



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 08:28 PM UTC

PDB ID : 2D5N / pdb_00002d5n
Title : Crystal structure of a bifunctional deaminase and reductase involved in riboflavin biosynthesis
Authors : Liaw, S.H.; Chen, S.J.; Chang, Y.C.
Deposited on : 2005-11-02
Resolution : 2.97 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

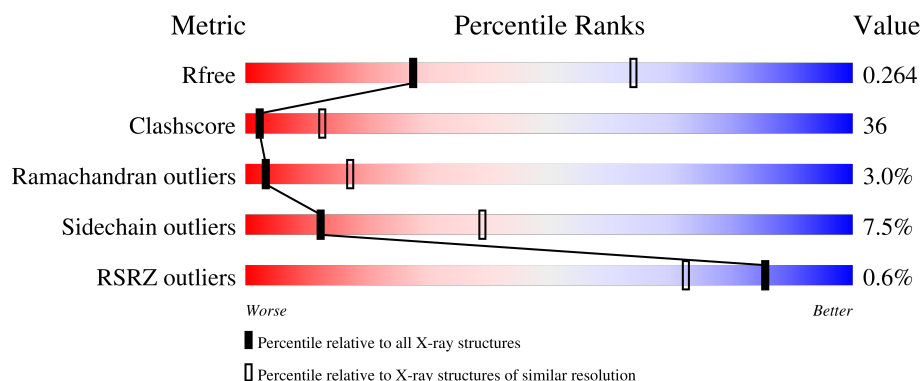
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	373	
1	B	373	
1	C	373	
1	D	373	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11257 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 Riboflavin biosynthesis protein ribD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2741	1740	469	517	15			
1	B	359	Total	C	N	O	S	0	0	0
			2741	1740	469	517	15			
1	C	359	Total	C	N	O	S	0	0	0
			2741	1740	469	517	15			
1	D	360	Total	C	N	O	S	0	0	0
			2747	1743	470	519	15			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	cloning artifact	UNP P17618
A	-10	ARG	-	cloning artifact	UNP P17618
A	-9	GLY	-	cloning artifact	UNP P17618
A	-8	SER	-	cloning artifact	UNP P17618
A	-7	HIS	-	cloning artifact	UNP P17618
A	-6	HIS	-	cloning artifact	UNP P17618
A	-5	HIS	-	cloning artifact	UNP P17618
A	-4	HIS	-	cloning artifact	UNP P17618
A	-3	HIS	-	cloning artifact	UNP P17618
A	-2	HIS	-	cloning artifact	UNP P17618
A	-1	GLY	-	cloning artifact	UNP P17618
A	0	SER	-	cloning artifact	UNP P17618
B	-11	MET	-	cloning artifact	UNP P17618
B	-10	ARG	-	cloning artifact	UNP P17618
B	-9	GLY	-	cloning artifact	UNP P17618
B	-8	SER	-	cloning artifact	UNP P17618
B	-7	HIS	-	cloning artifact	UNP P17618
B	-6	HIS	-	cloning artifact	UNP P17618
B	-5	HIS	-	cloning artifact	UNP P17618
B	-4	HIS	-	cloning artifact	UNP P17618
B	-3	HIS	-	cloning artifact	UNP P17618

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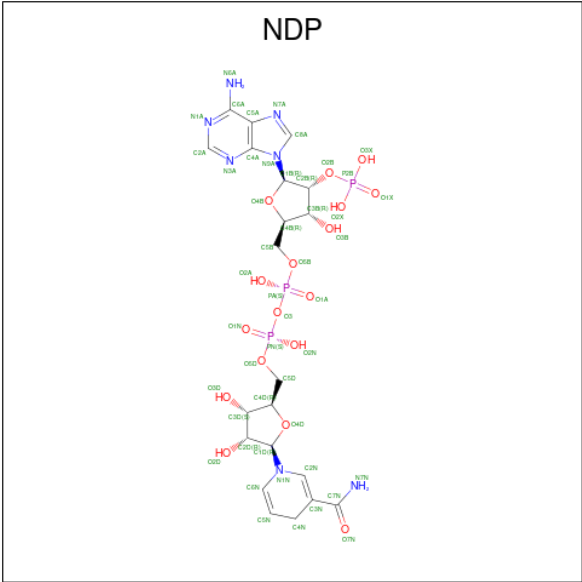
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	cloning artifact	UNP P17618
B	-1	GLY	-	cloning artifact	UNP P17618
B	0	SER	-	cloning artifact	UNP P17618
C	-11	MET	-	cloning artifact	UNP P17618
C	-10	ARG	-	cloning artifact	UNP P17618
C	-9	GLY	-	cloning artifact	UNP P17618
C	-8	SER	-	cloning artifact	UNP P17618
C	-7	HIS	-	cloning artifact	UNP P17618
C	-6	HIS	-	cloning artifact	UNP P17618
C	-5	HIS	-	cloning artifact	UNP P17618
C	-4	HIS	-	cloning artifact	UNP P17618
C	-3	HIS	-	cloning artifact	UNP P17618
C	-2	HIS	-	cloning artifact	UNP P17618
C	-1	GLY	-	cloning artifact	UNP P17618
C	0	SER	-	cloning artifact	UNP P17618
D	-11	MET	-	cloning artifact	UNP P17618
D	-10	ARG	-	cloning artifact	UNP P17618
D	-9	GLY	-	cloning artifact	UNP P17618
D	-8	SER	-	cloning artifact	UNP P17618
D	-7	HIS	-	cloning artifact	UNP P17618
D	-6	HIS	-	cloning artifact	UNP P17618
D	-5	HIS	-	cloning artifact	UNP P17618
D	-4	HIS	-	cloning artifact	UNP P17618
D	-3	HIS	-	cloning artifact	UNP P17618
D	-2	HIS	-	cloning artifact	UNP P17618
D	-1	GLY	-	cloning artifact	UNP P17618
D	0	SER	-	cloning artifact	UNP P17618

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

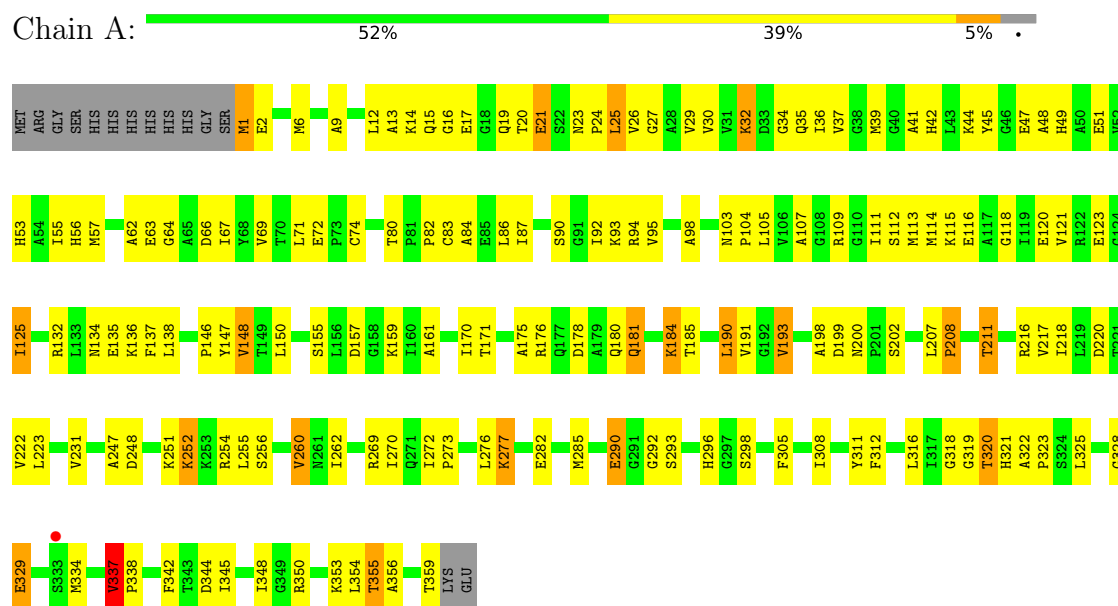
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total	O	0	0
			66	66		
4	B	64	Total	O	0	0
			64	64		
4	C	54	Total	O	0	0
			54	54		
4	D	51	Total	O	0	0
			51	51		

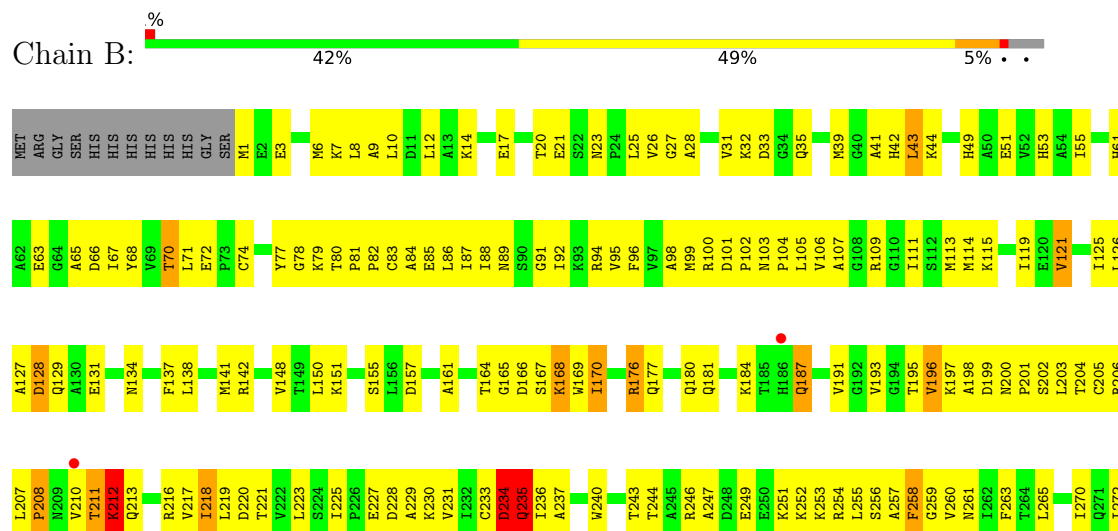
3 Residue-property plots

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: Riboflavin biosynthesis protein ribD

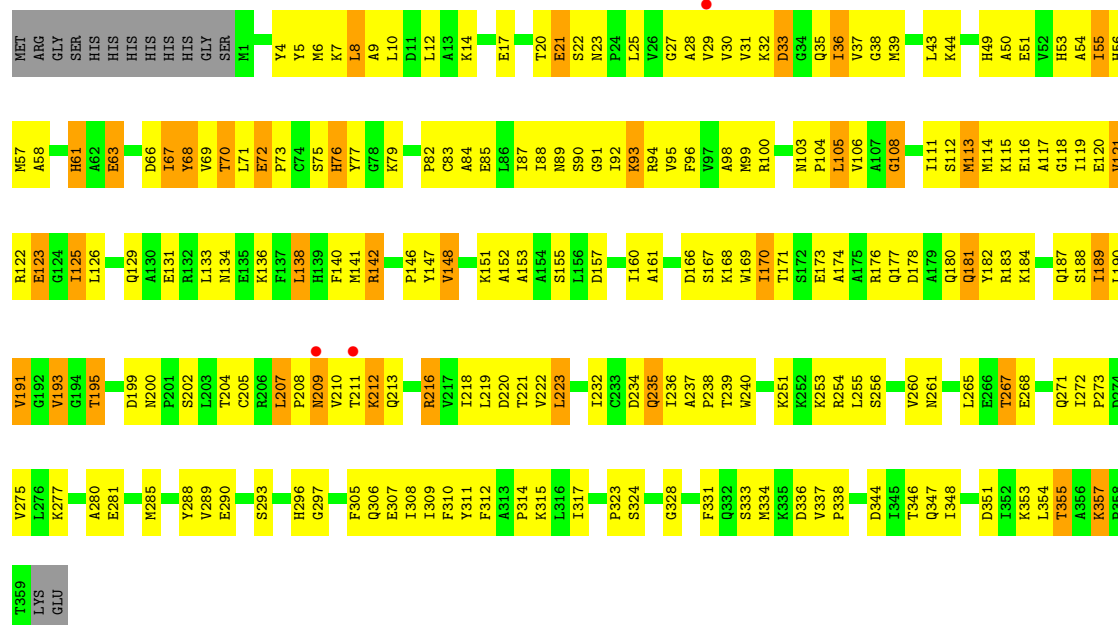


• Molecule 1: Riboflavin biosynthesis protein ribD

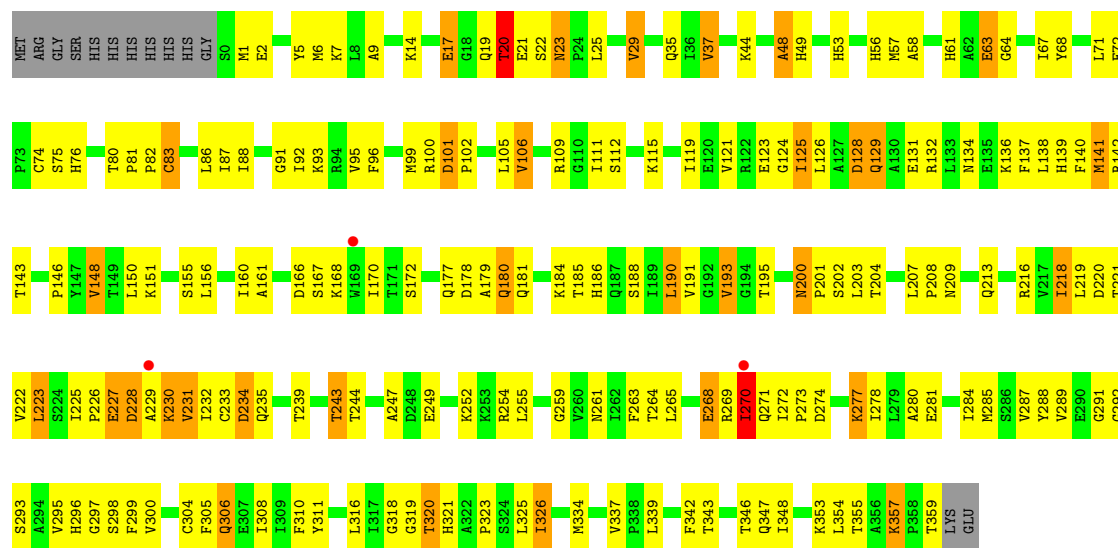
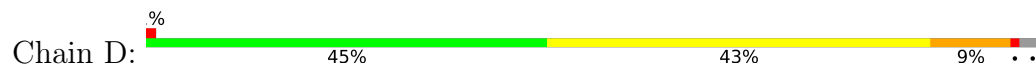




• Molecule 1: Riboflavin biosynthesis protein ribD



• Molecule 1: Riboflavin biosynthesis protein ribD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.13Å 107.95Å 186.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.97 30.00 – 2.97	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.00-2.97) 97.4 (30.00-2.97)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.96Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.270 0.214 , 0.264	Depositor DCC
R_{free} test set	3573 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	71.8	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11257	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: NDP, ZN

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	0.50	0/2792	0.99	9/3778 (0.2%)
1	B	0.47	0/2792	0.98	4/3778 (0.1%)
1	C	0.47	0/2792	1.02	15/3778 (0.4%)
1	D	0.47	0/2798	1.01	19/3786 (0.5%)
All	All	0.48	0/11174	1.00	47/15120 (0.3%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	293	SER	N-CA-C	-10.24	99.95	111.82
1	D	320	THR	N-CA-C	-7.50	100.89	110.19
1	D	229	ALA	N-CA-C	7.43	117.69	107.73
1	D	293	SER	N-CA-C	-7.39	102.59	111.69
1	B	170	ILE	N-CA-C	-7.32	104.08	110.74
1	B	291	GLY	N-CA-C	7.24	124.21	111.25
1	D	227	GLU	N-CA-C	-6.91	103.94	112.38
1	D	101	ASP	CA-C-N	6.74	125.98	118.97
1	D	101	ASP	C-N-CA	6.74	125.98	118.97
1	C	178	ASP	N-CA-C	-6.38	104.25	111.14
1	A	320	THR	N-CA-C	-6.24	105.16	112.89
1	C	202	SER	N-CA-C	-6.02	106.07	113.41
1	C	70	THR	N-CA-C	-5.82	106.31	113.41
1	D	106	VAL	CB-CA-C	-5.79	105.97	111.06
1	D	304	CYS	N-CA-C	5.78	118.30	109.62
1	A	262	ILE	N-CA-C	5.76	116.09	107.51
1	D	37	VAL	N-CA-C	5.71	117.22	111.00
1	D	326	ILE	N-CA-C	5.71	115.80	106.72
1	D	23	ASN	CA-C-N	5.70	125.67	120.03
1	D	23	ASN	C-N-CA	5.70	125.67	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	VAL	CA-C-N	5.62	125.55	119.76
1	A	337	VAL	C-N-CA	5.62	125.55	119.76
1	C	117	ALA	N-CA-C	-5.62	106.51	113.19
1	D	7	LYS	N-CA-C	-5.58	105.19	111.28
1	D	357	LYS	CA-C-N	5.56	125.88	119.93
1	D	357	LYS	C-N-CA	5.56	125.88	119.93
1	C	72	GLU	CA-C-N	5.51	126.73	119.84
1	C	72	GLU	C-N-CA	5.51	126.73	119.84
1	C	61	HIS	N-CA-C	-5.50	106.54	113.20
1	C	4	TYR	N-CA-C	-5.44	105.04	110.97
1	A	252	LYS	N-CA-C	-5.37	104.84	111.33
1	C	20	THR	N-CA-C	-5.30	106.31	112.89
1	D	200	ASN	CA-C-N	5.30	125.28	120.03
1	D	200	ASN	C-N-CA	5.30	125.28	120.03
1	C	121	VAL	N-CA-C	5.29	115.13	106.72
1	D	218	ILE	N-CA-C	5.27	115.44	107.80
1	D	148	VAL	N-CA-C	5.22	115.10	107.37
1	C	357	LYS	CA-C-N	5.18	125.91	120.11
1	C	357	LYS	C-N-CA	5.18	125.91	120.11
1	A	155	SER	N-CA-C	-5.14	103.74	110.53
1	B	121	VAL	N-CA-C	5.14	115.26	107.75
1	C	148	VAL	N-CA-C	5.14	115.49	107.99
1	B	165	GLY	N-CA-C	-5.10	108.21	115.30
1	A	198	ALA	N-CA-C	5.08	116.89	111.36
1	C	123	GLU	N-CA-C	5.05	117.48	109.50
1	A	34	GLY	N-CA-C	-5.02	108.35	115.43
1	A	148	VAL	N-CA-C	5.00	115.52	108.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2741	0	2782	168	0
1	B	2741	0	2782	248	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2741	0	2782	232	0
1	D	2747	0	2787	187	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	B	48	0	26	10	0
4	A	66	0	0	17	2
4	B	64	0	0	4	1
4	C	54	0	0	3	0
4	D	51	0	0	5	0
All	All	11257	0	11159	795	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 36.

All (795) 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:309:ILE:HG12	1:B:355:THR:HG22	1.33	1.06
1:A:94:ARG:HA	4:A:1377:HOH:O	1.55	1.06
1:A:355:THR:HG22	4:A:1415:HOH:O	1.58	1.01
1:C:21:GLU:HG3	1:C:22:SER:H	1.26	1.00
1:D:270:ILE:HD13	1:D:270:ILE:H	1.24	0.98
1:B:308:ILE:HB	4:B:1362:HOH:O	1.64	0.97
1:B:181:GLN:HA	1:B:207:LEU:HD11	1.45	0.96
1:A:125:ILE:HD12	1:A:125:ILE:H	1.30	0.95
1:C:184:LYS:HZ1	1:C:207:LEU:HB2	1.32	0.95
1:B:166:ASP:OD1	1:B:168:LYS:HG3	1.66	0.94
1:C:207:LEU:HD12	1:C:207:LEU:H	1.32	0.94
1:D:148:VAL:H	1:D:306:GLN:NE2	1.65	0.94
1:A:328:GLY:H	1:B:320:THR:HG22	1.36	0.91
1:D:148:VAL:HB	1:D:305:PHE:HA	1.52	0.91
1:D:141:MET:HE3	1:D:141:MET:HA	1.50	0.91
1:D:111:ILE:HG23	1:D:121:VAL:HG11	1.53	0.90
1:A:318:GLY:HA3	1:B:330:GLY:HA2	1.52	0.90
1:C:232:ILE:HD13	1:C:255:LEU:HD22	1.54	0.89
1:D:19:GLN:HG2	1:D:44:LYS:HD2	1.55	0.89
1:B:3:GLU:HB2	1:B:126:LEU:HD11	1.55	0.89
1:D:190:LEU:HB3	1:D:289:VAL:HG22	1.51	0.89
1:C:36:ILE:HD12	1:C:36:ILE:H	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:LYS:HD2	1:C:152:ALA:N	1.90	0.87
1:C:82:PRO:HD2	1:C:85:GLU:OE2	1.76	0.86
1:C:25:LEU:H	1:C:134:ASN:HD21	1.19	0.85
1:A:95:VAL:HG11	1:A:114:MET:HE1	1.59	0.84
1:B:148:VAL:H	1:B:306:GLN:HE21	1.18	0.84
1:D:272:ILE:HB	1:D:273:PRO:HD3	1.57	0.83
1:D:25:LEU:H	1:D:134:ASN:HD21	1.25	0.83
1:C:32:LYS:HD2	1:C:61:HIS:O	1.78	0.83
1:C:309:ILE:CD1	1:C:355:THR:HB	2.09	0.83
1:A:64:GLY:HA2	1:A:93:LYS:HG2	1.58	0.83
1:A:184:LYS:NZ	1:A:207:LEU:HD12	1.93	0.82
1:C:94:ARG:HD3	1:C:96:PHE:CE2	2.14	0.82
1:B:206:ARG:HB2	1:B:206:ARG:NH1	1.94	0.82
1:A:134:ASN:O	1:A:138:LEU:HD13	1.77	0.82
1:C:204:THR:HB	1:C:213:GLN:NE2	1.95	0.82
1:C:180:GLN:HB3	1:C:207:LEU:HD11	1.62	0.81
1:B:301:LYS:HZ3	1:B:329:GLU:HG3	1.45	0.81
1:C:223:LEU:HD12	1:C:251:LYS:HD3	1.63	0.81
1:C:111:ILE:O	1:C:115:LYS:HB2	1.82	0.80
1:B:207:LEU:HB3	1:B:208:PRO:CD	2.11	0.80
1:D:190:LEU:CB	1:D:289:VAL:HG22	2.10	0.79
1:A:328:GLY:N	1:B:320:THR:HG22	1.96	0.79
1:B:88:ILE:HD11	1:B:114:MET:HA	1.65	0.78
1:C:167:SER:HA	1:D:334:MET:HE2	1.64	0.78
1:B:161:ALA:HB3	1:B:323:PRO:CG	2.14	0.77
1:B:25:LEU:H	1:B:134:ASN:HD21	1.32	0.77
1:A:211:THR:HA	4:A:1369:HOH:O	1.85	0.76
1:B:72:GLU:OE1	1:B:111:ILE:HG12	1.86	0.75
1:B:207:LEU:HB3	1:B:208:PRO:HD2	1.68	0.75
1:C:105:LEU:HD23	1:C:105:LEU:H	1.51	0.75
1:A:62:ALA:O	1:A:92:ILE:HD13	1.87	0.75
1:B:137:PHE:HD1	1:B:138:LEU:HD12	1.51	0.75
1:C:309:ILE:HD13	1:C:355:THR:HB	1.68	0.75
1:A:72:GLU:OE2	1:A:111:ILE:HG12	1.87	0.74
1:C:94:ARG:HD3	1:C:96:PHE:CZ	2.22	0.74
1:C:181:GLN:HG3	1:C:182:TYR:N	2.02	0.74
1:B:234:ASP:O	1:B:236:ILE:N	2.20	0.73
1:A:120:GLU:N	4:A:1377:HOH:O	2.22	0.73
1:D:137:PHE:HD1	1:D:138:LEU:HD12	1.54	0.73
1:A:150:LEU:HB2	1:A:308:ILE:HD13	1.70	0.73
1:B:8:LEU:O	1:B:12:LEU:HD13	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:VAL:HG22	1:D:109:ARG:NH2	2.04	0.73
1:B:199:ASP:HB2	1:B:201:PRO:HD3	1.70	0.72
1:B:216:ARG:HD2	1:B:231:VAL:HG12	1.70	0.72
1:C:184:LYS:NZ	1:C:207:LEU:HB2	2.03	0.72
1:C:204:THR:HB	1:C:213:GLN:HE22	1.52	0.72
1:D:178:ASP:O	1:D:181:GLN:HG2	1.88	0.72
1:C:103:ASN:HD22	1:C:104:PRO:HD2	1.55	0.72
1:B:292:GLY:HA3	3:B:381:NDP:PA	2.29	0.72
1:A:44:LYS:HE3	1:C:35:GLN:NE2	2.05	0.72
1:B:243:THR:HG22	1:B:244:THR:N	2.04	0.72
1:D:193:VAL:HG13	1:D:220:ASP:HA	1.70	0.72
1:D:270:ILE:HD13	1:D:270:ILE:N	2.01	0.71
1:D:22:SER:HA	1:D:285:MET:HE1	1.73	0.70
1:B:161:ALA:HB3	1:B:323:PRO:HG3	1.72	0.70
1:A:184:LYS:HZ2	1:A:207:LEU:HD12	1.55	0.70
1:A:125:ILE:HD12	1:A:125:ILE:N	2.06	0.70
1:B:111:ILE:HG23	1:B:121:VAL:HG11	1.74	0.70
1:B:184:LYS:HB2	1:B:205:CYS:SG	2.32	0.70
1:B:187:GLN:HB3	1:B:284:ILE:HG23	1.74	0.70
1:C:99:MET:HE1	1:C:138:LEU:HD11	1.74	0.70
1:C:181:GLN:O	1:C:184:LYS:HG2	1.92	0.70
1:A:84:ALA:HB3	1:A:113:MET:HE2	1.73	0.69
1:B:216:ARG:NH1	1:B:231:VAL:HA	2.07	0.69
1:A:49:HIS:HD2	1:A:83:CYS:SG	2.15	0.69
1:C:220:ASP:OD2	1:C:223:LEU:HA	1.92	0.69
1:D:218:ILE:HD11	1:D:231:VAL:HG11	1.73	0.69
1:C:85:GLU:HB3	1:C:89:ASN:HD21	1.58	0.69
1:D:22:SER:HA	1:D:285:MET:CE	2.23	0.69
1:C:87:ILE:HA	1:C:92:ILE:HD12	1.74	0.69
1:D:270:ILE:H	1:D:270:ILE:CD1	1.99	0.69
1:B:301:LYS:NZ	1:B:329:GLU:HG3	2.07	0.68
1:B:234:ASP:O	1:B:236:ILE:HG12	1.92	0.68
1:B:275:VAL:O	1:B:279:LEU:HG	1.94	0.68
1:D:93:LYS:HB2	4:D:1388:HOH:O	1.93	0.68
1:C:6:MET:HE1	1:C:69:VAL:O	1.94	0.68
1:C:87:ILE:HG23	1:C:92:ILE:HD12	1.74	0.68
1:B:70:THR:O	1:B:98:ALA:HB3	1.94	0.68
1:A:329:GLU:HG2	4:A:1365:HOH:O	1.93	0.68
1:B:265:LEU:CD1	1:B:270:ILE:HG23	2.24	0.68
1:A:69:VAL:HG12	1:A:71:LEU:H	1.58	0.67
1:B:261:ASN:HB3	1:B:263:PHE:HE1	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:LYS:HD2	1:B:17:GLU:OE2	1.95	0.67
1:A:318:GLY:HA3	1:B:330:GLY:CA	2.24	0.67
1:B:98:ALA:O	1:B:127:ALA:HB2	1.95	0.67
4:A:1383:HOH:O	1:B:325:LEU:HB2	1.93	0.67
1:B:166:ASP:OD2	1:B:168:LYS:HE2	1.95	0.67
1:C:21:GLU:HG3	1:C:22:SER:N	2.07	0.67
1:C:93:LYS:O	1:C:119:ILE:HG23	1.94	0.67
1:C:25:LEU:N	1:C:134:ASN:HD21	1.91	0.67
1:B:63:GLU:HG3	1:B:91:GLY:HA3	1.77	0.67
1:B:134:ASN:O	1:B:138:LEU:HD13	1.95	0.67
1:B:79:LYS:HA	4:B:1367:HOH:O	1.95	0.66
1:A:170:ILE:HG12	1:B:334:MET:HE2	1.77	0.66
1:B:71:LEU:HD13	1:B:72:GLU:N	2.10	0.66
1:D:346:THR:HG22	1:D:347:GLN:N	2.09	0.66
1:A:334:MET:HA	1:A:337:VAL:HG12	1.77	0.66
1:B:137:PHE:CD1	1:B:138:LEU:HD12	2.31	0.66
1:B:270:ILE:HB	3:B:381:NDP:C2A	2.26	0.65
1:A:64:GLY:HA2	1:A:93:LYS:CG	2.26	0.65
1:A:190:LEU:HA	1:A:217:VAL:O	1.95	0.65
1:B:41:ALA:O	1:B:43:LEU:HD22	1.97	0.65
1:B:206:ARG:HB2	1:B:206:ARG:HH11	1.60	0.65
1:B:211:THR:O	1:B:212:LYS:HB2	1.97	0.65
1:A:53:HIS:HB3	1:C:57:MET:HE2	1.78	0.65
4:A:1374:HOH:O	1:C:35:GLN:HB3	1.97	0.65
1:C:180:GLN:HA	1:C:183:ARG:HD2	1.78	0.65
1:D:300:VAL:HG21	1:D:326:ILE:HD13	1.78	0.65
1:A:150:LEU:HD12	1:A:308:ILE:HD11	1.79	0.65
1:A:334:MET:HE2	1:B:170:ILE:HA	1.79	0.65
3:B:381:NDP:H52A	3:B:381:NDP:H8A	1.79	0.65
1:D:231:VAL:HB	1:D:239:THR:HG21	1.79	0.65
1:A:311:TYR:OH	1:A:353:LYS:HE2	1.98	0.64
1:D:190:LEU:HD13	1:D:191:VAL:N	2.12	0.64
1:D:230:LYS:O	1:D:234:ASP:HB3	1.96	0.64
1:D:346:THR:HG22	1:D:347:GLN:H	1.62	0.64
1:A:125:ILE:H	1:A:125:ILE:CD1	2.04	0.64
1:A:51:GLU:O	1:A:55:ILE:HG12	1.97	0.64
1:A:25:LEU:HB2	1:A:134:ASN:OD1	1.98	0.64
1:A:251:LYS:HG3	1:A:254:ARG:HH21	1.60	0.64
1:B:308:ILE:HG22	1:B:356:ALA:O	1.97	0.64
1:C:136:LYS:HG2	1:C:147:TYR:CG	2.32	0.64
1:C:6:MET:HB3	1:C:126:LEU:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:SER:HA	1:C:82:PRO:HB3	1.79	0.64
1:A:207:LEU:O	1:A:208:PRO:O	2.16	0.64
1:C:207:LEU:H	1:C:207:LEU:CD1	2.07	0.64
1:B:221:THR:HB	3:B:381:NDP:O3X	1.98	0.64
1:B:254:ARG:HG2	1:B:258:PHE:CE1	2.33	0.63
1:B:42:HIS:HD2	1:B:49:HIS:HA	1.62	0.63
1:D:141:MET:HA	1:D:141:MET:CE	2.26	0.63
1:B:84:ALA:O	1:B:88:ILE:HG12	1.99	0.63
1:D:243:THR:HG22	1:D:244:THR:H	1.63	0.63
1:C:151:LYS:HG3	1:C:288:TYR:OH	1.99	0.63
1:C:277:LYS:HE3	1:C:281:GLU:OE2	1.99	0.63
1:A:270:ILE:N	1:A:270:ILE:HD12	2.14	0.63
1:B:292:GLY:HA3	3:B:381:NDP:O2A	1.99	0.63
1:C:181:GLN:HG3	1:C:182:TYR:H	1.63	0.63
1:B:129:GLN:C	1:B:131:GLU:H	2.06	0.63
1:C:235:GLN:NE2	4:C:1395:HOH:O	2.32	0.63
1:D:277:LYS:NZ	1:D:277:LYS:HB3	2.13	0.63
1:B:243:THR:HG22	1:B:244:THR:H	1.62	0.62
1:C:188:SER:C	1:C:189:ILE:HD13	2.23	0.62
1:D:111:ILE:HG22	1:D:115:LYS:HE3	1.81	0.62
1:D:125:ILE:HD12	1:D:125:ILE:H	1.63	0.62
1:A:255:LEU:O	1:A:260:VAL:HG13	1.98	0.62
1:B:216:ARG:CZ	1:B:231:VAL:HA	2.30	0.62
1:C:347:GLN:HG3	1:C:351:ASP:O	2.00	0.62
1:A:184:LYS:HZ3	1:A:207:LEU:HB2	1.63	0.62
1:A:312:PHE:CE2	1:A:354:LEU:HD12	2.33	0.62
1:B:161:ALA:HB3	1:B:323:PRO:HG2	1.80	0.62
1:D:49:HIS:ND1	1:D:74:CYS:SG	2.71	0.62
1:D:310:PHE:CE2	1:D:325:LEU:HD13	2.35	0.62
1:C:6:MET:HE3	1:C:98:ALA:HB2	1.80	0.62
1:B:240:TRP:CD1	1:B:261:ASN:HB2	2.34	0.62
1:B:308:ILE:HD11	1:B:310:PHE:CE1	2.34	0.62
1:D:134:ASN:O	1:D:138:LEU:HD13	2.00	0.62
1:B:103:ASN:HD22	1:B:104:PRO:HD2	1.64	0.62
1:D:146:PRO:HD3	1:D:280:ALA:HB2	1.81	0.61
1:D:148:VAL:H	1:D:306:GLN:HE21	1.44	0.61
1:B:79:LYS:O	1:B:80:THR:HG23	2.00	0.61
1:B:308:ILE:CG2	1:B:356:ALA:HB3	2.29	0.61
1:C:77:TYR:HA	1:C:82:PRO:HG3	1.81	0.61
1:C:88:ILE:HG13	1:C:89:ASN:N	2.15	0.61
1:B:204:THR:HB	1:B:213:GLN:HE22	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:THR:HG21	1:B:247:ALA:HB2	1.83	0.61
1:B:291:GLY:O	1:B:295:VAL:HB	2.00	0.61
1:B:12:LEU:HD21	1:B:39:MET:HB3	1.83	0.61
1:D:148:VAL:H	1:D:306:GLN:HE22	1.46	0.61
1:C:161:ALA:HB3	1:C:323:PRO:CG	2.30	0.61
1:B:148:VAL:H	1:B:306:GLN:NE2	1.95	0.61
1:A:193:VAL:HG22	1:A:220:ASP:HA	1.82	0.61
1:B:125:ILE:HD12	1:B:125:ILE:H	1.66	0.61
1:C:173:GLU:HA	1:C:176:ARG:HD3	1.83	0.61
1:B:218:ILE:N	1:B:218:ILE:HD12	2.16	0.60
1:A:223:LEU:HD12	1:A:247:ALA:HB1	1.82	0.60
1:B:234:ASP:OD2	1:B:234:ASP:C	2.44	0.60
1:B:67:ILE:HG22	1:B:92:ILE:HG21	1.83	0.60
1:B:103:ASN:HD22	1:B:104:PRO:CD	2.14	0.60
1:D:343:THR:HG21	1:D:357:LYS:HG3	1.83	0.60
1:B:193:VAL:O	1:B:197:LYS:HG2	2.02	0.60
1:D:63:GLU:HB2	4:D:1394:HOH:O	2.01	0.60
1:D:297:GLY:HA2	1:D:326:ILE:HG23	1.83	0.60
1:A:6:MET:HE3	1:A:98:ALA:HB2	1.82	0.60
1:A:49:HIS:CD2	1:A:83:CYS:SG	2.94	0.60
1:D:150:LEU:CD2	1:D:289:VAL:HB	2.32	0.60
1:C:311:TYR:HE1	1:C:353:LYS:HD2	1.66	0.60
1:B:103:ASN:ND2	1:B:105:LEU:H	2.00	0.59
1:B:254:ARG:HG3	1:B:254:ARG:HH11	1.67	0.59
1:C:5:TYR:OH	1:C:31:VAL:HG21	2.01	0.59
1:B:199:ASP:CB	1:B:201:PRO:HD3	2.33	0.59
1:C:67:ILE:CG2	1:C:95:VAL:HG23	2.32	0.59
1:C:152:ALA:HB3	1:C:310:PHE:CE1	2.38	0.59
1:C:67:ILE:HG23	1:C:95:VAL:HG23	1.85	0.59
1:B:151:LYS:HD3	1:B:151:LYS:C	2.28	0.59
1:C:83:CYS:O	1:C:87:ILE:HG13	2.02	0.59
1:D:37:VAL:HG11	1:D:61:HIS:HB3	1.83	0.59
1:A:19:GLN:HE22	1:C:36:ILE:CD1	2.16	0.59
1:D:193:VAL:CG1	1:D:220:ASP:HA	2.33	0.59
1:B:292:GLY:HA2	3:B:381:NDP:H51N	1.84	0.58
4:A:1383:HOH:O	1:B:325:LEU:CB	2.49	0.58
1:B:74:CYS:SG	1:B:83:CYS:N	2.67	0.58
1:C:161:ALA:HB3	1:C:323:PRO:HG3	1.84	0.58
1:D:72:GLU:OE1	1:D:111:ILE:HG12	2.03	0.58
1:D:190:LEU:HD11	1:D:219:LEU:HD22	1.85	0.58
1:C:125:ILE:HD13	1:C:125:ILE:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:VAL:HG21	1:C:195:THR:HG21	1.85	0.58
1:D:80:THR:HB	1:D:81:PRO:HD2	1.83	0.58
1:B:44:LYS:NZ	1:D:35:GLN:HE22	2.02	0.58
1:B:284:ILE:N	1:B:284:ILE:HD12	2.19	0.58
1:B:302:GLU:HA	1:B:302:GLU:OE2	2.03	0.58
1:D:150:LEU:HD23	1:D:289:VAL:HB	1.84	0.58
1:C:103:ASN:HD22	1:C:104:PRO:CD	2.17	0.58
1:A:118:GLY:HA3	4:A:1403:HOH:O	2.04	0.58
1:A:83:CYS:O	1:A:87:ILE:HG12	2.04	0.57
1:B:177:GLN:O	1:B:180:GLN:HB2	2.04	0.57
1:D:269:ARG:HB2	4:D:1368:HOH:O	2.02	0.57
1:B:134:ASN:HB2	1:B:138:LEU:HD13	1.86	0.57
1:C:10:LEU:HD23	1:C:70:THR:HG21	1.87	0.57
1:C:187:GLN:NE2	1:C:285:MET:HE2	2.19	0.57
1:B:167:SER:O	1:B:169:TRP:N	2.37	0.57
1:C:157:ASP:HA	1:D:325:LEU:CD1	2.34	0.57
1:A:19:GLN:HE22	1:C:36:ILE:HD12	1.70	0.57
1:B:176:ARG:HH11	1:B:176:ARG:HG2	1.70	0.57
1:B:200:ASN:N	1:B:201:PRO:CD	2.67	0.57
1:B:270:ILE:HB	3:B:381:NDP:H2A	1.87	0.57
1:B:348:ILE:HD12	1:B:348:ILE:N	2.20	0.57
1:B:204:THR:O	1:B:206:ARG:HG3	2.05	0.57
1:C:193:VAL:HG13	1:C:220:ASP:HB2	1.86	0.57
1:B:191:VAL:CG1	1:B:195:THR:HB	2.34	0.57
1:D:178:ASP:OD1	1:D:348:ILE:HG13	2.04	0.57
1:C:180:GLN:CB	1:C:207:LEU:HD11	2.35	0.56
1:A:150:LEU:HD12	1:A:308:ILE:CD1	2.35	0.56
1:B:217:VAL:C	1:B:218:ILE:HD12	2.30	0.56
1:B:243:THR:CG2	1:B:244:THR:N	2.67	0.56
1:D:83:CYS:O	1:D:87:ILE:HG13	2.05	0.56
1:A:20:THR:HB	1:A:23:ASN:HB2	1.87	0.56
1:B:335:LYS:HD2	1:B:335:LYS:C	2.30	0.56
1:C:207:LEU:HD12	1:C:207:LEU:N	2.13	0.56
1:C:25:LEU:H	1:C:134:ASN:ND2	1.96	0.56
1:D:334:MET:O	1:D:337:VAL:HG12	2.05	0.56
1:A:290:GLU:O	1:A:296:HIS:CE1	2.58	0.56
1:B:243:THR:CG2	1:B:244:THR:H	2.18	0.56
1:C:205:CYS:SG	1:C:210:VAL:HG11	2.46	0.56
1:B:31:VAL:O	1:B:65:ALA:HB1	2.06	0.56
1:C:234:ASP:O	1:C:235:GLN:C	2.48	0.56
1:B:1:MET:HE2	1:B:1:MET:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ILE:HD12	1:B:125:ILE:N	2.21	0.56
1:D:101:ASP:OD1	1:D:102:PRO:HD2	2.06	0.56
1:C:28:ALA:HB3	1:C:50:ALA:O	2.05	0.55
1:C:55:ILE:HD11	1:C:92:ILE:HD11	1.87	0.55
1:A:66:ASP:OD2	1:A:94:ARG:HB2	2.06	0.55
1:C:94:ARG:HD3	1:C:96:PHE:HE2	1.64	0.55
1:C:131:GLU:OE1	1:C:142:ARG:NH2	2.32	0.55
1:B:176:ARG:HG2	1:B:176:ARG:NH1	2.21	0.55
1:B:258:PHE:N	1:B:258:PHE:HD1	2.05	0.55
1:D:17:GLU:HA	1:D:25:LEU:HD21	1.88	0.55
1:C:166:ASP:OD1	1:C:168:LYS:HG3	2.07	0.55
1:B:103:ASN:HD21	1:B:105:LEU:HD13	1.70	0.55
1:C:148:VAL:HB	1:C:305:PHE:HA	1.89	0.55
1:A:170:ILE:CG1	1:B:334:MET:HE2	2.36	0.55
1:B:240:TRP:CH2	1:B:284:ILE:HD11	2.42	0.55
1:B:308:ILE:HG21	1:B:356:ALA:HB3	1.87	0.55
1:C:265:LEU:HD11	1:C:275:VAL:HG22	1.89	0.55
1:D:296:HIS:O	1:D:300:VAL:HG23	2.05	0.55
1:C:120:GLU:HB3	4:C:1383:HOH:O	2.07	0.55
1:C:190:LEU:HD21	1:C:219:LEU:HD21	1.88	0.55
1:D:23:ASN:HD22	1:D:23:ASN:N	2.03	0.55
1:C:111:ILE:HG23	1:C:121:VAL:HG11	1.89	0.55
1:B:301:LYS:HZ3	1:B:329:GLU:CG	2.18	0.54
1:C:72:GLU:CD	1:C:111:ILE:HG12	2.32	0.54
1:C:221:THR:HG22	1:C:222:VAL:HG13	1.88	0.54
1:B:233:CYS:O	1:B:235:GLN:N	2.39	0.54
1:C:324:SER:HB3	4:C:1387:HOH:O	2.07	0.54
1:A:84:ALA:CB	1:A:113:MET:HE2	2.37	0.54
1:A:222:VAL:HG22	1:A:222:VAL:O	2.06	0.54
1:D:72:GLU:CD	1:D:111:ILE:HG12	2.33	0.54
1:A:1:MET:N	4:A:1368:HOH:O	2.40	0.54
1:B:193:VAL:HG11	1:B:220:ASP:CG	2.33	0.54
1:D:320:THR:HG22	1:D:321:HIS:H	1.72	0.54
1:D:243:THR:HG21	1:D:247:ALA:HB2	1.88	0.54
1:B:278:ILE:O	1:B:281:GLU:HB2	2.07	0.54
1:D:220:ASP:CG	1:D:223:LEU:HA	2.31	0.54
1:B:293:SER:OG	1:B:327:SER:HB2	2.08	0.54
1:A:105:LEU:O	1:A:105:LEU:HG	2.07	0.54
1:B:200:ASN:OD1	1:B:229:ALA:HA	2.07	0.54
1:C:10:LEU:HD23	1:C:70:THR:CG2	2.38	0.54
1:D:161:ALA:HB3	1:D:323:PRO:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:THR:O	1:C:212:LYS:HB2	2.07	0.54
1:B:17:GLU:HA	1:B:25:LEU:HD21	1.89	0.53
1:B:258:PHE:N	1:B:258:PHE:CD1	2.76	0.53
1:D:111:ILE:O	1:D:115:LYS:HG3	2.07	0.53
1:A:1:MET:HA	1:A:1:MET:CE	2.38	0.53
1:A:137:PHE:HD1	1:A:138:LEU:HD12	1.73	0.53
1:A:344:ASP:HB3	1:A:355:THR:CG2	2.39	0.53
1:B:35:GLN:OE1	1:D:19:GLN:HB2	2.09	0.53
1:C:93:LYS:NZ	1:C:93:LYS:HB3	2.23	0.53
1:A:9:ALA:O	1:A:27:GLY:HA3	2.08	0.53
1:A:190:LEU:HD23	1:A:191:VAL:N	2.23	0.53
1:C:103:ASN:HD21	1:C:105:LEU:HD21	1.74	0.53
1:D:99:MET:HE1	1:D:138:LEU:HD21	1.91	0.53
1:A:32:LYS:HE3	1:A:63:GLU:O	2.09	0.53
1:B:25:LEU:H	1:B:134:ASN:ND2	2.04	0.53
1:D:202:SER:O	1:D:204:THR:HG23	2.07	0.53
1:B:137:PHE:HD1	1:B:138:LEU:CD1	2.21	0.53
1:C:125:ILE:HD13	1:C:125:ILE:H	1.73	0.53
1:C:223:LEU:HD12	1:C:251:LYS:CD	2.37	0.53
1:C:235:GLN:HA	1:C:235:GLN:OE1	2.08	0.53
1:C:312:PHE:CE2	1:C:354:LEU:HD12	2.42	0.53
1:D:19:GLN:O	1:D:20:THR:HG23	2.09	0.53
1:A:207:LEU:HB3	1:A:208:PRO:HD2	1.90	0.53
1:C:168:LYS:HE3	1:C:169:TRP:CZ3	2.44	0.53
1:A:184:LYS:NZ	1:A:184:LYS:HB2	2.23	0.52
1:C:9:ALA:HB2	1:C:29:VAL:HG12	1.90	0.52
1:C:157:ASP:HA	1:D:325:LEU:HD12	1.91	0.52
1:A:26:VAL:O	1:A:41:ALA:HA	2.09	0.52
1:C:153:ALA:HB1	1:C:171:THR:CG2	2.39	0.52
1:D:232:ILE:HD12	1:D:255:LEU:HD22	1.92	0.52
1:A:184:LYS:HZ3	1:A:207:LEU:HD12	1.71	0.52
1:B:206:ARG:HH11	1:B:206:ARG:CB	2.21	0.52
1:B:251:LYS:HA	1:B:254:ARG:NH2	2.24	0.52
1:B:254:ARG:HH11	1:B:254:ARG:CG	2.21	0.52
1:D:337:VAL:HG13	1:D:337:VAL:O	2.08	0.52
1:D:101:ASP:OD2	1:D:106:VAL:HB	2.09	0.52
1:D:218:ILE:CD1	1:D:231:VAL:HG21	2.39	0.52
1:B:20:THR:HB	1:B:23:ASN:HB2	1.90	0.52
1:C:87:ILE:CG2	1:C:92:ILE:HD12	2.39	0.52
1:D:191:VAL:HG13	1:D:195:THR:HB	1.90	0.52
1:D:291:GLY:O	1:D:295:VAL:HB	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLN:OE1	1:C:44:LYS:HE3	2.10	0.52
1:A:277:LYS:NZ	1:A:277:LYS:HB3	2.24	0.52
1:B:150:LEU:HD23	1:B:289:VAL:HB	1.89	0.52
1:C:87:ILE:HG23	1:C:92:ILE:CD1	2.38	0.52
1:D:265:LEU:HD12	1:D:265:LEU:N	2.25	0.52
1:A:190:LEU:HG	1:A:217:VAL:HG12	1.92	0.52
1:A:193:VAL:HG13	1:A:220:ASP:HB2	1.90	0.52
1:B:234:ASP:O	1:B:235:GLN:C	2.52	0.52
1:D:19:GLN:HE21	1:D:44:LYS:HD2	1.75	0.52
1:D:216:ARG:O	1:D:239:THR:HA	2.09	0.52
1:A:251:LYS:HG3	1:A:254:ARG:NH2	2.25	0.52
1:A:325:LEU:HD12	1:B:157:ASP:HA	1.91	0.52
1:B:55:ILE:HD11	1:B:92:ILE:HD11	1.92	0.52
1:B:308:ILE:HD11	1:B:310:PHE:CZ	2.45	0.52
1:C:12:LEU:HD21	1:C:39:MET:HB3	1.91	0.52
1:A:16:GLY:O	1:A:19:GLN:HB2	2.09	0.52
1:C:136:LYS:HG2	1:C:147:TYR:CD2	2.45	0.52
1:C:169:TRP:O	1:C:315:LYS:HE3	2.10	0.51
1:C:160:ILE:HG12	1:C:323:PRO:O	2.09	0.51
1:D:177:GLN:HG3	4:D:1365:HOH:O	2.10	0.51
1:A:344:ASP:HB3	1:A:355:THR:HG23	1.92	0.51
1:B:7:LYS:HA	1:B:10:LEU:HD12	1.91	0.51
1:D:271:GLN:HG2	1:D:273:PRO:HD2	1.91	0.51
1:B:35:GLN:CD	1:D:19:GLN:HB2	2.36	0.51
1:C:90:SER:OG	1:C:92:ILE:HG13	2.09	0.51
1:C:187:GLN:HE22	1:C:285:MET:HG3	1.74	0.51
1:A:146:PRO:HA	1:A:285:MET:O	2.11	0.51
1:B:164:THR:O	1:B:164:THR:HG22	2.11	0.51
1:D:48:ALA:HB3	1:D:53:HIS:CE1	2.45	0.51
1:D:177:GLN:O	1:D:180:GLN:HB2	2.11	0.51
1:B:28:ALA:HA	1:B:68:TYR:O	2.11	0.51
1:B:102:PRO:HG2	1:B:137:PHE:HE1	1.76	0.51
1:C:8:LEU:HD22	1:C:12:LEU:HD13	1.92	0.51
1:C:37:VAL:HG22	1:C:37:VAL:O	2.10	0.51
1:D:222:VAL:HG22	1:D:222:VAL:O	2.10	0.51
1:A:109:ARG:HG3	4:A:1391:HOH:O	2.09	0.51
1:C:129:GLN:H	1:C:129:GLN:CD	2.18	0.51
1:B:184:LYS:NZ	1:B:210:VAL:HA	2.26	0.51
1:C:36:ILE:H	1:C:36:ILE:CD1	2.15	0.51
1:D:9:ALA:HB2	1:D:29:VAL:HG12	1.93	0.50
1:D:226:PRO:C	1:D:228:ASP:N	2.68	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:MET:CE	1:B:170:ILE:HA	2.41	0.50
1:B:169:TRP:HE3	1:B:169:TRP:HA	1.76	0.50
1:D:128:ASP:O	1:D:132:ARG:HG3	2.11	0.50
1:D:146:PRO:HG3	1:D:284:ILE:O	2.10	0.50
1:D:190:LEU:HD21	1:D:219:LEU:HD13	1.94	0.50
1:A:20:THR:O	1:A:21:GLU:HB2	2.10	0.50
1:A:57:MET:HG3	1:C:53:HIS:CE1	2.47	0.50
1:B:1:MET:N	4:B:1384:HOH:O	2.43	0.50
1:A:159:LYS:NZ	4:A:1383:HOH:O	2.35	0.50
1:C:25:LEU:HD23	1:C:133:LEU:HD11	1.93	0.50
1:C:66:ASP:CG	1:C:94:ARG:HD2	2.37	0.50
1:A:71:LEU:O	1:A:72:GLU:C	2.55	0.50
1:A:112:SER:O	1:A:116:GLU:HB2	2.11	0.50
1:B:131:GLU:OE2	1:B:138:LEU:HD23	2.11	0.50
1:D:148:VAL:HG23	1:D:306:GLN:HE22	1.76	0.50
1:A:74:CYS:O	1:A:82:PRO:HB2	2.11	0.50
1:A:175:ALA:O	1:A:178:ASP:N	2.44	0.50
1:C:151:LYS:HD2	1:C:151:LYS:C	2.37	0.50
1:B:53:HIS:CG	1:D:57:MET:HE3	2.47	0.50
1:A:325:LEU:CD1	1:B:157:ASP:HA	2.42	0.50
1:B:335:LYS:HD2	1:B:336:ASP:N	2.26	0.50
1:C:37:VAL:HG22	1:C:58:ALA:HA	1.94	0.50
1:C:116:GLU:C	1:C:118:GLY:H	2.19	0.50
1:B:169:TRP:HA	1:B:169:TRP:CE3	2.46	0.49
1:A:318:GLY:CA	1:B:330:GLY:HA2	2.35	0.49
1:C:49:HIS:ND1	1:C:83:CYS:SG	2.77	0.49
1:D:63:GLU:HA	1:D:91:GLY:HA3	1.93	0.49
1:A:150:LEU:HB2	1:A:308:ILE:CD1	2.40	0.49
1:A:320:THR:HG23	1:A:321:HIS:CD2	2.47	0.49
1:B:308:ILE:O	1:B:308:ILE:HG23	2.12	0.49
1:C:68:TYR:N	1:C:68:TYR:CD2	2.79	0.49
1:D:188:SER:OG	1:D:287:VAL:HG22	2.11	0.49
1:A:6:MET:HE1	1:A:69:VAL:O	2.12	0.49
1:A:136:LYS:HE3	1:A:185:THR:O	2.13	0.49
1:B:55:ILE:HG13	1:B:86:LEU:CD1	2.43	0.49
1:D:160:ILE:O	1:D:160:ILE:HG22	2.12	0.49
1:A:44:LYS:HE3	1:C:35:GLN:HE21	1.74	0.49
1:A:157:ASP:OD2	1:A:159:LYS:HD3	2.13	0.49
1:A:193:VAL:HG11	1:A:220:ASP:CG	2.38	0.49
1:C:14:LYS:HE3	1:C:17:GLU:OE2	2.13	0.49
1:C:56:HIS:ND1	1:C:56:HIS:C	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:VAL:HG21	1:D:299:PHE:CZ	2.47	0.49
1:B:312:PHE:CE2	1:B:354:LEU:HD12	2.48	0.49
1:C:95:VAL:HG11	1:C:114:MET:HE3	1.95	0.49
1:C:208:PRO:O	1:C:209:ASN:HB2	2.12	0.49
1:B:25:LEU:N	1:B:134:ASN:HD21	2.06	0.49
1:B:66:ASP:HA	1:B:94:ARG:O	2.13	0.49
1:C:180:GLN:O	1:C:183:ARG:HB2	2.11	0.49
1:D:200:ASN:O	1:D:230:LYS:HG3	2.13	0.49
1:A:29:VAL:O	1:A:67:ILE:HA	2.13	0.49
1:C:267:THR:HG22	1:C:268:GLU:H	1.78	0.49
1:D:272:ILE:CG1	1:D:298:SER:HB3	2.43	0.49
1:A:312:PHE:HE2	1:A:354:LEU:HD12	1.75	0.49
1:B:3:GLU:CB	1:B:126:LEU:HD11	2.37	0.49
1:B:14:LYS:HE3	4:B:1374:HOH:O	2.11	0.49
1:B:195:THR:O	1:B:196:VAL:C	2.56	0.49
1:B:255:LEU:O	1:B:260:VAL:HB	2.13	0.49
1:C:67:ILE:HG23	1:C:67:ILE:O	2.13	0.49
1:C:129:GLN:CD	1:C:129:GLN:N	2.71	0.49
1:A:184:LYS:HZ2	1:A:184:LYS:HB2	1.78	0.48
1:A:199:ASP:O	1:A:200:ASN:C	2.56	0.48
1:B:65:ALA:O	1:B:92:ILE:HG23	2.13	0.48
1:C:95:VAL:HG12	1:C:121:VAL:HG22	1.95	0.48
1:C:170:ILE:HD11	1:D:334:MET:HE1	1.95	0.48
1:B:53:HIS:HB3	1:D:57:MET:HE3	1.95	0.48
1:D:223:LEU:HD23	1:D:225:ILE:HG22	1.95	0.48
1:A:74:CYS:SG	1:A:83:CYS:N	2.76	0.48
1:A:272:ILE:N	1:A:273:PRO:CD	2.76	0.48
1:C:87:ILE:CA	1:C:92:ILE:HD12	2.42	0.48
1:C:193:VAL:HG11	1:C:220:ASP:CG	2.39	0.48
1:C:333:SER:HB3	1:C:336:ASP:OD2	2.14	0.48
1:D:75:SER:HB2	1:D:109:ARG:HD2	1.95	0.48
1:D:156:LEU:HB3	1:D:316:LEU:HD23	1.95	0.48
1:A:67:ILE:CG2	1:A:95:VAL:HG22	2.44	0.48
1:A:180:GLN:HB3	1:A:207:LEU:HD21	1.95	0.48
1:D:19:GLN:CG	1:D:44:LYS:HD2	2.37	0.48
1:B:254:ARG:HG2	1:B:258:PHE:CZ	2.49	0.48
1:A:114:MET:O	1:A:115:LYS:C	2.57	0.48
1:C:68:TYR:N	1:C:68:TYR:HD2	2.12	0.48
1:D:14:LYS:O	1:D:17:GLU:HB2	2.13	0.48
1:A:20:THR:O	1:A:45:TYR:HD1	1.97	0.48
1:D:124:GLY:O	1:D:125:ILE:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:ASN:N	1:D:201:PRO:CD	2.76	0.48
1:D:343:THR:HG21	1:D:357:LYS:HE2	1.95	0.48
1:D:339:LEU:O	1:D:359:THR:HG22	2.14	0.47
1:A:19:GLN:CD	1:C:35:GLN:HB2	2.39	0.47
1:B:103:ASN:HD22	1:B:103:ASN:C	2.21	0.47
1:C:95:VAL:HG11	1:C:114:MET:CE	2.44	0.47
1:A:184:LYS:HZ3	1:A:207:LEU:CB	2.27	0.47
1:B:202:SER:CB	1:B:230:LYS:HD2	2.44	0.47
1:B:272:ILE:HB	1:B:273:PRO:HD3	1.96	0.47
1:D:287:VAL:HG12	1:D:289:VAL:HG23	1.96	0.47
1:A:90:SER:OG	1:A:92:ILE:HG12	2.14	0.47
1:A:175:ALA:O	1:A:176:ARG:C	2.56	0.47
1:B:191:VAL:HG13	1:B:291:GLY:HA3	1.97	0.47
1:B:345:ILE:HG23	1:B:354:LEU:HD23	1.97	0.47
1:A:32:LYS:HD3	1:A:32:LYS:C	2.39	0.47
1:A:202:SER:O	1:A:216:ARG:HD2	2.14	0.47
1:B:6:MET:HE1	1:B:96:PHE:O	2.15	0.47
1:B:210:VAL:O	1:B:212:LYS:N	2.47	0.47
1:A:42:HIS:HE1	1:A:47:GLU:O	1.97	0.47
1:B:102:PRO:HG2	1:B:137:PHE:CE1	2.49	0.47
1:B:184:LYS:HZ1	1:B:210:VAL:HA	1.80	0.47
1:B:198:ALA:C	1:B:199:ASP:OD1	2.57	0.47
1:C:84:ALA:O	1:C:88:ILE:HG23	2.14	0.47
1:C:112:SER:O	1:C:115:LYS:N	2.47	0.47
1:D:140:PHE:CG	1:D:285:MET:HG2	2.49	0.47
1:D:263:PHE:CD2	1:D:278:ILE:HG21	2.48	0.47
1:A:134:ASN:C	1:A:138:LEU:HD13	2.40	0.47
1:B:12:LEU:CD2	1:B:39:MET:HB3	2.44	0.47
1:C:103:ASN:HD21	1:C:105:LEU:CD2	2.27	0.47
1:C:314:PRO:HG3	1:D:342:PHE:CE2	2.49	0.47
1:D:19:GLN:CG	1:D:44:LYS:HA	2.45	0.47
1:C:33:ASP:N	1:C:33:ASP:OD2	2.48	0.47
1:C:240:TRP:CD1	1:C:261:ASN:HB2	2.50	0.47
1:D:140:PHE:CD2	1:D:285:MET:HG2	2.49	0.47
1:A:123:GLU:O	1:A:125:ILE:HD12	2.14	0.47
1:D:1:MET:HG3	1:D:5:TYR:CE2	2.50	0.47
1:D:64:GLY:HA2	1:D:93:LYS:HG2	1.96	0.47
1:D:311:TYR:CE1	1:D:353:LYS:HD2	2.50	0.47
1:C:9:ALA:HB2	1:C:29:VAL:CG1	2.45	0.46
1:C:103:ASN:HB3	1:C:106:VAL:HG22	1.97	0.46
1:A:222:VAL:HG12	4:A:1395:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ILE:HG23	1:B:67:ILE:O	2.15	0.46
1:B:301:LYS:CE	1:B:329:GLU:HB2	2.45	0.46
1:B:301:LYS:HD3	1:B:329:GLU:HB2	1.96	0.46
1:B:126:LEU:C	1:B:128:ASP:N	2.74	0.46
1:A:207:LEU:HB3	1:A:208:PRO:CD	2.46	0.46
1:B:254:ARG:HB2	1:B:254:ARG:NH1	2.31	0.46
1:C:85:GLU:O	1:C:88:ILE:N	2.47	0.46
1:B:129:GLN:C	1:B:131:GLU:N	2.72	0.46
1:B:168:LYS:O	1:B:169:TRP:HB2	2.16	0.46
1:B:227:GLU:CD	1:B:227:GLU:H	2.23	0.46
1:C:7:LYS:O	1:C:10:LEU:HB2	2.15	0.46
1:C:100:ARG:HH21	1:C:108:GLY:HA2	1.79	0.46
1:A:56:HIS:NE2	1:C:56:HIS:NE2	2.64	0.46
1:B:202:SER:HB2	1:B:230:LYS:HD2	1.96	0.46
1:B:85:GLU:HG2	1:B:89:ASN:HD21	1.80	0.46
1:B:193:VAL:HG13	1:B:219:LEU:O	2.16	0.46
1:B:213:GLN:HB3	1:B:237:ALA:HB2	1.98	0.46
1:B:301:LYS:NZ	1:B:329:GLU:CG	2.77	0.46
1:B:301:LYS:NZ	1:B:329:GLU:CB	2.79	0.46
1:B:198:ALA:O	1:B:199:ASP:OD1	2.33	0.46
1:D:88:ILE:HA	1:D:119:ILE:HD11	1.97	0.46
1:D:99:MET:HE1	1:D:138:LEU:CD2	2.46	0.46
1:C:85:GLU:HB3	1:C:89:ASN:ND2	2.27	0.46
1:A:134:ASN:HB2	1:A:138:LEU:CD1	2.46	0.45
1:B:95:VAL:HG23	1:B:119:ILE:HG21	1.98	0.45
1:B:329:GLU:OE1	1:B:329:GLU:HA	2.15	0.45
1:C:23:ASN:N	1:C:23:ASN:HD22	2.14	0.45
1:C:344:ASP:HB3	1:C:355:THR:CG2	2.45	0.45
1:A:30:VAL:HG12	1:A:37:VAL:CG2	2.47	0.45
1:C:71:LEU:HD13	1:C:99:MET:HE2	1.97	0.45
1:D:180:GLN:HE21	1:D:180:GLN:HB3	1.53	0.45
1:A:64:GLY:CA	1:A:93:LYS:HG2	2.40	0.45
1:C:37:VAL:HG21	1:C:61:HIS:CD2	2.52	0.45
1:C:85:GLU:O	1:C:88:ILE:HG12	2.17	0.45
1:C:307:GLU:CD	1:C:357:LYS:HZ3	2.24	0.45
1:C:315:LYS:HE2	1:D:339:LEU:HD13	1.98	0.45
1:D:226:PRO:C	1:D:228:ASP:H	2.25	0.45
1:D:277:LYS:HB3	1:D:277:LYS:HZ3	1.82	0.45
1:B:263:PHE:CD2	1:B:278:ILE:HG21	2.52	0.45
1:C:153:ALA:HB1	1:C:171:THR:HG23	1.97	0.45
1:C:331:PHE:CE1	1:C:338:PRO:HD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:SER:N	1:D:170:ILE:HD11	2.32	0.45
1:B:134:ASN:HB3	1:B:137:PHE:HB3	1.99	0.45
1:B:277:LYS:O	1:B:281:GLU:HG3	2.17	0.45
1:C:216:ARG:HD2	1:C:237:ALA:HB3	1.98	0.45
1:B:92:ILE:O	1:B:119:ILE:HD12	2.17	0.45
1:B:310:PHE:CE1	1:B:325:LEU:HD22	2.51	0.45
1:C:82:PRO:O	1:C:85:GLU:N	2.47	0.45
1:C:157:ASP:HA	1:D:325:LEU:HD13	1.99	0.45
1:A:193:VAL:CG2	1:A:220:ASP:HA	2.46	0.45
1:C:85:GLU:HG3	1:C:113:MET:HE2	1.99	0.45
1:C:237:ALA:HB1	1:C:238:PRO:CD	2.47	0.45
1:C:311:TYR:CE1	1:C:353:LYS:HD2	2.50	0.45
1:B:308:ILE:HG22	1:B:356:ALA:C	2.42	0.45
1:C:55:ILE:O	1:C:58:ALA:N	2.36	0.45
1:C:85:GLU:HA	1:C:88:ILE:HG12	1.99	0.45
1:D:252:LYS:HE3	1:D:264:THR:HG21	1.98	0.45
1:D:346:THR:CG2	1:D:347:GLN:N	2.78	0.45
1:A:32:LYS:HB2	1:A:37:VAL:HG11	1.99	0.45
1:A:348:ILE:HD11	1:A:353:LYS:HE3	1.99	0.45
1:C:55:ILE:CD1	1:C:92:ILE:HD11	2.46	0.45
1:C:82:PRO:C	1:C:84:ALA:N	2.75	0.45
1:C:170:ILE:CD1	1:D:334:MET:HE1	2.46	0.45
1:D:100:ARG:HE	1:D:123:GLU:CD	2.24	0.45
1:D:181:GLN:O	1:D:184:LYS:HB3	2.16	0.45
1:A:14:LYS:C	1:A:16:GLY:H	2.25	0.44
1:C:346:THR:O	1:C:353:LYS:HB3	2.17	0.44
1:A:334:MET:HA	1:A:337:VAL:CG1	2.47	0.44
1:B:204:THR:HB	1:B:213:GLN:NE2	2.32	0.44
1:C:88:ILE:CG1	1:C:89:ASN:N	2.79	0.44
1:C:189:ILE:HD13	1:C:189:ILE:N	2.32	0.44
1:D:19:GLN:HG2	1:D:44:LYS:CD	2.37	0.44
1:D:72:GLU:HG3	1:D:111:ILE:CD1	2.47	0.44
1:B:257:ALA:C	1:B:259:GLY:H	2.25	0.44
1:B:293:SER:H	3:B:381:NDP:H52N	1.82	0.44
1:C:334:MET:C	1:C:336:ASP:H	2.25	0.44
1:D:326:ILE:O	1:D:326:ILE:HG22	2.17	0.44
1:B:53:HIS:CB	1:D:57:MET:HE3	2.47	0.44
1:B:200:ASN:CG	1:B:200:ASN:O	2.60	0.44
1:B:223:LEU:HB2	1:B:243:THR:HG21	1.99	0.44
1:C:5:TYR:CZ	1:C:31:VAL:HG21	2.52	0.44
1:C:6:MET:O	1:C:10:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:LYS:HG2	1:C:33:ASP:OD2	2.17	0.44
1:D:23:ASN:N	1:D:23:ASN:ND2	2.66	0.44
1:D:190:LEU:HD21	1:D:219:LEU:CD1	2.47	0.44
1:A:49:HIS:HD2	1:A:74:CYS:SG	2.40	0.44
1:A:148:VAL:HB	1:A:305:PHE:HA	2.00	0.44
1:B:246:ARG:HG3	1:B:246:ARG:HH11	1.83	0.44
1:C:116:GLU:C	1:C:118:GLY:N	2.74	0.44
1:D:230:LYS:O	1:D:232:ILE:N	2.50	0.44
1:B:261:ASN:HB3	1:B:263:PHE:CE1	2.45	0.44
1:A:311:TYR:CZ	1:A:353:LYS:HE2	2.52	0.44
1:C:174:ALA:HB1	1:C:348:ILE:HG22	2.00	0.44
1:D:204:THR:HB	1:D:213:GLN:NE2	2.33	0.44
1:D:300:VAL:HG21	1:D:326:ILE:CD1	2.45	0.44
1:A:12:LEU:CD1	1:A:39:MET:HB3	2.48	0.44
1:A:308:ILE:O	1:A:355:THR:HA	2.18	0.44
1:A:342:PHE:HA	1:A:356:ALA:HB2	2.00	0.44
1:C:28:ALA:H	1:C:50:ALA:HB1	1.82	0.44
1:C:337:VAL:HG23	1:C:337:VAL:O	2.16	0.44
1:D:76:HIS:O	1:D:82:PRO:HB3	2.18	0.44
1:D:134:ASN:HB3	1:D:137:PHE:HB3	2.00	0.44
1:D:151:LYS:HE2	1:D:179:ALA:HB1	2.00	0.44
1:D:160:ILE:O	1:D:160:ILE:CG2	2.66	0.44
1:D:272:ILE:HB	1:D:273:PRO:CD	2.39	0.44
1:A:329:GLU:O	1:B:319:GLY:HA2	2.17	0.44
1:B:80:THR:HB	1:B:81:PRO:HD2	2.00	0.44
1:B:348:ILE:HD13	1:B:353:LYS:HB2	2.00	0.44
1:C:6:MET:CB	1:C:126:LEU:HD12	2.45	0.44
1:C:99:MET:HE1	1:C:138:LEU:CD1	2.47	0.44
1:D:137:PHE:CD1	1:D:138:LEU:HD12	2.43	0.44
1:D:274:ASP:O	1:D:278:ILE:HG12	2.18	0.44
1:B:99:MET:HE2	1:B:100:ARG:O	2.16	0.43
1:A:157:ASP:HB2	4:A:1383:HOH:O	2.18	0.43
1:D:272:ILE:CB	1:D:273:PRO:HD3	2.35	0.43
1:A:134:ASN:HB2	1:A:138:LEU:HD11	1.99	0.43
1:B:61:HIS:NE2	1:D:44:LYS:HE2	2.33	0.43
1:B:234:ASP:CG	1:B:236:ILE:HG12	2.44	0.43
1:B:311:TYR:OH	1:B:353:LYS:HE3	2.17	0.43
1:C:96:PHE:CD2	1:C:96:PHE:N	2.86	0.43
1:C:344:ASP:HB3	1:C:355:THR:HG23	2.00	0.43
1:A:17:GLU:HA	1:A:25:LEU:HD11	1.99	0.43
1:A:181:GLN:HA	1:A:207:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:LYS:HE2	1:C:184:LYS:HB3	1.82	0.43
1:A:32:LYS:HB2	1:A:37:VAL:CG1	2.47	0.43
1:A:269:ARG:C	1:A:270:ILE:HD12	2.44	0.43
1:C:63:GLU:HA	1:C:91:GLY:O	2.19	0.43
1:C:180:GLN:O	1:C:181:GLN:C	2.62	0.43
1:C:216:ARG:HH22	1:C:234:ASP:CG	2.26	0.43
1:C:312:PHE:HE2	1:C:354:LEU:HD12	1.82	0.43
1:C:331:PHE:CD1	1:C:337:VAL:HG12	2.54	0.43
1:A:359:THR:HG22	4:A:1416:HOH:O	2.19	0.43
1:B:42:HIS:CD2	1:B:49:HIS:HD2	2.37	0.43
1:B:82:PRO:O	1:B:85:GLU:N	2.52	0.43
1:B:221:THR:O	1:B:243:THR:HG23	2.18	0.43
1:A:161:ALA:O	1:A:323:PRO:HD2	2.18	0.43
1:A:319:GLY:HA3	1:A:322:ALA:HB2	2.00	0.43
1:C:29:VAL:HG13	1:C:68:TYR:HB2	1.99	0.43
1:C:328:GLY:O	1:D:319:GLY:HA2	2.18	0.43
1:A:55:ILE:HD11	1:A:67:ILE:HD12	2.00	0.43
1:B:254:ARG:CG	1:B:254:ARG:NH1	2.81	0.43
1:C:95:VAL:CG1	1:C:121:VAL:HG22	2.48	0.43
1:D:190:LEU:HD13	1:D:191:VAL:H	1.82	0.43
1:D:277:LYS:O	1:D:281:GLU:HG3	2.18	0.43
1:B:252:LYS:O	1:B:256:SER:HB3	2.19	0.43
1:C:12:LEU:CD2	1:C:39:MET:HB3	2.49	0.43
1:A:290:GLU:O	1:A:296:HIS:NE2	2.51	0.43
1:B:138:LEU:O	1:B:142:ARG:HG3	2.19	0.43
1:C:28:ALA:HA	1:C:68:TYR:O	2.19	0.43
1:D:22:SER:HA	1:D:285:MET:HE2	2.00	0.43
1:D:337:VAL:O	1:D:337:VAL:CG1	2.67	0.43
1:B:126:LEU:C	1:B:128:ASP:H	2.27	0.42
1:D:6:MET:HE1	1:D:96:PHE:O	2.20	0.42
1:D:208:PRO:O	1:D:209:ASN:HB2	2.19	0.42
1:D:230:LYS:C	1:D:232:ILE:N	2.77	0.42
1:C:28:ALA:HB3	1:C:50:ALA:C	2.44	0.42
1:C:146:PRO:HA	1:C:285:MET:O	2.19	0.42
1:C:152:ALA:HB3	1:C:310:PHE:CD1	2.54	0.42
1:C:181:GLN:NE2	1:C:182:TYR:CE2	2.88	0.42
1:D:131:GLU:OE1	1:D:142:ARG:NH2	2.45	0.42
1:D:139:HIS:O	1:D:143:THR:HG23	2.19	0.42
1:D:272:ILE:HG12	1:D:298:SER:HB3	2.00	0.42
1:B:83:CYS:O	1:B:87:ILE:HG13	2.19	0.42
1:A:14:LYS:HG3	1:A:14:LYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ILE:O	1:C:43:LEU:HD13	2.18	0.42
1:A:248:ASP:O	1:A:252:LYS:HG3	2.19	0.42
1:B:202:SER:O	1:B:203:LEU:HB2	2.18	0.42
1:C:140:PHE:HE1	1:C:280:ALA:HB1	1.85	0.42
1:C:199:ASP:O	1:C:200:ASN:C	2.62	0.42
1:D:150:LEU:HB2	1:D:308:ILE:HD13	2.02	0.42
1:D:184:LYS:HD2	1:D:207:LEU:HD23	2.01	0.42
1:D:268:GLU:C	1:D:269:ARG:HG2	2.44	0.42
1:B:51:GLU:OE1	1:B:83:CYS:CB	2.67	0.42
1:B:103:ASN:ND2	1:B:103:ASN:C	2.74	0.42
1:B:258:PHE:HD1	1:B:258:PHE:H	1.66	0.42
1:C:8:LEU:HD22	1:C:12:LEU:CD1	2.49	0.42
1:C:28:ALA:CB	1:C:51:GLU:HA	2.49	0.42
1:C:173:GLU:O	1:C:177:GLN:HB2	2.20	0.42
1:C:239:THR:O	1:C:260:VAL:HG13	2.19	0.42
1:C:306:GLN:N	1:C:306:GLN:CD	2.78	0.42
1:D:227:GLU:OE2	1:D:254:ARG:HD2	2.20	0.42
1:A:13:ALA:HB2	1:A:27:GLY:N	2.34	0.42
1:A:170:ILE:HG12	1:B:334:MET:CE	2.46	0.42
1:B:9:ALA:O	1:B:27:GLY:HA3	2.20	0.42
1:A:345:ILE:HD12	1:A:345:ILE:N	2.34	0.42
1:B:176:ARG:HD3	1:B:176:ARG:N	2.35	0.42
1:B:220:ASP:CG	1:B:223:LEU:HA	2.44	0.42
1:B:234:ASP:O	1:B:234:ASP:CG	2.62	0.42
1:C:100:ARG:NH1	1:C:123:GLU:OE2	2.53	0.42
1:A:292:GLY:O	1:A:293:SER:C	2.63	0.42
1:B:284:ILE:N	1:B:284:ILE:CD1	2.83	0.42
1:B:296:HIS:HB3	1:B:326:ILE:HD12	2.02	0.42
1:C:9:ALA:HB1	1:C:27:GLY:O	2.20	0.42
1:D:67:ILE:HG22	1:D:95:VAL:HG22	2.01	0.42
1:A:157:ASP:HB3	1:A:316:LEU:HD22	2.02	0.42
1:B:210:VAL:HG23	1:B:211:THR:N	2.35	0.42
1:C:191:VAL:O	1:C:218:ILE:HA	2.20	0.42
1:C:234:ASP:O	1:C:236:ILE:N	2.52	0.42
1:C:234:ASP:O	1:C:236:ILE:HG13	2.19	0.42
1:D:202:SER:O	1:D:203:LEU:C	2.63	0.42
1:A:123:GLU:C	1:A:125:ILE:HD12	2.45	0.41
1:B:213:GLN:HB3	1:B:237:ALA:CB	2.49	0.41
1:C:8:LEU:C	1:C:8:LEU:HD13	2.45	0.41
1:D:56:HIS:C	1:D:58:ALA:N	2.77	0.41
1:D:216:ARG:CZ	1:D:231:VAL:HA	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLN:O	1:C:36:ILE:HD13	2.20	0.41
1:A:190:LEU:HD23	1:A:190:LEU:C	2.45	0.41
1:B:206:ARG:NH1	1:B:206:ARG:CB	2.76	0.41
1:B:218:ILE:N	1:B:218:ILE:CD1	2.82	0.41
1:C:272:ILE:HB	1:C:273:PRO:HD3	2.02	0.41
1:C:290:GLU:O	1:C:296:HIS:NE2	2.54	0.41
1:D:230:LYS:HB2	4:D:1404:HOH:O	2.19	0.41
1:B:102:PRO:HB2	1:B:141:MET:CB	2.49	0.41
1:B:106:VAL:O	1:B:107:ALA:C	2.62	0.41
1:B:115:LYS:HE3	1:B:115:LYS:HB2	1.85	0.41
1:C:72:GLU:HA	1:C:73:PRO:HD3	1.92	0.41
1:C:234:ASP:OD2	1:C:234:ASP:C	2.63	0.41
1:D:72:GLU:HB2	1:D:100:ARG:HA	2.02	0.41
1:D:218:ILE:HD11	1:D:231:VAL:HG21	2.01	0.41
1:B:102:PRO:HB2	1:B:141:MET:HB2	2.02	0.41
1:B:308:ILE:O	1:B:355:THR:HA	2.20	0.41
1:C:28:ALA:O	1:C:54:ALA:HB2	2.21	0.41
1:A:115:LYS:HE2	1:A:121:VAL:HB	2.02	0.41
1:A:132:ARG:O	1:A:135:GLU:HB2	2.20	0.41
1:A:147:TYR:N	1:A:285:MET:O	2.44	0.41
1:B:77:TYR:CE2	1:B:113:MET:HE2	2.55	0.41
1:B:103:ASN:HD22	1:B:104:PRO:N	2.18	0.41
1:B:125:ILE:H	1:B:125:ILE:CD1	2.32	0.41
1:C:272:ILE:N	1:C:273:PRO:CD	2.83	0.41
1:D:125:ILE:HG22	1:D:126:LEU:HG	2.02	0.41
1:D:161:ALA:HB3	1:D:323:PRO:CG	2.50	0.41
1:D:343:THR:CG2	1:D:357:LYS:HG3	2.50	0.41
1:C:69:VAL:HG21	1:C:73:PRO:HD3	2.01	0.41
1:D:29:VAL:HG13	1:D:68:TYR:HB2	2.02	0.41
1:A:24:PRO:HD3	1:A:137:PHE:CE2	2.56	0.41
1:A:191:VAL:O	1:A:218:ILE:HA	2.20	0.41
1:B:292:GLY:HA2	3:B:381:NDP:C5D	2.51	0.41
1:C:30:VAL:HB	1:C:38:GLY:HA3	2.01	0.41
1:D:136:LYS:HE3	1:D:185:THR:O	2.19	0.41
1:D:289:VAL:HG21	1:D:299:PHE:CE2	2.56	0.41
1:A:176:ARG:HD2	4:A:1385:HOH:O	2.21	0.41
1:B:12:LEU:HD12	1:B:12:LEU:N	2.36	0.41
1:D:23:ASN:ND2	1:D:23:ASN:H	2.18	0.41
1:A:30:VAL:O	1:A:37:VAL:HG22	2.21	0.41
1:A:103:ASN:HA	1:A:104:PRO:HD3	1.94	0.41
1:B:32:LYS:HE2	1:B:33:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:GLY:HA3	3:B:381:NDP:O1A	2.20	0.41
1:C:170:ILE:HG22	1:C:171:THR:N	2.35	0.41
1:C:190:LEU:HD12	1:C:289:VAL:HG13	2.01	0.41
1:C:296:HIS:O	1:C:297:GLY:C	2.63	0.41
1:D:75:SER:CB	1:D:109:ARG:HD2	2.51	0.41
1:D:166:ASP:OD1	1:D:168:LYS:HG3	2.20	0.41
1:D:233:CYS:O	1:D:235:GLN:N	2.54	0.41
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.87	0.41
1:A:334:MET:HB2	1:B:168:LYS:HB2	2.03	0.41
1:B:347:GLN:C	1:B:348:ILE:HD12	2.45	0.41
1:C:181:GLN:NE2	1:C:182:TYR:CD2	2.87	0.41
1:C:253:LYS:HA	1:C:256:SER:OG	2.21	0.41
1:C:308:ILE:HD11	1:C:310:PHE:CZ	2.56	0.41
1:D:186:HIS:CD2	1:D:288:TYR:HB2	2.56	0.41
1:B:6:MET:HG2	1:B:125:ILE:O	2.21	0.40
1:B:155:SER:HB3	1:B:317:ILE:HG13	2.03	0.40
1:C:96:PHE:HA	1:C:122:ARG:O	2.21	0.40
1:C:155:SER:HB3	1:C:317:ILE:HG12	2.02	0.40
1:D:37:VAL:HG11	1:D:61:HIS:CB	2.50	0.40
1:D:129:GLN:HE21	1:D:129:GLN:HB3	1.68	0.40
1:A:25:LEU:HA	4:A:1375:HOH:O	2.21	0.40
1:A:107:ALA:C	1:A:109:ARG:H	2.29	0.40
1:A:337:VAL:HA	1:A:338:PRO:HD3	1.87	0.40
1:B:51:GLU:O	1:B:55:ILE:HG12	2.21	0.40
1:B:86:LEU:HD13	1:B:86:LEU:O	2.21	0.40
1:D:9:ALA:HB2	1:D:29:VAL:CG1	2.51	0.40
1:A:32:LYS:C	1:A:32:LYS:CD	2.94	0.40
1:B:79:LYS:O	1:B:80:THR:CG2	2.69	0.40
1:D:20:THR:O	1:D:21:GLU:HB2	2.21	0.40
1:A:1:MET:HA	1:A:1:MET:HE3	2.03	0.40
1:B:26:VAL:HG12	1:B:27:GLY:N	2.36	0.40
1:C:174:ALA:CB	1:C:348:ILE:HG22	2.52	0.40
1:C:253:LYS:O	1:C:254:ARG:C	2.63	0.40
1:D:19:GLN:HE21	1:D:44:LYS:NZ	2.19	0.40
1:D:101:ASP:HA	1:D:102:PRO:HD3	1.79	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)
4:A:1398:HOH:O	4:B:1422:HOH:O[3_645]	1.93	0.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1410:HOH:O	4:A:1419:HOH:O[3_645]	2.19	0.01

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	357/373 (96%)	310 (87%)	41 (12%)	6 (2%)	7	30
1	B	357/373 (96%)	303 (85%)	44 (12%)	10 (3%)	4	19
1	C	357/373 (96%)	303 (85%)	43 (12%)	11 (3%)	3	16
1	D	358/373 (96%)	309 (86%)	33 (9%)	16 (4%)	2	10
All	All	1429/1492 (96%)	1225 (86%)	161 (11%)	43 (3%)	3	17

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	PRO
1	A	329	GLU
1	B	168	LYS
1	B	208	PRO
1	B	211	THR
1	B	212	LYS
1	B	234	ASP
1	B	235	GLN
1	C	67	ILE
1	C	209	ASN
1	C	212	LYS
1	C	235	GLN
1	D	20	THR
1	D	167	SER
1	A	211	THR
1	B	78	GLY

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Mol	Chain	Res	Type
1	B	196	VAL
1	B	292	GLY
1	C	79	LYS
1	D	17	GLU
1	D	92	ILE
1	D	125	ILE
1	D	234	ASP
1	A	48	ALA
1	C	21	GLU
1	C	108	GLY
1	A	21	GLU
1	B	21	GLU
1	C	76	HIS
1	D	172	SER
1	D	221	THR
1	D	230	LYS
1	D	259	GLY
1	A	290	GLU
1	C	170	ILE
1	D	48	ALA
1	D	270	ILE
1	C	113	MET
1	D	228	ASP
1	D	231	VAL
1	D	318	GLY
1	C	55	ILE
1	D	292	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	293/305 (96%)	272 (93%)	21 (7%)	13	41
1	B	293/305 (96%)	274 (94%)	19 (6%)	15	45
1	C	293/305 (96%)	270 (92%)	23 (8%)	11	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	294/305 (96%)	269 (92%)	25 (8%)	10	34
All	All	1173/1220 (96%)	1085 (92%)	88 (8%)	12	39

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLU
1	A	25	LEU
1	A	32	LYS
1	A	80	THR
1	A	86	LEU
1	A	125	ILE
1	A	171	THR
1	A	181	GLN
1	A	184	LYS
1	A	190	LEU
1	A	193	VAL
1	A	231	VAL
1	A	256	SER
1	A	260	VAL
1	A	277	LYS
1	A	282	GLU
1	A	298	SER
1	A	337	VAL
1	A	350	ARG
1	A	355	THR
1	B	43	LEU
1	B	70	THR
1	B	101	ASP
1	B	109	ARG
1	B	128	ASP
1	B	176	ARG
1	B	187	GLN
1	B	212	LYS
1	B	218	ILE
1	B	225	ILE
1	B	228	ASP
1	B	234	ASP
1	B	235	GLN
1	B	249	GLU
1	B	253	LYS

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Mol	Chain	Res	Type
1	B	258	PHE
1	B	320	THR
1	B	325	LEU
1	B	335	LYS
1	C	8	LEU
1	C	33	ASP
1	C	36	ILE
1	C	63	GLU
1	C	68	TYR
1	C	76	HIS
1	C	93	LYS
1	C	105	LEU
1	C	125	ILE
1	C	138	LEU
1	C	141	MET
1	C	142	ARG
1	C	181	GLN
1	C	189	ILE
1	C	191	VAL
1	C	193	VAL
1	C	195	THR
1	C	207	LEU
1	C	216	ARG
1	C	223	LEU
1	C	267	THR
1	C	271	GLN
1	C	355	THR
1	D	2	GLU
1	D	20	THR
1	D	29	VAL
1	D	63	GLU
1	D	71	LEU
1	D	83	CYS
1	D	86	LEU
1	D	105	LEU
1	D	112	SER
1	D	128	ASP
1	D	129	GLN
1	D	141	MET
1	D	180	GLN
1	D	190	LEU
1	D	193	VAL

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Mol	Chain	Res	Type
1	D	223	LEU
1	D	243	THR
1	D	249	GLU
1	D	261	ASN
1	D	268	GLU
1	D	270	ILE
1	D	277	LYS
1	D	306	GLN
1	D	354	LEU
1	D	355	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	19	GLN
1	A	49	HIS
1	A	89	ASN
1	A	177	GLN
1	A	187	GLN
1	A	235	GLN
1	A	296	HIS
1	A	321	HIS
1	A	341	GLN
1	A	347	GLN
1	B	23	ASN
1	B	35	GLN
1	B	42	HIS
1	B	53	HIS
1	B	89	ASN
1	B	103	ASN
1	B	134	ASN
1	B	187	GLN
1	B	261	ASN
1	B	271	GLN
1	B	296	HIS
1	B	306	GLN
1	B	341	GLN
1	B	347	GLN
1	C	15	GLN
1	C	23	ASN
1	C	35	GLN

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Mol	Chain	Res	Type
1	C	76	HIS
1	C	89	ASN
1	C	103	ASN
1	C	134	ASN
1	C	187	GLN
1	C	209	ASN
1	C	261	ASN
1	C	332	GLN
1	C	341	GLN
1	D	19	GLN
1	D	23	ASN
1	D	35	GLN
1	D	53	HIS
1	D	56	HIS
1	D	89	ASN
1	D	129	GLN
1	D	134	ASN
1	D	180	GLN
1	D	181	GLN
1	D	186	HIS
1	D	271	GLN
1	D	306	GLN
1	D	341	GLN
1	D	347	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	NDP	B	381	-	51,52,52	1.27	6 (11%)	71,80,80	0.89	1 (1%)

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	NDP	B	381	-	-	11/34/77/77	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	381	NDP	C4N-C3N	-3.33	1.43	1.50
3	B	381	NDP	C4N-C5N	-2.94	1.41	1.49
3	B	381	NDP	C6N-C5N	2.53	1.40	1.33
3	B	381	NDP	PA-O3	2.42	1.62	1.59
3	B	381	NDP	PN-O3	-2.42	1.56	1.59
3	B	381	NDP	C5A-N7A	-2.11	1.35	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	381	NDP	C1D-N1N-C2N	-2.83	116.47	121.14

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	381	NDP	C5D-O5D-PN-O3
3	B	381	NDP	C5D-O5D-PN-O1N
3	B	381	NDP	C5D-O5D-PN-O2N
3	B	381	NDP	C2D-C1D-N1N-C6N

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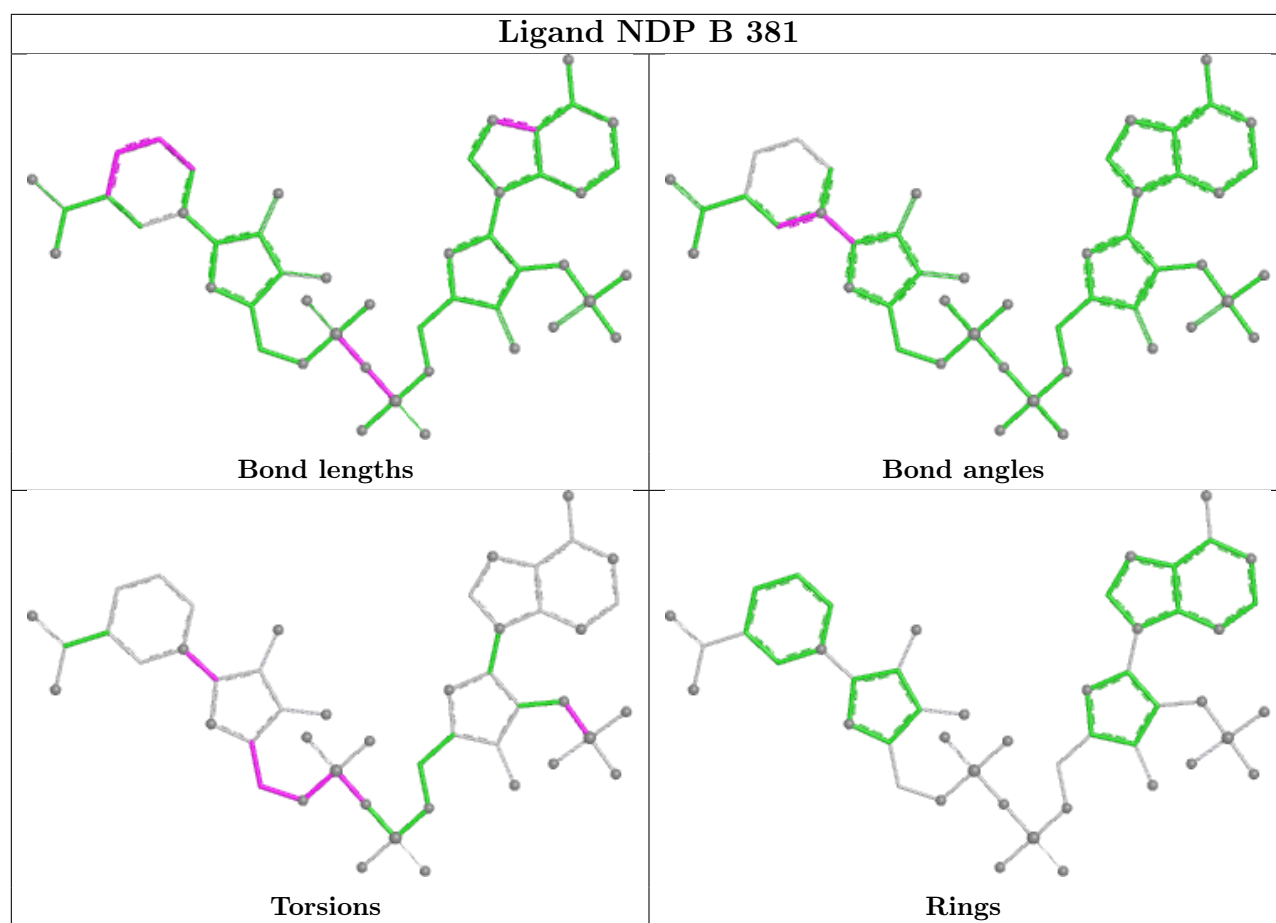
Mol	Chain	Res	Type	Atoms
3	B	381	NDP	C2D-C1D-N1N-C2N
3	B	381	NDP	O4D-C4D-C5D-O5D
3	B	381	NDP	PA-O3-PN-O5D
3	B	381	NDP	O4D-C1D-N1N-C6N
3	B	381	NDP	C4D-C5D-O5D-PN
3	B	381	NDP	O4D-C1D-N1N-C2N
3	B	381	NDP	C2B-O2B-P2B-O2X

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	381	NDP	10	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	359/373 (96%)	-0.56	1 (0%) 90 82	37, 58, 78, 99	0
1	B	359/373 (96%)	-0.36	2 (0%) 85 72	45, 66, 98, 128	0
1	C	359/373 (96%)	-0.28	3 (0%) 82 67	41, 70, 99, 122	0
1	D	360/373 (96%)	-0.35	3 (0%) 82 67	44, 66, 110, 123	0
All	All	1437/1492 (96%)	-0.39	9 (0%) 85 72	37, 64, 99, 128	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	209	ASN	4.2
1	C	29	VAL	3.1
1	B	210	VAL	2.6
1	A	333	SER	2.5
1	B	186	HIS	2.2
1	D	169	TRP	2.2
1	D	229	ALA	2.1
1	D	270	ILE	2.1
1	C	211	THR	2.0

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

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

6.3 Carbohydrates [i](#)

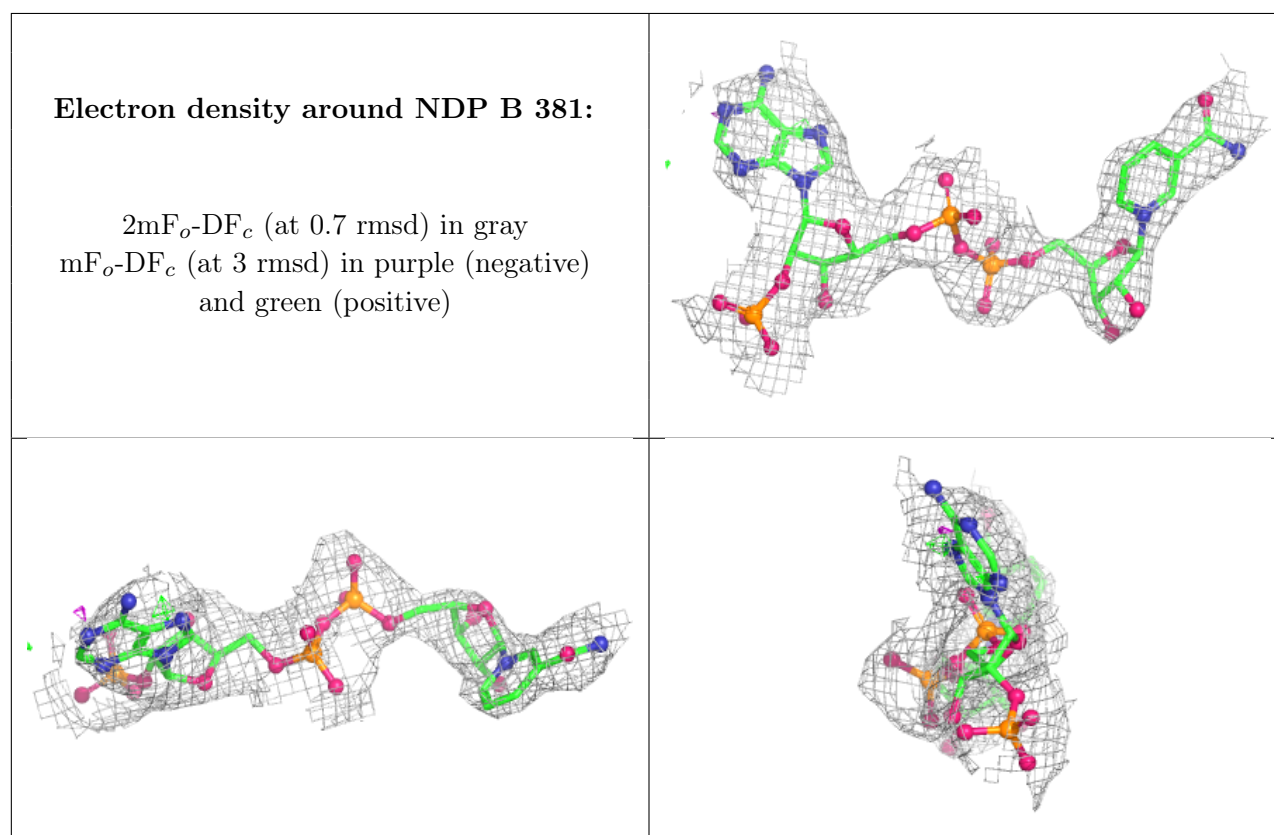
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NDP	B	381	48/48	0.94	0.08	76,85,88,91	0
2	ZN	D	1360	1/1	0.96	0.06	78,78,78,78	0
2	ZN	C	1360	1/1	0.99	0.03	92,92,92,92	0
2	ZN	A	1360	1/1	0.99	0.03	73,73,73,73	0
2	ZN	B	1360	1/1	0.99	0.01	63,63,63,63	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.