



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:30 AM UTC

PDB ID : 3DLA / pdb_00003dla
Title : X-ray crystal structure of glutamine-dependent NAD⁺ synthetase from Mycobacterium tuberculosis bound to NaAD⁺ and DON
Authors : LaRonde-LeBlanc, N.A.; Resto, M.; Gerratana, B.
Deposited on : 2008-06-26
Resolution : 2.35 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

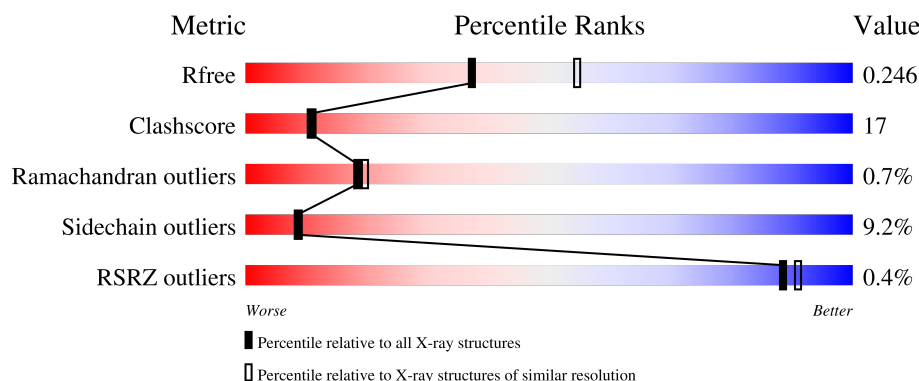
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	680	 73% 20% 5% 2%
1	B	680	 71% 20% 5% 2%
1	C	680	 62% 29% 5% 2%
1	D	680	 69% 24% 5% 2%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	C	683	-	-	X	-
4	GOL	D	682	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22006 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.

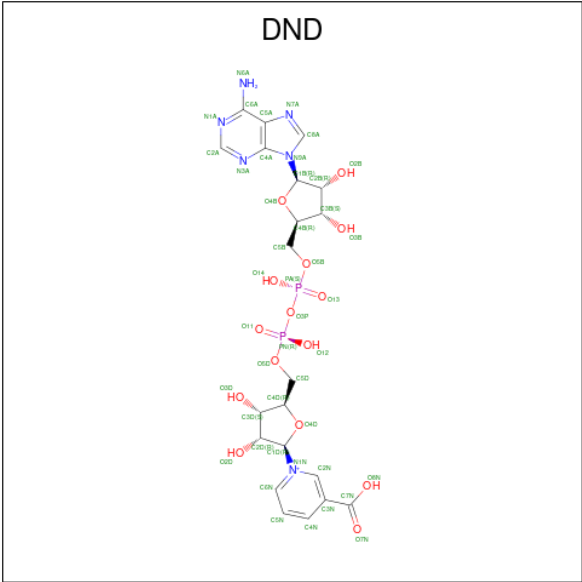
- Molecule 1 is a protein called Glutamine-dependent NAD(+) synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	651	Total	C	N	O	S	0	1	0
			5014	3180	892	926	16			
1	B	649	Total	C	N	O	S	0	0	0
			5017	3179	896	926	16			
1	C	657	Total	C	N	O	S	8	2	0
			5117	3242	911	947	17			
1	D	657	Total	C	N	O	S	0	0	0
			5099	3229	910	944	16			

There are 4 discrepancies between the modelled and reference sequences:

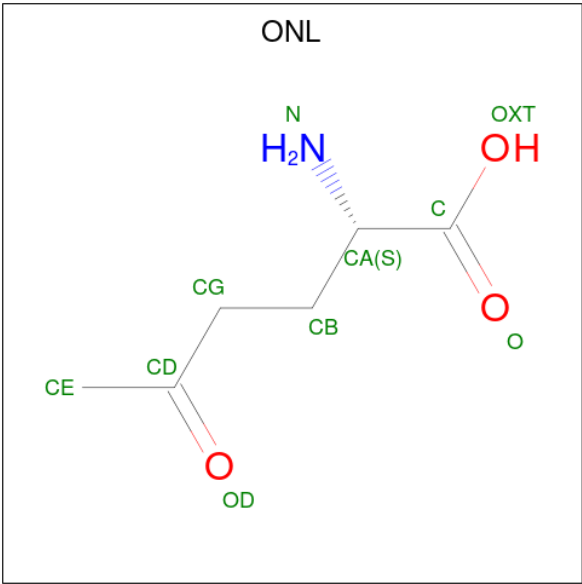
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P0A5L6
B	0	SER	-	expression tag	UNP P0A5L6
C	0	SER	-	expression tag	UNP P0A5L6
D	0	SER	-	expression tag	UNP P0A5L6

- Molecule 2 is NICOTINIC ACID ADENINE DINUCLEOTIDE (CCD ID: DND) (formula: $C_{21}H_{27}N_6O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	6	15	2		

- Molecule 3 is 5-OXO-L-NORLEUCINE (CCD ID: ONL) (formula: C₆H₁₁NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			20	12	2	6		
3	A	1	Total	C	N	O	0	0
			10	6	1	3		
3	A	1	Total	C	N	O	0	0
			10	6	1	3		
3	A	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

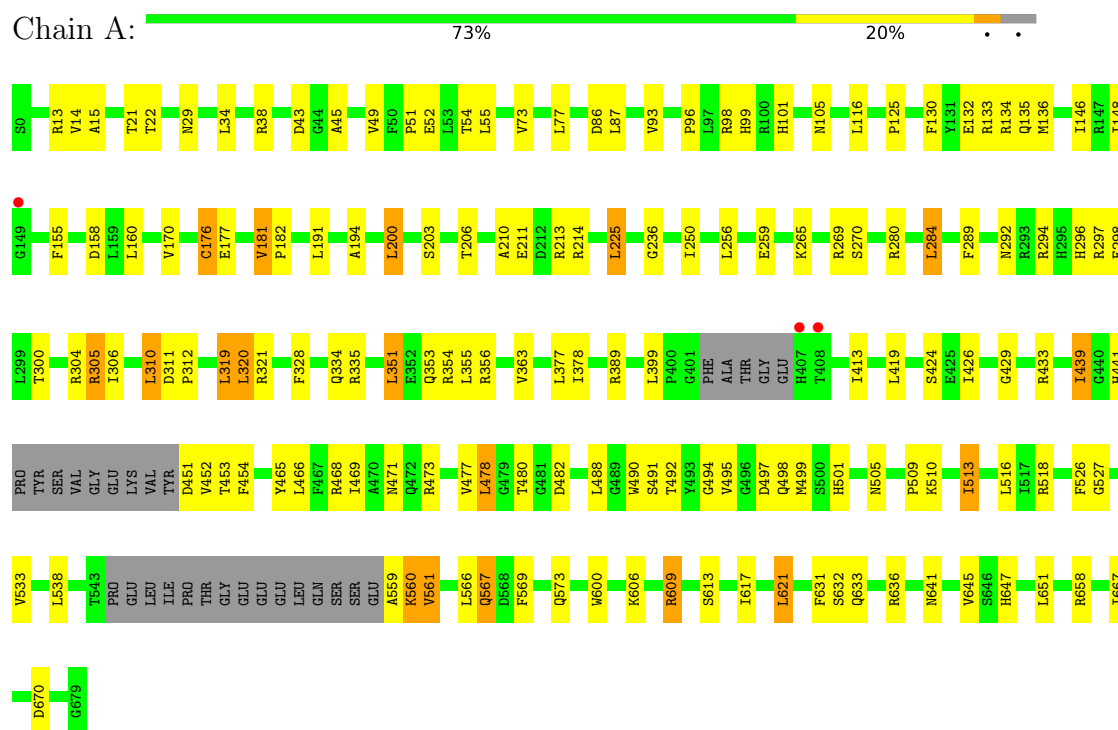
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	334	Total O 334 334	0	0
5	B	384	Total O 384 384	0	0
5	C	366	Total O 366 366	0	0
5	D	359	Total O 359 359	0	0

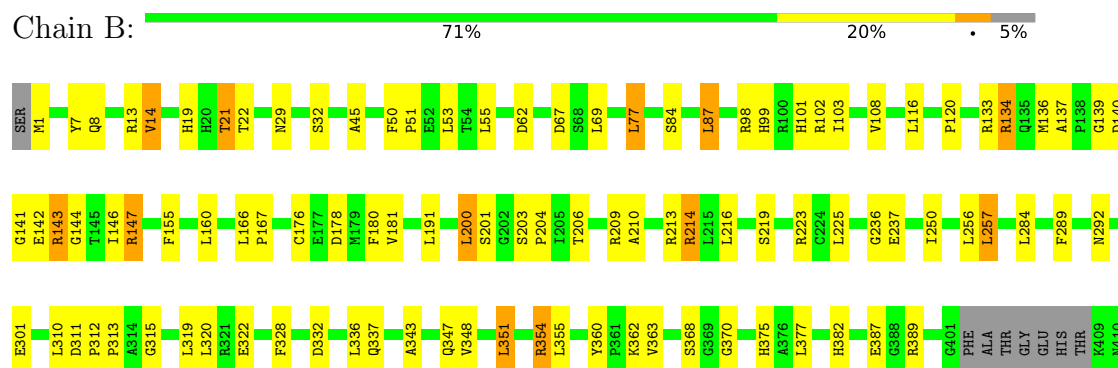
3 Residue-property plots

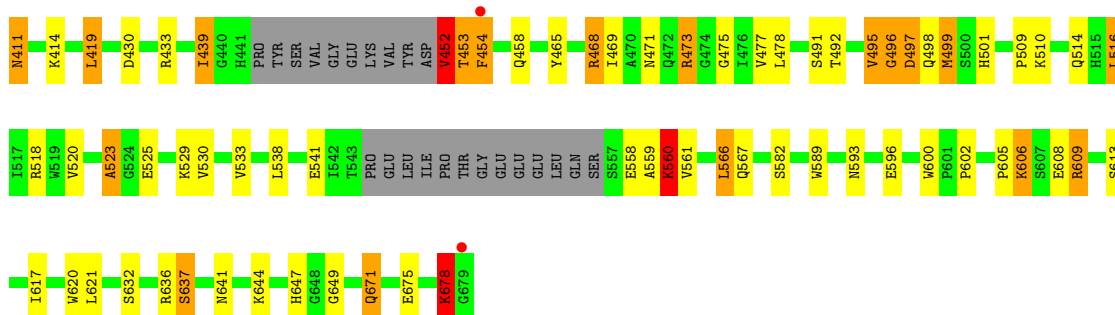
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glutamine-dependent NAD(+) synthetase



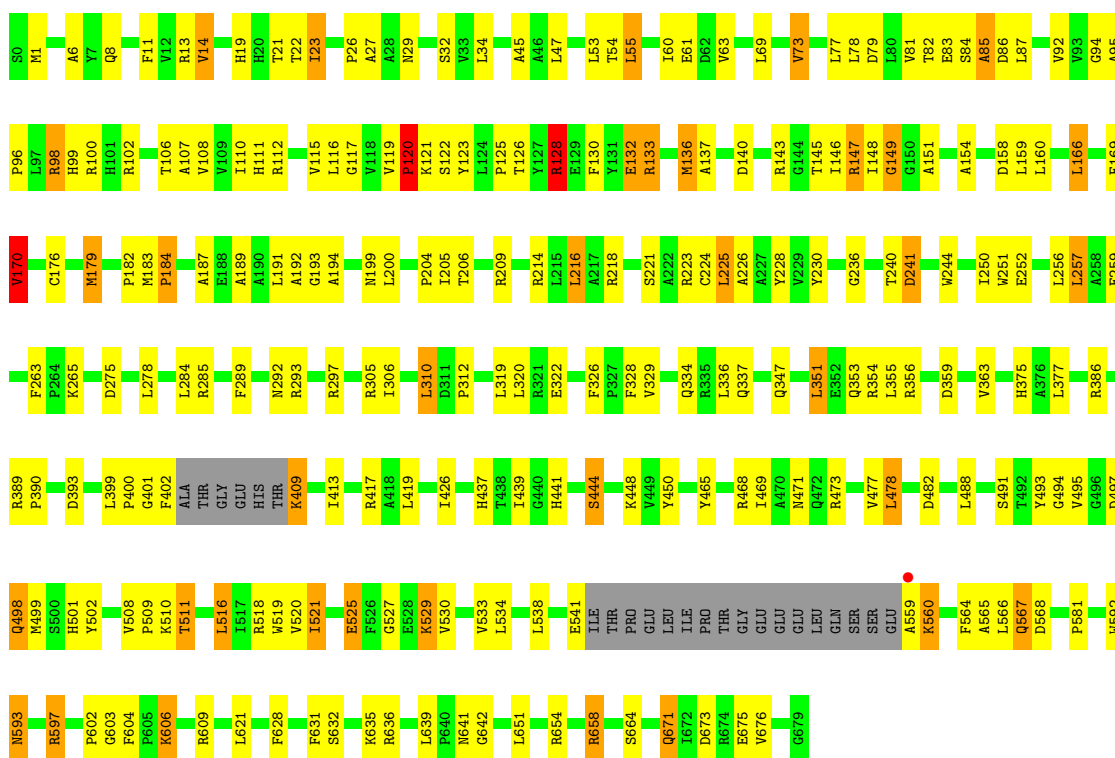
- Molecule 1: Glutamine-dependent NAD(+) synthetase





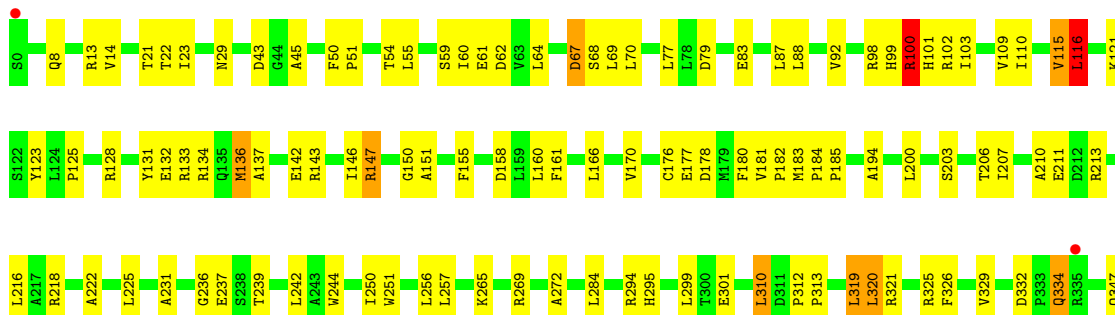
• Molecule 1: Glutamine-dependent NAD(+) synthetase

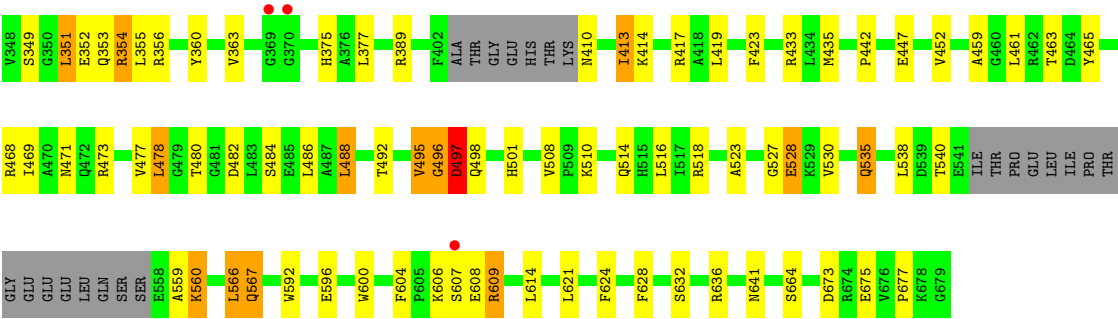
Chain C: 62% 29% 5%



• Molecule 1: Glutamine-dependent NAD(+) synthetase

Chain D: 69% 24%





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.13Å 178.13Å 215.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.70 – 2.35 29.70 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.70-2.35) 99.2 (29.70-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	172.61 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.184 , 0.246 0.187 , 0.246	Depositor DCC
R_{free} test set	7144 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 23.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22006	wwPDB-VP
Average B, all atoms (Å ²)	6.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.72% 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: ONL, GOL, DND

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	0.80	0/5128	0.99	6/6963 (0.1%)
1	B	0.90	0/5132	1.06	9/6969 (0.1%)
1	C	1.02	5/5237 (0.1%)	1.17	23/7111 (0.3%)
1	D	0.94	3/5219 (0.1%)	1.07	7/7089 (0.1%)
All	All	0.92	8/20716 (0.0%)	1.08	45/28132 (0.2%)

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	B	0	3
1	C	0	2
1	D	0	1
All	All	0	6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	123	TYR	N-CA	8.40	1.56	1.46
1	D	103	ILE	C-O	7.24	1.33	1.24
1	C	73	VAL	CA-CB	6.79	1.61	1.54
1	C	187	ALA	CA-CB	6.29	1.63	1.53
1	D	121	LYS	N-CA	5.99	1.53	1.46
1	C	560	LYS	CA-C	5.96	1.60	1.53
1	C	132	GLU	N-CA	5.29	1.53	1.46
1	C	241	ASP	N-CA	5.07	1.51	1.46

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	170	VAL	CB-CA-C	-7.45	101.31	110.99
1	C	216	LEU	CA-CB-CG	-6.75	92.67	116.30
1	C	631	PHE	N-CA-C	6.70	118.59	111.28
1	C	95	ALA	CA-C-N	6.67	128.18	119.84
1	C	95	ALA	C-N-CA	6.67	128.18	119.84
1	B	67	ASP	N-CA-C	6.42	119.09	111.33
1	B	166	LEU	CA-C-N	6.30	125.99	119.56
1	B	166	LEU	C-N-CA	6.30	125.99	119.56
1	C	166	LEU	CA-C-N	6.21	126.67	119.47
1	C	166	LEU	C-N-CA	6.21	126.67	119.47
1	A	609	ARG	CA-C-N	6.17	126.36	120.31
1	A	609	ARG	C-N-CA	6.17	126.36	120.31
1	C	628	PHE	N-CA-C	6.11	117.63	110.97
1	D	158	ASP	CB-CA-C	-6.07	103.67	111.50
1	C	263	PHE	CA-C-N	-6.04	114.39	120.31
1	C	263	PHE	C-N-CA	-6.04	114.39	120.31
1	C	184	PRO	N-CA-C	5.85	116.90	110.64
1	C	158	ASP	N-CA-C	5.64	118.95	112.97
1	C	593	ASN	N-CA-C	5.59	118.14	111.71
1	C	676	VAL	N-CA-C	5.59	113.40	107.76
1	B	523	ALA	N-CA-C	-5.56	104.61	111.33
1	C	289	PHE	N-CA-C	-5.51	104.97	110.97
1	C	189	ALA	N-CA-C	-5.46	105.49	111.82
1	D	527	GLY	N-CA-C	5.44	117.58	112.08
1	C	216	LEU	N-CA-C	5.42	117.18	111.28
1	B	452	VAL	CA-C-N	5.39	131.40	121.70
1	B	452	VAL	C-N-CA	5.39	131.40	121.70
1	D	115	VAL	N-CA-C	-5.38	100.70	108.87
1	C	521	ILE	CB-CA-C	-5.37	105.10	111.81
1	A	645	VAL	N-CA-C	5.33	115.83	111.62
1	D	203	SER	CA-C-N	-5.28	114.32	119.76
1	D	203	SER	C-N-CA	-5.28	114.32	119.76
1	A	181	VAL	CA-C-N	-5.27	113.25	119.84
1	A	181	VAL	C-N-CA	-5.27	113.25	119.84
1	B	315	GLY	N-CA-C	5.27	120.69	112.31
1	B	332	ASP	CA-C-N	5.24	124.87	119.05
1	B	332	ASP	C-N-CA	5.24	124.87	119.05
1	C	73	VAL	N-CA-C	5.19	115.81	110.36
1	D	116	LEU	N-CA-C	-5.18	107.09	113.41
1	C	192	ALA	N-CA-C	-5.11	106.89	113.23
1	A	631	PHE	N-CA-C	5.10	116.64	111.14
1	D	628	PHE	N-CA-C	5.09	116.63	111.14
1	C	560	LYS	CB-CA-C	5.07	119.28	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	VAL	CB-CA-C	-5.04	105.43	111.88
1	C	145	THR	N-CA-C	5.01	116.91	109.69

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	496	GLY	Peptide
1	B	559	ALA	Peptide
1	B	560	LYS	Peptide
1	C	559	ALA	Peptide
1	C	560	LYS	Peptide
1	D	496	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5014	0	4904	123	0
1	B	5017	0	4919	164	1
1	C	5117	0	5015	234	0
1	D	5099	0	4994	182	0
2	A	44	0	25	6	0
2	B	44	0	25	0	0
2	C	44	0	25	2	0
2	D	44	0	25	3	0
3	A	50	0	38	11	0
4	A	12	0	16	0	0
4	B	24	0	32	4	0
4	C	24	0	32	10	0
4	D	30	0	40	11	0
5	A	334	0	0	37	2
5	B	384	0	0	46	1
5	C	366	0	0	77	0
5	D	359	0	0	58	0
All	All	22006	0	20090	679	2

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 17.

All (679) 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:B:495:VAL:HB	5:B:993:HOH:O	1.22	1.29
1:C:183[B]:MET:HE3	5:C:800:HOH:O	1.25	1.29
1:D:110:ILE:HA	5:D:970:HOH:O	1.36	1.24
1:D:147:ARG:HH11	1:D:147:ARG:CG	1.50	1.22
1:C:170:VAL:HG22	5:C:854:HOH:O	1.42	1.19
1:C:94:GLY:CA	5:C:961:HOH:O	1.89	1.19
1:D:51:PRO:HA	5:D:851:HOH:O	1.44	1.18
1:D:88:LEU:HG	5:D:973:HOH:O	1.41	1.18
1:A:211:GLU:HG3	5:A:1065:HOH:O	1.40	1.18
1:C:278:LEU:HB2	5:C:956:HOH:O	1.43	1.14
1:D:181:VAL:HG22	5:D:954:HOH:O	1.47	1.14
1:C:240:THR:HG22	5:C:860:HOH:O	1.51	1.10
1:C:221:SER:HA	5:C:966:HOH:O	1.49	1.09
1:B:354:ARG:NH1	5:B:750:HOH:O	1.79	1.08
1:D:147:ARG:HH11	1:D:147:ARG:HG3	1.07	1.05
1:C:581:PRO:HD2	1:C:671:GLN:HG2	1.39	1.04
1:C:94:GLY:HA3	5:C:961:HOH:O	1.51	1.03
1:C:78:LEU:HG	5:C:980:HOH:O	1.57	1.02
1:D:294:ARG:HD3	4:D:682:GOL:O3	1.58	1.02
1:C:204:PRO:HG3	1:C:244:TRP:CH2	1.95	1.02
1:C:529:LYS:H	1:C:529:LYS:HD3	1.22	1.01
1:C:593:ASN:HB2	5:C:996:HOH:O	1.60	1.01
1:C:94:GLY:HA2	5:C:961:HOH:O	1.55	0.99
1:A:125:PRO:O	5:A:1066:HOH:O	1.80	0.99
1:B:8:GLN:HB3	5:B:932:HOH:O	1.62	0.99
1:D:363:VAL:HG13	1:D:478:LEU:CD2	1.92	0.98
1:C:477:VAL:H	1:C:501:HIS:HD2	1.03	0.98
1:C:354:ARG:HH22	1:C:641:ASN:HD22	1.12	0.97
1:B:477:VAL:H	1:B:501:HIS:HD2	1.13	0.96
1:A:527:GLY:HA3	5:A:912:HOH:O	1.67	0.93
1:A:567:GLN:HA	1:A:567:GLN:HE21	1.34	0.93
1:C:73:VAL:HG11	5:C:743:HOH:O	1.68	0.93
1:D:477:VAL:H	1:D:501:HIS:HD2	1.12	0.93
1:D:146:ILE:HG22	1:D:155:PHE:HB2	1.49	0.92
1:D:354:ARG:HH22	1:D:641:ASN:HD22	0.97	0.92
1:B:181:VAL:HG22	5:B:859:HOH:O	1.69	0.92
1:C:123:TYR:CE2	5:C:901:HOH:O	2.23	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:ARG:HD2	1:C:251:TRP:CZ3	2.06	0.90
1:A:468:ARG:HH11	1:A:471:ASN:ND2	1.70	0.90
1:B:257:LEU:HD13	5:B:753:HOH:O	1.72	0.89
1:D:468:ARG:NH1	1:D:471:ASN:ND2	2.19	0.89
1:A:477:VAL:H	1:A:501:HIS:HD2	1.21	0.88
1:C:100:ARG:HB2	5:C:1002:HOH:O	1.73	0.88
1:C:529:LYS:H	1:C:529:LYS:CD	1.84	0.88
1:D:354:ARG:HH22	1:D:641:ASN:ND2	1.70	0.88
1:D:147:ARG:CG	1:D:147:ARG:NH1	2.22	0.88
1:C:477:VAL:H	1:C:501:HIS:CD2	1.90	0.87
1:C:122:SER:HB3	5:C:901:HOH:O	1.75	0.86
1:B:468:ARG:HH11	1:B:471:ASN:ND2	1.74	0.85
1:D:147:ARG:HH11	1:D:147:ARG:HG2	1.39	0.85
1:C:437:HIS:HA	1:C:444:SER:OG	1.78	0.84
1:B:354:ARG:NH2	1:B:641:ASN:HD22	1.74	0.84
1:D:147:ARG:HG3	1:D:147:ARG:NH1	1.83	0.84
1:A:22:THR:H	1:A:29:ASN:HD21	1.22	0.83
1:C:110:ILE:HG13	5:C:983:HOH:O	1.75	0.83
1:D:115:VAL:HA	5:D:970:HOH:O	1.76	0.83
1:B:136:MET:SD	5:B:885:HOH:O	2.36	0.83
1:D:272:ALA:HB1	5:D:857:HOH:O	1.78	0.83
1:B:558:GLU:HG2	5:B:928:HOH:O	1.79	0.82
1:A:335:ARG:HG2	5:A:851:HOH:O	1.80	0.82
1:C:96:PRO:HD2	5:C:743:HOH:O	1.80	0.82
1:C:102:ARG:HD3	1:C:137:ALA:HB2	1.62	0.81
1:C:241:ASP:OD2	5:C:860:HOH:O	1.98	0.81
1:A:561:VAL:HG23	5:A:1001:HOH:O	1.78	0.81
1:D:567:GLN:HE21	1:D:567:GLN:HA	1.44	0.81
1:B:289:PHE:HA	5:B:1003:HOH:O	1.79	0.81
1:D:216:LEU:HD13	5:D:874:HOH:O	1.77	0.81
1:B:311:ASP:HB2	5:B:856:HOH:O	1.81	0.80
5:A:1115:HOH:O	1:B:141:GLY:HA3	1.80	0.80
1:D:69:LEU:C	1:D:69:LEU:HD13	2.06	0.80
1:A:633:GLN:OE1	1:A:636:ARG:NH1	2.13	0.80
1:D:23:ILE:HG21	5:D:972:HOH:O	1.80	0.80
1:B:477:VAL:H	1:B:501:HIS:CD2	1.98	0.79
1:D:147:ARG:HE	1:D:150:GLY:HA2	1.47	0.79
1:D:363:VAL:HG13	1:D:478:LEU:HD23	1.64	0.79
1:A:297:ARG:NH2	1:B:142:GLU:OE2	2.15	0.79
1:A:560:LYS:HD2	5:A:914:HOH:O	1.81	0.79
1:C:606:LYS:HA	1:C:609:ARG:HD3	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:GLN:CB	5:B:932:HOH:O	2.26	0.78
1:C:567:GLN:HE21	1:C:567:GLN:HA	1.47	0.78
1:C:597:ARG:HG3	1:C:597:ARG:HH11	1.47	0.78
1:B:560:LYS:HE2	1:B:620:TRP:HH2	1.48	0.78
1:B:22:THR:H	1:B:29:ASN:HD21	1.32	0.78
1:C:204:PRO:HG3	1:C:244:TRP:CZ3	2.18	0.77
1:D:484:SER:O	1:D:488:LEU:HD22	1.84	0.77
1:A:477:VAL:H	1:A:501:HIS:CD2	2.02	0.77
1:D:459:ALA:HB1	5:D:974:HOH:O	1.83	0.77
1:D:477:VAL:H	1:D:501:HIS:CD2	1.99	0.76
1:C:359:ASP:HB2	5:C:878:HOH:O	1.86	0.76
1:D:354:ARG:NH2	1:D:641:ASN:HD22	1.79	0.76
1:B:354:ARG:HH21	1:B:641:ASN:HD22	1.34	0.76
1:C:47:LEU:HD12	5:C:886:HOH:O	1.86	0.76
1:A:132:GLU:HB2	5:A:1066:HOH:O	1.86	0.75
1:A:191:LEU:O	1:B:101:HIS:HE1	1.70	0.75
1:C:511:THR:HB	1:C:568:ASP:OD2	1.87	0.74
1:D:147:ARG:NH1	1:D:147:ARG:HG2	1.97	0.74
1:A:133:ARG:HG2	5:A:932:HOH:O	1.88	0.74
1:B:468:ARG:NH2	1:C:495:VAL:O	2.21	0.74
1:C:658:ARG:HD2	5:C:922:HOH:O	1.87	0.74
1:C:468:ARG:NH1	1:C:471:ASN:ND2	2.36	0.73
1:D:109:VAL:O	5:D:970:HOH:O	2.06	0.73
1:A:353:GLN:HE21	1:A:356:ARG:HH21	1.34	0.73
1:A:468:ARG:NH1	1:A:471:ASN:HD21	1.87	0.73
1:C:354:ARG:HH22	1:C:641:ASN:ND2	1.87	0.73
1:D:389:ARG:HD3	5:D:814:HOH:O	1.87	0.73
1:A:354:ARG:HH22	1:A:641:ASN:HD22	1.33	0.72
1:B:21:THR:HG22	5:B:687:HOH:O	1.88	0.72
1:D:463:THR:HG21	5:D:881:HOH:O	1.89	0.72
1:C:146:ILE:HD13	1:C:148:ILE:HD11	1.69	0.72
1:C:183[B]:MET:CE	5:C:800:HOH:O	1.99	0.72
1:C:204:PRO:CG	5:C:869:HOH:O	2.37	0.72
1:C:99:HIS:HD2	5:C:707:HOH:O	1.71	0.72
1:C:110:ILE:CD1	5:C:983:HOH:O	2.37	0.72
1:A:468:ARG:HH11	1:A:471:ASN:HD21	1.38	0.72
1:C:179:MET:O	5:C:797:HOH:O	2.07	0.72
1:B:523:ALA:HB3	5:B:737:HOH:O	1.88	0.72
1:C:92:VAL:HG23	5:C:886:HOH:O	1.89	0.72
1:D:673:ASP:HB3	5:D:1022:HOH:O	1.90	0.71
2:A:680:DND:H10	2:A:680:DND:H5	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:VAL:CG1	1:D:478:LEU:HD23	2.21	0.71
1:B:453:THR:HG23	1:B:454:PHE:H	1.54	0.71
1:C:23:ILE:CD1	5:C:960:HOH:O	2.39	0.70
1:D:102:ARG:HD3	1:D:137:ALA:HB2	1.73	0.70
1:C:285:ARG:HE	4:C:681:GOL:H31	1.56	0.70
1:C:110:ILE:CG1	5:C:983:HOH:O	2.32	0.70
4:D:683:GOL:H32	5:D:1006:HOH:O	1.91	0.70
1:A:468:ARG:NH2	1:D:495:VAL:O	2.24	0.70
5:A:852:HOH:O	1:B:101:HIS:HD2	1.75	0.70
1:D:61:GLU:OE2	5:D:855:HOH:O	2.09	0.70
1:A:203:SER:O	5:A:971:HOH:O	2.09	0.69
1:C:275:ASP:CG	5:C:956:HOH:O	2.33	0.69
1:D:70:LEU:HG	5:D:726:HOH:O	1.90	0.69
1:B:21:THR:HB	5:B:708:HOH:O	1.92	0.69
1:A:495:VAL:HG12	1:D:495:VAL:HB	1.74	0.69
1:B:77:LEU:HD11	1:B:108:VAL:HG21	1.75	0.69
1:A:294:ARG:HD3	5:D:1005:HOH:O	1.93	0.69
1:D:43:ASP:OD2	1:D:269:ARG:NH2	2.26	0.69
1:D:363:VAL:CG1	1:D:478:LEU:CD2	2.70	0.69
1:D:218:ARG:HD2	1:D:251:TRP:CZ3	2.28	0.69
1:D:468:ARG:HH11	1:D:471:ASN:ND2	1.90	0.69
1:C:305:ARG:HD3	5:C:899:HOH:O	1.92	0.68
1:A:354:ARG:HH22	1:A:641:ASN:ND2	1.89	0.68
1:A:363:VAL:HG13	1:A:478:LEU:HG	1.76	0.68
1:C:100:ARG:CZ	5:C:1002:HOH:O	2.41	0.68
1:B:301:GLU:HG2	5:B:1000:HOH:O	1.93	0.68
1:C:98:ARG:HG3	5:C:770:HOH:O	1.92	0.68
1:C:106:THR:HG22	1:C:120:PRO:HB3	1.74	0.68
1:C:204:PRO:HG2	5:C:869:HOH:O	1.90	0.68
1:C:597:ARG:HH11	1:C:597:ARG:CG	2.06	0.68
3:A:801[A]:ONL:HG1	1:B:180:PHE:CZ	2.29	0.68
1:B:178:ASP:O	5:B:859:HOH:O	2.11	0.68
1:C:21:THR:O	1:C:236:GLY:HA3	1.93	0.68
1:B:608:GLU:HB2	5:B:985:HOH:O	1.94	0.67
1:C:306:ILE:HG12	5:C:988:HOH:O	1.95	0.67
1:C:126:THR:OG1	1:C:133:ARG:HB2	1.95	0.67
1:A:297:ARG:NH1	5:A:1115:HOH:O	2.28	0.67
5:B:1003:HOH:O	1:D:182:PRO:CD	2.43	0.67
1:D:23:ILE:CG2	5:D:972:HOH:O	2.41	0.67
1:C:179:MET:HE2	1:C:228:TYR:CE2	2.30	0.67
1:B:605:PRO:HD2	5:B:985:HOH:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ARG:HD2	5:C:780:HOH:O	1.95	0.67
1:A:133:ARG:CG	5:A:932:HOH:O	2.41	0.66
1:D:535:GLN:HG2	5:D:864:HOH:O	1.96	0.66
1:A:22:THR:H	1:A:29:ASN:ND2	1.94	0.66
1:D:528:GLU:HG3	5:D:989:HOH:O	1.94	0.66
1:C:305:ARG:CD	5:C:899:HOH:O	2.43	0.66
1:C:353:GLN:HE21	1:C:356:ARG:HH21	1.44	0.66
1:D:22:THR:H	1:D:29:ASN:HD21	1.44	0.66
1:D:353:GLN:HE21	1:D:356:ARG:HH21	1.42	0.65
1:D:294:ARG:HD3	4:D:682:GOL:HO3	1.62	0.65
1:B:491:SER:HA	1:B:497:ASP:OD2	1.96	0.65
1:C:96:PRO:CD	5:C:743:HOH:O	2.41	0.65
1:C:389:ARG:HD3	5:C:685:HOH:O	1.95	0.65
1:B:473:ARG:HG2	5:B:990:HOH:O	1.96	0.65
1:C:110:ILE:HD12	5:C:983:HOH:O	1.97	0.65
1:A:567:GLN:HE21	1:A:567:GLN:CA	2.09	0.64
1:B:292:ASN:HD21	1:D:183:MET:H	1.42	0.64
1:C:297:ARG:NH2	1:D:142:GLU:OE2	2.30	0.64
1:C:23:ILE:HG13	5:C:960:HOH:O	1.96	0.64
1:D:14:VAL:HG23	1:D:250:ILE:HD13	1.78	0.64
1:B:389:ARG:HD3	5:B:694:HOH:O	1.97	0.64
1:B:465:TYR:HD1	1:C:439:ILE:HD11	1.63	0.64
1:C:441:HIS:O	1:C:444:SER:HB2	1.97	0.64
1:D:363:VAL:HG13	1:D:478:LEU:HD21	1.77	0.64
1:D:45:ALA:O	5:D:973:HOH:O	2.14	0.64
1:D:497:ASP:HB2	5:D:974:HOH:O	1.97	0.64
1:C:214:ARG:NH1	1:C:259:GLU:OE2	2.30	0.64
1:C:182:PRO:O	1:C:184:PRO:HD3	1.98	0.64
1:C:179:MET:HE3	1:C:199:ASN:ND2	2.13	0.63
1:A:647:HIS:HD2	5:A:870:HOH:O	1.80	0.63
3:A:801[A]:ONL:HG1	1:B:180:PHE:HZ	1.61	0.63
1:B:593:ASN:HB2	5:B:1038:HOH:O	1.98	0.63
1:B:452:VAL:HA	1:B:453:THR:HB	1.81	0.63
1:A:495:VAL:HG23	1:D:468:ARG:NH2	2.12	0.63
1:B:468:ARG:HH11	1:B:471:ASN:HD21	1.45	0.63
1:D:98:ARG:HG3	5:D:711:HOH:O	1.98	0.63
2:C:680:DND:H4	5:C:1032:HOH:O	1.99	0.63
1:C:126:THR:O	4:C:683:GOL:C1	2.46	0.63
1:C:354:ARG:NH2	1:C:641:ASN:HD22	1.91	0.62
1:C:19:HIS:HB2	1:C:32:SER:OG	1.99	0.62
1:B:223:ARG:HG3	5:D:874:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ARG:NH2	5:B:858:HOH:O	2.31	0.62
5:B:1003:HOH:O	1:D:182:PRO:HD3	2.00	0.62
1:C:214:ARG:HG3	5:C:832:HOH:O	1.98	0.62
1:D:463:THR:CG2	5:D:881:HOH:O	2.46	0.62
1:B:1:MET:N	5:B:1066:HOH:O	2.28	0.62
1:A:158:ASP:OD1	1:A:304:ARG:NH2	2.32	0.62
1:C:521:ILE:HD11	1:C:534:LEU:HB3	1.81	0.62
1:B:210:ALA:HA	1:B:213:ARG:HD2	1.83	0.61
1:B:439:ILE:HD13	1:C:465:TYR:CD1	2.36	0.61
1:A:101:HIS:HD2	5:A:810:HOH:O	1.82	0.61
1:A:439:ILE:HD11	1:D:465:TYR:HD1	1.66	0.61
1:C:437:HIS:HA	1:C:444:SER:HG	1.66	0.61
1:C:27:ALA:HB2	4:C:682:GOL:H12	1.82	0.61
1:C:494:GLY:H	1:C:498:GLN:NE2	1.98	0.61
1:D:468:ARG:HH11	1:D:471:ASN:HD22	1.46	0.61
1:B:347:GLN:OE1	1:B:375:HIS:HE1	1.84	0.61
1:C:518:ARG:HD3	5:C:766:HOH:O	2.00	0.61
1:D:468:ARG:NH1	1:D:471:ASN:HD21	1.99	0.60
1:B:558:GLU:O	1:B:561:VAL:HG22	2.00	0.60
1:B:453:THR:HG21	5:B:996:HOH:O	2.00	0.60
1:A:351:LEU:HD22	1:A:355:LEU:HG	1.84	0.60
1:A:495:VAL:O	1:D:468:ARG:NH2	2.35	0.60
1:A:497:ASP:OD2	2:A:680:DND:H12	2.02	0.60
1:A:567:GLN:NE2	5:A:854:HOH:O	2.32	0.60
1:B:21:THR:HG21	1:B:237:GLU:HG2	1.84	0.59
1:D:514:GLN:HE21	1:D:518:ARG:HH12	1.51	0.59
1:D:59:SER:OG	5:D:972:HOH:O	1.98	0.59
1:C:326:PHE:CB	1:C:329:VAL:HB	2.33	0.59
1:D:417:ARG:HD2	5:D:960:HOH:O	2.01	0.59
1:A:49:VAL:HG13	1:A:200:LEU:HD22	1.85	0.59
1:C:53:LEU:HD22	1:C:96:PRO:HD3	1.83	0.59
1:A:14:VAL:HG23	1:A:250:ILE:HD13	1.84	0.58
1:C:529:LYS:CD	1:C:529:LYS:N	2.63	0.58
1:B:99:HIS:HE1	5:B:902:HOH:O	1.84	0.58
1:B:411:ASN:HA	1:B:414:LYS:HB2	1.84	0.58
1:D:21:THR:O	1:D:236:GLY:HA3	2.02	0.58
2:D:680:DND:H4	5:D:978:HOH:O	2.03	0.58
1:B:468:ARG:NH1	1:B:471:ASN:HD21	2.01	0.58
1:C:107:ALA:N	1:C:119:VAL:O	2.30	0.58
1:B:147:ARG:HB2	4:B:682:GOL:H31	1.83	0.58
1:A:158:ASP:CG	1:A:304:ARG:HH21	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ARG:CD	5:D:874:HOH:O	2.51	0.58
1:C:567:GLN:HA	1:C:567:GLN:NE2	2.18	0.58
1:D:492:THR:HB	5:D:974:HOH:O	2.03	0.58
1:A:353:GLN:HE21	1:A:356:ARG:NH2	2.02	0.58
5:B:1003:HOH:O	1:D:182:PRO:HD2	2.02	0.58
1:B:62:ASP:OD2	1:B:134:ARG:NH1	2.37	0.58
1:B:102:ARG:HD3	1:B:137:ALA:HB2	1.85	0.58
1:C:285:ARG:NH1	5:C:1035:HOH:O	2.14	0.58
1:B:50:PHE:O	1:B:200:LEU:HB3	2.04	0.57
1:C:55:LEU:HB2	1:C:94:GLY:O	2.04	0.57
1:A:468:ARG:NH1	1:A:471:ASN:ND2	2.43	0.57
1:B:22:THR:H	1:B:29:ASN:ND2	1.98	0.57
1:C:147:ARG:HD2	5:C:851:HOH:O	2.04	0.57
1:B:98:ARG:HG3	5:B:699:HOH:O	2.03	0.57
1:D:64:LEU:O	5:D:726:HOH:O	2.17	0.57
1:A:441:HIS:NE2	1:A:453:THR:HG21	2.19	0.57
1:D:353:GLN:HE21	1:D:356:ARG:NH2	2.02	0.57
1:C:363:VAL:HG13	1:C:478:LEU:HG	1.86	0.57
1:D:360:TYR:HB3	1:D:389:ARG:HD2	1.87	0.57
1:C:69:LEU:HD13	1:C:69:LEU:C	2.30	0.57
1:D:64:LEU:C	5:D:726:HOH:O	2.48	0.57
1:A:191:LEU:O	1:B:101:HIS:CE1	2.54	0.56
1:C:126:THR:O	4:C:683:GOL:H11	2.04	0.56
1:D:125:PRO:HD2	1:D:132:GLU:CD	2.31	0.56
1:B:468:ARG:NH1	1:B:471:ASN:ND2	2.51	0.56
1:C:1:MET:HB3	1:C:675:GLU:OE1	2.05	0.56
1:B:541:GLU:HG2	5:B:775:HOH:O	2.06	0.56
1:C:525:GLU:HG3	5:C:955:HOH:O	2.05	0.56
1:D:182:PRO:O	1:D:184:PRO:HD3	2.05	0.56
1:C:81:VAL:HG22	1:C:110:ILE:HG12	1.89	0.56
1:D:514:GLN:HE21	1:D:518:ARG:NH1	2.04	0.56
1:C:482:ASP:HB2	1:C:508:VAL:O	2.06	0.55
1:A:310:LEU:HB3	1:A:312:PRO:HD3	1.88	0.55
1:C:84:SER:O	1:C:85:ALA:C	2.49	0.55
1:B:354:ARG:NH2	5:B:1007:HOH:O	2.22	0.55
1:B:605:PRO:HB2	5:B:935:HOH:O	2.05	0.55
1:D:468:ARG:NH1	1:D:471:ASN:HD22	1.97	0.55
1:A:305:ARG:HD3	5:A:891:HOH:O	2.05	0.55
1:B:439:ILE:HD13	1:C:465:TYR:HD1	1.72	0.55
1:C:409:LYS:HD3	5:C:1017:HOH:O	2.06	0.55
1:B:430:ASP:OD1	1:B:433:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ILE:HG22	1:A:155:PHE:HB2	1.89	0.54
2:A:680:DND:H10	2:A:680:DND:C3D	2.38	0.54
1:D:604:PHE:O	1:D:609:ARG:NH1	2.38	0.54
1:B:499:MET:HE3	1:C:499:MET:HE3	1.89	0.54
1:C:191:LEU:HD11	1:C:292:ASN:ND2	2.23	0.54
1:A:567:GLN:HA	1:A:567:GLN:NE2	2.14	0.54
1:A:658:ARG:NH1	5:A:982:HOH:O	2.14	0.54
1:B:491:SER:HB2	1:B:497:ASP:OD2	2.08	0.54
1:A:490:TRP:CZ2	1:A:559:ALA:HA	2.43	0.54
1:C:14:VAL:HG12	1:C:250:ILE:HD13	1.89	0.54
1:A:561:VAL:HG13	5:A:844:HOH:O	2.07	0.54
1:C:347:GLN:OE1	1:C:375:HIS:HE1	1.91	0.54
1:C:530:VAL:HG23	5:C:897:HOH:O	2.07	0.54
1:B:452:VAL:HA	1:B:453:THR:CB	2.37	0.53
1:C:23:ILE:HD12	5:C:960:HOH:O	2.05	0.53
1:B:133:ARG:HD2	5:B:1035:HOH:O	2.08	0.53
1:B:644:LYS:HE3	1:B:649:GLY:HA2	1.90	0.53
1:C:78:LEU:HD21	1:C:149:GLY:HA3	1.90	0.53
1:C:351:LEU:HD22	1:C:355:LEU:HG	1.89	0.53
1:A:310:LEU:HD13	1:A:312:PRO:HB3	1.91	0.53
1:A:492:THR:OG1	2:A:680:DND:H11	2.08	0.53
1:D:413:ILE:CD1	1:D:417:ARG:HE	2.21	0.53
1:A:284:LEU:HD21	1:B:103:ILE:HG23	1.90	0.53
1:B:223:ARG:NH1	5:B:864:HOH:O	2.36	0.53
1:B:560:LYS:HB2	5:B:926:HOH:O	2.09	0.53
1:C:337:GLN:NE2	1:C:519:TRP:HE1	2.06	0.53
1:B:200:LEU:HD23	1:B:200:LEU:H	1.73	0.53
1:A:632:SER:OG	1:A:636:ARG:NH2	2.42	0.53
1:C:252:GLU:HB2	1:C:257:LEU:CD2	2.39	0.53
1:D:210:ALA:HA	1:D:213:ARG:HD2	1.90	0.53
1:C:191:LEU:O	1:D:101:HIS:HE1	1.92	0.52
1:C:675:GLU:HG3	5:C:908:HOH:O	2.09	0.52
1:A:334:GLN:HB2	5:A:1038:HOH:O	2.09	0.52
1:A:439:ILE:CD1	1:D:465:TYR:CD1	2.93	0.52
1:B:120:PRO:HB2	1:B:139:GLY:HA3	1.91	0.52
1:B:167:PRO:HA	5:B:836:HOH:O	2.10	0.52
1:D:482:ASP:HB2	1:D:508:VAL:O	2.10	0.52
1:D:13:ARG:HB3	1:D:45:ALA:HA	1.91	0.52
1:D:22:THR:H	1:D:29:ASN:ND2	2.06	0.52
1:B:146:ILE:HG22	1:B:155:PHE:HB2	1.90	0.52
1:A:73:VAL:HG11	1:A:96:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:597:ARG:CG	1:C:597:ARG:NH1	2.71	0.52
1:A:86:ASP:HB2	5:A:1057:HOH:O	2.09	0.52
3:A:800:ONL:CB	5:A:1020:HOH:O	2.57	0.52
1:C:108:VAL:HG12	5:C:983:HOH:O	2.08	0.52
1:A:319:LEU:HD13	1:A:321:ARG:HB3	1.91	0.51
1:A:482:ASP:HA	1:A:505:ASN:O	2.09	0.51
1:D:559:ALA:O	1:D:560:LYS:HD2	2.10	0.51
1:A:99:HIS:HD2	5:A:813:HOH:O	1.92	0.51
1:C:204:PRO:CG	1:C:244:TRP:CZ3	2.92	0.51
1:A:181:VAL:O	1:A:182:PRO:C	2.53	0.51
1:B:468:ARG:HH11	1:B:471:ASN:HD22	1.56	0.51
1:B:632:SER:OG	1:B:636:ARG:NH2	2.43	0.51
1:C:102:ARG:NH2	5:C:710:HOH:O	2.43	0.51
1:D:69:LEU:C	1:D:69:LEU:CD1	2.79	0.51
1:D:69:LEU:HD12	5:D:726:HOH:O	2.10	0.51
1:D:116:LEU:HB3	1:D:161:PHE:CE1	2.46	0.51
1:C:224:CYS:HB2	5:C:966:HOH:O	2.09	0.51
1:D:98:ARG:NH2	5:D:794:HOH:O	2.38	0.51
1:B:310:LEU:HB3	1:B:312:PRO:HD3	1.93	0.51
1:C:170:VAL:HB	1:C:194:ALA:HA	1.93	0.51
1:C:170:VAL:HG21	1:C:193:GLY:O	2.11	0.51
1:D:146:ILE:CG2	1:D:155:PHE:HB2	2.34	0.51
4:D:682:GOL:H11	5:D:1005:HOH:O	2.10	0.51
1:A:177:GLU:OE1	3:A:800:ONL:HA	2.11	0.51
1:A:452:VAL:HG23	5:A:1043:HOH:O	2.11	0.51
1:B:495:VAL:O	1:C:468:ARG:NH2	2.43	0.51
1:A:451:ASP:O	1:A:453:THR:HG22	2.11	0.51
1:C:204:PRO:HB2	5:C:869:HOH:O	2.11	0.51
1:A:132:GLU:CB	5:A:1066:HOH:O	2.52	0.51
5:C:696:HOH:O	1:D:101:HIS:HD2	1.94	0.51
1:B:525:GLU:HB2	5:B:737:HOH:O	2.11	0.50
1:B:99:HIS:CD2	4:B:682:GOL:H2	2.46	0.50
1:C:126:THR:O	4:C:683:GOL:H12	2.09	0.50
1:C:497:ASP:OD1	2:C:680:DND:H11	2.11	0.50
3:A:803:ONL:HG1	5:A:1019:HOH:O	2.11	0.50
1:D:128:ARG:HD3	5:D:854:HOH:O	2.11	0.50
1:D:360:TYR:CG	1:D:389:ARG:HD2	2.46	0.50
1:D:349:SER:HA	1:D:352:GLU:OE2	2.11	0.50
1:A:225:LEU:HD22	1:A:289:PHE:CD2	2.47	0.50
1:A:399:LEU:HD11	1:A:466:LEU:HD21	1.93	0.50
1:B:21:THR:O	1:B:236:GLY:HA3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:PRO:HB2	5:C:800:HOH:O	2.12	0.50
1:C:401:GLY:O	1:C:402:PHE:C	2.55	0.50
1:D:180:PHE:N	5:D:954:HOH:O	2.44	0.50
1:C:409:LYS:HE2	5:C:776:HOH:O	2.11	0.50
1:C:493:TYR:HB2	1:C:635:LYS:HG2	1.93	0.50
1:D:319:LEU:HD13	1:D:321:ARG:HB3	1.92	0.50
1:D:413:ILE:HG12	1:D:423:PHE:CE2	2.47	0.50
3:A:801[A]:ONL:HB1	1:B:209:ARG:HD3	1.94	0.50
1:C:328:PHE:CG	1:C:509:PRO:HG3	2.46	0.50
1:A:296:HIS:O	1:A:300:THR:HG23	2.12	0.49
1:C:166:LEU:HD22	1:C:169:PHE:HB2	1.93	0.49
1:D:614:LEU:HD21	1:D:677:PRO:HD2	1.93	0.49
1:C:525:GLU:CD	1:C:525:GLU:H	2.20	0.49
1:C:179:MET:HG3	1:C:228:TYR:OH	2.11	0.49
1:A:354:ARG:NH2	1:A:641:ASN:HD22	2.06	0.49
1:C:92:VAL:CG1	1:C:200:LEU:HD11	2.42	0.49
1:D:410:ASN:O	1:D:413:ILE:HG22	2.12	0.49
1:A:560:LYS:HB2	5:A:1007:HOH:O	2.13	0.49
1:B:492:THR:HB	1:B:496:GLY:HA3	1.93	0.49
1:B:492:THR:H	1:B:497:ASP:HB3	1.76	0.49
1:C:106:THR:HA	1:C:120:PRO:HA	1.95	0.49
1:A:170:VAL:HG12	1:A:194:ALA:HA	1.95	0.49
1:B:180:PHE:N	5:B:859:HOH:O	2.46	0.49
1:B:348:VAL:HG21	1:B:382:HIS:HD2	1.77	0.49
1:A:363:VAL:CG1	1:A:478:LEU:HG	2.41	0.49
1:A:469:ILE:HG23	1:A:473:ARG:HD2	1.93	0.49
1:C:337:GLN:NE2	5:C:852:HOH:O	2.35	0.49
1:D:295:HIS:CE1	5:D:887:HOH:O	2.66	0.49
1:C:154:ALA:HB1	1:C:159:LEU:HD21	1.95	0.48
1:C:468:ARG:HA	1:C:468:ARG:HD3	1.57	0.48
1:D:62:ASP:OD1	1:D:134:ARG:HD3	2.12	0.48
1:D:497:ASP:OD2	2:D:680:DND:H11	2.12	0.48
1:A:13:ARG:HB3	1:A:45:ALA:HA	1.95	0.48
1:B:14:VAL:HG12	1:B:250:ILE:HD13	1.95	0.48
1:C:636:ARG:HA	1:C:639:LEU:HD13	1.96	0.48
1:B:69:LEU:C	1:B:69:LEU:HD13	2.38	0.48
1:C:204:PRO:CB	5:C:869:HOH:O	2.60	0.48
1:C:305:ARG:HD2	5:C:885:HOH:O	2.13	0.48
1:C:658:ARG:NH2	5:D:855:HOH:O	2.45	0.48
1:A:439:ILE:CD1	1:D:465:TYR:HD1	2.25	0.48
1:C:326:PHE:HB2	1:C:329:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:PRO:HD2	1:C:426:ILE:O	2.13	0.48
1:B:204:PRO:O	1:B:209:ARG:HD2	2.13	0.48
1:C:73:VAL:HG21	5:C:743:HOH:O	2.13	0.48
1:C:390:PRO:O	1:C:393:ASP:HB2	2.13	0.48
1:D:496:GLY:O	1:D:498:GLN:N	2.46	0.48
1:A:210:ALA:HA	1:A:213:ARG:HD2	1.95	0.48
1:B:21:THR:HA	1:B:29:ASN:ND2	2.29	0.48
1:B:491:SER:CA	1:B:497:ASP:OD2	2.60	0.48
1:C:34:LEU:HD13	1:C:83:GLU:HB3	1.96	0.48
1:C:61:GLU:OE2	4:C:684:GOL:H31	2.13	0.48
1:D:180:PHE:HA	5:D:874:HOH:O	2.13	0.48
1:C:204:PRO:HD2	5:C:869:HOH:O	2.12	0.48
1:A:51:PRO:O	1:A:54:THR:OG1	2.32	0.48
1:A:214:ARG:NH1	1:A:259:GLU:OE2	2.47	0.47
1:B:22:THR:N	1:B:29:ASN:HD21	2.07	0.47
1:C:13:ARG:HB3	1:C:45:ALA:HA	1.95	0.47
1:C:221:SER:HB3	1:C:228:TYR:HB2	1.95	0.47
1:C:658:ARG:HH21	1:D:61:GLU:CD	2.22	0.47
1:D:632:SER:OG	1:D:636:ARG:NH2	2.47	0.47
1:A:353:GLN:NE2	1:A:356:ARG:HH21	2.05	0.47
1:B:465:TYR:CD1	1:C:439:ILE:HD11	2.46	0.47
1:C:353:GLN:HE21	1:C:356:ARG:NH2	2.11	0.47
1:D:310:LEU:HD13	1:D:312:PRO:HB3	1.96	0.47
1:D:13:ARG:CZ	1:D:320:LEU:HD22	2.44	0.47
1:A:43:ASP:OD2	1:A:269:ARG:NH2	2.47	0.47
1:B:178:ASP:C	5:B:859:HOH:O	2.57	0.47
1:D:231:ALA:O	5:D:851:HOH:O	2.20	0.47
1:A:21:THR:O	1:A:236:GLY:HA3	2.15	0.47
1:A:490:TRP:NE1	2:A:680:DND:H13	2.30	0.47
1:B:468:ARG:HA	1:B:468:ARG:HD3	1.55	0.47
1:C:221:SER:HB2	1:C:226:ALA:O	2.15	0.47
1:C:326:PHE:HB3	1:C:329:VAL:HB	1.97	0.47
1:C:123:TYR:CZ	5:C:901:HOH:O	2.58	0.47
1:C:154:ALA:HB1	1:C:159:LEU:CD2	2.45	0.47
1:C:337:GLN:HE21	1:C:519:TRP:HE1	1.62	0.47
1:B:589:TRP:O	1:B:593:ASN:HB3	2.15	0.47
1:A:636:ARG:HD3	1:A:651:LEU:HB3	1.96	0.46
1:B:133:ARG:HH22	4:D:682:GOL:H2	1.80	0.46
1:B:214:ARG:HG3	1:B:214:ARG:HH11	1.80	0.46
1:C:122:SER:HB3	1:C:123:TYR:CD2	2.50	0.46
1:D:200:LEU:HA	5:D:851:HOH:O	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ARG:CD	1:C:137:ALA:HB2	2.41	0.46
1:D:326:PHE:CB	1:D:329:VAL:HB	2.45	0.46
1:A:453:THR:HG23	1:A:454:PHE:H	1.81	0.46
1:B:360:TYR:HB3	1:B:389:ARG:HD2	1.98	0.46
1:C:218:ARG:HD2	1:C:251:TRP:CH2	2.50	0.46
1:D:353:GLN:NE2	1:D:356:ARG:HH21	2.11	0.46
1:A:13:ARG:CZ	1:A:320:LEU:HD22	2.46	0.46
1:A:613:SER:O	1:A:617:ILE:HG12	2.15	0.46
3:A:803:ONL:OD	1:D:177:GLU:HB2	2.15	0.46
1:B:600:TRP:CD2	1:B:609:ARG:HG2	2.50	0.46
1:C:98:ARG:HD2	5:C:789:HOH:O	2.16	0.46
1:D:237:GLU:HB2	1:D:244:TRP:CD1	2.51	0.46
3:A:802:ONL:HG2	1:C:130:PHE:CZ	2.51	0.46
1:C:23:ILE:CG1	5:C:960:HOH:O	2.55	0.46
1:C:329:VAL:CG2	1:C:511:THR:HG23	2.46	0.46
1:B:180:PHE:CD2	1:B:216:LEU:HD12	2.50	0.46
1:B:678:LYS:HA	1:B:678:LYS:HD2	1.83	0.46
1:C:8:GLN:HB3	5:C:1044:HOH:O	2.15	0.46
1:C:133:ARG:HD2	1:C:133:ARG:HA	1.63	0.46
1:D:530:VAL:HG23	5:D:720:HOH:O	2.15	0.46
1:C:147:ARG:HA	1:C:151:ALA:O	2.16	0.46
1:C:509:PRO:HB2	1:C:568:ASP:OD2	2.15	0.46
1:D:301:GLU:HG3	5:D:747:HOH:O	2.16	0.46
1:C:148:ILE:O	1:C:149:GLY:C	2.58	0.45
1:C:502:TYR:CZ	1:C:642:GLY:HA2	2.51	0.45
1:D:131:TYR:HB2	5:D:855:HOH:O	2.15	0.45
1:B:336:LEU:HD23	1:B:602:PRO:HG2	1.99	0.45
1:B:53:LEU:HD21	1:B:136:MET:HE1	1.99	0.45
1:B:140:ASP:HB2	5:D:887:HOH:O	2.16	0.45
1:C:604:PHE:O	1:C:609:ARG:HD2	2.16	0.45
1:D:604:PHE:O	1:D:609:ARG:HD2	2.16	0.45
1:A:34:LEU:O	1:A:38:ARG:HG3	2.15	0.45
1:A:328:PHE:CG	1:A:509:PRO:HG3	2.51	0.45
1:A:378:ILE:HG23	1:A:526:PHE:CE2	2.51	0.45
1:C:205:ILE:HD12	1:C:209:ARG:HB3	1.98	0.45
1:D:136:MET:HE3	1:D:136:MET:HB2	1.84	0.45
1:D:442:PRO:HB2	1:D:447:GLU:HB2	1.98	0.45
1:A:311:ASP:HB2	5:A:902:HOH:O	2.15	0.45
1:C:204:PRO:CD	5:C:869:HOH:O	2.60	0.45
1:D:133:ARG:HD2	1:D:133:ARG:HA	1.78	0.45
2:D:680:DND:H21	5:D:845:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ARG:HA	1:D:151:ALA:O	2.17	0.45
1:D:514:GLN:NE2	1:D:518:ARG:HH12	2.12	0.45
1:D:433:ARG:HB3	4:D:683:GOL:C1	2.47	0.45
1:D:523:ALA:HB3	5:D:703:HOH:O	2.16	0.45
1:A:98:ARG:NH1	5:A:967:HOH:O	2.38	0.45
1:A:130:PHE:CZ	3:A:800:ONL:HG2	2.52	0.45
1:C:63:VAL:HG12	1:C:63:VAL:O	2.17	0.45
1:D:180:PHE:CD2	1:D:216:LEU:HD12	2.53	0.45
1:A:465:TYR:CE1	1:D:435:MET:HG3	2.51	0.44
1:B:50:PHE:HB3	1:B:51:PRO:CD	2.48	0.44
1:B:328:PHE:CD2	1:B:509:PRO:HG3	2.53	0.44
1:B:354:ARG:HD3	1:B:354:ARG:HA	1.69	0.44
1:C:179:MET:O	1:C:179:MET:HG2	2.17	0.44
1:D:332:ASP:OD2	1:D:334:GLN:HG2	2.16	0.44
1:D:79:ASP:O	1:D:83:GLU:HG2	2.17	0.44
1:D:237:GLU:HB3	1:D:244:TRP:CE2	2.53	0.44
1:A:191:LEU:HD11	1:A:292:ASN:ND2	2.33	0.44
1:C:183[B]:MET:HB2	5:C:800:HOH:O	2.16	0.44
1:D:92:VAL:CG1	1:D:200:LEU:HD11	2.47	0.44
1:D:178:ASP:O	1:D:185:PRO:HD2	2.18	0.44
1:D:410:ASN:HB3	1:D:414:LYS:HD2	2.00	0.44
1:B:19:HIS:HB2	1:B:32:SER:OG	2.17	0.44
1:B:133:ARG:HH22	4:D:682:GOL:C2	2.31	0.44
1:C:22:THR:H	1:C:29:ASN:ND2	2.16	0.44
1:C:22:THR:H	1:C:29:ASN:HD21	1.66	0.44
1:C:468:ARG:NH1	1:C:471:ASN:HD22	2.11	0.44
1:C:516:LEU:O	1:C:520:VAL:HG23	2.16	0.44
1:D:600:TRP:CE2	1:D:609:ARG:HG2	2.53	0.44
4:D:682:GOL:C1	5:D:1005:HOH:O	2.65	0.44
1:C:399:LEU:HA	1:C:426:ILE:O	2.18	0.44
1:D:181:VAL:CG2	5:D:954:HOH:O	2.31	0.44
1:D:347:GLN:OE1	1:D:375:HIS:HE1	2.01	0.44
1:B:606:LYS:HA	1:B:609:ARG:HD3	2.00	0.44
1:C:252:GLU:HB2	1:C:257:LEU:HD21	1.98	0.44
1:A:265:LYS:HD3	1:A:265:LYS:HA	1.88	0.44
1:B:514:GLN:HG3	1:B:518:ARG:HH12	1.81	0.44
1:C:223:ARG:HA	5:C:1023:HOH:O	2.18	0.44
1:C:518:ARG:NH1	1:C:603:GLY:HA3	2.32	0.44
1:C:632:SER:OG	1:C:636:ARG:NH2	2.51	0.44
1:B:13:ARG:HB3	1:B:45:ALA:HA	1.99	0.44
1:C:494:GLY:H	1:C:498:GLN:HE21	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:468:ARG:HH12	1:D:471:ASN:HD21	1.65	0.44
1:C:84:SER:C	1:C:86:ASP:N	2.76	0.44
1:C:115:VAL:HG12	1:C:117:GLY:H	1.83	0.44
1:C:182:PRO:C	1:C:184:PRO:HD3	2.43	0.43
1:D:182:PRO:C	1:D:184:PRO:HD3	2.43	0.43
1:D:325:ARG:HB3	1:D:592:TRP:CZ2	2.52	0.43
1:B:453:THR:HG23	1:B:454:PHE:N	2.27	0.43
1:C:111:HIS:CE1	1:C:112:ARG:HG3	2.53	0.43
1:C:121:LYS:HE2	1:C:123:TYR:O	2.18	0.43
1:A:670:ASP:HB2	5:A:1008:HOH:O	2.18	0.43
1:B:354:ARG:NE	5:B:1007:HOH:O	2.42	0.43
1:B:370:GLY:HA3	5:B:1049:HOH:O	2.19	0.43
1:B:582:SER:HB2	1:B:671:GLN:HE22	1.83	0.43
1:C:22:THR:N	1:C:29:ASN:HD21	2.16	0.43
1:D:211:GLU:HG3	5:D:956:HOH:O	2.17	0.43
1:A:280:ARG:HD3	5:A:821:HOH:O	2.18	0.43
1:B:419:LEU:HD13	1:B:530:VAL:HG21	1.99	0.43
1:C:125:PRO:HD2	1:C:132:GLU:CD	2.42	0.43
1:D:566:LEU:HD12	1:D:566:LEU:HA	1.77	0.43
1:B:7:TYR:CE2	1:B:313:PRO:HD2	2.54	0.43
1:B:567:GLN:NE2	1:B:620:TRP:O	2.51	0.43
1:C:448:LYS:HB3	1:C:450:TYR:CZ	2.54	0.43
1:A:15:ALA:HA	1:A:270:SER:O	2.18	0.43
1:A:294:ARG:HH11	4:D:682:GOL:H11	1.83	0.43
1:A:298:GLU:CB	5:A:1137:HOH:O	2.66	0.43
1:C:386:ARG:NH1	5:C:761:HOH:O	2.50	0.43
1:C:511:THR:HG21	5:C:687:HOH:O	2.19	0.43
1:B:1:MET:HB2	1:B:675:GLU:OE1	2.18	0.43
1:B:452:VAL:HA	1:B:453:THR:HG22	2.01	0.43
1:C:6:ALA:O	1:C:11:PHE:HB2	2.18	0.43
1:D:170:VAL:HG12	1:D:194:ALA:HA	2.00	0.43
1:D:239:THR:HA	1:D:242:LEU:O	2.19	0.43
1:B:637:SER:O	1:C:654:ARG:NH1	2.50	0.43
1:C:285:ARG:HE	4:C:681:GOL:C3	2.29	0.43
1:A:439:ILE:HG13	1:D:469:ILE:HD13	2.01	0.43
1:A:518:ARG:CZ	5:A:1059:HOH:O	2.66	0.43
1:B:219:SER:HB2	5:B:864:HOH:O	2.18	0.43
1:B:368:SER:HB3	4:B:681:GOL:H12	2.01	0.43
1:C:125:PRO:HA	4:C:683:GOL:O2	2.19	0.43
1:C:336:LEU:HD22	1:C:602:PRO:HD2	2.01	0.43
1:D:23:ILE:HB	1:D:60:ILE:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:ARG:HD2	5:D:713:HOH:O	2.19	0.42
1:A:453:THR:HG23	1:A:454:PHE:N	2.34	0.42
1:B:214:ARG:HH11	1:B:214:ARG:CG	2.32	0.42
1:C:636:ARG:HD3	1:C:651:LEU:HB3	2.01	0.42
1:A:468:ARG:HA	1:A:468:ARG:HD3	1.60	0.42
1:B:439:ILE:HD12	1:B:439:ILE:HA	1.89	0.42
1:B:613:SER:HB2	5:B:827:HOH:O	2.18	0.42
1:C:26:PRO:HD2	5:C:844:HOH:O	2.18	0.42
1:C:79:ASP:O	1:C:83:GLU:HG2	2.19	0.42
1:D:125:PRO:HD2	1:D:132:GLU:OE1	2.18	0.42
1:B:1:MET:CE	5:B:932:HOH:O	2.67	0.42
1:B:191:LEU:HD21	1:B:292:ASN:HD22	1.83	0.42
1:B:343:ALA:HB2	1:D:207:ILE:HD11	2.01	0.42
1:B:560:LYS:HB3	1:B:560:LYS:NZ	2.35	0.42
1:C:23:ILE:HB	1:C:60:ILE:CG2	2.49	0.42
1:C:468:ARG:HH11	1:C:471:ASN:ND2	2.13	0.42
1:D:88:LEU:HD21	1:D:313:PRO:HD3	2.01	0.42
1:B:469:ILE:HG23	1:B:473:ARG:HD3	2.02	0.42
1:C:26:PRO:HA	1:C:55:LEU:O	2.20	0.42
1:C:468:ARG:HH11	1:C:471:ASN:HD22	1.67	0.42
1:C:491:SER:OG	1:C:498:GLN:HB2	2.19	0.42
1:D:51:PRO:O	1:D:54:THR:OG1	2.33	0.42
1:B:21:THR:HA	1:B:29:ASN:HD21	1.85	0.42
1:B:99:HIS:HD2	4:B:682:GOL:H2	1.83	0.42
1:C:96:PRO:HA	5:C:822:HOH:O	2.20	0.42
1:C:136:MET:HE3	1:C:136:MET:HB2	1.49	0.42
1:D:468:ARG:HA	1:D:468:ARG:HD3	1.75	0.42
1:A:617:ILE:O	1:A:621:LEU:HB2	2.20	0.42
1:B:452:VAL:HA	1:B:453:THR:CG2	2.49	0.42
1:B:454:PHE:O	1:B:458:GLN:HG3	2.19	0.42
1:C:252:GLU:HB2	1:C:257:LEU:HD22	2.02	0.42
1:D:70:LEU:CD2	5:D:726:HOH:O	2.68	0.42
1:D:528:GLU:N	1:D:528:GLU:CD	2.78	0.42
1:A:510:LYS:HA	1:A:513:ILE:HD12	2.00	0.42
1:B:439:ILE:HD13	1:C:465:TYR:CE1	2.55	0.42
1:C:179:MET:HE1	1:C:230:TYR:CD2	2.55	0.42
1:D:50:PHE:HB3	1:D:51:PRO:CD	2.50	0.42
1:D:67:ASP:CG	5:D:696:HOH:O	2.63	0.42
1:D:222:ALA:O	1:D:225:LEU:HD12	2.19	0.42
1:B:387:GLU:OE2	1:D:265:LYS:NZ	2.53	0.42
1:B:647:HIS:CE1	5:B:973:HOH:O	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:THR:C	4:C:683:GOL:H11	2.45	0.42
1:C:310:LEU:HD13	1:C:312:PRO:HB3	2.02	0.42
1:D:92:VAL:HG12	1:D:200:LEU:HD11	2.01	0.42
1:D:142:GLU:C	1:D:143:ARG:HG2	2.44	0.42
1:A:52:GLU:OE2	1:A:105:ASN:ND2	2.50	0.41
1:A:294:ARG:NH2	1:B:140:ASP:O	2.53	0.41
1:B:84:SER:HA	1:B:87:LEU:HB2	2.01	0.41
1:A:497:ASP:CG	2:A:680:DND:H12	2.45	0.41
1:A:561:VAL:HG12	5:A:921:HOH:O	2.20	0.41
3:A:800:ONL:HB2	5:A:1020:HOH:O	2.18	0.41
1:B:439:ILE:CD1	1:C:465:TYR:HD1	2.32	0.41
1:C:488:LEU:HD11	1:C:567:GLN:HG3	2.01	0.41
1:D:310:LEU:HD22	1:D:310:LEU:O	2.20	0.41
1:D:567:GLN:HE22	1:D:624:PHE:HB2	1.85	0.41
1:B:292:ASN:HD21	1:D:183:MET:N	2.14	0.41
1:B:491:SER:CB	1:B:497:ASP:OD2	2.68	0.41
1:B:514:GLN:HE21	1:B:518:ARG:HH12	1.67	0.41
1:D:452:VAL:HG23	5:D:776:HOH:O	2.19	0.41
1:A:494:GLY:H	1:A:498:GLN:HE21	1.66	0.41
1:A:606:LYS:HA	1:A:609:ARG:HD3	2.03	0.41
1:D:675:GLU:OE1	1:D:675:GLU:HA	2.19	0.41
1:C:27:ALA:HB2	4:C:682:GOL:C1	2.49	0.41
1:C:92:VAL:HG12	1:C:200:LEU:HD21	2.03	0.41
1:C:55:LEU:HD12	1:C:55:LEU:HA	1.74	0.41
1:C:468:ARG:NH1	1:C:471:ASN:HD21	2.14	0.41
1:B:516:LEU:O	1:B:520:VAL:HG23	2.19	0.41
1:C:293:ARG:NE	1:D:100:ARG:HE	2.18	0.41
1:C:565:ALA:HB1	1:C:592:TRP:CZ2	2.56	0.41
1:D:147:ARG:NE	1:D:150:GLY:HA2	2.25	0.41
1:D:363:VAL:CG1	1:D:478:LEU:HD21	2.45	0.41
1:A:439:ILE:HD11	1:D:465:TYR:CD1	2.50	0.41
1:B:214:ARG:HG3	5:B:851:HOH:O	2.20	0.41
1:B:566:LEU:HA	1:B:566:LEU:HD12	1.57	0.41
1:C:510:LYS:HD3	1:C:564:PHE:CE2	2.56	0.41
1:D:468:ARG:HH12	1:D:471:ASN:ND2	2.12	0.41
1:A:569:PHE:O	1:A:573:GLN:HG2	2.21	0.41
1:A:600:TRP:CD2	1:A:609:ARG:HG2	2.55	0.41
5:A:852:HOH:O	1:B:101:HIS:CD2	2.61	0.41
1:B:143:ARG:HB3	1:B:144:GLY:H	1.78	0.41
1:B:362:LYS:O	1:B:475:GLY:HA2	2.21	0.41
1:B:439:ILE:HD11	1:C:469:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:GLU:CG	5:B:775:HOH:O	2.65	0.41
1:C:108:VAL:C	5:C:983:HOH:O	2.63	0.41
1:C:183[B]:MET:HE3	1:C:183[B]:MET:HB2	1.58	0.41
1:C:224:CYS:SG	5:C:826:HOH:O	2.31	0.41
1:D:433:ARG:HB3	4:D:683:GOL:H12	2.02	0.41
1:A:429:GLY:O	1:A:433:ARG:HG3	2.21	0.41
1:B:84:SER:HA	1:B:87:LEU:HD22	2.02	0.41
1:D:294:ARG:HH11	4:D:682:GOL:H12	1.86	0.41
1:A:176:CYS:HB3	1:A:177:GLU:H	1.64	0.40
1:B:146:ILE:CG2	1:B:155:PHE:HB2	2.51	0.40
1:C:140:ASP:HB3	5:C:901:HOH:O	2.21	0.40
1:C:191:LEU:O	1:D:101:HIS:CE1	2.72	0.40
1:C:224:CYS:O	1:C:225:LEU:C	2.65	0.40
1:D:99:HIS:HE1	5:D:750:HOH:O	2.04	0.40
1:D:486:LEU:HD12	5:D:975:HOH:O	2.19	0.40
1:D:567:GLN:HE21	1:D:567:GLN:CA	2.22	0.40
1:A:134:ARG:HD3	1:A:135:GLN:NE2	2.36	0.40
3:A:801[A]:ONL:CE	1:B:203:SER:HB2	2.51	0.40
1:C:96:PRO:CA	5:C:822:HOH:O	2.69	0.40
1:D:326:PHE:HB3	1:D:329:VAL:HB	2.03	0.40
1:B:328:PHE:CG	1:B:509:PRO:HG3	2.56	0.40
1:B:351:LEU:HD22	1:B:355:LEU:HG	2.03	0.40
1:D:351:LEU:HD22	1:D:355:LEU:HG	2.03	0.40
1:D:606:LYS:HA	1:D:609:ARG:HD3	2.03	0.40
1:A:389:ARG:HD3	5:A:1046:HOH:O	2.22	0.40
1:C:353:GLN:NE2	1:C:356:ARG:HH21	2.15	0.40
1:D:8:GLN:HB3	5:D:966:HOH:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ARG:NE	5:A:809:HOH:O[8_665]	1.91	0.29
5:A:815:HOH:O	5:B:796:HOH:O[8_665]	2.11	0.09

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	644/680 (95%)	615 (96%)	28 (4%)	1 (0%)	43	52
1	B	641/680 (94%)	613 (96%)	24 (4%)	4 (1%)	21	24
1	C	653/680 (96%)	619 (95%)	27 (4%)	7 (1%)	11	11
1	D	651/680 (96%)	622 (96%)	24 (4%)	5 (1%)	16	17
All	All	2589/2720 (95%)	2469 (95%)	103 (4%)	17 (1%)	18	20

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	453	THR
1	B	497	ASP
1	B	176	CYS
1	C	128	ARG
1	C	176	CYS
1	D	176	CYS
1	D	497	ASP
1	D	608	GLU
1	C	85	ALA
1	A	176	CYS
1	B	678	LYS
1	C	120	PRO
1	C	149	GLY
1	C	54	THR
1	D	67	ASP
1	D	100	ARG
1	C	527	GLY

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	512/549 (93%)	472 (92%)	40 (8%)	11	12
1	B	515/549 (94%)	463 (90%)	52 (10%)	7	6
1	C	529/549 (96%)	474 (90%)	55 (10%)	7	6
1	D	527/549 (96%)	482 (92%)	45 (8%)	10	11
All	All	2083/2196 (95%)	1891 (91%)	192 (9%)	8	9

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	77	LEU
1	A	87	LEU
1	A	93	VAL
1	A	116	LEU
1	A	136	MET
1	A	148	ILE
1	A	160	LEU
1	A	200	LEU
1	A	206	THR
1	A	225	LEU
1	A	256	LEU
1	A	284	LEU
1	A	305	ARG
1	A	306	ILE
1	A	310	LEU
1	A	319	LEU
1	A	320	LEU
1	A	351	LEU
1	A	377	LEU
1	A	413	ILE
1	A	419	LEU
1	A	424	SER
1	A	426	ILE
1	A	439	ILE
1	A	478	LEU
1	A	480	THR
1	A	488	LEU

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Mol	Chain	Res	Type
1	A	491	SER
1	A	499	MET
1	A	513	ILE
1	A	516	LEU
1	A	533	VAL
1	A	538	LEU
1	A	560	LYS
1	A	561	VAL
1	A	566	LEU
1	A	567	GLN
1	A	621	LEU
1	A	667	ILE
1	B	14	VAL
1	B	21	THR
1	B	55	LEU
1	B	77	LEU
1	B	87	LEU
1	B	116	LEU
1	B	134	ARG
1	B	143	ARG
1	B	147	ARG
1	B	160	LEU
1	B	200	LEU
1	B	201	SER
1	B	206	THR
1	B	214	ARG
1	B	225	LEU
1	B	256	LEU
1	B	257	LEU
1	B	284	LEU
1	B	319	LEU
1	B	320	LEU
1	B	322	GLU
1	B	337	GLN
1	B	351	LEU
1	B	354	ARG
1	B	363	VAL
1	B	377	LEU
1	B	411	ASN
1	B	419	LEU
1	B	439	ILE
1	B	452	VAL

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Mol	Chain	Res	Type
1	B	454	PHE
1	B	468	ARG
1	B	473	ARG
1	B	478	LEU
1	B	495	VAL
1	B	498	GLN
1	B	499	MET
1	B	510	LYS
1	B	516	LEU
1	B	529	LYS
1	B	533	VAL
1	B	538	LEU
1	B	560	LYS
1	B	566	LEU
1	B	596	GLU
1	B	606	LYS
1	B	609	ARG
1	B	617	ILE
1	B	621	LEU
1	B	637	SER
1	B	671	GLN
1	B	678	LYS
1	C	14	VAL
1	C	23	ILE
1	C	55	LEU
1	C	77	LEU
1	C	82	THR
1	C	87	LEU
1	C	98	ARG
1	C	116	LEU
1	C	120	PRO
1	C	128	ARG
1	C	133	ARG
1	C	136	MET
1	C	143	ARG
1	C	147	ARG
1	C	160	LEU
1	C	170	VAL
1	C	179	MET
1	C	206	THR
1	C	216	LEU
1	C	225	LEU

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Mol	Chain	Res	Type
1	C	256	LEU
1	C	257	LEU
1	C	265	LYS
1	C	284	LEU
1	C	310	LEU
1	C	319	LEU
1	C	320	LEU
1	C	322	GLU
1	C	334	GLN
1	C	351	LEU
1	C	377	LEU
1	C	409	LYS
1	C	413	ILE
1	C	417	ARG
1	C	419	LEU
1	C	444	SER
1	C	473	ARG
1	C	478	LEU
1	C	498	GLN
1	C	511	THR
1	C	516	LEU
1	C	525	GLU
1	C	529	LYS
1	C	533	VAL
1	C	538	LEU
1	C	541	GLU
1	C	566	LEU
1	C	567	GLN
1	C	597	ARG
1	C	606	LYS
1	C	621	LEU
1	C	658	ARG
1	C	664	SER
1	C	671	GLN
1	C	673	ASP
1	D	55	LEU
1	D	68	SER
1	D	77	LEU
1	D	87	LEU
1	D	100	ARG
1	D	116	LEU
1	D	136	MET

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Mol	Chain	Res	Type
1	D	147	ARG
1	D	160	LEU
1	D	166	LEU
1	D	206	THR
1	D	256	LEU
1	D	257	LEU
1	D	284	LEU
1	D	299	LEU
1	D	310	LEU
1	D	319	LEU
1	D	320	LEU
1	D	334	GLN
1	D	351	LEU
1	D	354	ARG
1	D	377	LEU
1	D	413	ILE
1	D	419	LEU
1	D	461	LEU
1	D	473	ARG
1	D	478	LEU
1	D	480	THR
1	D	488	LEU
1	D	495	VAL
1	D	497	ASP
1	D	510	LYS
1	D	516	LEU
1	D	528	GLU
1	D	535	GLN
1	D	538	LEU
1	D	540	THR
1	D	560	LYS
1	D	566	LEU
1	D	567	GLN
1	D	596	GLU
1	D	607	SER
1	D	609	ARG
1	D	621	LEU
1	D	664	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	99	HIS
1	A	101	HIS
1	A	292	ASN
1	A	295	HIS
1	A	353	GLN
1	A	375	HIS
1	A	411	ASN
1	A	471	ASN
1	A	498	GLN
1	A	501	HIS
1	A	567	GLN
1	A	641	ASN
1	A	647	HIS
1	B	29	ASN
1	B	99	HIS
1	B	101	HIS
1	B	292	ASN
1	B	347	GLN
1	B	375	HIS
1	B	437	HIS
1	B	458	GLN
1	B	471	ASN
1	B	498	GLN
1	B	505	ASN
1	B	514	GLN
1	B	590	HIS
1	B	626	GLN
1	B	641	ASN
1	B	647	HIS
1	C	19	HIS
1	C	29	ASN
1	C	99	HIS
1	C	292	ASN
1	C	337	GLN
1	C	347	GLN
1	C	353	GLN
1	C	375	HIS
1	C	471	ASN
1	C	498	GLN
1	C	501	HIS
1	C	567	GLN
1	C	590	HIS

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Mol	Chain	Res	Type
1	C	599	ASN
1	C	641	ASN
1	D	19	HIS
1	D	29	ASN
1	D	101	HIS
1	D	353	GLN
1	D	375	HIS
1	D	471	ASN
1	D	498	GLN
1	D	501	HIS
1	D	514	GLN
1	D	535	GLN
1	D	567	GLN
1	D	590	HIS
1	D	619	HIS
1	D	626	GLN
1	D	641	ASN
1	D	647	HIS

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](#)

24 ligands are 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	$\# Z > 2$
3	ONL	A	802	1	8,9,9	0.84	0	8,11,11	1.34	2 (25%)
4	GOL	C	681	-	5,5,5	0.42	0	5,5,5	0.18	0
4	GOL	C	683	-	5,5,5	0.77	0	5,5,5	1.37	1 (20%)
2	DND	A	680	-	46,48,48	1.29	4 (8%)	64,73,73	1.63	10 (15%)
4	GOL	D	685	-	5,5,5	0.45	0	5,5,5	0.25	0
3	ONL	A	801[A]	1	8,9,9	0.83	0	8,11,11	1.47	2 (25%)
4	GOL	D	682	-	5,5,5	0.41	0	5,5,5	0.68	0
3	ONL	A	801[B]	1	8,9,9	0.77	1 (12%)	8,11,11	1.66	3 (37%)
3	ONL	A	800	1	8,9,9	0.70	0	8,11,11	1.40	2 (25%)
4	GOL	B	684	-	5,5,5	0.51	0	5,5,5	0.63	0
4	GOL	D	681	-	5,5,5	0.48	0	5,5,5	0.23	0
2	DND	C	680	-	46,48,48	1.21	4 (8%)	64,73,73	1.69	10 (15%)
4	GOL	B	683	-	5,5,5	0.59	0	5,5,5	1.04	0
4	GOL	A	804	-	5,5,5	0.44	0	5,5,5	0.36	0
3	ONL	A	803	1	8,9,9	0.72	0	8,11,11	1.18	1 (12%)
4	GOL	D	683	-	5,5,5	0.39	0	5,5,5	0.78	0
2	DND	D	680	-	46,48,48	0.97	1 (2%)	64,73,73	1.57	9 (14%)
4	GOL	A	805	-	5,5,5	0.49	0	5,5,5	1.00	0
4	GOL	C	684	-	5,5,5	0.53	0	5,5,5	0.79	0
4	GOL	D	684	-	5,5,5	0.48	0	5,5,5	0.32	0
4	GOL	B	682	-	5,5,5	0.54	0	5,5,5	0.32	0
4	GOL	B	681	-	5,5,5	0.40	0	5,5,5	0.66	0
4	GOL	C	682	-	5,5,5	0.41	0	5,5,5	0.55	0
2	DND	B	680	-	46,48,48	1.22	3 (6%)	64,73,73	1.76	11 (17%)

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
3	ONL	A	802	1	-	7/9/9/9	-
4	GOL	C	681	-	-	4/4/4/4	-
4	GOL	C	683	-	-	4/4/4/4	-
2	DND	A	680	-	-	15/30/62/62	0/5/5/5
4	GOL	D	685	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ONL	A	801[A]	1	-	6/9/9/9	-
4	GOL	D	682	-	-	4/4/4/4	-
3	ONL	A	801[B]	1	-	3/9/9/9	-
3	ONL	A	800	1	-	7/9/9/9	-
4	GOL	B	684	-	-	2/4/4/4	-
4	GOL	D	681	-	-	4/4/4/4	-
2	DND	C	680	-	-	10/30/62/62	0/5/5/5
4	GOL	B	683	-	-	2/4/4/4	-
4	GOL	A	804	-	-	4/4/4/4	-
3	ONL	A	803	1	-	5/9/9/9	-
4	GOL	D	683	-	-	2/4/4/4	-
2	DND	D	680	-	-	5/30/62/62	0/5/5/5
4	GOL	A	805	-	-	3/4/4/4	-
4	GOL	C	684	-	-	2/4/4/4	-
4	GOL	D	684	-	-	1/4/4/4	-
4	GOL	B	682	-	-	4/4/4/4	-
4	GOL	B	681	-	-	2/4/4/4	-
4	GOL	C	682	-	-	2/4/4/4	-
2	DND	B	680	-	-	19/30/62/62	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	680	DND	PA-O3P	4.54	1.64	1.59
2	A	680	DND	PN-O3P	4.42	1.64	1.59
2	A	680	DND	PA-O3P	4.12	1.63	1.59
2	C	680	DND	PN-O3P	3.67	1.63	1.59
2	C	680	DND	PA-O3P	3.60	1.63	1.59
2	A	680	DND	O4D-C1D	3.20	1.45	1.40
2	C	680	DND	O4D-C1D	3.06	1.44	1.40
2	D	680	DND	O4D-C1D	2.85	1.44	1.40
2	B	680	DND	PN-O3P	2.85	1.62	1.59
2	B	680	DND	O4D-C1D	2.79	1.44	1.40
2	C	680	DND	C8A-N7A	2.33	1.36	1.31
2	A	680	DND	C8A-N7A	2.22	1.36	1.31
3	A	801[B]	ONL	OXT-C	-2.08	1.24	1.30

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	680	DND	N1A-C2A-N3A	-6.30	119.05	128.58
2	A	680	DND	N1A-C2A-N3A	-5.97	119.55	128.58
2	C	680	DND	N1A-C2A-N3A	-5.89	119.67	128.58
2	D	680	DND	N1A-C2A-N3A	-5.68	119.98	128.58
2	B	680	DND	C5A-C4A-N3A	-5.63	118.96	126.72
2	C	680	DND	C5A-C4A-N3A	-5.33	119.38	126.72
2	D	680	DND	C5A-C4A-N3A	-5.07	119.74	126.72
2	A	680	DND	C5A-C4A-N3A	-4.60	120.38	126.72
2	B	680	DND	C2A-N3A-C4A	4.35	122.45	111.83
2	B	680	DND	N3A-C4A-N9A	4.03	134.03	127.17
2	C	680	DND	C2A-N3A-C4A	3.99	121.58	111.83
2	A	680	DND	C2A-N3A-C4A	3.91	121.38	111.83
2	A	680	DND	N9A-C8A-N7A	-3.66	108.74	113.94
2	D	680	DND	N3A-C4A-N9A	3.66	133.40	127.17
2	B	680	DND	N9A-C8A-N7A	-3.59	108.84	113.94
2	D	680	DND	C2A-N3A-C4A	3.59	120.61	111.83
2	C	680	DND	N3A-C4A-N9A	3.47	133.08	127.17
2	C	680	DND	N9A-C8A-N7A	-3.32	109.23	113.94
2	D	680	DND	N9A-C8A-N7A	-3.23	109.35	113.94
2	A	680	DND	C4A-N9A-C8A	3.17	109.07	105.74
2	A	680	DND	N3A-C4A-N9A	3.06	132.38	127.17
3	A	800	ONL	CB-CG-CD	-2.96	110.15	114.77
2	A	680	DND	C6N-N1N-C2N	-2.79	119.50	121.88
3	A	801[B]	ONL	CB-CG-CD	-2.79	110.42	114.77
2	B	680	DND	C4A-N9A-C8A	2.75	108.63	105.74
2	B	680	DND	C5A-N7A-C8A	2.73	107.74	103.45
2	C	680	DND	C4A-C5A-N7A	-2.71	107.48	110.58
2	A	680	DND	C4A-C5A-N7A	-2.66	107.54	110.58
3	A	801[A]	ONL	OXT-C-O	-2.60	118.18	124.08
2	C	680	DND	C4A-N9A-C8A	2.54	108.40	105.74
2	A	680	DND	C5A-N7A-C8A	2.52	107.41	103.45
4	C	683	GOL	O1-C1-C2	2.49	121.59	110.38
2	D	680	DND	C4A-N9A-C8A	2.47	108.34	105.74
2	C	680	DND	C5A-N7A-C8A	2.47	107.34	103.45
3	A	802	ONL	OXT-C-O	-2.47	118.47	124.08
2	B	680	DND	C4A-C5A-N7A	-2.45	107.78	110.58
3	A	802	ONL	CB-CG-CD	-2.43	110.98	114.77
2	B	680	DND	O14-PA-O3P	2.41	113.80	107.27
2	D	680	DND	C5A-N7A-C8A	2.40	107.22	103.45
3	A	803	ONL	OXT-C-O	-2.29	118.89	124.08
3	A	801[B]	ONL	OXT-C-O	-2.27	118.94	124.08
2	C	680	DND	C6N-N1N-C2N	-2.24	119.97	121.88
3	A	801[B]	ONL	CG-CB-CA	-2.21	108.79	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801[A]	ONL	CE-CD-CG	2.20	123.54	116.85
2	C	680	DND	O8N-C7N-C3N	2.17	120.40	114.84
3	A	800	ONL	OXT-C-O	-2.14	119.24	124.08
2	A	680	DND	C4A-N9A-C1B	-2.11	121.71	126.63
2	D	680	DND	O12-PN-O11	2.06	122.03	112.44
2	D	680	DND	C4A-C5A-N7A	-2.06	108.23	110.58
2	B	680	DND	O8N-C7N-C3N	2.01	120.01	114.84
2	B	680	DND	O3B-C3B-C4B	-2.00	105.33	111.08

There are no chirality outliers.

All (121) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	680	DND	O4D-C1D-N1N-C6N
2	A	680	DND	C4N-C3N-C7N-O7N
2	A	680	DND	C2N-C3N-C7N-O7N
2	B	680	DND	C5D-O5D-PN-O11
2	B	680	DND	C5D-O5D-PN-O3P
2	B	680	DND	O4D-C1D-N1N-C6N
2	B	680	DND	O4D-C1D-N1N-C2N
2	B	680	DND	C2D-C1D-N1N-C6N
2	B	680	DND	C2D-C1D-N1N-C2N
2	B	680	DND	C2N-C3N-C7N-O7N
2	B	680	DND	C2N-C3N-C7N-O8N
2	C	680	DND	PN-O3P-PA-O5B
2	C	680	DND	C2N-C3N-C7N-O7N
2	C	680	DND	C2N-C3N-C7N-O8N
3	A	801[A]	ONL	N-CA-CB-CG
3	A	801[A]	ONL	CE-CD-CG-CB
3	A	801[B]	ONL	C-CA-CB-CG
3	A	803	ONL	CA-CB-CG-CD
3	A	800	ONL	N-CA-CB-CG
4	A	804	GOL	C1-C2-C3-O3
4	A	805	GOL	O1-C1-C2-C3
4	B	682	GOL	C1-C2-C3-O3
4	B	683	GOL	C1-C2-C3-O3
4	B	683	GOL	O2-C2-C3-O3
4	B	684	GOL	O1-C1-C2-O2
4	B	684	GOL	O1-C1-C2-C3
4	C	682	GOL	C1-C2-C3-O3
4	C	683	GOL	C1-C2-C3-O3
4	C	684	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	D	682	GOL	O1-C1-C2-C3
4	D	682	GOL	C1-C2-C3-O3
4	D	683	GOL	O1-C1-C2-O2
4	D	683	GOL	O1-C1-C2-C3
4	D	685	GOL	O1-C1-C2-O2
4	D	685	GOL	O1-C1-C2-C3
4	D	685	GOL	C1-C2-C3-O3
2	A	680	DND	C4N-C3N-C7N-O8N
2	C	680	DND	C4N-C3N-C7N-O7N
2	C	680	DND	C4N-C3N-C7N-O8N
2	B	680	DND	C4N-C3N-C7N-O7N
2	B	680	DND	C4N-C3N-C7N-O8N
2	A	680	DND	C2N-C3N-C7N-O8N
3	A	801[B]	ONL	OXT-C-CA-N
3	A	802	ONL	OXT-C-CA-N
3	A	801[A]	ONL	OD-CD-CG-CB
4	B	682	GOL	O1-C1-C2-O2
4	D	685	GOL	O2-C2-C3-O3
2	C	680	DND	O4D-C4D-C5D-O5D
2	D	680	DND	O4D-C4D-C5D-O5D
3	A	800	ONL	OXT-C-CA-N
2	C	680	DND	C3D-C4D-C5D-O5D
3	A	800	ONL	CE-CD-CG-CB
4	A	804	GOL	O1-C1-C2-C3
4	B	681	GOL	O1-C1-C2-C3
4	B	682	GOL	O1-C1-C2-C3
4	C	681	GOL	O1-C1-C2-C3
4	C	681	GOL	C1-C2-C3-O3
4	C	683	GOL	O1-C1-C2-C3
4	D	681	GOL	O1-C1-C2-C3
4	D	681	GOL	C1-C2-C3-O3
4	A	805	GOL	O1-C1-C2-O2
4	B	682	GOL	O2-C2-C3-O3
4	C	681	GOL	O1-C1-C2-O2
4	C	682	GOL	O2-C2-C3-O3
4	C	684	GOL	O1-C1-C2-O2
4	D	682	GOL	O1-C1-C2-O2
4	D	682	GOL	O2-C2-C3-O3
2	D	680	DND	C3D-C4D-C5D-O5D
3	A	802	ONL	OD-CD-CG-CB
3	A	800	ONL	OD-CD-CG-CB
4	A	804	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	C	683	GOL	O1-C1-C2-O2
4	C	683	GOL	O2-C2-C3-O3
3	A	800	ONL	OXT-C-CA-CB
3	A	802	ONL	CE-CD-CG-CB
4	A	805	GOL	O2-C2-C3-O3
4	B	681	GOL	O2-C2-C3-O3
3	A	800	ONL	O-C-CA-CB
2	A	680	DND	O4D-C4D-C5D-O5D
3	A	800	ONL	O-C-CA-N
2	C	680	DND	C4B-C5B-O5B-PA
2	A	680	DND	C3D-C4D-C5D-O5D
4	D	684	GOL	O1-C1-C2-C3
3	A	801[A]	ONL	C-CA-CB-CG
2	B	680	DND	C3B-C4B-C5B-O5B
2	A	680	DND	C4B-C5B-O5B-PA
2	B	680	DND	C2B-C1B-N9A-C8A
2	A	680	DND	PA-O3P-PN-O11
3	A	801[A]	ONL	O-C-CA-CB
3	A	802	ONL	CA-CB-CG-CD
2	B	680	DND	C4D-C5D-O5D-PN
3	A	803	ONL	N-CA-CB-CG
3	A	801[A]	ONL	OXT-C-CA-CB
2	A	680	DND	C5B-O5B-PA-O13
2	B	680	DND	C5D-O5D-PN-O12
2	B	680	DND	C5B-O5B-PA-O13
2	D	680	DND	C5B-O5B-PA-O13
2	D	680	DND	C4B-C5B-O5B-PA
4	D	681	GOL	O2-C2-C3-O3
2	B	680	DND	C4B-C5B-O5B-PA
3	A	803	ONL	O-C-CA-N
2	A	680	DND	O4D-C1D-N1N-C2N
4	A	804	GOL	O1-C1-C2-O2
4	C	681	GOL	O2-C2-C3-O3
4	D	681	GOL	O1-C1-C2-O2
3	A	802	ONL	O-C-CA-CB
2	C	680	DND	C2B-C1B-N9A-C8A
3	A	803	ONL	C-CA-CB-CG
2	A	680	DND	PA-O3P-PN-O12
2	B	680	DND	PN-O3P-PA-O14
2	C	680	DND	PA-O3P-PN-O12
2	A	680	DND	C3B-C4B-C5B-O5B
3	A	802	ONL	OXT-C-CA-CB

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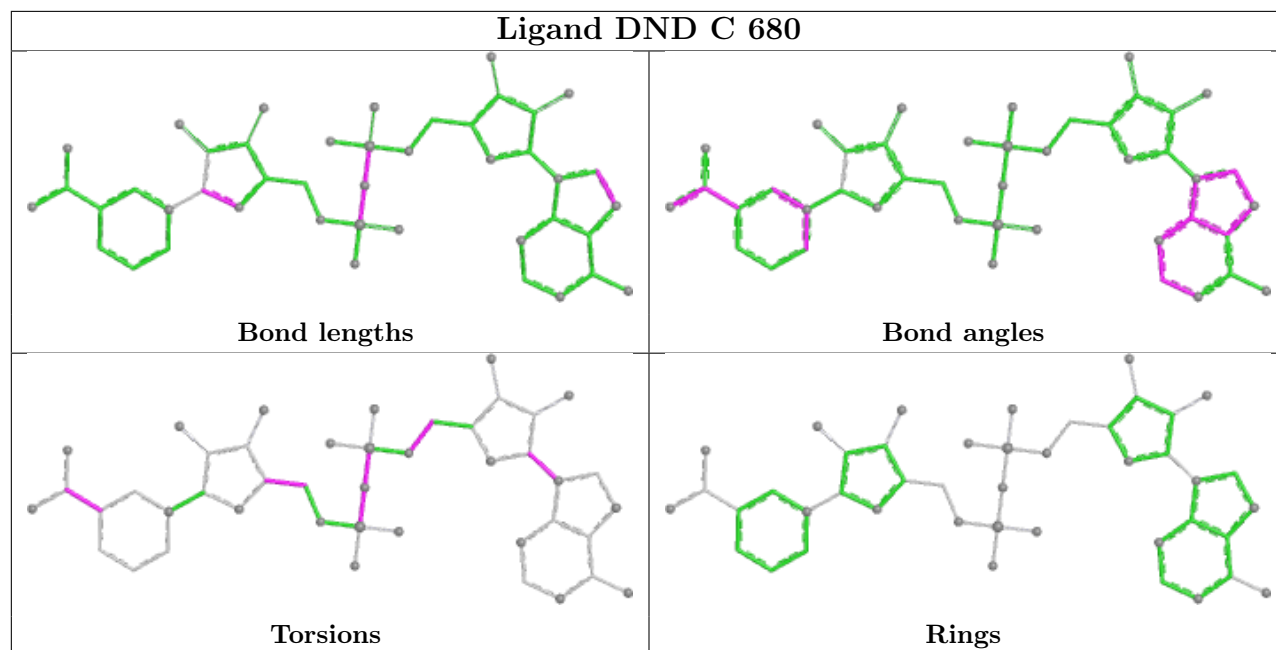
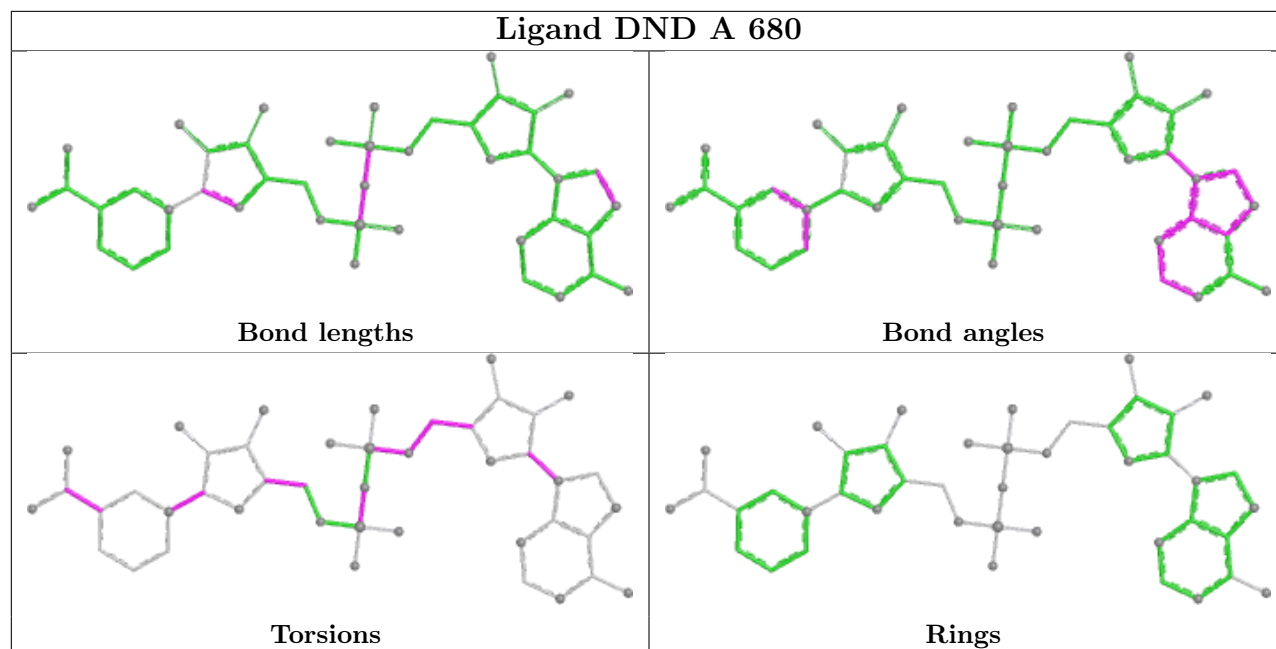
Mol	Chain	Res	Type	Atoms
2	A	680	DND	C2B-C1B-N9A-C8A
2	B	680	DND	O4D-C4D-C5D-O5D
2	A	680	DND	O4B-C1B-N9A-C8A
2	B	680	DND	O4B-C1B-N9A-C8A
3	A	803	ONL	OXT-C-CA-CB
3	A	801[B]	ONL	O-C-CA-N
3	A	802	ONL	O-C-CA-N
2	D	680	DND	PA-O3P-PN-O11

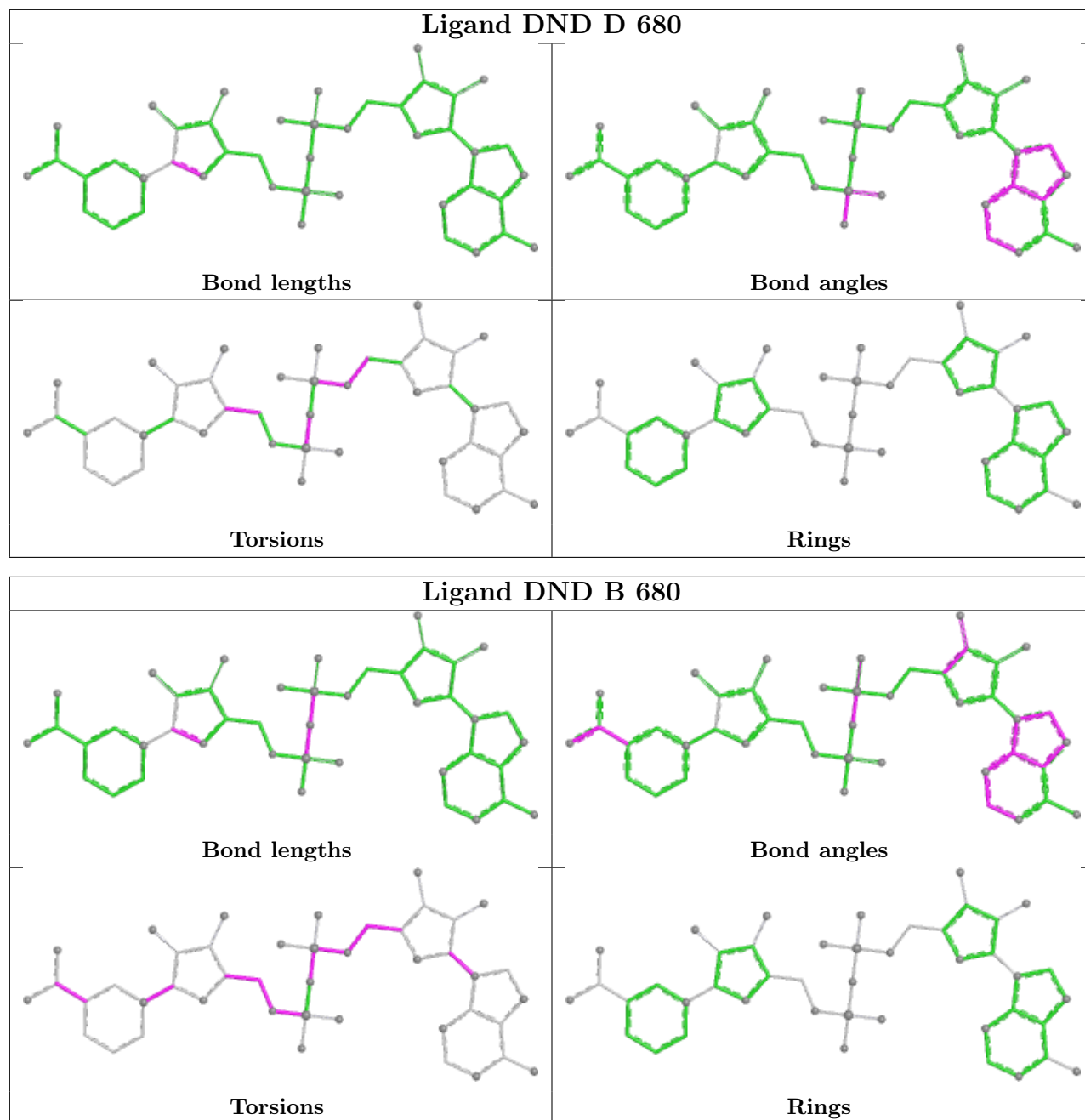
There are no ring outliers.

15 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	ONL	1	0
4	C	681	GOL	2	0
4	C	683	GOL	5	0
2	A	680	DND	6	0
3	A	801[A]	ONL	4	0
4	D	682	GOL	8	0
3	A	800	ONL	4	0
2	C	680	DND	2	0
3	A	803	ONL	2	0
4	D	683	GOL	3	0
2	D	680	DND	3	0
4	C	684	GOL	1	0
4	B	682	GOL	3	0
4	B	681	GOL	1	0
4	C	682	GOL	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	651/680 (95%)	-0.22	3 (0%) 87 90	2, 5, 19, 41	1 (0%)
1	B	649/680 (95%)	-0.21	2 (0%) 90 92	2, 3, 17, 34	0
1	C	656/680 (96%)	-0.24	1 (0%) 91 92	2, 3, 15, 26	1 (0%)
1	D	657/680 (96%)	-0.09	5 (0%) 82 86	2, 3, 17, 25	0
All	All	2613/2720 (96%)	-0.19	11 (0%) 88 91	2, 4, 17, 41	2 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	369	GLY	3.9
1	A	408	THR	3.8
1	B	454	PHE	3.1
1	D	370	GLY	2.7
1	D	0	SER	2.7
1	B	679	GLY	2.6
1	A	407	HIS	2.6
1	A	149	GLY	2.5
1	C	559	ALA	2.5
1	D	607	SER	2.3
1	D	335	ARG	2.1

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 ⓘ

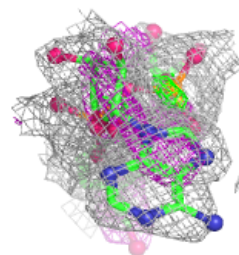
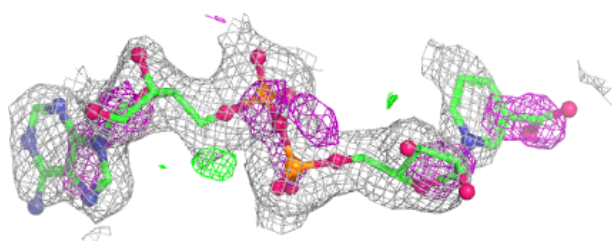
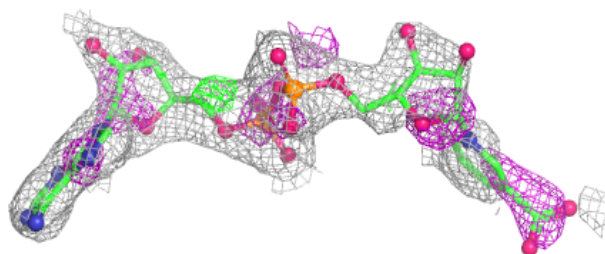
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	804	6/6	0.62	0.16	46,47,48,48	0
4	GOL	B	682	6/6	0.69	0.15	42,43,45,45	0
4	GOL	D	685	6/6	0.69	0.14	37,39,39,40	0
4	GOL	B	684	6/6	0.72	0.14	31,34,35,36	0
4	GOL	B	681	6/6	0.74	0.18	35,37,37,38	0
3	ONL	A	803	10/10	0.74	0.17	27,34,35,35	0
4	GOL	C	683	6/6	0.76	0.32	10,12,13,16	0
3	ONL	A	800	10/10	0.76	0.18	20,27,28,29	0
3	ONL	A	801[A]	10/10	0.77	0.16	2,2,2,2	10
3	ONL	A	801[B]	10/10	0.77	0.16	5,7,7,7	10
4	GOL	D	682	6/6	0.79	0.17	20,22,22,24	0
3	ONL	A	802	10/10	0.80	0.15	16,25,26,26	0
4	GOL	C	682	6/6	0.81	0.26	25,27,28,28	0
4	GOL	D	683	6/6	0.86	0.16	12,17,18,20	0
4	GOL	B	683	6/6	0.88	0.13	9,18,19,20	0
2	DND	A	680	44/44	0.89	0.11	25,29,59,61	0
4	GOL	C	681	6/6	0.89	0.12	21,25,27,28	0
4	GOL	C	684	6/6	0.89	0.12	8,11,12,14	0
4	GOL	D	681	6/6	0.91	0.16	16,18,19,19	0
4	GOL	A	805	6/6	0.91	0.14	7,9,9,10	0
4	GOL	D	684	6/6	0.92	0.18	5,6,7,8	0
2	DND	D	680	44/44	0.92	0.10	18,25,48,49	0
2	DND	C	680	44/44	0.93	0.09	14,18,36,36	0
2	DND	B	680	44/44	0.93	0.11	12,21,54,56	0

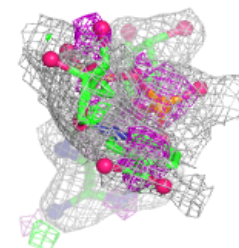
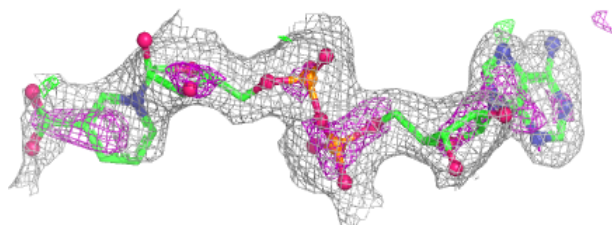
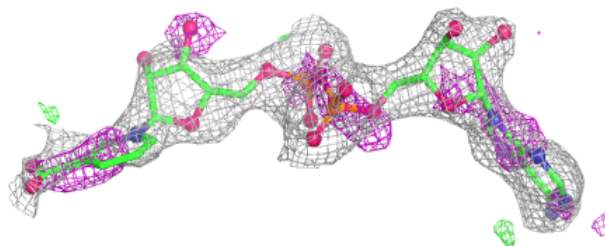
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DND A 680:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

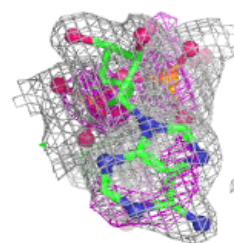
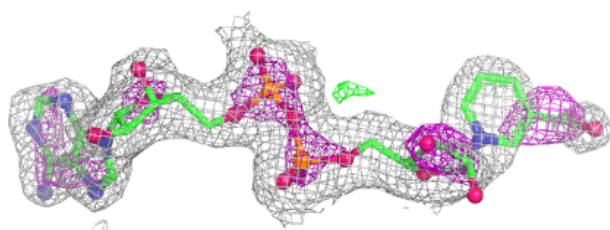
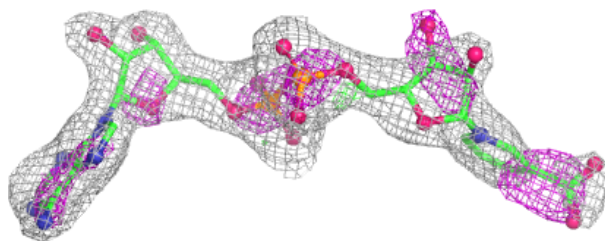
**Electron density around DND D 680:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

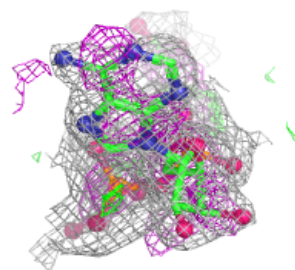
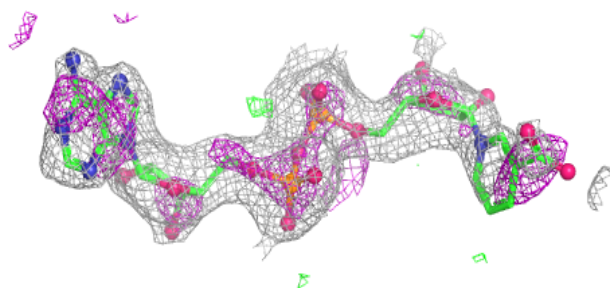
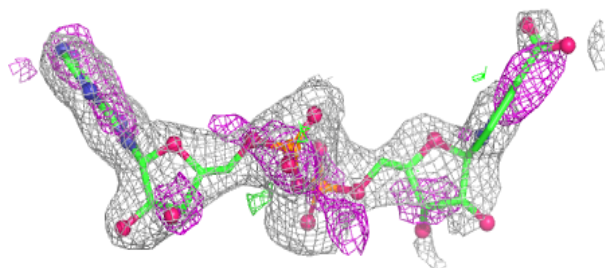


Electron density around DND C 680:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around DND B 680:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.