



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:56 PM GMT

PDB ID : 3DLA
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

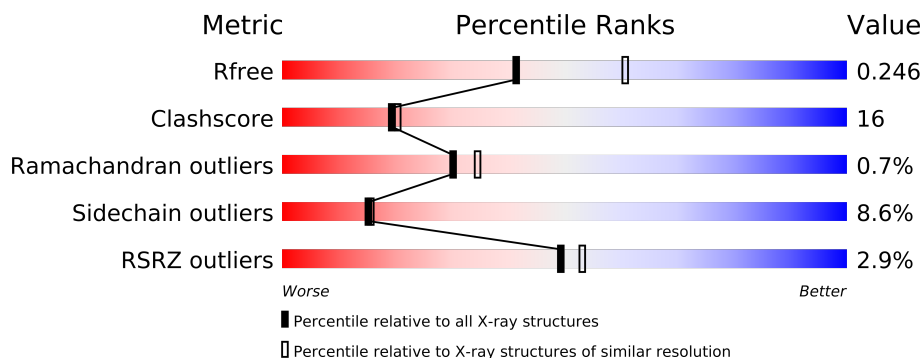
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	680	
1	B	680	
1	C	680	
1	D	680	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NXX	B	680	-	X
3	ONL	A	800	-	X
3	ONL	A	801[A]	-	X
3	ONL	A	801[B]	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	ONL	A	803	-	X
4	GOL	B	681	-	X
4	GOL	B	683	-	X
4	GOL	B	684	-	X
4	GOL	C	682	-	X
4	GOL	C	683	-	X
4	GOL	D	682	-	X
4	GOL	D	683	-	X
4	GOL	D	685	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22006 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

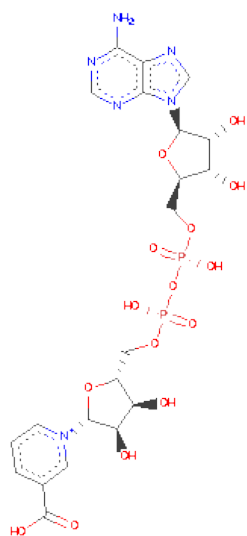
- Molecule 1 is a protein called Glutamine-dependent NAD(+) synthetase.

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:

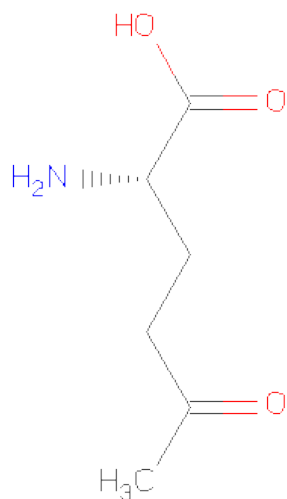
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP P0A5L6
B	0	SER	-	EXPRESSION TAG	UNP P0A5L6
C	0	SER	-	EXPRESSION TAG	UNP P0A5L6
D	0	SER	-	EXPRESSION TAG	UNP P0A5L6

- Molecule 2 is 1-[(2R,3R,4S,5R)-5-({[(R)-{[(R)-{(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHOXY}(HYDROXY)PHOSPHORYL]OXY}(HYDROXY)PHOSPHORYL]OXY}METHYL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]-3-CARBOXYPYRIDINIUM (three-letter code: NXX) (formula: C₂₁H₂₇N₆O₁₅P₂).



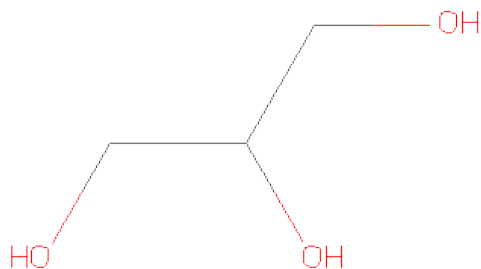
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	6	15	2		

- Molecule 3 is 5-OXO-L-NORLEUCINE (three-letter code: ONL) (formula: $C_6H_{11}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	4	Total	C	N	O	0	1
			50	30	5	15		

- Molecule 4 is GLYCEROL (three-letter code: 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		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is water.

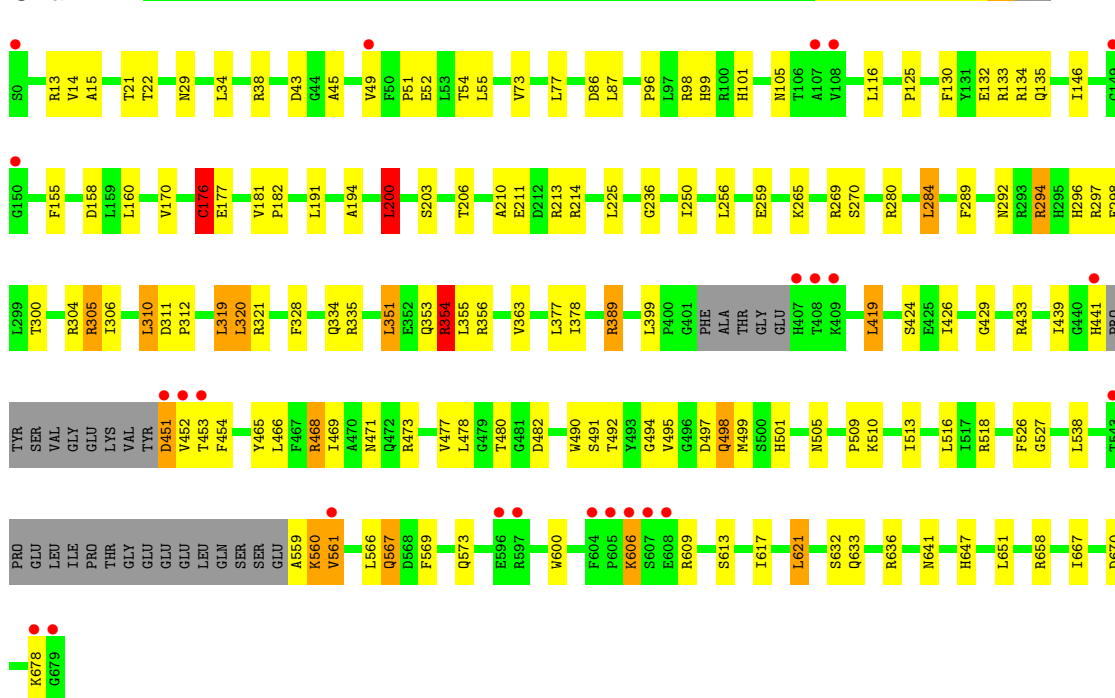
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	334	Total	O	0	0
			334	334		
5	B	384	Total	O	0	0
			384	384		
5	C	366	Total	O	0	0
			366	366		
5	D	359	Total	O	0	0
			359	359		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

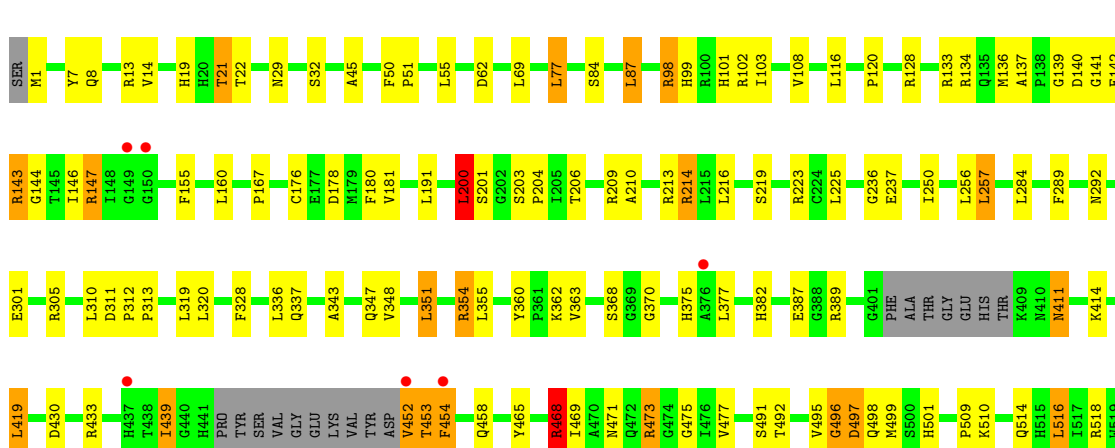
- Molecule 1: Glutamine-dependent NAD(+) synthetase

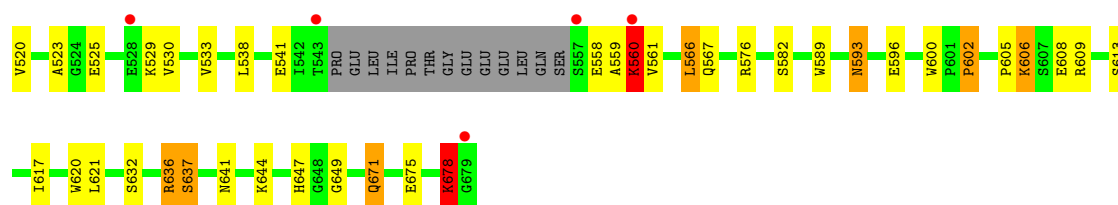
Chain A:



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

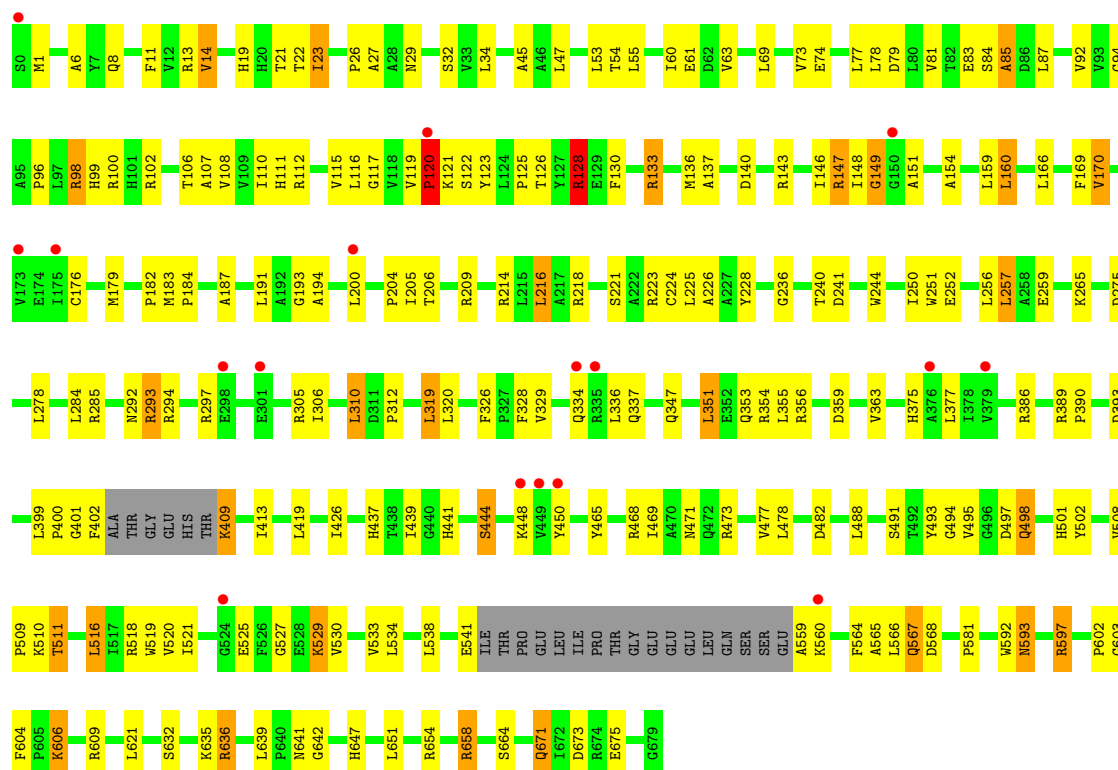
Chain B:





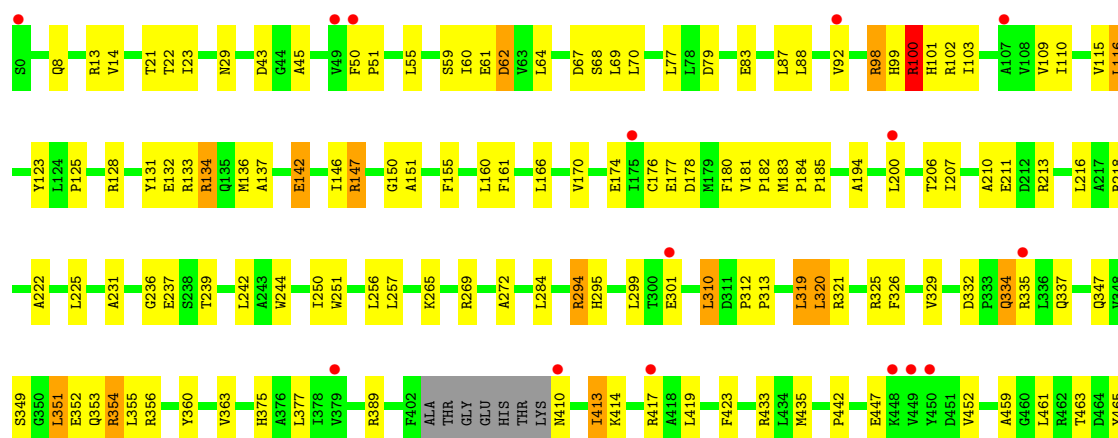
• Molecule 1: Glutamine-dependent NAD(+) synthetase

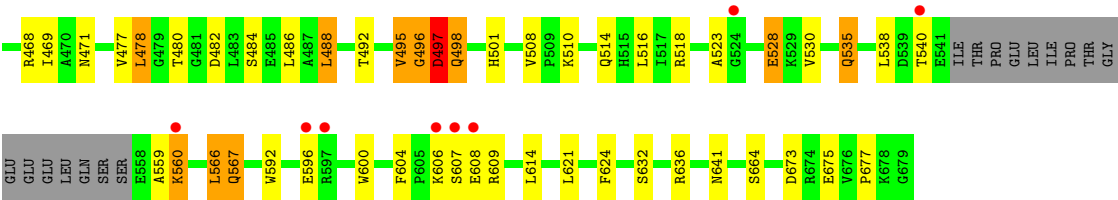
Chain C:



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

Chain D:





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) 99.3 (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 (5.29%)	DCC
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 , 17.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	4 of 142287 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NXX, ONL

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	0.64	0/5128	0.76	4/6963 (0.1%)
1	B	0.72	0/5132	0.82	7/6969 (0.1%)
1	C	0.84	2/5237 (0.0%)	0.90	9/7111 (0.1%)
1	D	0.77	4/5219 (0.1%)	0.84	7/7089 (0.1%)
All	All	0.75	6/20716 (0.0%)	0.83	27/28132 (0.1%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	142	GLU	CD-OE2	5.90	1.32	1.25
1	D	174	GLU	CG-CD	5.79	1.60	1.51
1	D	103	ILE	C-O	5.34	1.33	1.23
1	C	74	GLU	CD-OE2	5.15	1.31	1.25
1	D	123	TYR	N-CA	5.10	1.56	1.46
1	C	187	ALA	CA-CB	5.07	1.63	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	294	ARG	NE-CZ-NH2	-10.75	114.93	120.30
1	C	216	LEU	CA-CB-CG	-9.84	92.67	115.30
1	D	134	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	C	294	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	294	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	B	200	LEU	CA-CB-CG	7.44	132.41	115.30
1	B	468	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	D	98	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	200	LEU	CA-CB-CG	6.36	129.93	115.30
1	B	98	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	128	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	D	134	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	D	294	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	C	319	LEU	CA-CB-CG	5.98	129.06	115.30
1	C	98	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	305	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	C	636	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	636	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	D	100	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	576	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	C	170	VAL	CB-CA-C	-5.31	101.31	111.40
1	A	354	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	419	LEU	CA-CB-CG	5.24	127.36	115.30
1	D	62	ASP	CB-CG-OD1	5.24	123.01	118.30
1	C	160	LEU	CB-CG-CD1	5.14	119.73	111.00
1	D	294	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	C	293	ARG	NE-CZ-NH1	5.01	122.81	120.30

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5014	0	4904	122	0
1	B	5017	0	4919	162	1
1	C	5117	0	5015	224	0
1	D	5099	0	4994	178	0
2	A	44	0	24	5	0
2	B	44	0	24	0	0
2	C	44	0	24	2	0
2	D	44	0	24	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	9	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	20086	663	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (663) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:495:VAL:HB	5:B:993:HOH:O	1.22	1.29
1:D:110:ILE:HA	5:D:970:HOH:O	1.36	1.24
1:D:147:ARG:CG	1:D:147:ARG:HH11	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:88:LEU:HG	5:D:973:HOH:O	1.41	1.18
1:D:51:PRO:HA	5:D:851:HOH:O	1.44	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:C:183[B]:MET:CE	5:C:800:HOH:O	1.99	1.08
1:B:354:ARG:NH1	5:B:750:HOH:O	1.79	1.08
1:D:147:ARG:HG3	1:D:147:ARG:HH11	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:HD3	1:C:529:LYS:H	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
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:D:468:ARG:NH1	1:D:471:ASN:ND2	2.19	0.89
1:B:257:LEU:HD13	5:B:753:HOH:O	1.72	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:CD	1:C:529:LYS:H	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:183[B]:MET:HE2	5:C:800:HOH:O	1.64	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:HG2	1:D:147:ARG:HH11	1.39	0.85
1:C:437:HIS:HA	1:C:444:SER:OG	1.78	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:241:ASP:OD2	5:C:860:HOH:O	1.98	0.81
1:C:102:ARG:HD3	1:C:137:ALA:HB2	1.62	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:D:216:LEU:HD13	5:D:874:HOH:O	1.77	0.81
1:B:289:PHE:HA	5:B:1003:HOH:O	1.79	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: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:C:183[B]:MET:HE3	5:C:800:HOH:O	1.65	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
1:B:8:GLN:CB	5:B:932:HOH:O	2.26	0.78
1:C:567:GLN:HA	1:C:567:GLN:HE21	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:D:354:ARG:NH2	1:D:641:ASN:HD22	1.79	0.76
1:C:359:ASP:HB2	5:C:878:HOH:O	1.86	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:D:69:LEU:HD13	1:D:69:LEU:C	2.06	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:D:147:ARG:HG2	1:D:147:ARG:NH1	1.97	0.74
1:C:511:THR:HB	1:C:568:ASP:OD2	1.87	0.74
1:B:468:ARG:NH2	1:C:495:VAL:O	2.21	0.74
1:A:133:ARG:HG2	5:A:932:HOH:O	1.88	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:C:354:ARG:HH22	1:C:641:ASN:ND2	1.87	0.73
1:A:468:ARG:NH1	1:A:471:ASN:HD21	1.87	0.73
1:D:389:ARG:HD3	5:D:814:HOH:O	1.87	0.73
1:B:21:THR:HG22	5:B:687:HOH:O	1.88	0.72
1:A:354:ARG:HH22	1:A:641:ASN:HD22	1.33	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:204:PRO:CG	5:C:869:HOH:O	2.37	0.72
1:C:110:ILE:CD1	5:C:983:HOH:O	2.37	0.72
1:C:99:HIS:HD2	5:C:707:HOH:O	1.71	0.72
1:C:179:MET:O	5:C:797:HOH:O	2.07	0.72
1:A:468:ARG:HH11	1:A:471:ASN:HD21	1.38	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:NXX:H6N	2:A:680:NXX:H3M	1.73	0.71
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:D:102:ARG:HD3	1:D:137:ALA:HB2	1.73	0.70
1:C:23:ILE:CD1	5:C:960:HOH:O	2.39	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:363:VAL:CG1	1:D:478:LEU:CD2	2.70	0.69
1:D:43:ASP:OD2	1:D:269:ARG:NH2	2.26	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:C:100:ARG:CZ	5:C:1002:HOH:O	2.41	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:98:ARG:HG3	5:C:770:HOH:O	1.92	0.68
1:B:301:GLU:HG2	5:B:1000:HOH:O	1.93	0.68
1:C:204:PRO:HG2	5:C:869:HOH:O	1.90	0.68
1:C:106:THR:HG22	1:C:120:PRO:HB3	1.74	0.68
1:C:597:ARG:CG	1:C:597:ARG:HH11	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
5:B:1003:HOH:O	1:D:182:PRO:CD	2.43	0.67
1:A:297:ARG:NH1	5:A:1115:HOH:O	2.28	0.67
1:D:23:ILE:CG2	5:D:972:HOH:O	2.41	0.67
1:B:605:PRO:HD2	5:B:985:HOH:O	1.95	0.67
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:D:22:THR:H	1:D:29:ASN:HD21	1.44	0.66
1:C:353:GLN:HE21	1:C:356:ARG:HH21	1.44	0.66
1:D:353:GLN:HE21	1:D:356:ARG:HH21	1.42	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:275:ASP:CG	5:C:956:HOH:O	2.33	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:CA	1:A:567:GLN:HE21	2.09	0.64
1:D:294:ARG:HD3	4:D:682:GOL:HO3	1.63	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:D:363:VAL:HG13	1:D:478:LEU:HD21	1.77	0.64
1:C:441:HIS:O	1:C:444:SER:HB2	1.97	0.64
1:B:465:TYR:HD1	1:C:439:ILE:HD11	1.63	0.64
1:B:389:ARG:HD3	5:B:694:HOH:O	1.97	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
3:A:801[A]:ONL:HG1	1:B:180:PHE:HZ	1.61	0.63
1:A:647:HIS:HD2	5:A:870:HOH:O	1.80	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:NXX:H4M	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
5:B:1003:HOH:O	1:D:182:PRO:HD3	2.00	0.62
1:B:98:ARG:NH2	5:B:858:HOH:O	2.31	0.62
1:D:463:THR:CG2	5:D:881:HOH:O	2.46	0.62
1:C:214:ARG:HG3	5:C:832:HOH:O	1.98	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:D:468:ARG:HH11	1:D:471:ASN:HD22	1.46	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:C:518:ARG:HD3	5:C:766:HOH:O	2.00	0.61
1:B:347:GLN:OE1	1:B:375:HIS:HE1	1.84	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:567:GLN:NE2	5:A:854:HOH:O	2.32	0.60
1:A:495:VAL:O	1:D:468:ARG:NH2	2.35	0.60
1:A:497:ASP:OD2	2:A:680:NXX:H4N	2.02	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:C:53:LEU:HD22	1:C:96:PRO:HD3	1.83	0.59
1:A:49:VAL:HG13	1:A:200:LEU:HD22	1.85	0.59
1:C:529:LYS:CD	1:C:529:LYS:N	2.63	0.58
1:A:14:VAL:HG23	1:A:250:ILE:HD13	1.84	0.58
2:D:680:NXX:H4M	5:D:978:HOH:O	2.03	0.58
1:B:411:ASN:HA	1:B:414:LYS:HB2	1.84	0.58
1:B:99:HIS:HE1	5:B:902:HOH:O	1.84	0.58
1:D:21:THR:O	1:D:236:GLY:HA3	2.02	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: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
5:B:1003:HOH:O	1:D:182:PRO:HD2	2.02	0.58
1:A:353:GLN:HE21	1:A:356:ARG:NH2	2.02	0.58
1:C:285:ARG:NH1	5:C:1035:HOH:O	2.14	0.58
1:B:102:ARG:HD3	1:B:137:ALA:HB2	1.85	0.58
1:B:62:ASP:OD2	1:B:134:ARG:NH1	2.37	0.58
1:C:55:LEU:HB2	1:C:94:GLY:O	2.04	0.57
1:B:50:PHE:O	1:B:200:LEU:HB3	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:D:64:LEU:O	5:D:726:HOH:O	2.17	0.57
1:B:98:ARG:HG3	5:B:699:HOH:O	2.03	0.57
1:D:353:GLN:HE21	1:D:356:ARG:NH2	2.02	0.57
1:A:441:HIS:NE2	1:A:453:THR:HG21	2.19	0.57
1:D:360:TYR:HB3	1:D:389:ARG:HD2	1.87	0.57
1:C:363:VAL:HG13	1:C:478:LEU:HG	1.86	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:182:PRO:O	1:D:184:PRO:HD3	2.05	0.56
1:C:525:GLU:HG3	5:C:955:HOH:O	2.05	0.56
1:B:541:GLU:HG2	5:B:775:HOH:O	2.06	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: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: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:A:305:ARG:HD3	5:A:891:HOH:O	2.05	0.55
1:B:430:ASP:OD1	1:B:433:ARG:NH1	2.40	0.55
2:A:680:NXX:H6N	2:A:680:NXX:C3M	2.38	0.54
1:A:146:ILE:HG22	1:A:155:PHE:HB2	1.89	0.54
1:D:604:PHE:O	1:D:609:ARG:NH1	2.38	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:B:491:SER:HB2	1:B:497:ASP:OD2	2.08	0.54
1:A:658:ARG:NH1	5:A:982:HOH:O	2.14	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:A:158:ASP:CG	1:A:304:ARG:HH21	2.12	0.53
1:C:179:MET:HE2	1:C:228:TYR:CE2	2.43	0.53
1:C:78:LEU:HD21	1:C:149:GLY:HA3	1.90	0.53
1:B:133:ARG:HD2	5:B:1035:HOH:O	2.08	0.53
1:C:351:LEU:HD22	1:C:355:LEU:HG	1.89	0.53
1:B:644:LYS:HE3	1:B:649:GLY:HA2	1.90	0.53
1:A:492:THR:OG1	2:A:680:NXX:H5N	2.08	0.53
1:D:413:ILE:CD1	1:D:417:ARG:HE	2.21	0.53
1:A:310:LEU:HD13	1:A:312:PRO:HB3	1.91	0.53
1:B:223:ARG:NH1	5:B:864:HOH:O	2.36	0.53
1:A:284:LEU:HD21	1:B:103:ILE:HG23	1.90	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:632:SER:OG	1:A:636:ARG:NH2	2.42	0.53
1:D:210:ALA:HA	1:D:213:ARG:HD2	1.90	0.53
1:C:252:GLU:HB2	1:C:257:LEU:CD2	2.39	0.53
1:C:675:GLU:HG3	5:C:908:HOH:O	2.09	0.52
1:C:191:LEU:O	1:D:101:HIS:HE1	1.92	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: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:B:120:PRO:HB2	1:B:139:GLY:HA3	1.91	0.52
1:D:13:ARG:HB3	1:D:45:ALA:HA	1.91	0.52
1:D:64:LEU:C	5:D:726:HOH:O	2.48	0.52
1:D:22:THR:H	1:D:29:ASN:ND2	2.06	0.52
1:C:69:LEU:C	1:C:69:LEU:HD13	2.30	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
1:C:597:ARG:CG	1:C:597:ARG:NH1	2.71	0.52
1:C:108:VAL:HG12	5:C:983:HOH:O	2.08	0.52
3:A:800:ONL:CB	5:A:1020:HOH:O	2.57	0.52
1:A:86:ASP:HB2	5:A:1057:HOH:O	2.09	0.52
1:A:482:ASP:HA	1:A:505:ASN:O	2.09	0.51
1:A:319:LEU:HD13	1:A:321:ARG:HB3	1.91	0.51
1:D:559:ALA:O	1:D:560:LYS:HD2	2.10	0.51
1:C:204:PRO:CG	1:C:244:TRP:CZ3	2.92	0.51
1:A:99:HIS:HD2	5:A:813:HOH:O	1.92	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: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:D:125:PRO:HD2	1:D:132:GLU:CD	2.31	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:C:170:VAL:HG21	1:C:193:GLY:O	2.11	0.51
1:C:170:VAL:HB	1:C:194:ALA:HA	1.93	0.51
4:D:682:GOL:H11	5:D:1005:HOH:O	2.10	0.51
1:D:146:ILE:CG2	1:D:155:PHE:HB2	2.34	0.51
1:B:310:LEU:HB3	1:B:312:PRO:HD3	1.93	0.51
1:B:495:VAL:O	1:C:468:ARG:NH2	2.43	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:A:451:ASP:O	1:A:453:THR:HG22	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:C:84:SER:O	1:C:85:ALA:C	2.49	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:NXX:H5N	2.11	0.50
1:D:360:TYR:CG	1:D:389:ARG:HD2	2.46	0.50
1:D:128:ARG:HD3	5:D:854:HOH:O	2.11	0.50
3:A:803:ONL:HG1	5:A:1019:HOH:O	2.11	0.50
1:D:349:SER:HA	1:D:352:GLU:OE2	2.11	0.50
1:D:180:PHE:N	5:D:954:HOH:O	2.44	0.50
1:C:182:PRO:HB2	5:C:800:HOH:O	2.12	0.50
1:B:21:THR:O	1:B:236:GLY:HA3	2.11	0.50
1:A:399:LEU:HD11	1:A:466:LEU:HD21	1.93	0.50
1:A:225:LEU:HD22	1:A:289:PHE:CD2	2.47	0.50
1:C:409:LYS:HE2	5:C:776:HOH:O	2.11	0.50
1:D:319:LEU:HD13	1:D:321:ARG:HB3	1.92	0.50
1:C:493:TYR:HB2	1:C:635:LYS:HG2	1.93	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:C:166:LEU:HD22	1:C:169:PHE:HB2	1.93	0.49
1:A:296:HIS:O	1:A:300:THR:HG23	2.12	0.49
1:D:614:LEU:HD21	1:D:677:PRO:HD2	1.93	0.49
1:C:179:MET:HG3	1:C:228:TYR:OH	2.11	0.49
1:C:92:VAL:CG1	1:C:200:LEU:HD11	2.42	0.49
1:A:354:ARG:NH2	1:A:641:ASN:HD22	2.06	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:C:106:THR:HA	1:C:120:PRO:HA	1.95	0.49
1:B:492:THR:H	1:B:497:ASP:HB3	1.76	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:170:VAL:HG12	1:A:194:ALA:HA	1.95	0.49
1:D:295:HIS:CE1	5:D:887:HOH:O	2.66	0.49
1:A:363:VAL:CG1	1:A:478:LEU:HG	2.41	0.49
1:C:337:GLN:NE2	5:C:852:HOH:O	2.35	0.49
1:A:469:ILE:HG23	1:A:473:ARG:HD2	1.93	0.49
1:C:468:ARG:HD3	1:C:468:ARG:HA	1.57	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:497:ASP:OD2	2:D:680:NXX:H5N	2.12	0.48
1:D:62:ASP:OD1	1:D:134:ARG:HD3	2.12	0.48
1:C:154:ALA:HB1	1:C:159:LEU:HD21	1.95	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:C:204:PRO:CB	5:C:869:HOH:O	2.60	0.48
1:C:658:ARG:NH2	5:D:855:HOH:O	2.45	0.48
1:C:305:ARG:HD2	5:C:885:HOH:O	2.13	0.48
1:C:326:PHE:HB2	1:C:329:VAL:HB	1.95	0.48
1:A:439:ILE:CD1	1:D:465:TYR:HD1	2.25	0.48
1:C:400:PRO:HD2	1:C:426:ILE:O	2.13	0.48
1:C:73:VAL:HG21	5:C:743:HOH:O	2.13	0.48
1:B:204:PRO:O	1:B:209:ARG:HD2	2.13	0.48
1:D:496:GLY:O	1:D:498:GLN:N	2.46	0.48
1:C:390:PRO:O	1:C:393:ASP:HB2	2.13	0.48
1:B:21:THR:HA	1:B:29:ASN:ND2	2.29	0.48
1:A:210:ALA:HA	1:A:213:ARG:HD2	1.95	0.48
1:D:180:PHE:HA	5:D:874:HOH:O	2.13	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: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:C:221:SER:HB3	1:C:228:TYR:HB2	1.95	0.47
1:B:22:THR:N	1:B:29:ASN:HD21	2.07	0.47
1:A:214:ARG:NH1	1:A:259:GLU:OE2	2.47	0.47
1:D:632:SER:OG	1:D:636:ARG:NH2	2.47	0.47
1:C:13:ARG:HB3	1:C:45:ALA:HA	1.95	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:D:231:ALA:O	5:D:851:HOH:O	2.20	0.47
1:C:221:SER:HB2	1:C:226:ALA:O	2.15	0.47
1:B:468:ARG:HD3	1:B:468:ARG:HA	1.55	0.47
1:C:326:PHE:HB3	1:C:329:VAL:HB	1.97	0.47
1:A:490:TRP:NE1	2:A:680:NXX:H2N	2.30	0.47
1:A:21:THR:O	1:A:236:GLY:HA3	2.15	0.47
1:D:69:LEU:CD1	1:D:69:LEU:C	2.79	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:123:TYR:CZ	5:C:901:HOH:O	2.58	0.47
1:C:337:GLN:HE21	1:C:519:TRP:HE1	1.62	0.47
1:C:154:ALA:HB1	1:C:159:LEU:CD2	2.45	0.47
1:B:589:TRP:O	1:B:593:ASN:HB3	2.15	0.47
1:A:181:VAL:O	1:A:182:PRO:C	2.53	0.47
1:D:200:LEU:HA	5:D:851:HOH:O	2.13	0.46
1:B:133:ARG:HH22	4:D:682:GOL:H2	1.80	0.46
1:C:122:SER:HB3	1:C:123:TYR:CD2	2.50	0.46
1:A:636:ARG:HD3	1:A:651:LEU:HB3	1.96	0.46
1:B:214:ARG:HG3	1:B:214:ARG:HH11	1.80	0.46
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: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:B:360:TYR:HB3	1:B:389:ARG:HD2	1.98	0.46
1:A:453:THR:HG23	1:A:454:PHE:H	1.81	0.46
1:C:179:MET:HE2	1:C:228:TYR:CZ	2.51	0.46
1:C:98:ARG:HD2	5:C:789:HOH:O	2.16	0.46
3:A:803:ONL:OD	1:D:177:GLU:HB2	2.15	0.46
1:A:13:ARG:CZ	1:A:320:LEU:HD22	2.46	0.46
1:B:600:TRP:CD2	1:B:609:ARG:HG2	2.50	0.46
1:A:613:SER:O	1:A:617:ILE:HG12	2.15	0.46
1:D:237:GLU:HB2	1:D:244:TRP:CD1	2.51	0.46
1:C:329:VAL:CG2	1:C:511:THR:HG23	2.46	0.46
1:C:23:ILE:CG1	5:C:960:HOH:O	2.55	0.46
3:A:802:ONL:HG2	1:C:130:PHE:CZ	2.51	0.46
1:B:180:PHE:CD2	1:B:216:LEU:HD12	2.50	0.46
1:C:133:ARG:HA	1:C:133:ARG:HD2	1.63	0.46
1:D:530:VAL:HG23	5:D:720:HOH:O	2.15	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:509:PRO:HB2	1:C:568:ASP:OD2	2.15	0.46
1:C:147:ARG:HA	1:C:151:ALA:O	2.16	0.46
1:D:301:GLU:HG3	5:D:747:HOH:O	2.16	0.46
1:D:131:TYR:HB2	5:D:855:HOH:O	2.15	0.45
1:C:502:TYR:CZ	1:C:642:GLY:HA2	2.51	0.45
1:C:401:GLY:O	1:C:402:PHE:C	2.55	0.45
1:B:336:LEU:HD23	1:B:602:PRO:HG2	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:378:ILE:HG23	1:A:526:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:34:LEU:O	1:A:38:ARG:HG3	2.15	0.45
1:D:442:PRO:HB2	1:D:447:GLU:HB2	1.98	0.45
1:A:328:PHE:CG	1:A:509:PRO:HG3	2.51	0.45
1:C:205:ILE:HD12	1:C:209:ARG:HB3	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
2:D:680:NXX:H2B	5:D:845:HOH:O	2.16	0.45
1:D:133:ARG:HA	1:D:133:ARG:HD2	1.78	0.45
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:C:525:GLU:H	1:C:525:GLU:CD	2.20	0.45
1:D:523:ALA:HB3	5:D:703:HOH:O	2.16	0.45
1:D:180:PHE:CD2	1:D:216:LEU:HD12	2.53	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:A:98:ARG:NH1	5:A:967:HOH:O	2.38	0.45
1:C:179:MET:HG2	1:C:179:MET:O	2.17	0.44
1:B:354:ARG:HD3	1:B:354:ARG:HA	1.69	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:A:465:TYR:CE1	1:D:435:MET:HG3	2.51	0.44
1:D:332:ASP:OD2	1:D:334:GLN:HG2	2.16	0.44
1:D:237:GLU:HB3	1:D:244:TRP:CE2	2.53	0.44
1:D:79:ASP:O	1:D:83:GLU:HG2	2.17	0.44
1:D:92:VAL:CG1	1:D:200:LEU:HD11	2.47	0.44
1:C:183[B]:MET:HB2	5:C:800:HOH:O	2.16	0.44
1:A:191:LEU:HD11	1:A:292:ASN:ND2	2.33	0.44
1:D:410:ASN:HB3	1:D:414:LYS:HD2	2.00	0.44
1:D:178:ASP:O	1:D:185:PRO:HD2	2.18	0.44
1:C:468:ARG:NH1	1:C:471:ASN:HD22	2.11	0.44
1:B:133:ARG:HH22	4:D:682:GOL:C2	2.31	0.44
4:D:682:GOL:C1	5:D:1005:HOH:O	2.65	0.44
1:D:600:TRP:CE2	1:D:609:ARG:HG2	2.53	0.44
1:C:516:LEU:O	1:C:520:VAL:HG23	2.16	0.44
1:B:19:HIS:HB2	1:B:32:SER:OG	2.17	0.44
1:C:22:THR:H	1:C:29:ASN:HD21	1.66	0.44
1:C:22:THR:H	1:C:29:ASN:ND2	2.16	0.44
1:D:181:VAL:CG2	5:D:954:HOH:O	2.31	0.44
1:C:399:LEU:HA	1:C:426:ILE:O	2.18	0.44
1:D:347:GLN:OE1	1:D:375:HIS:HE1	2.01	0.44
1:C:252:GLU:HB2	1:C:257:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:606:LYS:HA	1:B:609:ARG:HD3	2.00	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:C:223:ARG:HA	5:C:1023:HOH:O	2.18	0.44
1:B:514:GLN:HG3	1:B:518:ARG:HH12	1.81	0.44
1:A:265:LYS:HD3	1:A:265:LYS:HA	1.88	0.44
1:D:468:ARG:HH12	1:D:471:ASN:HD21	1.65	0.44
1:C:494:GLY:H	1:C:498:GLN:HE21	1.66	0.44
1:B:13:ARG:HB3	1:B:45:ALA:HA	1.99	0.44
1:B:69:LEU:C	1:B:69:LEU:HD13	2.38	0.44
1:C:115:VAL:HG12	1:C:117:GLY:H	1.83	0.44
1:D:325:ARG:HB3	1:D:592:TRP:CZ2	2.52	0.43
1:C:121:LYS:HE2	1:C:123:TYR:O	2.18	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:B:354:ARG:NE	5:B:1007:HOH:O	2.42	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:B:370:GLY:HA3	5:B:1049:HOH:O	2.19	0.43
1:A:670:ASP:HB2	5:A:1008:HOH:O	2.18	0.43
1:B:582:SER:HB2	1:B:671:GLN:HE22	1.83	0.43
1:B:419:LEU:HD13	1:B:530:VAL:HG21	1.99	0.43
1:A:280:ARG:HD3	5:A:821:HOH:O	2.18	0.43
1:D:566:LEU:HD12	1:D:566:LEU:HA	1.77	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:B:7:TYR:CE2	1:B:313:PRO:HD2	2.54	0.43
1:A:294:ARG:HH11	4:D:682:GOL:H11	1.83	0.43
1:C:511:THR:HG21	5:C:687:HOH:O	2.19	0.43
1:A:15:ALA:HA	1:A:270:SER:O	2.18	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:B:1:MET:HB2	1:B:675:GLU:OE1	2.18	0.43
1:C:658:ARG:HH21	1:D:61:GLU:CD	2.22	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:239:THR:HA	1:D:242:LEU:O	2.19	0.43
1:D:170:VAL:HG12	1:D:194:ALA:HA	2.00	0.43
1:C:285:ARG:HE	4:C:681:GOL:C3	2.29	0.43
1:B:637:SER:O	1:C:654:ARG:NH1	2.50	0.43
1:B:219:SER:HB2	5:B:864:HOH:O	2.18	0.43
1:C:125:PRO:HA	4:C:683:GOL:O2	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:439:ILE:HG13	1:D:469:ILE:HD13	2.01	0.43
1:C:336:LEU:HD22	1:C:602:PRO:HD2	2.01	0.43
1:B:368:SER:HB3	4:B:681:GOL:H12	2.01	0.43
1:A:518:ARG:CZ	5:A:1059:HOH:O	2.66	0.43
1:B:178:ASP:C	5:B:859:HOH:O	2.57	0.42
1:D:23:ILE:HB	1:D:60:ILE:HG22	2.00	0.42
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:C:636:ARG:HD3	1:C:651:LEU:HB3	2.01	0.42
1:B:214:ARG:CG	1:B:214:ARG:HH11	2.32	0.42
1:C:26:PRO:HD2	5:C:844:HOH:O	2.18	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:D:125:PRO:HD2	1:D:132:GLU:OE1	2.18	0.42
1:C:79:ASP:O	1:C:83:GLU:HG2	2.19	0.42
1:B:613:SER:HB2	5:B:827:HOH:O	2.18	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:1:MET:CE	5:B:932:HOH:O	2.67	0.42
1:B:560:LYS:NZ	1:B:560:LYS:HB3	2.35	0.42
1:C:23:ILE:HB	1:C:60:ILE:CG2	2.49	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:C:468:ARG:HH11	1:C:471:ASN:HD22	1.67	0.42
1:C:26:PRO:HA	1:C:55:LEU:O	2.20	0.42
1:B:469:ILE:HG23	1:B:473:ARG:HD3	2.02	0.42
1:C:491:SER:OG	1:C:498:GLN:HB2	2.19	0.42
1:C:96:PRO:HA	5:C:822:HOH:O	2.20	0.42
1:D:468:ARG:HA	1:D:468:ARG:HD3	1.75	0.42
1:B:21:THR:HA	1:B:29:ASN:HD21	1.85	0.42
1:D:183:MET:HB3	1:D:183:MET:HE2	1.75	0.42
1:B:99:HIS:HD2	4:B:682:GOL:H2	1.83	0.42
1:D:70:LEU:CD2	5:D:726:HOH:O	2.68	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:A:617:ILE:O	1:A:621:LEU:HB2	2.20	0.42
1:B:439:ILE:HD13	1:C:465:TYR:CE1	2.55	0.42
1:A:510:LYS:HA	1:A:513:ILE:HD12	2.00	0.42
1:D:50:PHE:HB3	1:D:51:PRO:CD	2.50	0.42
1:D:222:ALA:O	1:D:225:LEU:HD12	2.19	0.42
1:D:92:VAL:HG12	1:D:200:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:310:LEU:HD13	1:C:312:PRO:HB3	2.02	0.42
1:B:647:HIS:CE1	5:B:973:HOH:O	2.73	0.42
1:B:387:GLU:OE2	1:D:265:LYS:NZ	2.53	0.42
1:A:294:ARG:NH2	1:B:140:ASP:O	2.53	0.41
1:A:52:GLU:OE2	1:A:105:ASN:ND2	2.50	0.41
1:B:84:SER:HA	1:B:87:LEU:HB2	2.01	0.41
1:A:561:VAL:HG12	5:A:921:HOH:O	2.20	0.41
1:D:567:GLN:HE22	1:D:624:PHE:HB2	1.85	0.41
1:C:488:LEU:HD11	1:C:567:GLN:HG3	2.01	0.41
1:B:439:ILE:CD1	1:C:465:TYR:HD1	2.32	0.41
3:A:800:ONL:HB2	5:A:1020:HOH:O	2.18	0.41
1:D:310:LEU:HD22	1:D:310:LEU:O	2.20	0.41
1:B:491:SER:CB	1:B:497:ASP:OD2	2.68	0.41
1:B:292:ASN:HD21	1:D:183:MET:N	2.14	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:D:675:GLU:HA	1:D:675:GLU:OE1	2.19	0.41
1:A:606:LYS:HA	1:A:609:ARG:HD3	2.03	0.41
1:C:92:VAL:HG12	1:C:200:LEU:HD21	2.03	0.41
1:C:27:ALA:HB2	4:C:682:GOL:C1	2.49	0.41
1:C:468:ARG:NH1	1:C:471:ASN:HD21	2.14	0.41
1:C:55:LEU:HA	1:C:55:LEU:HD12	1.74	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:B:516:LEU:O	1:B:520:VAL:HG23	2.19	0.41
1:C:565:ALA:HB1	1:C:592:TRP:CZ2	2.56	0.41
1:C:293:ARG:NE	1:D:100:ARG:HE	2.18	0.41
1:D:468:ARG:HH12	1:D:471:ASN:ND2	2.12	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:C:510:LYS:HD3	1:C:564:PHE:CE2	2.56	0.41
1:B:566:LEU:HA	1:B:566:LEU:HD12	1.57	0.41
1:C:224:CYS:SG	5:C:826:HOH:O	2.31	0.41
1:C:148:ILE:O	1:C:149:GLY:C	2.58	0.41
5:A:852:HOH:O	1:B:101:HIS:CD2	2.61	0.41
1:D:433:ARG:HB3	4:D:683:GOL:H12	2.02	0.41
1:B:439:ILE:HD11	1:C:469:ILE:HD11	2.02	0.41
1:B:541:GLU:CG	5:B:775:HOH:O	2.65	0.41
1:A:600:TRP:CD2	1:A:609:ARG:HG2	2.55	0.41
1:A:569:PHE:O	1:A:573:GLN:HG2	2.21	0.41
1:B:362:LYS:O	1:B:475:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:143:ARG:HB3	1:B:144:GLY:H	1.78	0.41
1:D:294:ARG:HH11	4:D:682:GOL:H12	1.86	0.41
1:B:84:SER:HA	1:B:87:LEU:HD22	2.02	0.41
1:A:429:GLY:O	1:A:433:ARG:HG3	2.21	0.41
1:C:140:ASP:HB3	5:C:901:HOH:O	2.21	0.40
1:D:567:GLN:CA	1:D:567:GLN:HE21	2.22	0.40
1:C:191:LEU:O	1:D:101:HIS:CE1	2.72	0.40
1:B:146:ILE:CG2	1:B:155:PHE:HB2	2.51	0.40
1:A:176:CYS:HB3	1:A:177:GLU:H	1.64	0.40
1:D:486:LEU:HD12	5:D:975:HOH:O	2.19	0.40
1:D:99:HIS:HE1	5:D:750:HOH:O	2.04	0.40
1:C:96:PRO:CA	5:C:822:HOH:O	2.69	0.40
3:A:801[A]:ONL:CE	1:B:203:SER:HB2	2.51	0.40
1:D:326:PHE:HB3	1:D:329:VAL:HB	2.03	0.40
1:A:134:ARG:HD3	1:A:135:GLN:NE2	2.36	0.40
1:B:328:PHE:CG	1:B:509:PRO:HG3	2.56	0.40
1:D:606:LYS:HA	1:D:609:ARG:HD3	2.03	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:C:353:GLN:NE2	1:C:356:ARG:HH21	2.15	0.40
1:D:136:MET:HE3	5:D:859:HOH:O	2.21	0.40
1:A:389:ARG:HD3	5:A:1046:HOH:O	2.22	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	Distance(Å)	Clash(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

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	644/680 (95%)	615 (96%)	28 (4%)	1 (0%)	56	70
1	B	641/680 (94%)	613 (96%)	24 (4%)	4 (1%)	33	39
1	C	653/680 (96%)	619 (95%)	27 (4%)	7 (1%)	21	21
1	D	651/680 (96%)	622 (96%)	24 (4%)	5 (1%)	27	31
All	All	2589/2720 (95%)	2469 (95%)	103 (4%)	17 (1%)	30	34

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 ⓘ

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%)	474 (93%)	38 (7%)	20	22
1	B	515/549 (94%)	467 (91%)	48 (9%)	13	13
1	C	529/549 (96%)	481 (91%)	48 (9%)	14	13
1	D	527/549 (96%)	483 (92%)	44 (8%)	16	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2083/2196 (95%)	1905 (92%)	178 (8%)	15	16

All (178) 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	116	LEU
1	A	160	LEU
1	A	176	CYS
1	A	200	LEU
1	A	206	THR
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	354	ARG
1	A	377	LEU
1	A	389	ARG
1	A	419	LEU
1	A	424	SER
1	A	426	ILE
1	A	451	ASP
1	A	468	ARG
1	A	480	THR
1	A	491	SER
1	A	498	GLN
1	A	499	MET
1	A	516	LEU
1	A	538	LEU
1	A	560	LYS
1	A	561	VAL
1	A	566	LEU
1	A	567	GLN
1	A	606	LYS
1	A	621	LEU
1	A	667	ILE

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Mol	Chain	Res	Type
1	A	678	LYS
1	B	21	THR
1	B	55	LEU
1	B	77	LEU
1	B	87	LEU
1	B	116	LEU
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	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
1	B	454	PHE
1	B	468	ARG
1	B	473	ARG
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	593	ASN
1	B	596	GLU

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Mol	Chain	Res	Type
1	B	602	PRO
1	B	606	LYS
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	77	LEU
1	C	87	LEU
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	206	THR
1	C	216	LEU
1	C	225	LEU
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	334	GLN
1	C	351	LEU
1	C	377	LEU
1	C	409	LYS
1	C	413	ILE
1	C	419	LEU
1	C	444	SER
1	C	473	ARG
1	C	498	GLN
1	C	511	THR
1	C	516	LEU
1	C	529	LYS
1	C	533	VAL

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Mol	Chain	Res	Type
1	C	538	LEU
1	C	541	GLU
1	C	566	LEU
1	C	567	GLN
1	C	593	ASN
1	C	597	ARG
1	C	606	LYS
1	C	621	LEU
1	C	647	HIS
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	116	LEU
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	335	ARG
1	D	337	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	478	LEU
1	D	480	THR
1	D	488	LEU
1	D	495	VAL

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Mol	Chain	Res	Type
1	D	497	ASP
1	D	498	GLN
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	621	LEU
1	D	664	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) 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	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	590	HIS
1	A	593	ASN
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	375	HIS
1	B	441	HIS
1	B	456	ASN
1	B	471	ASN

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Mol	Chain	Res	Type
1	B	498	GLN
1	B	501	HIS
1	B	514	GLN
1	B	590	HIS
1	B	626	GLN
1	B	641	ASN
1	B	647	HIS
1	C	29	ASN
1	C	99	HIS
1	C	292	ASN
1	C	295	HIS
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
1	C	641	ASN
1	D	29	ASN
1	D	101	HIS
1	D	347	GLN
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	567	GLN
1	D	590	HIS
1	D	593	ASN
1	D	626	GLN
1	D	641	ASN
1	D	647	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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$
2	NXX	A	680	-	48,48,48	0.97	5 (10%)	73,73,73	1.85	11 (15%)
3	ONL	A	800	1	9,9,9	0.70	0	11,11,11	1.57	2 (18%)
3	ONL	A	801[A]	1	9,9,9	0.81	0	11,11,11	1.73	3 (27%)
3	ONL	A	801[B]	1	9,9,9	0.77	0	11,11,11	1.80	4 (36%)
3	ONL	A	802	1	9,9,9	0.74	0	11,11,11	1.42	2 (18%)
3	ONL	A	803	1	9,9,9	0.66	0	11,11,11	1.26	2 (18%)
4	GOL	A	804	-	5,5,5	0.35	0	5,5,5	0.45	0
4	GOL	A	805	-	5,5,5	0.39	0	5,5,5	1.00	0
2	NXX	B	680	-	48,48,48	0.91	2 (4%)	73,73,73	1.85	7 (9%)
4	GOL	B	681	-	5,5,5	0.31	0	5,5,5	0.70	0
4	GOL	B	682	-	5,5,5	0.48	0	5,5,5	0.25	0
4	GOL	B	683	-	5,5,5	0.48	0	5,5,5	1.00	0
4	GOL	B	684	-	5,5,5	0.40	0	5,5,5	0.72	0
2	NXX	C	680	-	48,48,48	0.97	2 (4%)	73,73,73	1.92	8 (10%)
4	GOL	C	681	-	5,5,5	0.38	0	5,5,5	0.19	0
4	GOL	C	682	-	5,5,5	0.29	0	5,5,5	0.62	0
4	GOL	C	683	-	5,5,5	0.65	0	5,5,5	1.37	1 (20%)
4	GOL	C	684	-	5,5,5	0.45	0	5,5,5	0.78	0
2	NXX	D	680	-	48,48,48	0.85	2 (4%)	73,73,73	1.84	7 (9%)
4	GOL	D	681	-	5,5,5	0.42	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	D	682	-	5,5,5	0.33	0	5,5,5	0.68	0
4	GOL	D	683	-	5,5,5	0.33	0	5,5,5	0.72	0
4	GOL	D	684	-	5,5,5	0.45	0	5,5,5	0.28	0
4	GOL	D	685	-	5,5,5	0.36	0	5,5,5	0.30	0

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	NXX	A	680	-	-	0/30/62/62	0/3/5/5
3	ONL	A	800	1	-	0/9/9/9	0/0/0/0
3	ONL	A	801[A]	1	-	0/9/9/9	0/0/0/0
3	ONL	A	801[B]	1	-	0/9/9/9	0/0/0/0
3	ONL	A	802	1	-	0/9/9/9	0/0/0/0
3	ONL	A	803	1	-	0/9/9/9	0/0/0/0
4	GOL	A	804	-	-	0/4/4/4	0/0/0/0
4	GOL	A	805	-	-	0/4/4/4	0/0/0/0
2	NXX	B	680	-	-	0/30/62/62	0/3/5/5
4	GOL	B	681	-	-	0/4/4/4	0/0/0/0
4	GOL	B	682	-	-	0/4/4/4	0/0/0/0
4	GOL	B	683	-	-	0/4/4/4	0/0/0/0
4	GOL	B	684	-	-	0/4/4/4	0/0/0/0
2	NXX	C	680	-	-	0/30/62/62	0/3/5/5
4	GOL	C	681	-	-	0/4/4/4	0/0/0/0
4	GOL	C	682	-	-	0/4/4/4	0/0/0/0
4	GOL	C	683	-	-	0/4/4/4	0/0/0/0
4	GOL	C	684	-	-	0/4/4/4	0/0/0/0
2	NXX	D	680	-	-	0/30/62/62	0/3/5/5
4	GOL	D	681	-	-	0/4/4/4	0/0/0/0
4	GOL	D	682	-	-	0/4/4/4	0/0/0/0
4	GOL	D	683	-	-	0/4/4/4	0/0/0/0
4	GOL	D	684	-	-	0/4/4/4	0/0/0/0
4	GOL	D	685	-	-	0/4/4/4	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	680	NXX	O4B-C1B	2.80	1.45	1.41
2	A	680	NXX	O4B-C1B	2.63	1.45	1.41
2	B	680	NXX	PA-O3A	2.50	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	680	NXX	O4M-C1M	2.44	1.45	1.41
2	A	680	NXX	PN-O3A	2.43	1.64	1.59
2	C	680	NXX	O4M-C1M	2.31	1.44	1.41
2	A	680	NXX	PA-O3A	2.25	1.63	1.59
2	A	680	NXX	C4A-N9A	-2.19	1.34	1.37
2	D	680	NXX	O4M-C1M	2.14	1.44	1.41
2	D	680	NXX	O4B-C1B	2.13	1.44	1.41
2	B	680	NXX	O4M-C1M	2.09	1.44	1.41

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	680	NXX	N3A-C2A-N1A	-11.56	119.05	128.71
2	A	680	NXX	N3A-C2A-N1A	-10.96	119.55	128.71
2	C	680	NXX	N3A-C2A-N1A	-10.82	119.67	128.71
2	D	680	NXX	N3A-C2A-N1A	-10.44	119.98	128.71
2	D	680	NXX	C2M-C1M-N1N	-5.50	104.55	113.86
2	C	680	NXX	C2M-C1M-N1N	-5.36	104.79	113.86
2	C	680	NXX	O4M-C1M-N1N	5.15	113.22	107.95
2	A	680	NXX	O4M-C1M-N1N	4.93	113.00	107.95
2	B	680	NXX	N3A-C4A-N9A	4.76	134.03	125.43
2	D	680	NXX	O4M-C1M-N1N	4.59	112.65	107.95
2	D	680	NXX	N3A-C4A-N9A	4.41	133.40	125.43
2	C	680	NXX	N3A-C4A-N9A	4.23	133.08	125.43
2	A	680	NXX	N3A-C4A-N9A	3.85	132.38	125.43
3	A	800	ONL	CB-CG-CD	-3.76	110.15	114.53
3	A	801[B]	ONL	CB-CG-CD	-3.53	110.42	114.53
3	A	801[A]	ONL	C-CA-N	3.11	114.51	109.36
2	B	680	NXX	C5A-C4A-N3A	-3.10	118.96	125.70
3	A	802	ONL	CB-CG-CD	-3.05	110.98	114.53
3	A	801[B]	ONL	CG-CB-CA	-3.02	108.79	114.43
2	B	680	NXX	C2A-N3A-C4A	2.96	122.45	114.01
2	C	680	NXX	C5A-C4A-N3A	-2.90	119.38	125.70
2	A	680	NXX	C1B-N9A-C4A	-2.85	121.71	126.64
2	A	680	NXX	C8A-N9A-C4A	2.84	109.07	106.90
2	C	680	NXX	O4B-C1B-N9A	2.81	111.06	108.44
2	A	680	NXX	O4B-C1B-N9A	2.77	111.02	108.44
2	D	680	NXX	C5A-C4A-N3A	-2.74	119.74	125.70
2	B	680	NXX	C3M-C2M-C1M	2.71	105.14	100.91
2	A	680	NXX	C2M-C1M-N1N	-2.68	109.32	113.86
2	C	680	NXX	C2A-N3A-C4A	2.66	121.58	114.01
3	A	801[A]	ONL	OXT-C-O	-2.60	118.18	124.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	680	NXX	C2A-N3A-C4A	2.59	121.38	114.01
2	D	680	NXX	O4B-C1B-N9A	2.52	110.78	108.44
3	A	802	ONL	OXT-C-O	-2.48	118.47	124.07
2	A	680	NXX	C5A-C4A-N3A	-2.44	120.38	125.70
4	C	683	GOL	O1-C1-C2	2.43	121.59	109.71
2	C	680	NXX	C4A-C5A-N7A	-2.38	107.48	109.52
2	D	680	NXX	C2A-N3A-C4A	2.32	120.61	114.01
2	A	680	NXX	C4A-C5A-N7A	-2.31	107.54	109.52
3	A	803	ONL	OXT-C-O	-2.29	118.89	124.07
3	A	801[B]	ONL	OXT-C-O	-2.27	118.94	124.07
2	B	680	NXX	C8A-N9A-C4A	2.27	108.63	106.90
2	A	680	NXX	C6N-N1N-C2N	-2.25	119.50	122.04
3	A	801[A]	ONL	CE-CD-CG	2.22	123.54	117.04
3	A	803	ONL	CB-CG-CD	-2.20	111.97	114.53
3	A	800	ONL	OXT-C-O	-2.14	119.24	124.07
3	A	801[B]	ONL	OD-CD-CG	-2.07	117.31	121.50
2	B	680	NXX	C4A-C5A-N7A	-2.03	107.78	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	651/680 (95%)	-0.05	24 (3%) 39 43	2, 5, 19, 41	0
1	B	649/680 (95%)	-0.12	11 (1%) 67 70	2, 3, 17, 34	0
1	C	657/680 (96%)	-0.01	17 (2%) 53 56	2, 3, 15, 26	0
1	D	657/680 (96%)	0.01	23 (3%) 42 46	2, 3, 17, 25	0
All	All	2614/2720 (96%)	-0.04	75 (2%) 49 53	2, 4, 17, 41	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	408	THR	8.3
1	A	407	HIS	4.9
1	A	0	SER	4.8
1	A	451	ASP	4.7
1	C	450	TYR	4.7
1	B	679	GLY	4.6
1	B	454	PHE	4.2
1	C	0	SER	4.1
1	D	607	SER	4.1
1	A	543	THR	3.8
1	B	452	VAL	3.8
1	D	450	TYR	3.4
1	D	0	SER	3.4
1	A	604	PHE	3.4
1	D	417	ARG	3.3
1	A	453	THR	3.2
1	B	557	SER	3.2
1	D	597	ARG	3.1
1	D	448	LYS	3.1
1	A	149	GLY	3.1
1	A	452	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	449	VAL	3.0
1	D	540	THR	3.0
1	D	449	VAL	3.0
1	B	543	THR	3.0
1	D	560	LYS	2.9
1	C	298[A]	GLU	2.9
1	A	679	GLY	2.8
1	C	150	GLY	2.8
1	A	150	GLY	2.8
1	A	608	GLU	2.8
1	D	524	GLY	2.7
1	D	606	LYS	2.7
1	A	597	ARG	2.6
1	D	335	ARG	2.6
1	C	200	LEU	2.6
1	A	441	HIS	2.6
1	D	200	LEU	2.6
1	D	379	VAL	2.5
1	A	606	LYS	2.5
1	D	608	GLU	2.5
1	C	334	GLN	2.5
1	A	607	SER	2.5
1	A	605	PRO	2.4
1	A	409	LYS	2.4
1	C	560	LYS	2.4
1	D	301	GLU	2.4
1	D	49	VAL	2.4
1	A	561	VAL	2.4
1	D	50	PHE	2.4
1	C	173	VAL	2.3
1	C	301	GLU	2.3
1	B	560	LYS	2.3
1	C	335	ARG	2.3
1	B	149	GLY	2.3
1	D	92	VAL	2.3
1	D	410	ASN	2.3
1	C	524	GLY	2.3
1	B	150	GLY	2.3
1	A	107	ALA	2.3
1	D	107	ALA	2.2
1	A	678	LYS	2.2
1	B	376	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	49	VAL	2.1
1	C	376	ALA	2.1
1	D	175	ILE	2.1
1	C	175	ILE	2.1
1	C	448	LYS	2.1
1	C	379	VAL	2.1
1	B	437	HIS	2.0
1	A	108	VAL	2.0
1	A	596	GLU	2.0
1	B	528	GLU	2.0
1	D	596	GLU	2.0
1	C	120	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	C	683	6/6	0.40	12.42	10,12,13,16	0
3	ONL	A	801[B]	10/10	0.31	9.33	5,7,7,7	10
4	GOL	C	682	6/6	0.54	8.21	25,27,28,28	0
3	ONL	A	801[A]	10/10	0.31	8.20	2,2,2,2	10
4	GOL	D	685	6/6	0.30	7.76	37,39,39,40	0
4	GOL	B	681	6/6	0.23	5.43	35,37,37,38	0
4	GOL	B	683	6/6	0.21	4.20	9,18,19,20	0
4	GOL	D	683	6/6	0.19	4.16	12,17,18,20	0
2	NXX	B	680	44/44	0.19	2.90	12,21,54,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	B	684	6/6	0.25	2.90	31,34,35,36	0
3	ONL	A	803	10/10	0.22	2.53	27,34,35,35	0
4	GOL	D	682	6/6	0.16	2.26	20,22,22,24	0
3	ONL	A	800	10/10	0.20	2.17	20,27,28,29	0
4	GOL	D	681	6/6	0.14	1.91	16,18,19,19	0
3	ONL	A	802	10/10	0.18	1.76	16,25,26,26	0
4	GOL	C	684	6/6	0.15	1.73	8,11,12,14	0
2	NXX	A	680	44/44	0.20	1.69	25,29,59,61	0
2	NXX	D	680	44/44	0.18	1.47	18,25,48,49	0
4	GOL	A	804	6/6	0.19	1.33	46,47,48,48	0
4	GOL	A	805	6/6	0.13	1.28	7,9,9,10	0
2	NXX	C	680	44/44	0.17	1.27	14,18,36,36	0
4	GOL	C	681	6/6	0.15	1.23	21,25,27,28	0
4	GOL	B	682	6/6	0.18	1.16	42,43,45,45	0
4	GOL	D	684	6/6	0.12	0.54	5,6,7,8	0

6.5 Other polymers ⓘ

There are no such residues in this entry.