3	1:C:507:VAL:C	2.40	0.46
1:C:289:ALA:HA	1:C:294:LEU:HD11	1.96	0.46
1:D:69:LEU:HD13	1:D:107:ILE:HD12	1.98	0.46
1:D:89:PHE:CE1	1:D:107:ILE:HD13	2.50	0.46
1:D:93:SER:HB2	1:D:96:ASP:OD2	2.15	0.46
1:A:489:LYS:NZ	1:A:489:LYS:CB	2.76	0.46
1:B:325:MET:HE2	1:B:327:ILE:HD11	1.98	0.46
1:C:464:GLU:HG3	3:C:948:HOH:O	2.15	0.46
1:D:40:ARG:HD3	1:D:507:VAL:C	2.40	0.46
1:D:597:ARG:HA	1:D:597:ARG:HD3	1.64	0.46
1:B:323:SER:OG	1:B:347:GLU:HB3	2.16	0.46
1:C:726:VAL:HG13	1:C:726:VAL:O	2.15	0.46
1:D:65:ASP:CG	1:D:464:GLU:HB2	2.40	0.46
1:D:726:VAL:CG1	1:D:726:VAL:O	2.64	0.46
1:A:325:MET:HE2	1:A:327:ILE:CG1	2.46	0.46
1:B:519:LEU:O	1:B:520:ASN:C	2.58	0.46
1:C:111:GLY:O	1:C:137:LEU:HD12	2.16	0.46
1:C:471:ARG:HG2	1:C:480:TYR:CD2	2.50	0.46
1:C:679:ASN:ND2	3:C:978:HOH:O	2.49	0.46
1:D:571:GLU:CD	1:D:760:LYS:HD3	2.40	0.46
1:A:39:SER:CB	1:A:40:ARG:HE	2.25	0.46
1:A:322:TYR:CE2	1:A:348:MET:HE2	2.51	0.46
1:B:171:ASP:HA	1:B:186:THR:CG2	2.45	0.46
1:B:657:SER:OG	1:B:689:MET:HE1	2.15	0.46
1:C:93:SER:HB2	1:C:96:ASP:OD2	2.15	0.46
1:D:486:VAL:HG13	1:D:487:ASN:H	1.80	0.46
1:D:522:THR:HG22	1:D:523:LYS:N	2.30	0.46
1:A:65:ASP:OD2	1:A:466:LYS:HB2	2.14	0.46
1:A:114:ILE:HD12	1:A:137:LEU:HD21	1.98	0.46
1:A:141:GLN:HG2	3:A:1198:HOH:O	2.15	0.46
1:A:243:ASP:HB3	3:A:1258:HOH:O	2.15	0.46
1:D:132:TYR:HB2	3:D:1456:HOH:O	2.15	0.46
1:D:483:HIS:HD2	3:D:878:HOH:O	1.98	0.46
1:A:519:LEU:O	1:A:520:ASN:C	2.59	0.46
1:C:704:HIS:HD2	1:C:716:SER:OG	1.98	0.46
1:D:403:GLU:OE1	1:D:585:TYR:HA	2.15	0.46
1:A:463:LYS:HA	1:A:463:LYS:HD3	1.74	0.46
1:A:528:MET:HE3	1:A:530:LEU:HD21	1.97	0.46
1:B:341:VAL:C	1:B:343:ARG:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:546:VAL:CG2	1:D:547:TYR:N	2.78	0.46
1:C:79:PHE:CD1	1:C:86:SER:HB3	2.51	0.45
1:A:482:LEU:HD23	1:A:482:LEU:HA	1.79	0.45
1:B:76:ILE:HB	1:B:90:LEU:HD13	1.98	0.45
1:C:71:LYS:HE2	3:C:1041:HOH:O	2.15	0.45
1:C:496:ASP:HB2	3:C:1258:HOH:O	2.16	0.45
1:D:341:VAL:C	1:D:343:ARG:N	2.74	0.45
1:B:435:GLN:NE2	1:B:441:LYS:HD2	2.32	0.45
1:C:286:GLN:NE2	1:C:288:THR:HG22	2.32	0.45
1:A:75:ASN:HB3	1:A:92:ASN:N	2.32	0.45
1:A:323:SER:OG	1:A:347:GLU:HB3	2.16	0.45
1:B:532:PRO:HD3	1:B:569:SER:HA	1.99	0.45
1:B:726:VAL:O	1:B:726:VAL:CG1	2.63	0.45
1:D:726:VAL:O	1:D:726:VAL:HG13	2.15	0.45
1:A:136:ASP:CG	1:A:139:LYS:HG2	2.42	0.45
1:A:726:VAL:O	1:A:726:VAL:CG1	2.65	0.45
1:B:114:ILE:HD12	1:B:137:LEU:HD21	1.99	0.45
1:B:486:VAL:HG13	1:B:487:ASN:N	2.31	0.45
1:C:244:GLU:CD	1:D:689:MET:HG3	2.42	0.45
1:C:314:GLN:HE22	1:C:373:LYS:NZ	2.14	0.45
1:C:536:LYS:CB	1:C:536:LYS:NZ	2.80	0.45
1:D:306:ALA:CB	1:D:310:ARG:HD2	2.47	0.45
1:D:435:GLN:HG2	1:D:438:ASP:H	1.80	0.45
1:B:39:SER:CB	1:B:40:ARG:HE	2.25	0.45
1:B:74:ASN:HB3	1:B:92:ASN:OD1	2.16	0.45
1:D:498:SER:O	1:D:502:LYS:HG2	2.16	0.45
1:B:194:ILE:HD12	3:B:4346:HOH:O	2.17	0.45
1:B:718:GLN:HE22	1:B:721:LYS:NZ	2.15	0.45
1:D:183:TYR:CE2	1:D:276:LEU:HG	2.52	0.45
1:D:253:ARG:HD2	3:D:1225:HOH:O	2.17	0.45
1:D:321:ASN:ND2	3:D:951:HOH:O	2.48	0.45
1:D:611:ARG:NH1	3:D:1422:HOH:O	2.50	0.45
1:D:697:GLN:HG3	3:D:1267:HOH:O	2.15	0.45
1:A:76:ILE:HB	1:A:90:LEU:HD13	1.97	0.45
1:A:241:TYR:CE2	1:B:714:GLN:HA	2.52	0.45
1:A:589:LYS:HD2	3:A:1645:HOH:O	2.17	0.45
1:B:136:ASP:CG	1:B:139:LYS:HG2	2.42	0.45
1:B:173:TYR:CE2	1:B:184:ARG:HG3	2.52	0.45
1:C:65:ASP:CG	1:C:464:GLU:HB2	2.41	0.45
1:D:289:ALA:HB3	3:D:1357:HOH:O	2.17	0.45
1:A:69:LEU:HD13	1:A:107:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ASN:ND2	1:A:93:SER:N	2.65	0.45
1:A:147:ARG:HA	3:A:1151:HOH:O	2.16	0.45
1:A:486:VAL:HG13	1:A:487:ASN:N	2.32	0.45
1:B:75:ASN:HB3	1:B:92:ASN:N	2.32	0.45
1:B:429:ARG:NE	3:B:4044:HOH:O	2.36	0.45
1:B:718:GLN:HA	1:B:718:GLN:NE2	2.31	0.45
1:C:403:GLU:OE1	1:C:585:TYR:HA	2.17	0.45
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.52	0.45
1:C:110:ASP:OD2	1:C:162:HIS:ND1	2.51	0.45
1:D:393:ASP:HA	3:D:1433:HOH:O	2.16	0.45
1:A:392:LYS:HD3	3:A:1547:HOH:O	2.17	0.44
1:A:528:MET:HE1	1:A:618:PHE:CE1	2.52	0.44
1:B:92:ASN:ND2	1:B:93:SER:N	2.64	0.44
1:B:310:ARG:NH1	1:B:329:ASP:OD1	2.50	0.44
1:C:76:ILE:CD1	1:C:90:LEU:HD11	2.37	0.44
1:C:651:ILE:HG21	1:C:755:MET:HE3	1.99	0.44
1:D:110:ASP:OD2	1:D:162:HIS:ND1	2.50	0.44
1:A:310:ARG:NH1	1:A:329:ASP:OD1	2.50	0.44
1:C:69:LEU:HD11	1:C:107:ILE:HD12	1.96	0.44
1:C:172:ILE:N	1:C:186:THR:HG22	2.18	0.44
1:C:522:THR:HG22	1:C:523:LYS:N	2.32	0.44
1:C:571:GLU:CD	1:C:760:LYS:HD3	2.41	0.44
1:D:272:ASN:ND2	1:D:272:ASN:C	2.75	0.44
1:A:148:ILE:HG23	1:A:149:PRO:HD2	1.99	0.44
1:A:481:THR:OG1	1:A:483:HIS:CE1	2.65	0.44
1:B:489:LYS:NZ	1:B:489:LYS:CB	2.77	0.44
1:C:74:ASN:HB3	1:C:92:ASN:HB3	1.99	0.44
1:C:319:ILE:C	1:C:321:ASN:H	2.23	0.44
1:D:74:ASN:HB3	1:D:92:ASN:HB3	1.99	0.44
1:D:79:PHE:CD1	1:D:86:SER:HB3	2.52	0.44
1:D:283:THR:HG22	1:D:285:ILE:HD12	2.00	0.44
1:D:57:LEU:HD23	3:D:1030:HOH:O	2.17	0.44
1:A:731:GLN:HG2	3:A:1299:HOH:O	2.17	0.44
1:C:726:VAL:CG1	1:C:728:VAL:HG23	2.40	0.44
1:D:259:ALA:HB3	1:D:660:GLU:HA	2.00	0.44
1:D:286:GLN:NE2	1:D:288:THR:HG22	2.33	0.44
1:B:482:LEU:HD23	1:B:482:LEU:HA	1.76	0.44
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.48	0.44
1:C:306:ALA:CB	1:C:310:ARG:HD2	2.47	0.44
1:C:341:VAL:C	1:C:343:ARG:N	2.74	0.44
1:C:486:VAL:HG13	1:C:487:ASN:H	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:546:VAL:CG2	1:C:547:TYR:N	2.81	0.44
1:D:74:ASN:O	1:D:92:ASN:HB3	2.18	0.44
1:D:319:ILE:O	1:D:321:ASN:N	2.36	0.44
1:D:184:ARG:HD2	1:D:187:TRP:CE2	2.53	0.44
1:B:134:ILE:HG21	1:B:178:PRO:HB3	2.00	0.44
1:D:536:LYS:NZ	1:D:536:LYS:CB	2.81	0.44
1:D:718:GLN:HA	1:D:718:GLN:NE2	2.33	0.44
1:A:413:ASP:HB2	3:A:1644:HOH:O	2.17	0.44
1:C:248:TYR:CZ	1:D:234:PRO:HB2	2.53	0.44
1:A:134:ILE:HG21	1:A:178:PRO:HB3	1.99	0.43
1:B:761:GLN:HE21	1:B:761:GLN:HB3	1.60	0.43
1:C:425:MET:HA	1:C:426:PRO:HD2	1.77	0.43
1:C:483:HIS:HD2	3:C:1070:HOH:O	2.01	0.43
1:D:154:TRP:O	1:D:166:TYR:HA	2.18	0.43
1:A:173:TYR:CE2	1:A:184:ARG:HG3	2.53	0.43
1:C:283:THR:HG22	1:C:285:ILE:HD12	1.99	0.43
1:C:596:ARG:O	1:C:597:ARG:HD3	2.18	0.43
1:D:40:ARG:HD2	1:D:508:GLN:HG3	2.00	0.43
1:D:718:GLN:HA	1:D:718:GLN:HE21	1.82	0.43
1:A:74:ASN:O	1:A:92:ASN:HB3	2.17	0.43
1:A:176:ILE:HG22	1:A:177:GLU:HG2	2.00	0.43
1:A:440:THR:HG21	3:A:1678:HOH:O	2.17	0.43
1:B:205:GLU:OE2	2:B:4000:DLI:N22	2.51	0.43
1:C:183:TYR:CE2	1:C:276:LEU:HG	2.54	0.43
1:C:649:CYS:HB3	1:C:699:GLU:HB2	2.00	0.43
1:D:615:LYS:HG2	3:D:1209:HOH:O	2.19	0.43
1:A:40:ARG:HB2	1:A:41:LYS:H	1.55	0.43
1:A:76:ILE:CD1	1:A:90:LEU:HD11	2.42	0.43
1:A:108:SER:C	1:A:110:ASP:H	2.25	0.43
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.53	0.43
1:C:516:PHE:CE2	1:C:523:LYS:HE2	2.54	0.43
1:D:415:LEU:C	1:D:415:LEU:CD1	2.91	0.43
1:B:107:ILE:HG12	1:B:114:ILE:HG12	2.00	0.43
1:B:612:GLN:HE21	1:B:612:GLN:HB3	1.59	0.43
1:B:726:VAL:O	1:B:726:VAL:HG13	2.18	0.43
1:C:40:ARG:HH11	1:C:40:ARG:CG	2.28	0.43
1:C:154:TRP:O	1:C:166:TYR:HA	2.18	0.43
1:C:498:SER:O	1:C:502:LYS:HG2	2.18	0.43
1:C:693:GLU:HG2	3:C:1444:HOH:O	2.19	0.43
1:C:726:VAL:O	1:C:726:VAL:CG1	2.65	0.43
1:A:532:PRO:HD3	1:A:569:SER:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ALA:O	1:B:295:ILE:HG23	2.18	0.43
1:C:519:LEU:O	1:C:520:ASN:C	2.62	0.43
1:D:649:CYS:HB3	1:D:699:GLU:HB2	2.00	0.43
1:D:696:LYS:CG	1:D:728:VAL:HG22	2.49	0.43
1:B:76:ILE:CD1	1:B:90:LEU:HD11	2.42	0.43
1:B:125:ARG:HG2	1:B:126:HIS:CD2	2.54	0.43
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.48	0.43
1:D:422:TYR:CZ	1:D:423:LYS:HE3	2.54	0.43
1:C:422:TYR:CZ	1:C:423:LYS:HE3	2.54	0.43
1:C:438:ASP:OD2	1:C:440:THR:HG22	2.19	0.43
1:C:622:LYS:HB2	1:C:622:LYS:HZ2	1.84	0.43
1:D:75:ASN:ND2	3:D:974:HOH:O	2.52	0.43
1:D:125:ARG:HG2	1:D:126:HIS:CD2	2.54	0.43
1:B:62:TRP:CE3	1:B:68:TYR:HB3	2.54	0.43
1:B:148:ILE:HG23	1:B:149:PRO:HD2	1.99	0.43
1:B:176:ILE:HG22	1:B:177:GLU:HG2	2.00	0.43
1:C:40:ARG:HE	1:C:508:GLN:HG2	1.84	0.43
1:D:147:ARG:HH11	1:D:147:ARG:HG2	1.82	0.43
1:D:696:LYS:HG3	1:D:728:VAL:HG22	2.00	0.43
1:A:107:ILE:HG12	1:A:114:ILE:HG12	2.00	0.43
1:A:237:GLU:HA	1:A:252:VAL:O	2.19	0.43
1:B:74:ASN:HB3	1:B:92:ASN:CB	2.49	0.43
1:C:40:ARG:HD2	1:C:508:GLN:HG3	2.00	0.43
1:C:147:ARG:HG2	1:C:147:ARG:HH11	1.84	0.43
1:C:289:ALA:HA	1:C:294:LEU:CD1	2.49	0.43
1:C:536:LYS:HB3	1:C:536:LYS:HZ3	1.83	0.43
1:D:531:PRO:HB3	1:D:572:ASN:HD22	1.84	0.43
1:D:546:VAL:HG22	1:D:547:TYR:N	2.33	0.43
1:A:172:ILE:N	1:A:186:THR:HG22	2.21	0.42
1:B:74:ASN:O	1:B:92:ASN:HB3	2.17	0.42
1:B:289:ALA:HB2	3:B:4251:HOH:O	2.18	0.42
1:B:377:ASN:HB2	1:B:381:TYR:H	1.84	0.42
1:C:74:ASN:O	1:C:92:ASN:HB3	2.18	0.42
1:C:696:LYS:CG	1:C:728:VAL:HG22	2.49	0.42
1:D:425:MET:HA	1:D:426:PRO:HD2	1.78	0.42
1:A:177:GLU:CG	1:A:180:LEU:HD22	2.49	0.42
1:A:325:MET:O	1:A:344:GLN:HA	2.19	0.42
1:A:704:HIS:CE1	1:A:711:VAL:O	2.72	0.42
1:D:314:GLN:HE22	1:D:373:LYS:NZ	2.17	0.42
1:D:411:THR:C	1:D:413:ASP:N	2.76	0.42
1:A:82:GLU:HG2	1:A:83:TYR:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:ARG:HG3	1:C:476:GLY:HA3	2.02	0.42
1:D:64:SER:O	1:D:463:LYS:HG2	2.19	0.42
1:D:438:ASP:OD2	1:D:440:THR:HG22	2.19	0.42
1:A:92:ASN:HD22	1:A:93:SER:N	2.18	0.42
1:A:332:GLU:HB2	3:A:901:HOH:O	2.19	0.42
1:B:506:ASN:ND2	3:B:4532:HOH:O	2.52	0.42
1:D:289:ALA:HA	1:D:294:LEU:CD1	2.49	0.42
1:D:502:LYS:HD3	3:D:1160:HOH:O	2.18	0.42
1:D:519:LEU:O	1:D:520:ASN:C	2.61	0.42
1:A:693:GLU:HB2	3:A:975:HOH:O	2.18	0.42
1:B:92:ASN:HD22	1:B:93:SER:N	2.18	0.42
1:C:696:LYS:HG3	1:C:728:VAL:HG22	2.00	0.42
1:D:319:ILE:C	1:D:321:ASN:H	2.22	0.42
1:A:156:THR:CG2	1:A:214:LEU:HD11	2.50	0.42
1:A:536:LYS:CB	1:A:536:LYS:NZ	2.83	0.42
1:B:82:GLU:HG2	1:B:83:TYR:CZ	2.55	0.42
1:B:159:PRO:HB2	1:B:218:PRO:O	2.20	0.42
1:B:177:GLU:CG	1:B:180:LEU:HD22	2.49	0.42
1:D:40:ARG:NH1	1:D:40:ARG:CG	2.83	0.42
1:D:40:ARG:HE	1:D:508:GLN:HG2	1.84	0.42
1:D:276:LEU:HD22	1:D:276:LEU:N	2.22	0.42
1:D:292:SER:HA	3:D:1237:HOH:O	2.19	0.42
1:A:581:ARG:HG2	1:A:593:ALA:HB1	2.02	0.42
1:C:57:LEU:HB3	3:C:960:HOH:O	2.18	0.42
1:C:110:ASP:HB3	1:C:112:GLN:HB2	2.01	0.42
1:C:253:ARG:NH1	3:C:1509:HOH:O	2.34	0.42
1:C:259:ALA:HB3	1:C:660:GLU:HA	2.01	0.42
1:D:114:ILE:HD12	1:D:137:LEU:HD21	2.01	0.42
1:D:147:ARG:HB2	3:D:975:HOH:O	2.19	0.42
1:A:658:ARG:NH1	3:A:965:HOH:O	2.50	0.42
1:B:172:ILE:H	1:B:186:THR:CG2	2.21	0.42
1:C:125:ARG:HG2	1:C:126:HIS:CD2	2.55	0.42
1:C:236:ILE:HG12	1:C:712:HIS:CE1	2.55	0.42
1:C:415:LEU:C	1:C:415:LEU:CD1	2.93	0.42
1:D:148:ILE:CG2	1:D:149:PRO:HD2	2.49	0.42
1:D:382:ARG:NH2	3:D:766:HOH:O	2.51	0.42
1:A:333:SER:HB2	3:A:1026:HOH:O	2.19	0.42
1:C:98:PHE:CE2	1:C:100:HIS:HB2	2.55	0.42
1:C:523:LYS:HG2	3:C:808:HOH:O	2.19	0.42
1:C:532:PRO:HD3	1:C:569:SER:HA	2.02	0.42
1:C:658:ARG:HD2	1:C:661:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:PHE:CE2	1:D:100:HIS:HB2	2.55	0.42
1:D:111:GLY:O	1:D:137:LEU:HD12	2.19	0.42
1:D:489:LYS:NZ	1:D:489:LYS:CB	2.82	0.42
1:A:62:TRP:CE3	1:A:68:TYR:HB3	2.55	0.42
1:A:184:ARG:HD2	1:A:187:TRP:CD2	2.55	0.42
1:A:187:TRP:CD1	1:A:187:TRP:N	2.88	0.42
1:A:435:GLN:NE2	1:A:441:LYS:CD	2.83	0.42
1:B:85:ASN:ND2	3:B:4276:HOH:O	2.52	0.42
1:B:109:PRO:HA	3:B:4766:HOH:O	2.19	0.42
1:C:64:SER:O	1:C:463:LYS:HG2	2.19	0.42
1:C:95:PHE:HB3	1:C:98:PHE:HB2	2.02	0.42
1:C:530:LEU:HA	1:C:531:PRO:HD3	1.84	0.42
1:D:520:ASN:O	1:D:520:ASN:ND2	2.53	0.42
1:D:562:ASN:HB2	3:D:913:HOH:O	2.19	0.42
1:D:704:HIS:CE1	1:D:711:VAL:O	2.72	0.42
1:A:248:TYR:CE1	1:B:258:LYS:HD2	2.55	0.41
1:A:512:LYS:HD3	3:A:1141:HOH:O	2.19	0.41
1:A:546:VAL:HG22	1:A:547:TYR:N	2.35	0.41
1:B:546:VAL:HG22	1:B:547:TYR:N	2.35	0.41
1:C:152:THR:HG21	1:C:155:VAL:CG2	2.50	0.41
1:C:520:ASN:O	1:C:520:ASN:ND2	2.52	0.41
1:C:597:ARG:HD3	1:C:597:ARG:HA	1.63	0.41
1:B:183:TYR:CE1	1:B:277:SER:O	2.72	0.41
1:B:187:TRP:CD1	1:B:187:TRP:N	2.88	0.41
1:C:489:LYS:NZ	1:C:489:LYS:CB	2.82	0.41
1:C:531:PRO:HB3	1:C:572:ASN:HD22	1.84	0.41
1:D:95:PHE:HB3	1:D:98:PHE:HB2	2.02	0.41
1:D:622:LYS:HB2	1:D:622:LYS:HZ2	1.84	0.41
1:A:535:ASP:C	1:A:537:SER:N	2.79	0.41
1:A:718:GLN:HA	1:A:718:GLN:NE2	2.33	0.41
1:B:40:ARG:HB2	1:B:41:LYS:H	1.56	0.41
1:B:246:LEU:HD23	1:B:246:LEU:HA	1.87	0.41
1:C:370:SER:HB3	1:C:388:GLN:NE2	2.35	0.41
1:C:734:TRP:CD1	1:C:736:THR:HG22	2.55	0.41
1:D:137:LEU:HD23	1:D:137:LEU:HA	1.84	0.41
1:D:442:VAL:O	1:D:442:VAL:HG13	2.20	0.41
1:D:459:VAL:HG22	1:D:460:SER:N	2.34	0.41
1:B:137:LEU:O	1:B:140:ARG:NH1	2.54	0.41
1:C:561:LEU:HD12	1:C:561:LEU:HA	1.92	0.41
1:C:704:HIS:CE1	1:C:711:VAL:O	2.73	0.41
1:D:110:ASP:HB3	1:D:112:GLN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:579:ASP:HB3	1:D:583:SER:OG	2.20	0.41
1:B:156:THR:CG2	1:B:214:LEU:HD11	2.50	0.41
1:B:269:PHE:CE2	1:B:286:GLN:HB2	2.56	0.41
1:B:325:MET:HE2	1:B:327:ILE:CG1	2.50	0.41
1:C:76:ILE:HB	1:C:90:LEU:HD13	2.00	0.41
1:C:148:ILE:CG2	1:C:149:PRO:HD2	2.50	0.41
1:D:152:THR:HG21	1:D:155:VAL:CG2	2.50	0.41
1:D:532:PRO:HD3	1:D:569:SER:HA	2.01	0.41
1:C:411:THR:C	1:C:413:ASP:N	2.76	0.41
1:D:734:TRP:CD1	1:D:736:THR:HG22	2.55	0.41
1:A:137:LEU:O	1:A:140:ARG:NH1	2.53	0.41
1:A:597:ARG:HD2	1:A:597:ARG:HA	1.94	0.41
1:C:334:SER:CB	1:C:336:ARG:HD2	2.49	0.41
1:D:520:ASN:O	1:D:521:GLU:CB	2.68	0.41
1:A:74:ASN:HB3	1:A:92:ASN:CG	2.46	0.41
1:A:415:LEU:C	1:A:415:LEU:CD1	2.94	0.41
1:A:726:VAL:O	1:A:726:VAL:HG13	2.20	0.41
1:B:536:LYS:NZ	1:B:536:LYS:CB	2.83	0.41
1:A:74:ASN:HB3	1:A:92:ASN:CB	2.50	0.41
1:A:120:TYR:OH	1:A:122:LYS:HB2	2.21	0.41
1:A:183:TYR:CE1	1:A:277:SER:O	2.73	0.41
1:A:596:ARG:C	1:A:597:ARG:HD3	2.45	0.41
1:B:69:LEU:CD1	1:B:107:ILE:HD12	2.51	0.41
1:B:74:ASN:HB3	1:B:92:ASN:CG	2.46	0.41
1:B:184:ARG:HD2	1:B:187:TRP:CD2	2.56	0.41
1:B:214:LEU:HD12	1:B:214:LEU:O	2.20	0.41
1:B:387:PHE:CD2	1:B:394:CYS:HB3	2.56	0.41
1:B:627:TRP:CZ3	1:B:755:MET:HE1	2.56	0.41
1:C:361:GLU:HG2	3:C:882:HOH:O	2.20	0.41
1:C:485:SER:O	1:C:486:VAL:C	2.64	0.41
1:C:504:LEU:O	1:C:507:VAL:HG13	2.21	0.41
1:D:91:GLU:HA	3:D:974:HOH:O	2.20	0.41
1:D:331:ASP:CB	1:D:334:SER:HB2	2.49	0.41
1:D:505:GLN:HE21	1:D:505:GLN:HB3	1.59	0.41
1:A:691:ARG:NE	3:A:1580:HOH:O	2.27	0.41
1:B:176:ILE:HD11	1:B:276:LEU:HD21	2.02	0.41
1:B:535:ASP:C	1:B:537:SER:N	2.79	0.41
1:C:544:LEU:HD21	1:C:606:GLN:HG3	2.03	0.41
1:D:453:ARG:HG3	1:D:476:GLY:HA3	2.03	0.41
1:D:504:LEU:O	1:D:507:VAL:HG13	2.21	0.41
1:D:513:LYS:O	1:D:527:GLN:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:PHE:CE2	1:A:286:GLN:HB2	2.56	0.40
1:A:291:ALA:O	1:A:295:ILE:HG23	2.21	0.40
1:A:708:ASP:OD2	1:A:740:HIS:HA	2.21	0.40
1:B:708:ASP:OD2	1:B:740:HIS:HA	2.21	0.40
1:C:459:VAL:HG22	1:C:460:SER:N	2.36	0.40
1:C:513:LYS:O	1:C:527:GLN:HA	2.20	0.40
1:C:579:ASP:HB3	1:C:583:SER:OG	2.21	0.40
1:D:474:GLY:HA3	1:D:557:THR:O	2.21	0.40
1:D:516:PHE:CE2	1:D:523:LYS:HE2	2.56	0.40
1:A:159:PRO:HB2	1:A:218:PRO:O	2.21	0.40
1:A:319:ILE:HB	3:A:1427:HOH:O	2.20	0.40
1:A:614:SER:HB2	1:A:621:ASN:HB3	2.04	0.40
1:A:627:TRP:CZ3	1:A:755:MET:HE1	2.55	0.40
1:B:110:ASP:C	1:B:112:GLN:H	2.29	0.40
1:C:146:GLU:O	1:C:175:LYS:HE2	2.22	0.40
1:C:272:ASN:ND2	1:C:272:ASN:C	2.76	0.40
1:C:546:VAL:HG22	1:C:547:TYR:N	2.36	0.40
1:D:482:LEU:HD23	1:D:482:LEU:HA	1.91	0.40
1:A:110:ASP:C	1:A:112:GLN:H	2.30	0.40
1:A:203:TYR:HA	1:A:207:VAL:CG1	2.51	0.40
1:A:535:ASP:C	1:A:537:SER:H	2.29	0.40
1:B:237:GLU:HA	1:B:252:VAL:O	2.21	0.40
1:C:90:LEU:HD22	1:C:90:LEU:C	2.47	0.40
1:C:402:TRP:HA	3:C:805:HOH:O	2.21	0.40
1:C:520:ASN:O	1:C:521:GLU:CB	2.69	0.40
1:C:718:GLN:HA	1:C:718:GLN:HE21	1.86	0.40
1:D:195:TYR:O	1:D:227:GLN:HA	2.22	0.40
1:D:334:SER:CB	1:D:336:ARG:HD2	2.48	0.40
1:D:463:LYS:HD3	1:D:463:LYS:HA	1.85	0.40
1:D:544:LEU:HD21	1:D:606:GLN:HG3	2.03	0.40
1:A:114:ILE:HG13	1:A:137:LEU:HD11	2.04	0.40
1:A:150:ASN:O	1:A:151:ASN:HB2	2.21	0.40
1:A:172:ILE:H	1:A:186:THR:CG2	2.23	0.40
1:B:242:SER:OG	1:B:243:ASP:N	2.51	0.40
1:B:596:ARG:C	1:B:597:ARG:HD3	2.45	0.40
1:C:685:ASN:ND2	3:C:1440:HOH:O	2.55	0.40
1:C:718:GLN:HA	1:C:718:GLN:NE2	2.36	0.40
1:D:388:GLN:CB	1:D:391:LYS:HB2	2.52	0.40
1:D:658:ARG:HD2	1:D:661:TYR:CE1	2.56	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%)	668 (92%)	49 (7%)	7 (1%)	12	15
1	B	724/726 (100%)	667 (92%)	50 (7%)	7 (1%)	12	15
1	C	724/726 (100%)	672 (93%)	45 (6%)	7 (1%)	12	15
1	D	724/726 (100%)	671 (93%)	46 (6%)	7 (1%)	12	15
All	All	2896/2904 (100%)	2678 (92%)	190 (7%)	28 (1%)	12	15

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

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Mol	Chain	Res	Type
1	C	334	SER
1	D	334	SER
1	A	277	SER
1	B	277	SER
1	D	389	ILE
1	C	389	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	651/651 (100%)	606 (93%)	45 (7%)	14	20
1	B	651/651 (100%)	604 (93%)	47 (7%)	13	18
1	C	651/651 (100%)	609 (94%)	42 (6%)	15	22
1	D	651/651 (100%)	607 (93%)	44 (7%)	14	20
All	All	2604/2604 (100%)	2426 (93%)	178 (7%)	14	20

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	66	HIS
1	A	73	GLU
1	A	90	LEU
1	A	91	GLU
1	A	92	ASN
1	A	110	ASP
1	A	140	ARG
1	A	141	GLN
1	A	170	ASN
1	A	176	ILE
1	A	184	ARG
1	A	207	VAL
1	A	246	LEU
1	A	253	ARG

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Mol	Chain	Res	Type
1	A	254	VAL
1	A	272	ASN
1	A	276	LEU
1	A	303	VAL
1	A	336	ARG
1	A	373	LYS
1	A	388	GLN
1	A	391	LYS
1	A	413	ASP
1	A	415	LEU
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	581	ARG
1	A	597	ARG
1	A	603	VAL
1	A	673	LEU
1	A	689	MET
1	A	701	LEU
1	A	702	LEU
1	A	726	VAL
1	A	761	GLN
1	B	40	ARG
1	B	66	HIS
1	B	73	GLU
1	B	90	LEU
1	B	91	GLU
1	B	92	ASN
1	B	110	ASP
1	B	125	ARG
1	B	140	ARG
1	B	141	GLN
1	B	170	ASN
1	B	176	ILE

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Mol	Chain	Res	Type
1	B	184	ARG
1	B	207	VAL
1	B	246	LEU
1	B	253	ARG
1	B	254	VAL
1	B	272	ASN
1	B	276	LEU
1	B	303	VAL
1	B	336	ARG
1	B	373	LYS
1	B	388	GLN
1	B	391	LYS
1	B	413	ASP
1	B	415	LEU
1	B	425	MET
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	581	ARG
1	B	597	ARG
1	B	603	VAL
1	B	673	LEU
1	B	689	MET
1	B	701	LEU
1	B	702	LEU
1	B	726	VAL
1	B	761	GLN
1	C	40	ARG
1	C	90	LEU
1	C	91	GLU
1	C	110	ASP
1	C	145	GLU
1	C	170	ASN
1	C	184	ARG

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Mol	Chain	Res	Type
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	293	MET
1	C	303	VAL
1	C	313	LEU
1	C	336	ARG
1	C	373	LYS
1	C	388	GLN
1	C	413	ASP
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	507	VAL
1	C	514	LEU
1	C	536	LYS
1	C	543	LEU
1	C	561	LEU
1	C	597	ARG
1	C	603	VAL
1	C	622	LYS
1	C	679	ASN
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	760	LYS
1	D	40	ARG
1	D	90	LEU
1	D	91	GLU
1	D	110	ASP
1	D	145	GLU
1	D	170	ASN
1	D	184	ARG

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Mol	Chain	Res	Type
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	293	MET
1	D	303	VAL
1	D	313	LEU
1	D	336	ARG
1	D	373	LYS
1	D	388	GLN
1	D	413	ASP
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	507	VAL
1	D	514	LEU
1	D	536	LYS
1	D	543	LEU
1	D	561	LEU
1	D	597	ARG
1	D	603	VAL
1	D	622	LYS
1	D	656	VAL
1	D	679	ASN
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	760	LYS
1	D	761	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN

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Mol	Chain	Res	Type
1	A	75	ASN
1	A	92	ASN
1	A	112	GLN
1	A	126	HIS
1	A	169	ASN
1	A	170	ASN
1	A	272	ASN
1	A	314	GLN
1	A	345	HIS
1	A	369	ASN
1	A	430	ASN
1	A	435	GLN
1	A	483	HIS
1	A	487	ASN
1	A	533	HIS
1	A	572	ASN
1	A	586	GLN
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	66	HIS
1	B	72	GLN
1	B	75	ASN
1	B	92	ASN
1	B	103	ASN
1	B	169	ASN
1	B	170	ASN
1	B	247	GLN
1	B	272	ASN
1	B	314	GLN
1	B	344	GLN
1	B	345	HIS
1	B	369	ASN
1	B	430	ASN
1	B	435	GLN
1	B	483	HIS
1	B	487	ASN
1	B	533	HIS

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Mol	Chain	Res	Type
1	B	553	GLN
1	B	572	ASN
1	B	586	GLN
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	72	GLN
1	C	75	ASN
1	C	100	HIS
1	C	169	ASN
1	C	170	ASN
1	C	247	GLN
1	C	272	ASN
1	C	286	GLN
1	C	314	GLN
1	C	321	ASN
1	C	369	ASN
1	C	388	GLN
1	C	455	GLN
1	C	483	HIS
1	C	487	ASN
1	C	505	GLN
1	C	520	ASN
1	C	572	ASN
1	C	612	GLN
1	C	679	ASN
1	C	685	ASN
1	C	694	ASN
1	C	704	HIS
1	C	718	GLN
1	C	731	GLN
1	C	761	GLN
1	D	72	GLN
1	D	100	HIS
1	D	169	ASN
1	D	170	ASN
1	D	227	GLN

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Mol	Chain	Res	Type
1	D	247	GLN
1	D	272	ASN
1	D	286	GLN
1	D	314	GLN
1	D	369	ASN
1	D	388	GLN
1	D	455	GLN
1	D	483	HIS
1	D	487	ASN
1	D	505	GLN
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
1	D	731	GLN
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	DLI	B	4000	-	34,34,34	1.62	9 (26%)	42,51,51	2.06	16 (38%)

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	DLI	B	4000	-	-	6/18/30/30	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4000	DLI	C5-C6	3.54	1.43	1.37
2	B	4000	DLI	C5-C4	3.01	1.42	1.37
2	B	4000	DLI	C8-C7	-2.97	1.49	1.53
2	B	4000	DLI	C19-N18	2.96	1.41	1.35
2	B	4000	DLI	C3-C4	2.47	1.42	1.38
2	B	4000	DLI	C2-C1	2.15	1.41	1.37
2	B	4000	DLI	C23-C21	2.14	1.43	1.39
2	B	4000	DLI	C25-C26	2.08	1.42	1.38
2	B	4000	DLI	C2-C3	2.03	1.42	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4000	DLI	C10-S1-C26	4.82	109.85	104.55
2	B	4000	DLI	C2-C3-C4	4.76	120.40	116.42
2	B	4000	DLI	C20-C19-N18	-3.97	117.11	122.13
2	B	4000	DLI	C27-C26-S1	3.86	122.13	119.02
2	B	4000	DLI	C17-N18-C19	3.13	120.25	115.89
2	B	4000	DLI	F15-C1-C6	3.02	126.52	118.45
2	B	4000	DLI	N18-C17-N16	-2.87	124.23	128.58
2	B	4000	DLI	C5-C4-C3	-2.83	120.78	123.93
2	B	4000	DLI	F15-C1-C2	-2.80	113.03	118.64
2	B	4000	DLI	C25-C26-S1	-2.74	117.15	119.58
2	B	4000	DLI	O2-S1-C26	-2.37	106.39	108.23
2	B	4000	DLI	C20-C14-N11	-2.32	119.55	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4000	DLI	C17-N16-C14	2.32	116.90	114.95
2	B	4000	DLI	C12-N11-C8	2.29	114.96	111.64
2	B	4000	DLI	F10-C4-C5	2.10	122.84	118.64
2	B	4000	DLI	C21-C19-N18	2.01	120.60	116.87

There are no chirality outliers.

All (6) torsion outliers are listed below:

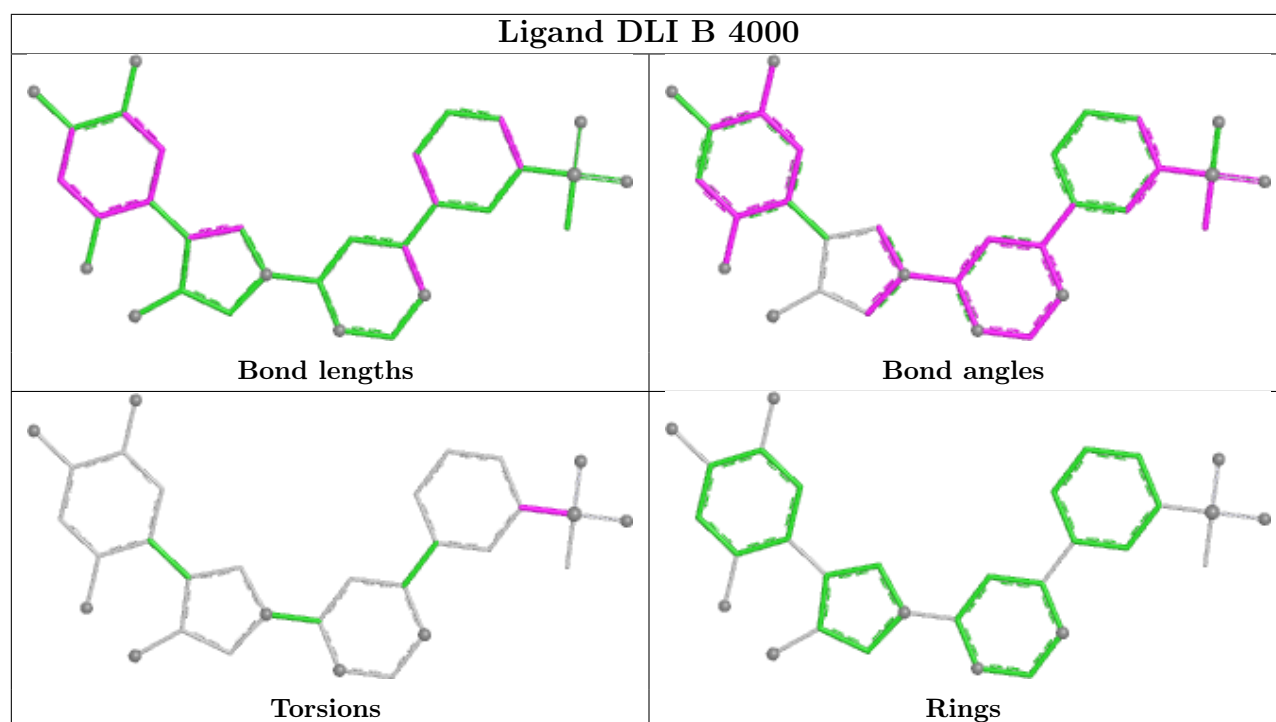
Mol	Chain	Res	Type	Atoms
2	B	4000	DLI	C25-C26-S1-C10
2	B	4000	DLI	C27-C26-S1-C10
2	B	4000	DLI	C25-C26-S1-O2
2	B	4000	DLI	C27-C26-S1-O2
2	B	4000	DLI	C25-C26-S1-O1
2	B	4000	DLI	C27-C26-S1-O1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4000	DLI	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%)	0.26	49 (6%) 24 26	15, 30, 71, 158	0
1	B	726/726 (100%)	0.41	77 (10%) 11 12	16, 31, 77, 132	0
1	C	726/726 (100%)	0.21	36 (4%) 34 35	16, 36, 82, 149	0
1	D	726/726 (100%)	0.24	50 (6%) 23 25	18, 35, 81, 135	0
All	All	2904/2904 (100%)	0.28	212 (7%) 21 23	15, 33, 79, 158	0

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	ALA	8.4
1	A	280	THR	7.0
1	D	289	ALA	6.7
1	B	341	VAL	6.4
1	A	281	ASN	6.2
1	C	289	ALA	5.8
1	B	111	GLY	5.8
1	A	277	SER	5.7
1	A	279	VAL	5.7
1	B	342	ALA	5.5
1	B	71	LYS	5.5
1	D	615	LYS	5.5
1	D	342	ALA	5.3
1	D	71	LYS	5.3
1	C	105	TYR	5.3
1	B	105	TYR	5.1
1	A	342	ALA	5.0
1	B	114	ILE	4.8
1	A	114	ILE	4.6
1	C	71	LYS	4.5
1	A	278	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	276	LEU	4.3
1	B	160	VAL	4.1
1	C	114	ILE	4.1
1	A	74	ASN	4.0
1	A	333	SER	4.0
1	D	764	SER	3.9
1	A	289	ALA	3.9
1	D	90	LEU	3.9
1	D	276	LEU	3.9
1	C	277	SER	3.8
1	D	279	VAL	3.8
1	B	39	SER	3.8
1	A	366	LEU	3.8
1	B	289	ALA	3.7
1	B	66	HIS	3.7
1	C	39	SER	3.6
1	A	140	ARG	3.6
1	C	764	SER	3.6
1	A	437	SER	3.5
1	B	69	LEU	3.5
1	B	275	SER	3.5
1	B	366	LEU	3.5
1	C	90	LEU	3.5
1	B	280	THR	3.4
1	B	330	TYR	3.4
1	A	283	THR	3.4
1	D	88	VAL	3.4
1	A	413	ASP	3.4
1	B	61	ARG	3.4
1	B	90	LEU	3.4
1	A	487	ASN	3.4
1	D	76	ILE	3.3
1	D	61	ARG	3.3
1	A	105	TYR	3.3
1	B	340	LEU	3.2
1	D	114	ILE	3.2
1	B	89	PHE	3.2
1	D	39	SER	3.2
1	A	377	ASN	3.2
1	D	89	PHE	3.2
1	C	182	SER	3.2
1	A	71	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	277	SER	3.1
1	B	764	SER	3.1
1	C	506	ASN	3.1
1	B	332	GLU	3.1
1	B	336	ARG	3.0
1	A	72	GLN	3.0
1	C	489	LYS	3.0
1	B	276	LEU	3.0
1	C	75	ASN	3.0
1	B	489	LYS	2.9
1	B	343	ARG	2.9
1	C	72	GLN	2.9
1	D	91	GLU	2.9
1	A	66	HIS	2.9
1	B	220	GLY	2.9
1	B	139	LYS	2.9
1	A	489	LYS	2.9
1	D	538	LYS	2.9
1	C	98	PHE	2.9
1	B	335	GLY	2.8
1	A	537	SER	2.8
1	B	72	GLN	2.8
1	B	486	VAL	2.8
1	D	40	ARG	2.8
1	A	110	ASP	2.8
1	C	276	LEU	2.8
1	B	413	ASP	2.8
1	A	392	LYS	2.8
1	C	392	LYS	2.8
1	D	41	LYS	2.8
1	B	279	VAL	2.8
1	C	74	ASN	2.7
1	B	63	ILE	2.7
1	C	521	GLU	2.7
1	A	103	ASN	2.7
1	B	76	ILE	2.7
1	B	339	CYS	2.7
1	A	159	PRO	2.7
1	B	334	SER	2.7
1	B	412	SER	2.7
1	D	277	SER	2.7
1	A	187	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	341	VAL	2.6
1	B	217	SER	2.6
1	B	91	GLU	2.6
1	A	39	SER	2.6
1	D	85	ASN	2.6
1	D	98	PHE	2.6
1	B	110	ASP	2.6
1	A	341	VAL	2.6
1	D	107	ILE	2.6
1	D	361	GLU	2.5
1	D	358	ARG	2.5
1	B	321	ASN	2.5
1	D	281	ASN	2.5
1	B	466	LYS	2.5
1	D	621	ASN	2.5
1	A	218	PRO	2.5
1	D	139	LYS	2.5
1	B	40	ARG	2.5
1	C	61	ARG	2.5
1	A	412	SER	2.5
1	B	389	ILE	2.5
1	D	366	LEU	2.5
1	A	41	LYS	2.5
1	B	103	ASN	2.5
1	D	280	THR	2.4
1	D	333	SER	2.4
1	A	75	ASN	2.4
1	D	99	GLY	2.4
1	B	615	LYS	2.4
1	A	90	LEU	2.4
1	A	441	LYS	2.4
1	C	523	LYS	2.4
1	C	538	LYS	2.4
1	B	281	ASN	2.4
1	B	78	VAL	2.4
1	B	435	GLN	2.4
1	D	141	GLN	2.4
1	A	506	ASN	2.3
1	B	134	ILE	2.3
1	C	391	LYS	2.3
1	C	330	TYR	2.3
1	D	83	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	342	ALA	2.3
1	D	94	THR	2.3
1	D	160	VAL	2.3
1	C	502	LYS	2.3
1	B	138	ASN	2.3
1	D	520	ASN	2.3
1	B	130	ALA	2.3
1	B	253	ARG	2.3
1	B	142	LEU	2.2
1	C	279	VAL	2.3
1	B	520	ASN	2.2
1	A	336	ARG	2.2
1	A	141	GLN	2.2
1	B	73	GLU	2.2
1	D	105	TYR	2.2
1	D	521	GLU	2.2
1	B	278	SER	2.2
1	A	321	ASN	2.2
1	A	139	LYS	2.2
1	A	538	LYS	2.2
1	D	72	GLN	2.2
1	B	416	TYR	2.2
1	B	92	ASN	2.2
1	C	147	ARG	2.2
1	D	140	ARG	2.2
1	C	73	GLU	2.2
1	D	147	ARG	2.2
1	A	520	ASN	2.2
1	C	103	ASN	2.2
1	D	66	HIS	2.2
1	B	87	SER	2.2
1	B	462	SER	2.2
1	B	161	GLY	2.1
1	B	333	SER	2.1
1	D	87	SER	2.1
1	C	76	ILE	2.1
1	D	622	LYS	2.1
1	A	91	GLU	2.1
1	A	379	GLU	2.1
1	D	110	ASP	2.1
1	A	507	VAL	2.1
1	C	341	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	442	VAL	2.1
1	B	307	THR	2.1
1	D	336	ARG	2.1
1	B	55	LEU	2.1
1	B	107	ILE	2.1
1	C	110	ASP	2.1
1	B	62	TRP	2.1
1	C	358	ARG	2.1
1	D	275	SER	2.1
1	B	180	LEU	2.1
1	B	74	ASN	2.1
1	B	344	GLN	2.1
1	C	138	ASN	2.1
1	B	135	TYR	2.1
1	B	98	PHE	2.1
1	B	52	THR	2.0
1	A	505	GLN	2.0
1	C	180	LEU	2.0
1	B	143	ILE	2.0
1	B	538	LYS	2.0
1	D	441	LYS	2.0
1	D	536	LYS	2.0
1	B	392	LYS	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](#)

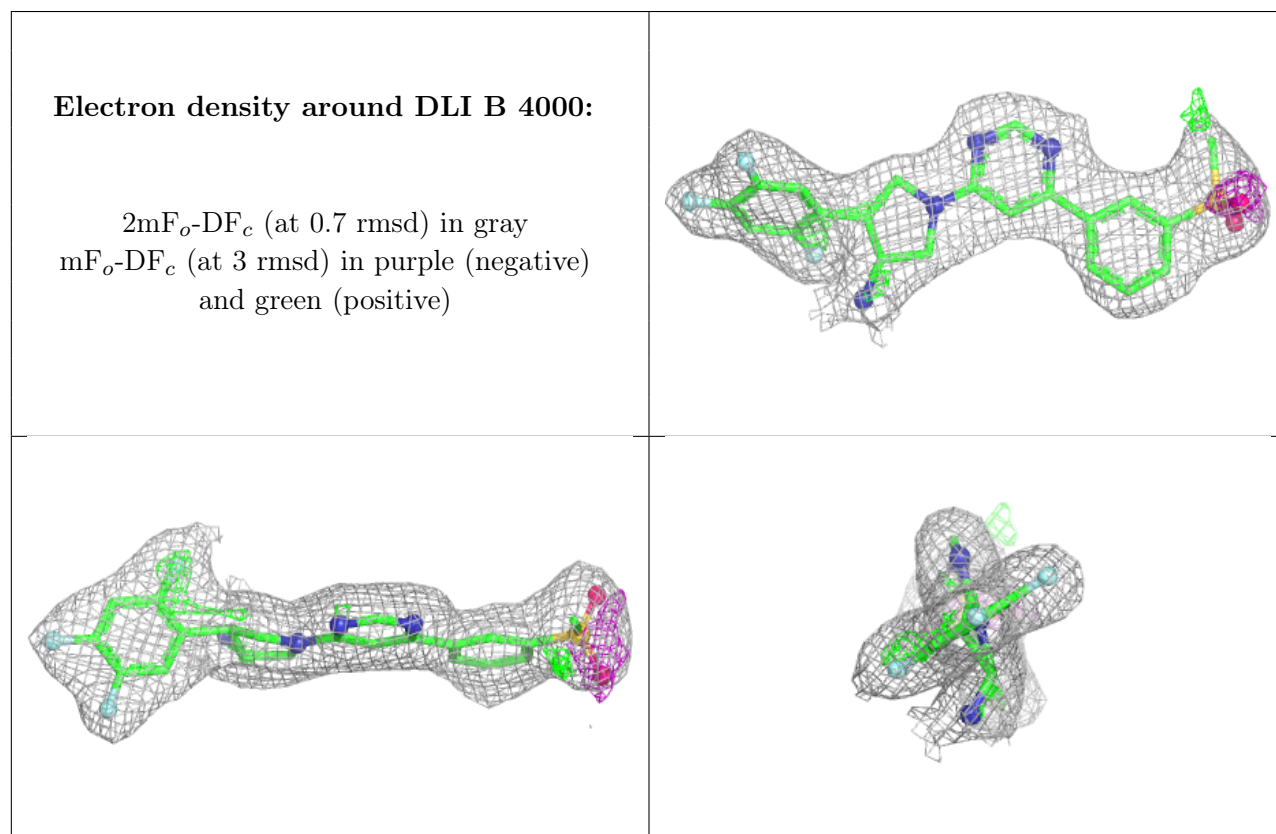
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DLI	B	4000	31/31	0.91	0.12	40,40,40,40	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 [i](#)

There are no such residues in this entry.