



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:17 AM UTC

PDB ID : 1R0L / pdb_00001r0l
Title : 1-deoxy-D-xylulose 5-phosphate reductoisomerase from zymomonas mobilis in complex with NADPH
Authors : Ricagno, S.; Grolle, S.; Bringer-Meyer, S.; Sahm, H.; Lindqvist, Y.; Schneider, G.
Deposited on : 2003-09-22
Resolution : 2.70 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

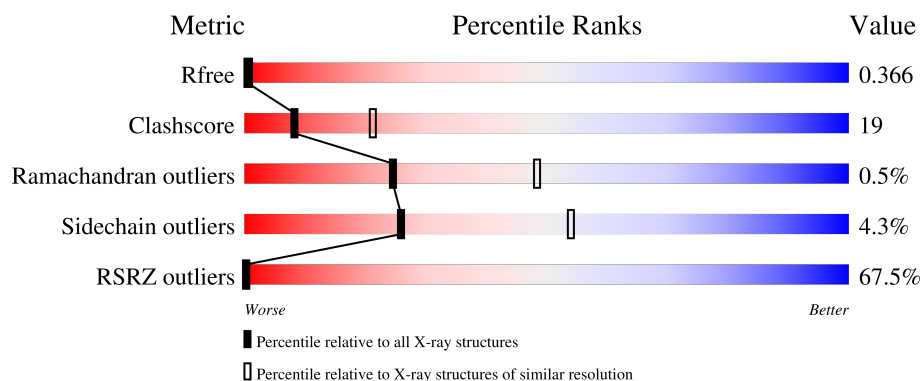
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	388	74% 61% 32% ..
1	B	388	45% 65% 30% ..
1	C	388	75% 63% 32% ..
1	D	388	70% 64% 31% ..

2 Entry composition ⓘ

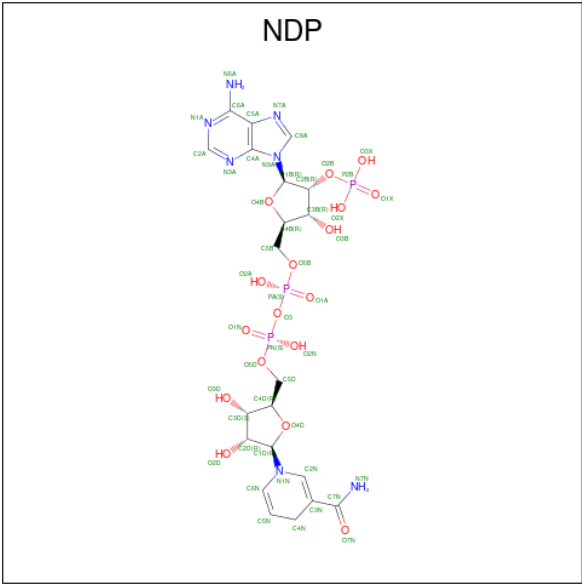
There are 3 unique types of molecules in this entry. The entry contains 11652 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1-deoxy-D-xylulose 5-phosphate reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2854	1798	496	544	16			
1	B	379	Total	C	N	O	S	0	0	0
			2867	1807	499	545	16			
1	C	378	Total	C	N	O	S	0	0	0
			2855	1799	495	544	17			
1	D	378	Total	C	N	O	S	0	0	0
			2860	1802	498	544	16			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

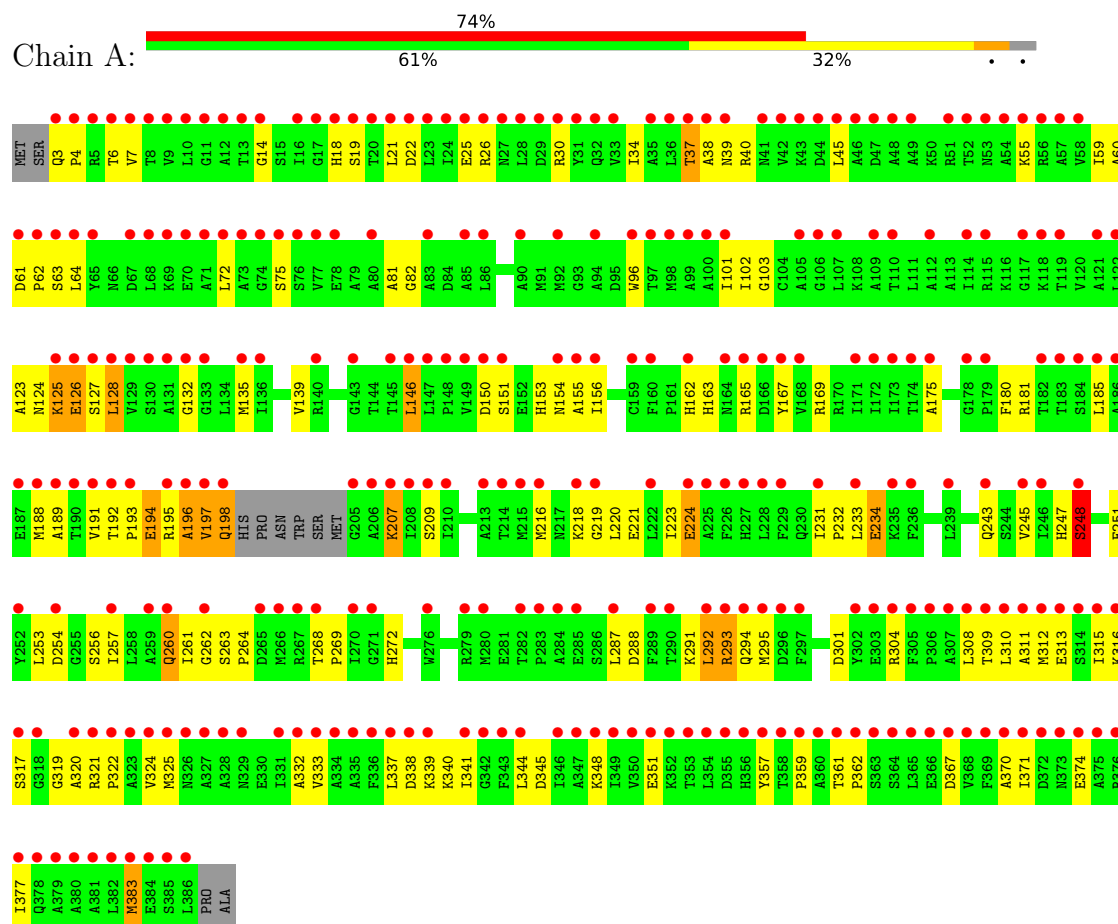
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	36	Total	O	0	0
			36	36		
3	C	22	Total	O	0	0
			22	22		
3	D	20	Total	O	0	0
			20	20		

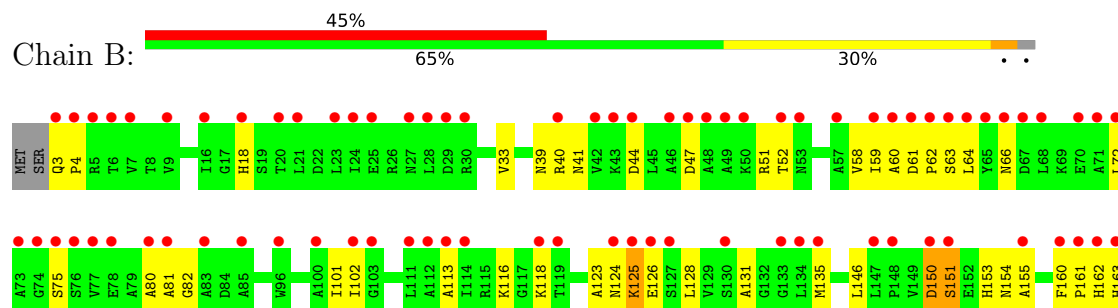
3 Residue-property plots

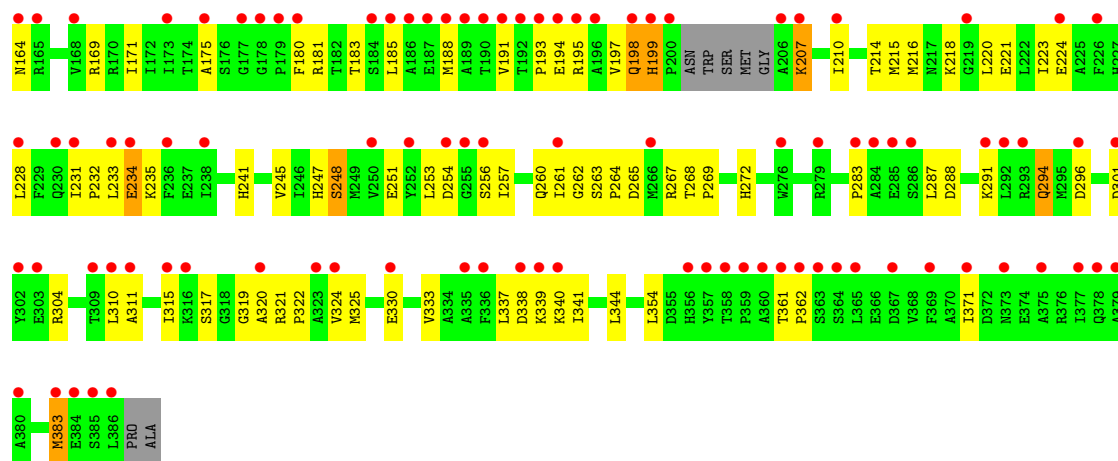
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

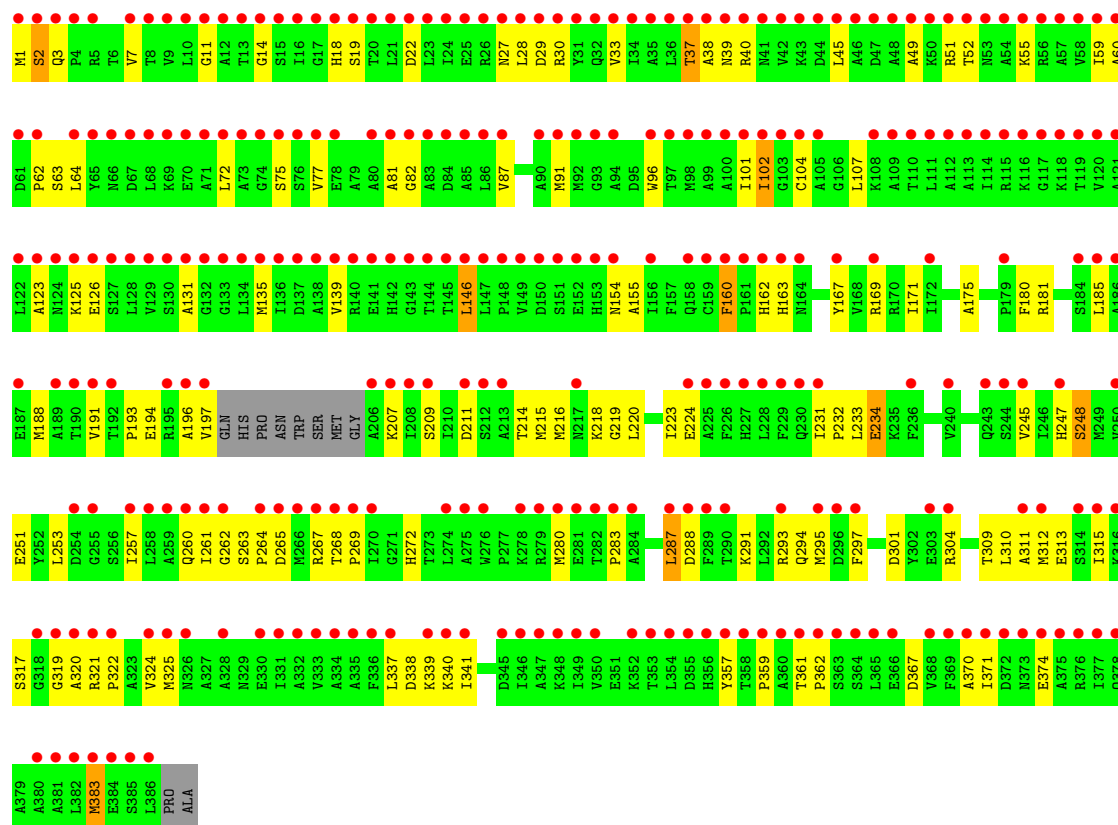
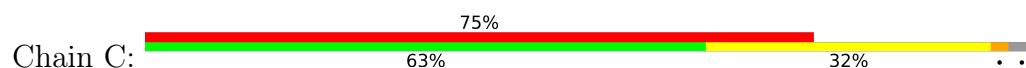


- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

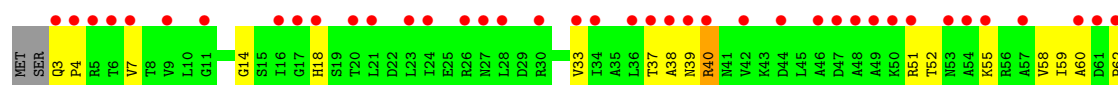


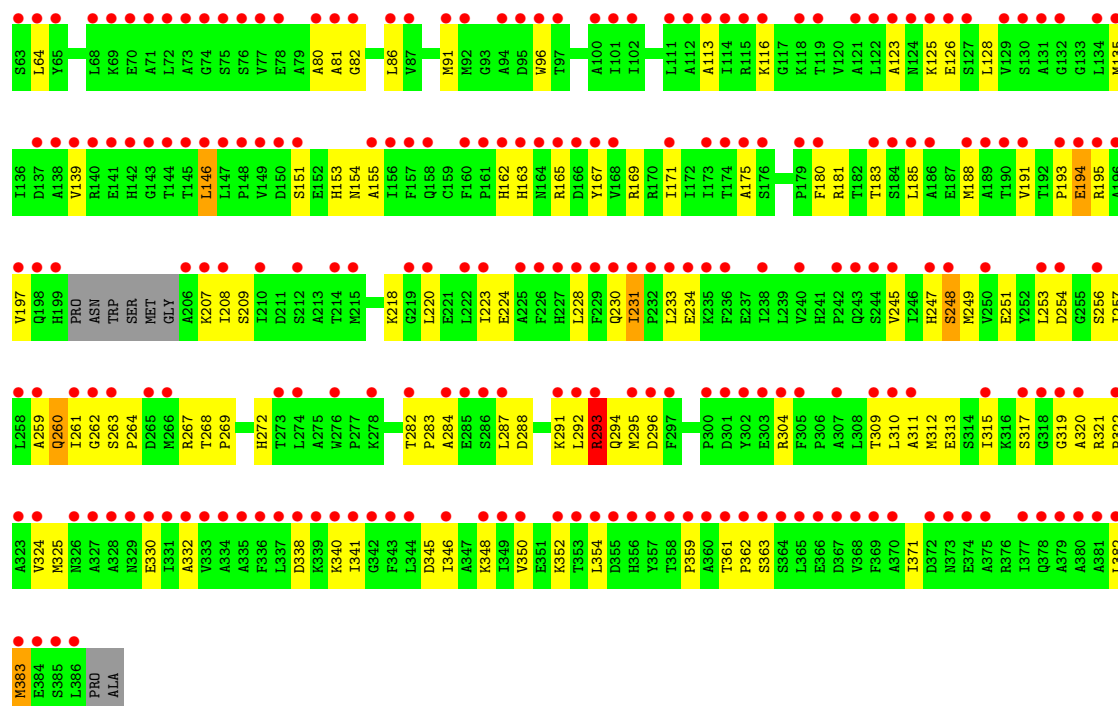


• Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase



• Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.70Å 93.20Å 98.60Å 90.00° 90.50° 90.00°	Depositor
Resolution (Å)	29.63 – 2.70 29.63 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.63-2.70) 98.8 (29.63-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.269 0.361 , 0.366	Depositor DCC
R_{free} test set	493 reflections (1.13%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	11652	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9583e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.56	2/2901 (0.1%)	1.00	10/3933 (0.3%)
1	B	0.59	1/2916 (0.0%)	1.00	10/3955 (0.3%)
1	C	0.50	0/2902	0.96	5/3934 (0.1%)
1	D	0.51	0/2908	0.96	4/3943 (0.1%)
All	All	0.54	3/11627 (0.0%)	0.98	29/15765 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	HIS	C-O	-9.51	1.12	1.24
1	A	198	GLN	CA-CB	5.24	1.64	1.53
1	A	125	LYS	C-N	5.09	1.40	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	HIS	C-N-CD	-10.41	82.32	125.00
1	C	2	SER	N-CA-C	10.26	122.35	107.88
1	A	198	GLN	OE1-CD-NE2	-10.03	112.57	122.60
1	B	207	LYS	N-CA-C	-8.76	103.11	113.88
1	D	123	ALA	N-CA-C	-8.32	103.65	113.88
1	B	123	ALA	N-CA-C	-7.30	104.90	113.88
1	A	123	ALA	N-CA-C	-7.28	104.92	113.88
1	B	199	HIS	CA-C-O	6.74	129.40	120.16
1	A	102	ILE	N-CA-C	6.74	118.85	109.55
1	A	198	GLN	CG-CD-NE2	6.67	126.41	116.40
1	C	123	ALA	N-CA-C	-6.48	105.92	113.88
1	C	102	ILE	N-CA-C	5.99	117.77	109.45
1	D	126	GLU	CA-CB-CG	-5.95	102.19	114.10
1	B	294	GLN	N-CA-C	5.91	118.84	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	LEU	N-CA-C	5.84	118.43	111.71
1	B	151	SER	N-CA-C	5.70	117.98	111.02
1	C	160	PHE	N-CA-C	5.68	117.23	110.07
1	B	199	HIS	CA-C-N	5.60	150.59	122.60
1	B	199	HIS	C-N-CA	5.60	150.59	122.60
1	D	363	SER	N-CA-C	-5.51	107.21	114.31
1	A	197	VAL	N-CA-C	-5.35	99.86	107.77
1	B	241	HIS	CA-C-N	5.33	126.50	119.84
1	B	241	HIS	C-N-CA	5.33	126.50	119.84
1	D	151	SER	N-CA-C	5.32	117.49	111.11
1	A	151	SER	N-CA-C	5.24	117.41	111.02
1	C	219	GLY	N-CA-C	-5.23	106.07	112.77
1	A	219	GLY	N-CA-C	-5.20	106.20	112.49
1	A	207	LYS	N-CA-C	-5.15	105.12	111.40
1	A	196	ALA	N-CA-C	5.02	118.95	111.87

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	2854	0	2891	125	0
1	B	2867	0	2902	107	14
1	C	2855	0	2897	116	15
1	D	2860	0	2895	106	0
2	A	27	0	11	1	0
2	B	27	0	11	2	0
2	C	27	0	11	1	0
2	D	27	0	11	3	0
3	A	30	0	0	3	0
3	B	36	0	0	6	1
3	C	22	0	0	4	0
3	D	20	0	0	2	0
All	All	11652	0	11629	446	15

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 19.

All (446) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LYS:HB2	1:C:224:GLU:OE2	1.50	1.11
1:D:40:ARG:HG2	1:D:64:LEU:HD11	1.48	0.95
1:C:126:GLU:HA	1:C:126:GLU:OE1	1.74	0.87
1:B:47:ASP:CG	1:B:51:ARG:HH22	1.85	0.84
1:A:3:GLN:HB3	1:A:4:PRO:HD3	1.59	0.84
1:A:247:HIS:HD2	1:A:260:GLN:HE22	1.25	0.82
1:C:207:LYS:HE2	1:C:211:ASP:OD2	1.81	0.80
1:D:220:LEU:O	1:D:224:GLU:HG3	1.81	0.79
1:C:251:GLU:HG3	1:C:257:ILE:HG12	1.63	0.79
1:C:294:GLN:NE2	1:D:294:GLN:HE22	1.80	0.79
1:A:125:LYS:HG3	1:A:126:GLU:N	1.95	0.79
1:D:185:LEU:HA	1:D:188:MET:HE3	1.66	0.77
1:B:154:ASN:HD21	1:B:272:HIS:CD2	2.03	0.77
1:A:124:ASN:ND2	1:A:126:GLU:HB2	2.01	0.76
1:B:51:ARG:HH21	1:B:51:ARG:HG3	1.49	0.76
1:D:154:ASN:HD21	1:D:272:HIS:CD2	2.04	0.76
1:A:124:ASN:HD21	1:A:126:GLU:HB2	1.51	0.75
1:C:220:LEU:O	1:C:224:GLU:HG3	1.87	0.75
1:B:154:ASN:HD21	1:B:272:HIS:HD2	1.37	0.73
1:A:247:HIS:CD2	1:A:260:GLN:HE22	2.05	0.73
1:B:267:ARG:CZ	1:B:283:PRO:HG2	2.19	0.73
1:C:125:LYS:CB	1:C:224:GLU:OE2	2.36	0.72
1:D:125:LYS:HB3	1:D:224:GLU:OE2	1.90	0.72
1:A:21:LEU:O	1:A:25:GLU:HG3	1.90	0.72
1:C:216:MET:HE1	1:C:325:MET:HE2	1.71	0.71
1:A:374:GLU:O	1:A:377:ILE:HG12	1.89	0.71
1:D:3:GLN:N	1:D:4:PRO:HD3	2.05	0.71
1:C:223:ILE:HG12	1:C:315:ILE:HG12	1.72	0.71
1:B:207:LYS:HE3	1:B:330:GLU:OE1	1.90	0.71
1:B:223:ILE:HG12	1:B:315:ILE:HG12	1.71	0.70
1:B:47:ASP:CG	1:B:51:ARG:NH2	2.50	0.69
1:C:297:PHE:O	1:D:293:ARG:HG2	1.93	0.69
1:D:309:THR:O	1:D:313:GLU:HG3	1.92	0.69
1:B:185:LEU:HA	1:B:188:MET:HE3	1.75	0.69
1:D:362:PRO:HG3	1:D:371:ILE:HD12	1.76	0.68
1:C:319:GLY:HA2	1:C:361:THR:HG22	1.76	0.68
1:D:39:ASN:HD22	1:D:60:ALA:HB3	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:PRO:HG3	1:A:371:ILE:HD12	1.75	0.68
1:A:154:ASN:HD21	1:A:272:HIS:CD2	2.10	0.68
1:D:7:VAL:HG13	1:D:96:TRP:HE3	1.59	0.68
1:A:223:ILE:HG12	1:A:315:ILE:CG1	2.24	0.68
1:A:301:ASP:OD2	1:A:304:ARG:HD3	1.93	0.67
1:B:40:ARG:HG2	1:B:40:ARG:HH11	1.60	0.67
1:B:39:ASN:HB2	2:B:401:NDP:C4A	2.24	0.67
1:C:37:THR:HG21	1:C:101:ILE:HD11	1.77	0.67
1:A:216:MET:HE1	1:A:325:MET:HE2	1.77	0.66
1:C:180:PHE:HZ	1:C:191:VAL:HG11	1.58	0.66
1:D:59:ILE:O	1:D:81:ALA:HA	1.95	0.66
1:D:233:LEU:HD21	1:D:315:ILE:HG21	1.78	0.66
1:C:319:GLY:CA	1:C:361:THR:HG22	2.26	0.66
1:C:126:GLU:OE1	1:C:126:GLU:CA	2.43	0.66
1:D:154:ASN:HD21	1:D:272:HIS:HD2	1.43	0.66
1:B:362:PRO:HG3	1:B:371:ILE:HD12	1.78	0.65
1:A:317:SER:HB3	1:A:321:ARG:HG3	1.77	0.65
1:D:251:GLU:HG3	1:D:257:ILE:HG12	1.78	0.65
1:C:267:ARG:CZ	1:C:283:PRO:HG2	2.25	0.65
1:A:223:ILE:CG1	1:A:315:ILE:HD11	2.26	0.65
1:C:338:ASP:OD1	1:C:340:LYS:HE3	1.97	0.65
1:A:7:VAL:HG13	1:A:96:TRP:HE3	1.63	0.64
1:B:233:LEU:HD21	1:B:315:ILE:HG21	1.80	0.64
1:A:207:LYS:HD2	1:A:333:VAL:HG11	1.79	0.64
1:A:223:ILE:HG12	1:A:315:ILE:HD11	1.78	0.64
1:A:357:TYR:CZ	1:A:374:GLU:HG2	2.31	0.64
1:B:338:ASP:OD1	1:B:340:LYS:HE3	1.97	0.64
1:A:309:THR:O	1:A:313:GLU:HG3	1.98	0.64
1:C:301:ASP:OD2	1:C:304:ARG:HD3	1.97	0.63
1:B:216:MET:SD	1:B:325:MET:HE2	2.38	0.63
1:C:39:ASN:HA	1:C:60:ALA:HB3	1.79	0.63
1:B:59:ILE:O	1:B:81:ALA:HA	1.99	0.63
1:B:223:ILE:HG12	1:B:315:ILE:CG1	2.28	0.63
1:B:267:ARG:NH1	1:B:283:PRO:HG2	2.14	0.62
1:A:125:LYS:HD3	3:A:407:HOH:O	1.98	0.62
1:C:55:LYS:NZ	1:C:55:LYS:HB3	2.14	0.62
1:B:51:ARG:HG3	1:B:51:ARG:NH2	2.13	0.62
1:C:223:ILE:HG12	1:C:315:ILE:CG1	2.29	0.62
1:A:216:MET:SD	1:A:325:MET:HE2	2.40	0.62
1:A:268:THR:HB	1:A:269:PRO:CD	2.30	0.62
1:C:197:VAL:HA	1:C:209:SER:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ASN:HB2	2:D:403:NDP:C4A	2.30	0.62
1:A:345:ASP:HA	1:A:348:LYS:HD2	1.82	0.61
1:C:180:PHE:CZ	1:C:191:VAL:HG11	2.35	0.61
1:A:62:PRO:HG3	1:A:82:GLY:HA2	1.81	0.61
1:B:194:GLU:N	1:B:194:GLU:OE1	2.34	0.61
1:A:207:LYS:CD	1:A:333:VAL:HG11	2.31	0.61
1:A:338:ASP:OD1	1:A:340:LYS:HE3	2.00	0.61
1:A:125:LYS:CG	1:A:126:GLU:N	2.63	0.61
1:C:383:MET:HE2	1:C:383:MET:O	2.01	0.60
1:D:86:LEU:HD11	2:D:403:NDP:H2A	1.82	0.60
1:D:345:ASP:HA	1:D:348:LYS:HD2	1.83	0.60
1:B:251:GLU:HG3	1:B:257:ILE:HG12	1.84	0.60
1:D:39:ASN:HA	1:D:60:ALA:HB3	1.83	0.60
1:A:103:GLY:HA2	1:A:126:GLU:HG3	1.83	0.60
1:B:193:PRO:O	1:B:197:VAL:HG22	2.02	0.60
1:B:150:ASP:OD2	1:B:153:HIS:ND1	2.35	0.60
1:D:193:PRO:O	1:D:197:VAL:HG22	2.02	0.60
1:A:221:GLU:HA	1:A:224:GLU:HG3	1.83	0.60
1:B:47:ASP:OD2	1:B:51:ARG:NH2	2.30	0.59
1:A:30:ARG:HB2	3:A:404:HOH:O	2.02	0.59
1:C:362:PRO:HG3	1:C:371:ILE:HD12	1.84	0.59
1:A:294:GLN:NE2	1:B:294:GLN:NE2	2.50	0.59
1:A:162:HIS:O	1:A:163:HIS:HB2	2.03	0.59
1:B:118:LYS:HE3	3:B:430:HOH:O	2.03	0.59
1:A:135:MET:O	1:A:139:VAL:HG23	2.03	0.59
1:A:220:LEU:O	1:A:224:GLU:CG	2.51	0.59
1:A:223:ILE:HG12	1:A:315:ILE:CD1	2.33	0.59
1:C:7:VAL:HG13	1:C:96:TRP:HE3	1.68	0.59
1:C:216:MET:CE	1:C:325:MET:HE2	2.33	0.59
1:B:3:GLN:HB2	1:B:4:PRO:HD3	1.85	0.59
1:A:223:ILE:HG12	1:A:315:ILE:HG12	1.84	0.58
1:C:175:ALA:CB	1:C:218:LYS:HE3	2.33	0.58
1:B:234:GLU:H	1:B:234:GLU:CD	2.11	0.58
1:A:216:MET:CE	1:A:325:MET:HE2	2.34	0.58
1:C:62:PRO:HG3	1:C:82:GLY:HA2	1.85	0.58
1:D:311:ALA:N	1:D:325:MET:HE1	2.18	0.58
1:A:207:LYS:HE2	1:A:333:VAL:HG21	1.85	0.57
1:D:223:ILE:HG12	1:D:315:ILE:HG12	1.86	0.57
1:B:216:MET:HE1	1:B:325:MET:HE2	1.86	0.57
1:C:72:LEU:O	1:C:75:SER:HB3	2.03	0.57
1:A:319:GLY:HA2	1:A:361:THR:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ARG:HA	1:B:64:LEU:CD1	2.34	0.57
1:D:58:VAL:HG22	1:D:80:ALA:HB3	1.86	0.57
1:B:310:LEU:CB	1:B:325:MET:HE3	2.35	0.57
1:C:311:ALA:N	1:C:325:MET:HE1	2.19	0.57
1:C:223:ILE:HG12	1:C:315:ILE:CD1	2.34	0.57
1:D:207:LYS:HE3	1:D:330:GLU:OE1	2.05	0.57
1:D:267:ARG:CZ	1:D:283:PRO:HG2	2.34	0.57
1:A:234:GLU:CD	1:A:234:GLU:H	2.13	0.56
1:B:47:ASP:OD1	1:B:51:ARG:NH2	2.37	0.56
1:D:338:ASP:OD1	1:D:340:LYS:HE3	2.05	0.56
1:A:180:PHE:CZ	1:A:191:VAL:HG11	2.40	0.56
1:B:311:ALA:O	1:B:315:ILE:HG13	2.05	0.56
1:D:40:ARG:HA	1:D:64:LEU:CD1	2.35	0.56
1:C:27:ASN:C	1:C:29:ASP:H	2.11	0.56
1:C:216:MET:SD	1:C:325:MET:HE2	2.45	0.56
1:D:175:ALA:CB	1:D:218:LYS:HE3	2.36	0.56
1:A:220:LEU:O	1:A:224:GLU:HG3	2.06	0.56
1:C:309:THR:O	1:C:313:GLU:HG3	2.05	0.56
1:B:39:ASN:HA	1:B:60:ALA:HB3	1.88	0.56
1:B:220:LEU:O	1:B:224:GLU:HG3	2.07	0.55
1:C:40:ARG:HA	1:C:64:LEU:CD1	2.35	0.55
1:C:27:ASN:C	1:C:29:ASP:N	2.63	0.55
1:D:362:PRO:HG3	1:D:371:ILE:CD1	2.37	0.55
1:B:320:ALA:O	1:B:324:VAL:HG23	2.07	0.55
1:D:325:MET:HB2	1:D:354:LEU:HD21	1.88	0.55
1:A:332:ALA:O	1:A:341:ILE:HD11	2.06	0.55
1:C:181:ARG:C	1:C:304:ARG:HH22	2.15	0.55
1:C:341:ILE:HG23	1:C:383:MET:HE3	1.88	0.55
1:C:185:LEU:HA	1:C:188:MET:HE3	1.88	0.55
1:D:268:THR:HB	1:D:269:PRO:CD	2.37	0.54
1:C:55:LYS:HB3	1:C:55:LYS:HZ3	1.71	0.54
1:C:162:HIS:O	1:C:163:HIS:HB2	2.08	0.54
1:C:311:ALA:O	1:C:315:ILE:HG13	2.07	0.54
1:D:3:GLN:N	1:D:4:PRO:CD	2.71	0.54
1:A:245:VAL:HG21	1:A:295:MET:HE2	1.88	0.54
1:B:338:ASP:HA	3:B:409:HOH:O	2.06	0.54
1:C:154:ASN:HD21	1:C:272:HIS:CD2	2.26	0.54
1:D:223:ILE:HG12	1:D:315:ILE:CG1	2.38	0.54
1:C:59:ILE:O	1:C:81:ALA:HA	2.09	0.53
1:C:317:SER:HB3	1:C:321:ARG:HG3	1.90	0.53
1:A:175:ALA:HB2	1:A:218:LYS:HE2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:HD22	1:A:294:GLN:O	2.09	0.53
1:A:319:GLY:CA	1:A:361:THR:HG22	2.39	0.53
1:D:310:LEU:CB	1:D:325:MET:HE3	2.39	0.53
1:C:155:ALA:HB1	1:C:260:GLN:HB3	1.89	0.53
1:B:39:ASN:ND2	1:B:40:ARG:HG3	2.24	0.53
1:B:58:VAL:HG22	1:B:80:ALA:HB3	1.90	0.53
1:C:312:MET:HE3	1:C:312:MET:O	2.09	0.53
1:B:254:ASP:OD1	1:B:256:SER:HB3	2.09	0.53
1:C:294:GLN:NE2	1:D:294:GLN:NE2	2.52	0.53
1:D:332:ALA:O	1:D:341:ILE:HD11	2.08	0.53
1:C:223:ILE:HG12	1:C:315:ILE:HD11	1.91	0.53
1:A:311:ALA:N	1:A:325:MET:HE1	2.24	0.52
1:A:154:ASN:HD21	1:A:272:HIS:HD2	1.55	0.52
1:A:59:ILE:O	1:A:81:ALA:HA	2.09	0.52
1:B:188:MET:HA	1:B:191:VAL:HG23	1.90	0.52
1:C:51:ARG:HH21	1:C:51:ARG:HG2	1.75	0.52
1:B:310:LEU:HB2	1:B:325:MET:HE3	1.92	0.52
1:A:294:GLN:HG2	1:B:296:ASP:OD1	2.10	0.52
1:D:311:ALA:O	1:D:315:ILE:HG13	2.09	0.52
1:D:55:LYS:NZ	1:D:55:LYS:HB3	2.25	0.52
1:D:254:ASP:OD1	1:D:256:SER:HB3	2.10	0.52
1:B:341:ILE:HG23	1:B:383:MET:HE3	1.92	0.52
1:A:40:ARG:HA	1:A:64:LEU:CD1	2.40	0.51
1:A:169:ARG:NH2	1:A:253:LEU:O	2.43	0.51
1:A:175:ALA:CB	1:A:218:LYS:HE2	2.40	0.51
1:B:61:ASP:OD2	1:B:63:SER:OG	2.21	0.51
1:C:197:VAL:HG12	1:C:197:VAL:O	2.10	0.51
1:A:39:ASN:HA	1:A:60:ALA:HB3	1.91	0.51
1:C:135:MET:O	1:C:139:VAL:HG23	2.10	0.51
1:A:40:ARG:HA	1:A:64:LEU:HD12	1.92	0.51
1:A:180:PHE:HZ	1:A:191:VAL:HG11	1.74	0.51
1:C:362:PRO:HG3	1:C:371:ILE:CD1	2.39	0.51
1:B:268:THR:HB	1:B:269:PRO:CD	2.41	0.51
1:D:263:SER:HB2	1:D:264:PRO:HD2	1.91	0.51
1:A:188:MET:HA	1:A:191:VAL:HG23	1.92	0.51
1:C:251:GLU:HG3	1:C:257:ILE:CG1	2.39	0.51
1:D:223:ILE:HG12	1:D:315:ILE:HD11	1.93	0.51
1:D:188:MET:HA	1:D:191:VAL:HG23	1.92	0.51
1:C:33:VAL:HG21	1:C:52:THR:HB	1.93	0.50
1:C:310:LEU:CB	1:C:325:MET:HE3	2.41	0.50
1:A:245:VAL:O	1:A:261:ILE:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ASP:OD1	1:A:256:SER:HB3	2.11	0.50
1:D:319:GLY:HA2	1:D:361:THR:HG22	1.93	0.50
1:B:162:HIS:O	1:B:163:HIS:HB2	2.11	0.50
1:D:51:ARG:HG2	1:D:51:ARG:HH21	1.77	0.50
1:B:221:GLU:HA	1:B:224:GLU:OE1	2.11	0.50
1:A:357:TYR:CE1	1:A:359:PRO:HD3	2.46	0.50
1:D:320:ALA:O	1:D:324:VAL:HG23	2.12	0.50
1:A:126:GLU:HA	1:A:126:GLU:OE1	2.11	0.49
1:C:40:ARG:HA	1:C:64:LEU:HD12	1.94	0.49
1:A:34:ILE:O	1:A:55:LYS:HB2	2.13	0.49
1:C:125:LYS:HE2	1:C:224:GLU:OE1	2.12	0.49
1:C:223:ILE:CG1	1:C:315:ILE:HD11	2.41	0.49
1:D:162:HIS:O	1:D:163:HIS:HB2	2.12	0.49
1:A:357:TYR:CE1	1:A:374:GLU:HG2	2.47	0.49
1:B:66:ASN:ND2	3:B:429:HOH:O	2.40	0.49
1:B:223:ILE:HG12	1:B:315:ILE:CD1	2.41	0.49
1:B:216:MET:CE	1:B:325:MET:HE2	2.43	0.49
1:D:153:HIS:HE1	1:D:224:GLU:OE1	1.96	0.49
1:C:11:GLY:H	1:C:37:THR:HG22	1.78	0.49
1:D:249:MET:HG2	1:D:259:ALA:HB2	1.94	0.49
1:B:267:ARG:NH1	1:B:283:PRO:CG	2.76	0.49
1:D:39:ASN:ND2	1:D:60:ALA:HB3	2.28	0.49
1:A:357:TYR:CD1	1:A:359:PRO:HD3	2.48	0.48
1:C:357:TYR:CE1	1:C:374:GLU:HG2	2.49	0.48
1:D:383:MET:O	1:D:383:MET:HE2	2.13	0.48
1:A:7:VAL:HG13	1:A:96:TRP:CE3	2.47	0.48
1:A:189:ALA:HB2	1:A:344:LEU:HD12	1.93	0.48
1:B:40:ARG:HA	1:B:64:LEU:HD12	1.93	0.48
1:C:101:ILE:HB	3:C:411:HOH:O	2.13	0.48
1:D:288:ASP:CG	1:D:291:LYS:HG2	2.38	0.48
1:B:101:ILE:O	1:B:124:ASN:ND2	2.46	0.48
1:B:261:ILE:HG22	1:B:262:GLY:N	2.28	0.48
1:C:207:LYS:CE	1:C:211:ASP:OD2	2.57	0.48
1:D:180:PHE:HB3	1:D:183:THR:HB	1.96	0.48
1:A:196:ALA:O	1:A:209:SER:HB3	2.14	0.48
1:A:362:PRO:HG3	1:A:371:ILE:CD1	2.43	0.48
1:B:321:ARG:HB2	1:B:322:PRO:CD	2.43	0.48
1:B:362:PRO:HG3	1:B:371:ILE:CD1	2.42	0.48
1:D:139:VAL:HG21	1:D:146:LEU:HD12	1.96	0.48
1:A:155:ALA:HB1	1:A:260:GLN:HB3	1.95	0.48
1:A:310:LEU:CB	1:A:325:MET:HE3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:ARG:NH2	1:D:253:LEU:O	2.46	0.48
1:D:175:ALA:HA	1:D:218:LYS:HE3	1.96	0.48
1:B:175:ALA:HB1	3:B:417:HOH:O	2.14	0.48
1:B:247:HIS:ND1	1:B:260:GLN:NE2	2.59	0.48
1:C:160:PHE:HE1	1:C:171:ILE:HD11	1.78	0.48
1:A:288:ASP:CG	1:A:291:LYS:HG3	2.39	0.48
1:B:265:ASP:OD1	1:B:267:ARG:HB2	2.14	0.48
1:C:37:THR:HG23	3:C:424:HOH:O	2.13	0.48
1:B:383:MET:HE2	1:B:383:MET:O	2.14	0.47
1:D:62:PRO:HG3	1:D:82:GLY:HA2	1.94	0.47
1:A:193:PRO:HB3	1:A:337:LEU:HD23	1.95	0.47
1:B:288:ASP:CG	1:B:291:LYS:HG2	2.39	0.47
1:A:294:GLN:NE2	1:B:294:GLN:CD	2.73	0.47
1:C:39:ASN:HB2	2:C:402:NDP:C4A	2.45	0.47
1:D:317:SER:HB3	1:D:321:ARG:HG3	1.95	0.47
1:A:245:VAL:CG2	1:A:295:MET:HE2	2.44	0.47
1:B:263:SER:HB2	1:B:264:PRO:HD2	1.95	0.47
1:C:154:ASN:HD21	1:C:272:HIS:HD2	1.63	0.47
1:D:223:ILE:HG12	1:D:315:ILE:CD1	2.44	0.47
1:C:357:TYR:CZ	1:C:374:GLU:HG2	2.48	0.47
1:D:167:TYR:O	1:D:253:LEU:HG	2.15	0.47
1:A:220:LEU:O	1:A:224:GLU:HG2	2.13	0.47
1:A:245:VAL:HG21	1:A:292:LEU:HD11	1.97	0.47
1:C:27:ASN:O	1:C:29:ASP:N	2.48	0.47
1:D:7:VAL:HG13	1:D:96:TRP:CE3	2.44	0.47
1:D:251:GLU:HG3	1:D:257:ILE:CG1	2.45	0.47
1:D:319:GLY:CA	1:D:361:THR:HG22	2.45	0.47
1:A:4:PRO:HA	1:A:30:ARG:O	2.14	0.47
1:B:337:LEU:C	1:B:339:LYS:H	2.21	0.47
1:C:214:THR:O	1:C:215:MET:HB2	2.14	0.47
1:B:180:PHE:CZ	1:B:191:VAL:HG11	2.50	0.47
1:A:223:ILE:HA	1:A:315:ILE:CD1	2.45	0.47
1:B:160:PHE:HE1	1:B:171:ILE:HD11	1.80	0.47
1:C:7:VAL:HG13	1:C:96:TRP:CE3	2.48	0.47
1:C:251:GLU:CG	1:C:257:ILE:HG12	2.41	0.47
1:A:223:ILE:HA	1:A:315:ILE:HD13	1.95	0.46
1:A:310:LEU:HB2	1:A:325:MET:HE3	1.96	0.46
1:C:247:HIS:O	1:C:248:SER:CB	2.62	0.46
1:D:247:HIS:ND1	1:D:260:GLN:NE2	2.52	0.46
1:A:181:ARG:C	1:A:304:ARG:HH22	2.24	0.46
1:A:320:ALA:O	1:A:324:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ASP:O	1:A:370:ALA:HB3	2.15	0.46
1:A:167:TYR:O	1:A:253:LEU:HG	2.14	0.46
1:C:310:LEU:HB3	1:C:325:MET:HE3	1.97	0.46
1:B:232:PRO:HD2	1:B:235:LYS:HD2	1.96	0.46
1:B:311:ALA:N	1:B:325:MET:HE1	2.29	0.46
1:C:38:ALA:HB3	1:C:45:LEU:HD22	1.96	0.46
1:C:265:ASP:OD1	1:C:267:ARG:HB2	2.15	0.46
1:B:72:LEU:O	1:B:75:SER:HB3	2.16	0.46
1:B:310:LEU:HB3	1:B:325:MET:HE3	1.97	0.46
1:D:181:ARG:C	1:D:304:ARG:HH22	2.23	0.46
1:A:3:GLN:OE1	1:A:3:GLN:HA	2.14	0.46
1:B:125:LYS:HB2	1:B:224:GLU:OE2	2.16	0.46
1:B:40:ARG:HG2	1:B:40:ARG:NH1	2.28	0.46
1:B:169:ARG:HD2	1:B:251:GLU:OE2	2.15	0.46
1:A:251:GLU:HG3	1:A:257:ILE:HG12	1.98	0.46
1:A:195:ARG:O	1:A:195:ARG:HG2	2.15	0.46
1:C:131:ALA:O	1:C:135:MET:HG2	2.16	0.46
1:A:294:GLN:HE22	1:B:294:GLN:NE2	2.14	0.46
1:B:155:ALA:HB1	1:B:260:GLN:HB3	1.97	0.46
1:B:223:ILE:HG12	1:B:315:ILE:HD11	1.97	0.46
1:C:245:VAL:HG21	1:C:295:MET:HE2	1.97	0.46
1:D:249:MET:HG2	1:D:259:ALA:CB	2.46	0.45
1:D:310:LEU:HB3	1:D:325:MET:HE3	1.98	0.45
1:C:268:THR:HB	1:C:269:PRO:CD	2.47	0.45
1:C:359:PRO:HG3	1:C:371:ILE:HG23	1.98	0.45
1:D:128:LEU:HD13	1:D:228:LEU:HG	1.99	0.45
1:B:125:LYS:CB	1:B:224:GLU:OE2	2.65	0.45
1:B:169:ARG:NH2	1:B:253:LEU:O	2.49	0.45
1:A:128:LEU:HA	1:A:132:GLY:HA2	1.98	0.45
1:C:193:PRO:O	1:C:197:VAL:HG23	2.16	0.45
1:C:191:VAL:HG11	1:C:196:ALA:HB2	1.99	0.45
1:D:169:ARG:HD2	1:D:251:GLU:OE2	2.17	0.45
1:A:139:VAL:HG21	1:A:146:LEU:HD12	1.99	0.45
1:B:223:ILE:CG1	1:B:315:ILE:HD11	2.47	0.45
1:D:171:ILE:HD11	1:D:231:ILE:HD12	1.99	0.45
1:B:223:ILE:HD13	1:B:322:PRO:HB3	1.99	0.45
1:D:207:LYS:HD2	1:D:207:LYS:O	2.16	0.45
1:A:357:TYR:CZ	1:A:374:GLU:CG	2.99	0.45
1:C:263:SER:HB2	1:C:264:PRO:HD2	1.98	0.45
1:C:288:ASP:CG	1:C:291:LYS:HG2	2.42	0.45
1:A:6:THR:HG21	3:A:410:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ALA:CB	1:B:218:LYS:HE3	2.47	0.45
1:B:33:VAL:HG21	1:B:52:THR:HB	1.99	0.44
1:B:62:PRO:HG3	1:B:82:GLY:HA2	1.99	0.44
1:B:197:VAL:O	1:B:198:GLN:C	2.60	0.44
1:B:126:GLU:H	1:B:126:GLU:CD	2.25	0.44
1:C:321:ARG:HB2	1:C:322:PRO:CD	2.47	0.44
1:B:245:VAL:O	1:B:261:ILE:HG23	2.17	0.44
1:B:317:SER:HB3	1:B:321:ARG:HG3	1.99	0.44
1:C:139:VAL:HG21	1:C:146:LEU:HD12	1.98	0.44
1:C:337:LEU:C	1:C:339:LYS:H	2.26	0.44
1:D:245:VAL:HG21	1:D:295:MET:HE2	1.99	0.44
1:D:245:VAL:O	1:D:261:ILE:HG23	2.17	0.44
1:D:269:PRO:O	1:D:272:HIS:HB3	2.17	0.44
1:A:247:HIS:O	1:A:248:SER:CB	2.64	0.44
1:A:233:LEU:HD21	1:A:315:ILE:HG21	1.98	0.44
1:B:198:GLN:O	1:B:199:HIS:HB3	2.17	0.44
1:C:59:ILE:O	1:C:59:ILE:HG23	2.17	0.44
1:B:210:ILE:HG21	1:B:333:VAL:HG13	2.00	0.44
1:C:231:ILE:HG23	1:C:232:PRO:HD2	2.00	0.44
1:D:18:HIS:ND1	3:D:411:HOH:O	2.36	0.44
1:A:341:ILE:HG23	1:A:383:MET:HE3	2.00	0.44
1:C:14:GLY:O	1:C:18:HIS:HB2	2.18	0.44
1:A:321:ARG:HB2	1:A:322:PRO:CD	2.48	0.43
1:C:167:TYR:O	1:C:253:LEU:HG	2.18	0.43
1:C:367:ASP:O	1:C:370:ALA:HB3	2.17	0.43
1:D:165:ARG:HD2	1:D:230:GLN:O	2.19	0.43
1:C:19:SER:O	1:C:22:ASP:HB3	2.18	0.43
1:C:234:GLU:CD	1:C:234:GLU:H	2.27	0.43
1:D:282:THR:C	1:D:284:ALA:H	2.26	0.43
1:A:59:ILE:O	1:A:59:ILE:HG23	2.18	0.43
1:B:128:LEU:HD13	1:B:228:LEU:HG	2.00	0.43
1:B:319:GLY:HA2	1:B:361:THR:HG22	2.00	0.43
1:A:3:GLN:HB3	1:A:4:PRO:CD	2.41	0.43
1:A:22:ASP:O	1:A:26:ARG:HG3	2.19	0.43
1:C:175:ALA:HA	1:C:218:LYS:HE3	2.01	0.43
1:A:192:THR:OG1	1:A:194:GLU:HG2	2.18	0.43
1:B:113:ALA:O	1:B:116:LYS:HB2	2.19	0.43
1:C:169:ARG:NH2	1:C:253:LEU:O	2.52	0.43
1:A:337:LEU:C	1:A:339:LYS:H	2.27	0.42
1:C:104:CYS:HA	1:C:107:LEU:HG	2.00	0.42
1:C:320:ALA:O	1:C:324:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:LEU:O	1:D:294:GLN:N	2.48	0.42
1:A:37:THR:HG21	1:A:101:ILE:HD11	2.01	0.42
1:A:39:ASN:HB2	2:A:400:NDP:C4A	2.49	0.42
1:C:218:LYS:HA	1:C:218:LYS:HD3	1.86	0.42
1:C:293:ARG:O	1:D:296:ASP:HA	2.18	0.42
1:D:194:GLU:H	1:D:194:GLU:HG2	1.26	0.42
1:A:19:SER:O	1:A:22:ASP:HB3	2.19	0.42
1:A:301:ASP:CG	1:A:304:ARG:HD3	2.44	0.42
1:C:37:THR:CG2	3:C:424:HOH:O	2.66	0.42
1:C:261:ILE:HG22	1:C:262:GLY:N	2.33	0.42
1:C:261:ILE:HG22	1:C:287:LEU:HD12	2.01	0.42
1:A:216:MET:O	1:A:220:LEU:HG	2.19	0.42
1:C:1:MET:O	1:C:2:SER:HB2	2.19	0.42
1:D:33:VAL:HG21	1:D:52:THR:HB	2.02	0.42
1:D:233:LEU:HB3	1:D:312:MET:HE1	2.01	0.42
1:B:163:HIS:ND1	3:B:434:HOH:O	2.30	0.42
1:B:214:THR:O	1:B:215:MET:HB2	2.20	0.42
1:D:165:ARG:CD	1:D:230:GLN:O	2.68	0.42
1:A:150:ASP:OD2	1:A:153:HIS:ND1	2.36	0.42
1:A:232:PRO:HB3	1:A:234:GLU:OE2	2.19	0.42
1:A:268:THR:HB	1:A:269:PRO:HD2	2.02	0.42
1:A:308:LEU:O	1:A:312:MET:HG3	2.20	0.42
1:C:181:ARG:O	1:C:304:ARG:NH2	2.42	0.42
1:D:293:ARG:HE	1:D:293:ARG:HB3	1.28	0.42
1:A:261:ILE:HG22	1:A:262:GLY:N	2.34	0.42
1:B:319:GLY:CA	1:B:361:THR:HG22	2.50	0.42
1:D:14:GLY:O	1:D:18:HIS:HB2	2.20	0.42
1:A:263:SER:HB2	1:A:264:PRO:HD2	2.01	0.41
1:B:41:ASN:ND2	1:B:44:ASP:OD2	2.53	0.41
1:B:160:PHE:CG	1:B:161:PRO:HD2	2.55	0.41
1:C:188:MET:HA	1:C:191:VAL:HG23	2.02	0.41
1:D:311:ALA:CA	1:D:325:MET:HE1	2.50	0.41
1:D:346:ILE:O	1:D:350:VAL:HG23	2.20	0.41
1:D:352:LYS:HB3	1:D:382:LEU:HD13	2.02	0.41
1:B:39:ASN:HB2	2:B:401:NDP:C5A	2.50	0.41
1:B:325:MET:HB2	1:B:354:LEU:HD21	2.02	0.41
1:D:128:LEU:CD1	1:D:228:LEU:HG	2.50	0.41
1:D:261:ILE:HG22	1:D:262:GLY:N	2.35	0.41
1:A:313:GLU:O	1:A:316:LYS:HB3	2.20	0.41
1:A:312:MET:HB3	1:A:312:MET:HE2	1.63	0.41
1:C:233:LEU:HD22	1:C:312:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ALA:O	1:D:116:LYS:HB2	2.21	0.41
1:D:218:LYS:HD3	1:D:218:LYS:HA	1.87	0.41
1:D:321:ARG:HB2	1:D:322:PRO:CD	2.50	0.41
1:A:38:ALA:HB3	1:A:45:LEU:HD22	2.03	0.41
1:D:208:ILE:HG23	1:D:209:SER:N	2.36	0.41
1:D:310:LEU:HB2	1:D:325:MET:HE3	2.01	0.41
1:D:359:PRO:HG3	1:D:371:ILE:HG23	2.02	0.41
1:D:38:ALA:HB1	2:D:403:NDP:O3X	2.20	0.41
1:B:344:LEU:HB2	3:B:428:HOH:O	2.19	0.41
1:A:72:LEU:O	1:A:75:SER:HB3	2.20	0.41
1:A:345:ASP:O	1:A:348:LYS:HB2	2.21	0.41
1:B:131:ALA:O	1:B:135:MET:HG2	2.21	0.41
1:C:280:MET:HG2	3:C:406:HOH:O	2.21	0.41
1:D:91:MET:O	1:D:116:LYS:HE3	2.21	0.41
1:D:223:ILE:CG1	1:D:315:ILE:HD11	2.50	0.41
1:D:224:GLU:OE2	3:D:404:HOH:O	2.22	0.41
1:D:251:GLU:CG	1:D:257:ILE:HG12	2.49	0.41
1:D:267:ARG:NH1	1:D:283:PRO:HG2	2.35	0.41
1:A:14:GLY:O	1:A:18:HIS:HB2	2.20	0.41
1:A:150:ASP:CG	1:A:153:HIS:HD1	2.25	0.41
1:A:156:ILE:HG13	1:A:248:SER:HB3	2.02	0.41
1:A:292:LEU:O	1:A:293:ARG:CB	2.66	0.41
1:D:155:ALA:HB3	1:D:248:SER:HB2	2.03	0.40
1:A:243:GLN:CD	1:A:243:GLN:H	2.29	0.40
1:C:49:ALA:HB1	1:C:77:VAL:HG11	2.03	0.40
1:C:87:VAL:O	1:C:91:MET:HG3	2.21	0.40
1:B:51:ARG:NH2	1:B:51:ARG:CG	2.76	0.40
1:B:180:PHE:HB3	1:B:183:THR:HB	2.02	0.40
1:C:102:ILE:C	1:C:102:ILE:HD12	2.46	0.40
1:B:181:ARG:C	1:B:304:ARG:HH22	2.28	0.40
1:B:301:ASP:OD2	1:B:304:ARG:HD3	2.21	0.40
1:C:223:ILE:HA	1:C:315:ILE:HD13	2.03	0.40
1:C:319:GLY:HA3	1:C:361:THR:HG22	1.99	0.40
1:D:135:MET:O	1:D:139:VAL:HG23	2.22	0.40
1:D:361:THR:HA	1:D:362:PRO:HD3	1.93	0.40
1:A:383:MET:O	1:A:383:MET:HE2	2.21	0.40
1:B:361:THR:HA	1:B:362:PRO:HD3	1.92	0.40
1:C:102:ILE:HD12	1:C:102:ILE:O	2.22	0.40
1:C:361:THR:HA	1:C:362:PRO:HD3	1.91	0.40
1:D:40:ARG:HA	1:D:64:LEU:HD12	2.02	0.40

All (15) symmetry-related close contacts are listed below. The label for Atom-2 includes the

symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ASN:N	1:C:1:MET:O[2_656]	0.73	1.47
1:B:164:ASN:N	1:C:1:MET:C[2_656]	1.46	0.74
1:B:163:HIS:C	1:C:1:MET:C[2_656]	1.50	0.70
1:B:164:ASN:CA	1:C:1:MET:O[2_656]	1.55	0.65
1:B:163:HIS:N	1:C:1:MET:CA[2_656]	1.59	0.61
1:B:163:HIS:CA	1:C:1:MET:CA[2_656]	1.81	0.39
1:B:163:HIS:C	1:C:1:MET:O[2_656]	1.82	0.38
1:B:162:HIS:CA	1:C:1:MET:SD[2_656]	1.85	0.35
1:B:163:HIS:C	1:C:2:SER:N[2_656]	1.87	0.33
1:B:163:HIS:O	1:C:2:SER:N[2_656]	1.99	0.21
1:B:163:HIS:CA	1:C:1:MET:C[2_656]	2.06	0.14
1:B:163:HIS:O	1:C:2:SER:CA[2_656]	2.08	0.12
1:B:163:HIS:CA	1:C:1:MET:N[2_656]	2.14	0.06
1:B:164:ASN:C	1:C:1:MET:O[2_656]	2.15	0.05
1:C:3:GLN:N	3:B:412:HOH:O[2_646]	2.16	0.04

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	374/388 (96%)	355 (95%)	17 (4%)	2 (0%)	24	48
1	B	375/388 (97%)	355 (95%)	19 (5%)	1 (0%)	36	60
1	C	374/388 (96%)	353 (94%)	19 (5%)	2 (0%)	24	48
1	D	374/388 (96%)	360 (96%)	12 (3%)	2 (0%)	24	48
All	All	1497/1552 (96%)	1423 (95%)	67 (4%)	7 (0%)	24	48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	SER
1	B	248	SER

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Mol	Chain	Res	Type
1	C	248	SER
1	D	248	SER
1	D	293	ARG
1	A	127	SER
1	C	28	LEU

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	299/308 (97%)	279 (93%)	20 (7%)	15	36
1	B	301/308 (98%)	288 (96%)	13 (4%)	26	54
1	C	300/308 (97%)	292 (97%)	8 (3%)	39	69
1	D	300/308 (97%)	289 (96%)	11 (4%)	30	59
All	All	1200/1232 (97%)	1148 (96%)	52 (4%)	26	54

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	61	ASP
1	A	63	SER
1	A	126	GLU
1	A	146	LEU
1	A	165	ARG
1	A	185	LEU
1	A	194	GLU
1	A	197	VAL
1	A	198	GLN
1	A	224	GLU
1	A	231	ILE
1	A	234	GLU
1	A	248	SER
1	A	260	GLN
1	A	287	LEU

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Mol	Chain	Res	Type
1	A	292	LEU
1	A	293	ARG
1	A	351	GLU
1	A	383	MET
1	B	18	HIS
1	B	102	ILE
1	B	125	LYS
1	B	146	LEU
1	B	150	ASP
1	B	151	SER
1	B	195	ARG
1	B	198	GLN
1	B	231	ILE
1	B	234	GLU
1	B	248	SER
1	B	287	LEU
1	B	383	MET
1	C	30	ARG
1	C	37	THR
1	C	63	SER
1	C	146	LEU
1	C	194	GLU
1	C	234	GLU
1	C	287	LEU
1	C	383	MET
1	D	37	THR
1	D	40	ARG
1	D	146	LEU
1	D	194	GLU
1	D	195	ARG
1	D	231	ILE
1	D	234	GLU
1	D	260	GLN
1	D	287	LEU
1	D	293	ARG
1	D	383	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	124	ASN

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Mol	Chain	Res	Type
1	A	227	HIS
1	A	247	HIS
1	A	260	GLN
1	A	272	HIS
1	A	294	GLN
1	A	329	ASN
1	B	53	ASN
1	B	158	GLN
1	B	227	HIS
1	B	260	GLN
1	B	272	HIS
1	B	294	GLN
1	B	329	ASN
1	C	53	ASN
1	C	260	GLN
1	C	272	HIS
1	C	294	GLN
1	D	32	GLN
1	D	39	ASN
1	D	53	ASN
1	D	142	HIS
1	D	227	HIS
1	D	260	GLN
1	D	272	HIS

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 ⓘ

4 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	NDP	A	400	-	29,29,52	1.57	5 (17%)	44,45,80	2.35	14 (31%)
2	NDP	D	403	-	29,29,52	2.97	11 (37%)	44,45,80	3.43	22 (50%)
2	NDP	B	401	-	29,29,52	1.60	7 (24%)	44,45,80	2.40	15 (34%)
2	NDP	C	402	-	29,29,52	1.39	3 (10%)	44,45,80	1.52	11 (25%)

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	NDP	A	400	-	-	2/15/31/77	0/3/3/5
2	NDP	D	403	-	-	2/15/31/77	0/3/3/5
2	NDP	B	401	-	-	2/15/31/77	0/3/3/5
2	NDP	C	402	-	-	3/15/31/77	0/3/3/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	403	NDP	O5B-C5B	-7.87	1.14	1.44
2	D	403	NDP	C3B-C4B	-7.28	1.34	1.53
2	D	403	NDP	C5B-C4B	-6.02	1.33	1.51
2	D	403	NDP	O4B-C1B	5.13	1.53	1.42
2	A	400	NDP	O3B-C3B	4.38	1.53	1.43
2	D	403	NDP	C8A-N7A	-4.14	1.23	1.31
2	A	400	NDP	P2B-O2B	-3.84	1.52	1.59
2	C	402	NDP	O3B-C3B	3.65	1.52	1.43
2	C	402	NDP	PA-O1A	-3.63	1.39	1.50
2	B	401	NDP	C3B-C4B	3.47	1.61	1.53
2	D	403	NDP	PA-O5B	3.47	1.71	1.60
2	B	401	NDP	PA-O1A	-3.44	1.39	1.50
2	B	401	NDP	O3B-C3B	3.31	1.51	1.43
2	D	403	NDP	O4B-C4B	3.19	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	403	NDP	O3B-C3B	3.10	1.50	1.43
2	A	400	NDP	PA-O1A	-2.99	1.41	1.50
2	B	401	NDP	C5B-C4B	-2.74	1.43	1.51
2	B	401	NDP	P2B-O2B	-2.55	1.55	1.59
2	A	400	NDP	C5B-C4B	-2.25	1.44	1.51
2	A	400	NDP	C3B-C4B	2.23	1.58	1.53
2	D	403	NDP	C2A-N3A	2.19	1.37	1.33
2	D	403	NDP	C2A-N1A	2.17	1.37	1.33
2	B	401	NDP	C4A-N3A	2.06	1.38	1.34
2	B	401	NDP	O5B-C5B	-2.06	1.36	1.44
2	C	402	NDP	C5B-C4B	-2.05	1.45	1.51
2	D	403	NDP	PA-O1A	-2.01	1.44	1.50

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	403	NDP	O3-PA-O2A	-10.21	69.50	107.80
2	B	401	NDP	O3X-P2B-O1X	-7.62	81.14	110.83
2	A	400	NDP	O3X-P2B-O1X	-7.58	81.30	110.83
2	D	403	NDP	O3X-P2B-O1X	-7.13	83.07	110.83
2	B	401	NDP	O3X-P2B-O2X	-6.70	82.69	107.80
2	D	403	NDP	O5B-PA-O1A	-6.38	89.20	106.44
2	D	403	NDP	O3X-P2B-O2X	-5.95	85.48	107.80
2	A	400	NDP	O3X-P2B-O2B	-5.82	83.15	105.85
2	D	403	NDP	O3-PA-O1A	5.77	133.33	110.83
2	A	400	NDP	O3X-P2B-O2X	-5.45	87.35	107.80
2	D	403	NDP	C2B-C1B-N9A	-5.30	105.03	113.75
2	D	403	NDP	O3-PA-O5B	5.25	120.35	106.67
2	D	403	NDP	O2A-PA-O5B	5.09	119.94	106.67
2	B	401	NDP	O3X-P2B-O2B	-4.96	86.54	105.85
2	D	403	NDP	O3X-P2B-O2B	-4.82	87.07	105.85
2	D	403	NDP	O2A-PA-O1A	4.60	128.77	110.83
2	C	402	NDP	O4B-C4B-C5B	-4.12	96.13	109.33
2	A	400	NDP	O4B-C4B-C5B	-4.06	96.34	109.33
2	B	401	NDP	O4B-C4B-C5B	-3.73	97.38	109.33
2	B	401	NDP	O5B-C5B-C4B	-3.69	96.42	108.99
2	B	401	NDP	O2X-P2B-O1X	3.66	125.11	110.83
2	D	403	NDP	O5B-C5B-C4B	3.53	121.03	108.99
2	C	402	NDP	O5B-C5B-C4B	-3.41	97.40	108.99
2	A	400	NDP	O2X-P2B-O1X	3.40	124.07	110.83
2	D	403	NDP	N3A-C2A-N1A	-3.39	123.44	128.58
2	D	403	NDP	C4A-N9A-C1B	3.36	134.50	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	403	NDP	O2X-P2B-O1X	3.32	123.75	110.83
2	D	403	NDP	C1B-N9A-C8A	-3.25	119.88	127.09
2	A	400	NDP	N3A-C2A-N1A	-3.25	123.66	128.58
2	A	400	NDP	O2A-PA-O1A	3.24	123.45	110.83
2	B	401	NDP	O2A-PA-O1A	3.18	123.21	110.83
2	C	402	NDP	O2A-PA-O1A	3.08	122.84	110.83
2	D	403	NDP	O2X-P2B-O2B	3.08	117.83	105.85
2	D	403	NDP	C4B-O4B-C1B	-3.02	102.79	109.47
2	A	400	NDP	O5B-C5B-C4B	-2.83	99.37	108.99
2	D	403	NDP	O3B-C3B-C4B	-2.64	103.49	111.08
2	B	401	NDP	O2B-C2B-C3B	2.58	120.92	111.68
2	B	401	NDP	O2A-PA-O5B	-2.55	100.01	106.67
2	A	400	NDP	O2X-P2B-O2B	2.55	115.79	105.85
2	C	402	NDP	N3A-C2A-N1A	-2.55	124.73	128.58
2	A	400	NDP	O2B-C2B-C1B	2.50	118.83	110.05
2	B	401	NDP	O2B-C2B-C1B	2.47	118.75	110.05
2	C	402	NDP	O2B-C2B-C1B	2.45	118.68	110.05
2	A	400	NDP	O2A-PA-O5B	-2.43	100.34	106.67
2	D	403	NDP	C3B-C2B-C1B	-2.39	98.23	102.81
2	C	402	NDP	C5A-N7A-C8A	2.34	107.13	103.45
2	D	403	NDP	C5A-N7A-C8A	2.32	107.10	103.45
2	B	401	NDP	N3A-C2A-N1A	-2.32	125.07	128.58
2	A	400	NDP	O2B-C2B-C3B	2.25	119.76	111.68
2	C	402	NDP	O2A-PA-O5B	-2.24	100.83	106.67
2	D	403	NDP	C2B-C3B-C4B	2.22	106.76	101.99
2	B	401	NDP	C5A-N7A-C8A	2.20	106.90	103.45
2	B	401	NDP	O2B-P2B-O1X	2.19	117.14	109.33
2	C	402	NDP	O2B-C2B-C3B	2.16	119.44	111.68
2	A	400	NDP	C3B-C2B-C1B	-2.14	98.70	102.81
2	A	400	NDP	O2B-P2B-O1X	2.10	116.82	109.33
2	C	402	NDP	C3B-C2B-C1B	-2.08	98.82	102.81
2	D	403	NDP	O2B-C2B-C1B	2.08	117.35	110.05
2	C	402	NDP	N9A-C8A-N7A	-2.06	111.01	113.94
2	C	402	NDP	C2A-N1A-C6A	2.04	122.08	118.73
2	B	401	NDP	O5B-PA-O1A	2.03	111.93	106.44
2	B	401	NDP	O2X-P2B-O2B	2.02	113.74	105.85

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	NDP	C3B-C2B-O2B-P2B

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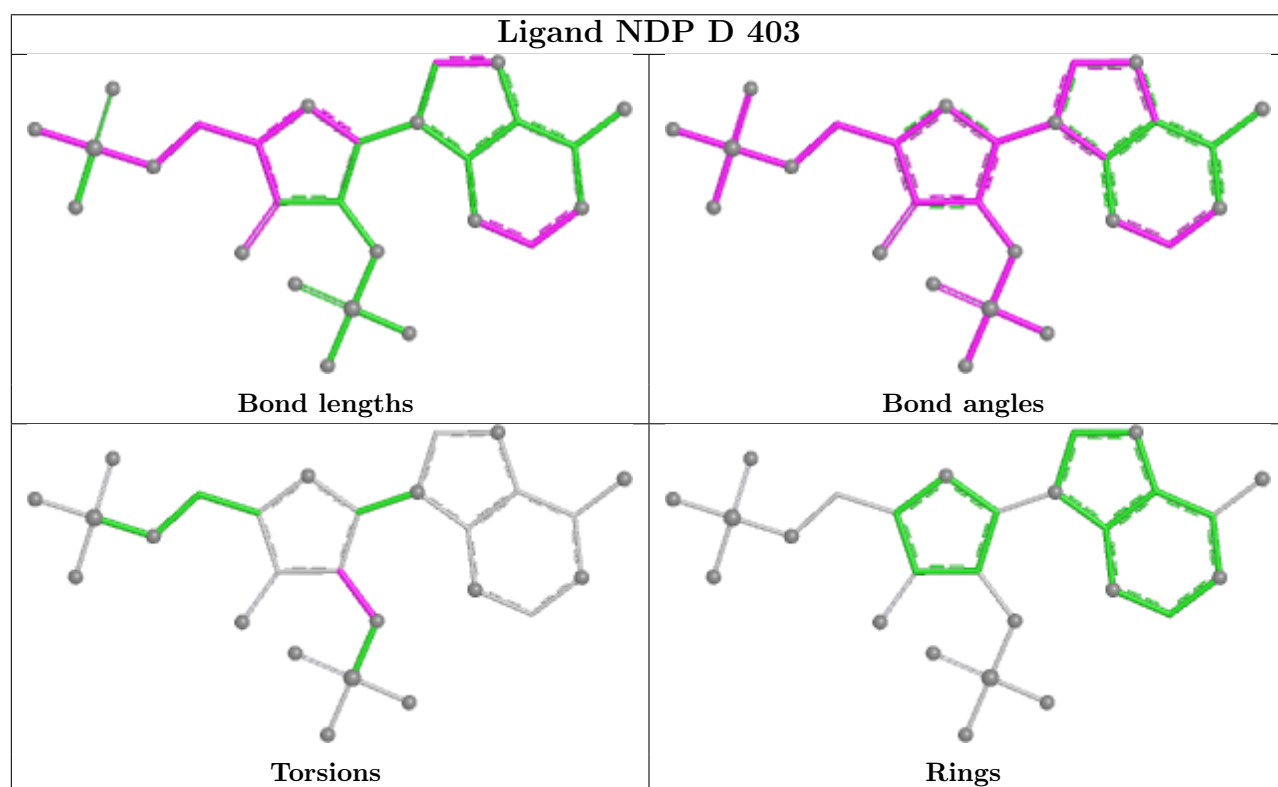
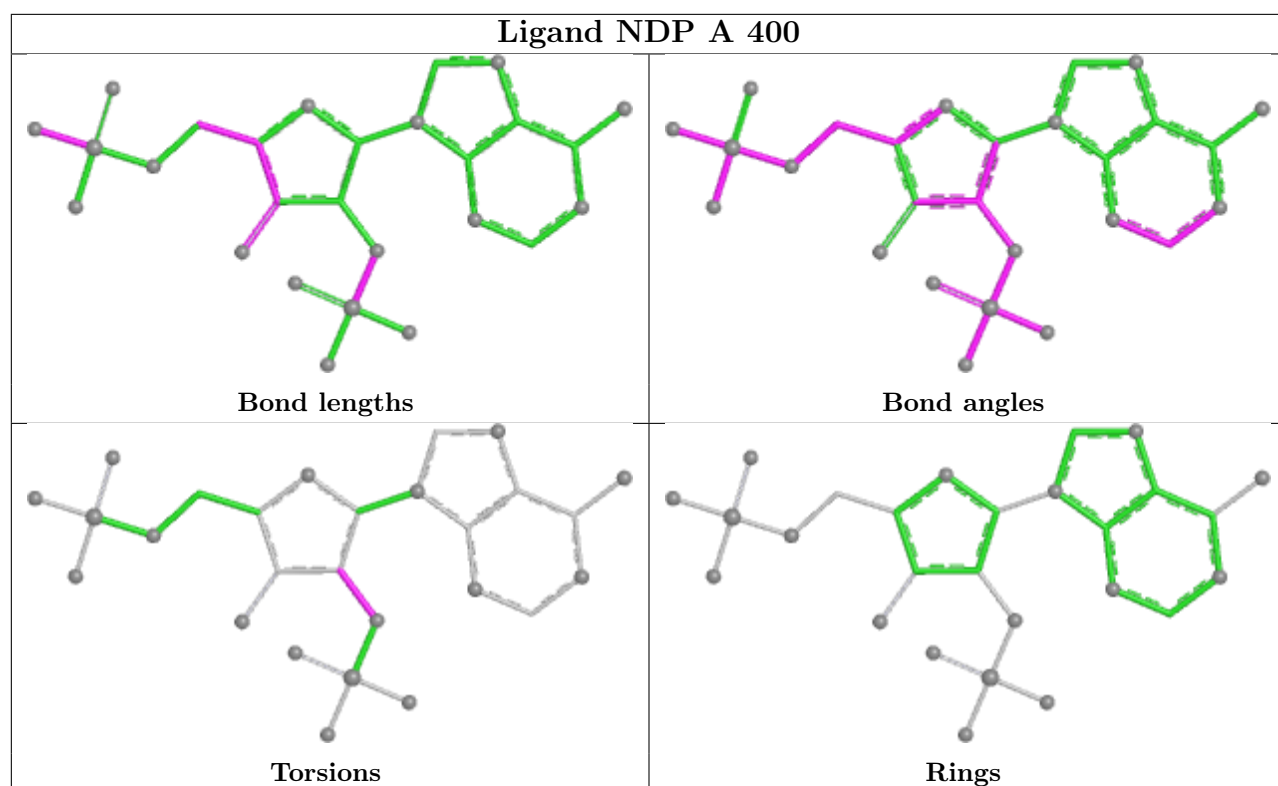
Mol	Chain	Res	Type	Atoms
2	B	401	NDP	C3B-C2B-O2B-P2B
2	C	402	NDP	C3B-C2B-O2B-P2B
2	A	400	NDP	C1B-C2B-O2B-P2B
2	D	403	NDP	C1B-C2B-O2B-P2B
2	D	403	NDP	C3B-C2B-O2B-P2B
2	B	401	NDP	C1B-C2B-O2B-P2B
2	C	402	NDP	C1B-C2B-O2B-P2B
2	C	402	NDP	C2B-O2B-P2B-O1X

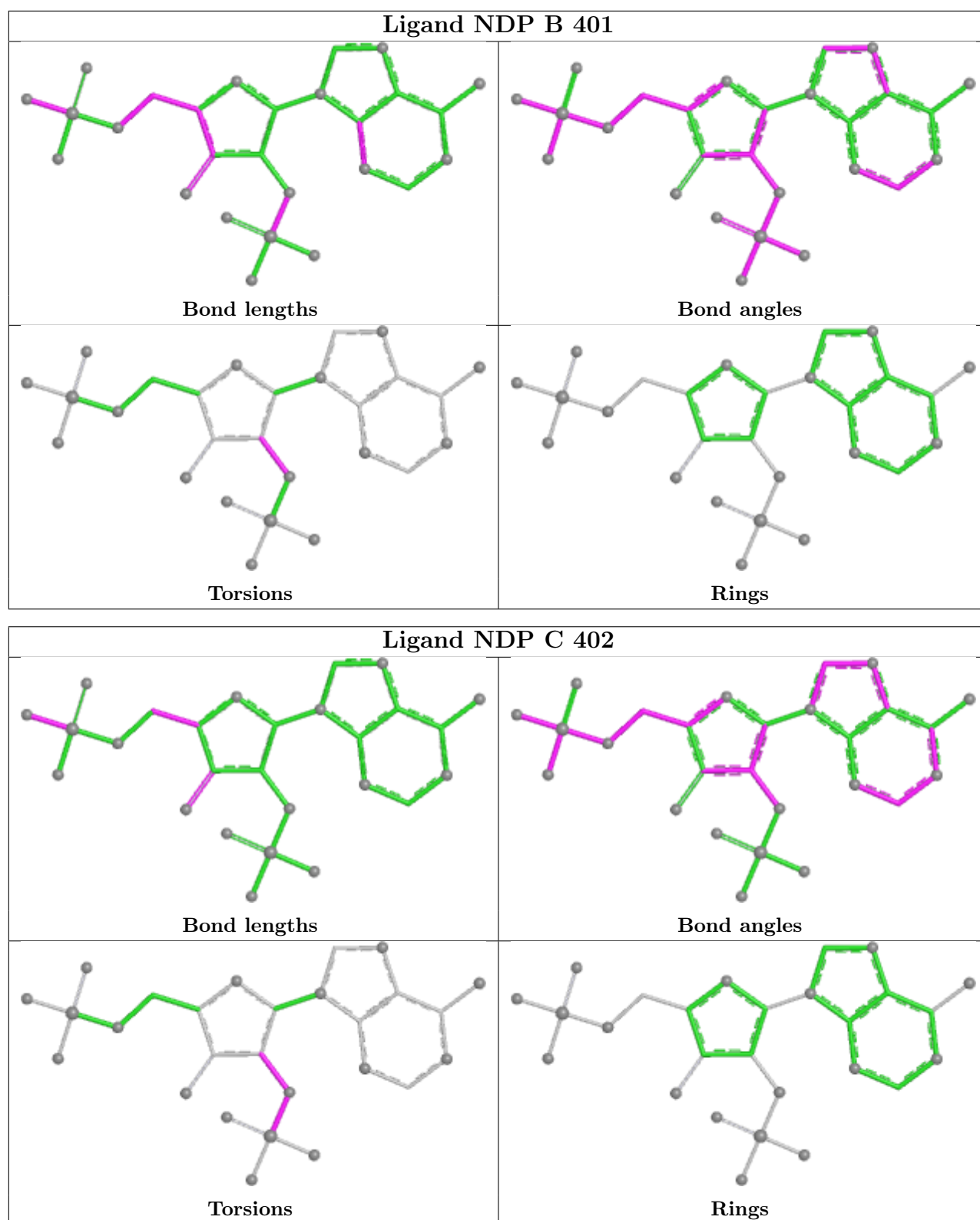
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	NDP	1	0
2	D	403	NDP	3	0
2	B	401	NDP	2	0
2	C	402	NDP	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	378/388 (97%)	2.99	286 (75%) 0 0	16, 43, 87, 104	0
1	B	379/388 (97%)	2.00	174 (45%) 0 0	17, 35, 63, 88	0
1	C	378/388 (97%)	3.03	291 (76%) 0 0	22, 44, 69, 94	0
1	D	378/388 (97%)	2.65	270 (71%) 0 0	22, 45, 74, 107	0
All	All	1513/1552 (97%)	2.67	1021 (67%) 0 0	16, 41, 75, 107	0

All (1021) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	365	LEU	8.6
1	A	68	LEU	8.4
1	A	375	ALA	7.9
1	C	2	SER	7.7
1	C	68	LEU	7.7
1	A	365	LEU	7.5
1	C	368	VAL	7.4
1	A	368	VAL	7.0
1	C	190	THR	7.0
1	A	357	TYR	6.9
1	C	52	THR	6.8
1	C	65	TYR	6.8
1	C	45	LEU	6.5
1	C	41	ASN	6.4
1	A	12	ALA	6.4
1	C	287	LEU	6.3
1	A	354	LEU	6.2
1	A	362	PRO	6.1
1	A	379	ALA	6.1
1	A	386	LEU	6.0
1	A	209	SER	6.0

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Mol	Chain	Res	Type	RSRZ
1	C	362	PRO	6.0
1	A	27	ASN	5.9
1	C	196	ALA	5.9
1	C	357	TYR	5.9
1	C	57	ALA	5.8
1	D	233	LEU	5.8
1	C	206	ALA	5.7
1	C	315	ILE	5.7
1	C	54	ALA	5.7
1	C	127	SER	5.7
1	C	150	ASP	5.6
1	A	356	HIS	5.6
1	C	117	GLY	5.6
1	D	4	PRO	5.6
1	A	323	ALA	5.6
1	C	24	ILE	5.6
1	C	143	GLY	5.6
1	C	161	PRO	5.6
1	A	184	SER	5.6
1	C	151	SER	5.6
1	A	190	THR	5.6
1	C	364	SER	5.5
1	C	64	LEU	5.5
1	D	359	PRO	5.5
1	C	386	LEU	5.5
1	C	101	ILE	5.5
1	A	23	LEU	5.5
1	A	364	SER	5.4
1	A	359	PRO	5.4
1	C	44	ASP	5.4
1	A	380	ALA	5.3
1	D	327	ALA	5.3
1	B	206	ALA	5.3
1	A	35	ALA	5.3
1	A	378	GLN	5.3
1	B	124	ASN	5.3
1	A	125	LYS	5.2
1	C	8	THR	5.2
1	D	124	ASN	5.2
1	D	135	MET	5.2
1	C	359	PRO	5.2
1	A	382	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	42	VAL	5.2
1	A	37	THR	5.2
1	D	373	ASN	5.1
1	D	206	ALA	5.1
1	A	315	ILE	5.1
1	A	371	ILE	5.1
1	C	341	ILE	5.1
1	C	1	MET	5.1
1	B	386	LEU	5.1
1	A	19	SER	5.1
1	A	127	SER	5.1
1	C	58	VAL	5.1
1	C	77	VAL	5.1
1	C	12	ALA	5.0
1	C	356	HIS	5.0
1	D	126	GLU	5.0
1	C	53	ASN	5.0
1	C	55	LYS	5.0
1	A	262	GLY	5.0
1	C	10	LEU	5.0
1	D	111	LEU	5.0
1	D	75	SER	4.9
1	D	356	HIS	4.9
1	C	38	ALA	4.9
1	A	331	ILE	4.9
1	D	57	ALA	4.9
1	A	215	MET	4.9
1	B	198	GLN	4.9
1	C	369	PHE	4.8
1	A	45	LEU	4.8
1	C	27	ASN	4.8
1	A	51	ARG	4.8
1	A	349	ILE	4.7
1	C	208	ILE	4.7
1	A	44	ASP	4.7
1	B	135	MET	4.7
1	A	360	ALA	4.7
1	D	307	ALA	4.7
1	A	189	ALA	4.7
1	C	380	ALA	4.7
1	A	140	ARG	4.7
1	C	265	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	149	VAL	4.7
1	A	126	GLU	4.7
1	C	11	GLY	4.7
1	B	200	PRO	4.7
1	A	332	ALA	4.6
1	B	199	HIS	4.6
1	A	185	LEU	4.6
1	B	111	LEU	4.6
1	C	20	THR	4.6
1	A	146	LEU	4.6
1	A	76	SER	4.6
1	D	180	PHE	4.6
1	A	65	TYR	4.6
1	D	184	SER	4.6
1	C	124	ASN	4.6
1	A	312	MET	4.6
1	A	341	ILE	4.6
1	A	343	PHE	4.6
1	C	48	ALA	4.5
1	C	49	ALA	4.5
1	A	64	LEU	4.5
1	B	64	LEU	4.5
1	D	147	LEU	4.5
1	A	325	MET	4.5
1	C	195	ARG	4.5
1	C	78	GLU	4.5
1	D	160	PHE	4.5
1	D	130	SER	4.5
1	A	52	THR	4.5
1	C	33	VAL	4.5
1	A	196	ALA	4.5
1	C	284	ALA	4.5
1	C	325	MET	4.5
1	D	363	SER	4.4
1	A	225	ALA	4.4
1	D	197	VAL	4.4
1	A	36	LEU	4.4
1	C	128	LEU	4.4
1	D	386	LEU	4.4
1	C	29	ASP	4.4
1	B	164	ASN	4.4
1	C	23	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	266	MET	4.4
1	C	96	TRP	4.4
1	D	286	SER	4.4
1	A	26	ARG	4.4
1	D	50	LYS	4.4
1	D	254	ASP	4.3
1	D	143	GLY	4.3
1	C	385	SER	4.3
1	A	318	GLY	4.3
1	A	195	ARG	4.3
1	B	130	SER	4.3
1	D	377	ILE	4.3
1	C	240	VAL	4.3
1	D	350	VAL	4.3
1	C	312	MET	4.3
1	D	146	LEU	4.3
1	A	322	PRO	4.3
1	B	126	GLU	4.3
1	C	297	PHE	4.3
1	C	37	THR	4.3
1	A	334	ALA	4.2
1	A	385	SER	4.2
1	C	374	GLU	4.2
1	D	315	ILE	4.2
1	A	149	VAL	4.2
1	C	67	ASP	4.2
1	D	284	ALA	4.2
1	A	208	ILE	4.2
1	C	34	ILE	4.2
1	A	353	THR	4.2
1	C	228	LEU	4.2
1	B	74	GLY	4.2
1	D	303	GLU	4.2
1	C	140	ARG	4.2
1	D	357	TYR	4.2
1	A	73	ALA	4.2
1	A	231	ILE	4.2
1	A	350	VAL	4.2
1	C	163	HIS	4.2
1	A	314	SER	4.1
1	D	199	HIS	4.1
1	A	302	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	62	PRO	4.1
1	C	99	ALA	4.1
1	B	47	ASP	4.1
1	D	346	ILE	4.1
1	B	30	ARG	4.1
1	B	256	SER	4.1
1	C	209	SER	4.1
1	A	191	VAL	4.1
1	D	332	ALA	4.1
1	D	76	SER	4.1
1	D	292	LEU	4.1
1	C	159	CYS	4.1
1	C	138	ALA	4.1
1	C	281	GLU	4.1
1	C	311	ALA	4.1
1	A	17	GLY	4.1
1	D	293	ARG	4.1
1	A	236	PHE	4.1
1	C	160	PHE	4.1
1	A	317	SER	4.1
1	C	76	SER	4.1
1	C	85	ALA	4.0
1	D	334	ALA	4.0
1	A	11	GLY	4.0
1	A	376	ARG	4.0
1	A	22	ASP	4.0
1	A	308	LEU	4.0
1	C	382	LEU	4.0
1	D	196	ALA	4.0
1	C	289	PHE	4.0
1	A	13	THR	4.0
1	B	363	SER	4.0
1	D	198	GLN	4.0
1	A	293	ARG	4.0
1	C	146	LEU	4.0
1	C	276	TRP	4.0
1	C	355	ASP	4.0
1	C	51	ARG	3.9
1	A	355	ASP	3.9
1	A	369	PHE	3.9
1	C	98	MET	3.9
1	C	39	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	42	VAL	3.9
1	A	55	LYS	3.9
1	A	117	GLY	3.9
1	A	129	VAL	3.9
1	A	186	ALA	3.9
1	A	337	LEU	3.9
1	A	377	ILE	3.9
1	C	326	ASN	3.9
1	A	75	SER	3.9
1	C	130	SER	3.9
1	A	10	LEU	3.9
1	A	101	ILE	3.9
1	D	64	LEU	3.9
1	B	380	ALA	3.9
1	D	81	ALA	3.9
1	A	205	GLY	3.9
1	A	197	VAL	3.9
1	A	46	ALA	3.8
1	C	191	VAL	3.8
1	C	32	GLN	3.8
1	C	358	THR	3.8
1	A	316	LYS	3.8
1	D	244	SER	3.8
1	B	284	ALA	3.8
1	D	112	ALA	3.8
1	A	179	PRO	3.8
1	D	69	LYS	3.8
1	C	71	ALA	3.8
1	A	358	THR	3.8
1	D	366	GLU	3.8
1	D	21	LEU	3.8
1	C	115	ARG	3.8
1	C	316	LYS	3.8
1	A	193	PRO	3.8
1	A	110	THR	3.7
1	D	145	THR	3.7
1	A	130	SER	3.7
1	D	320	ALA	3.7
1	C	279	ARG	3.7
1	D	168	VAL	3.7
1	D	250	VAL	3.7
1	C	378	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	184	SER	3.7
1	D	40	ARG	3.7
1	D	193	PRO	3.7
1	A	150	ASP	3.7
1	A	361	THR	3.7
1	A	83	ALA	3.7
1	C	207	LYS	3.7
1	A	306	PRO	3.7
1	A	287	LEU	3.7
1	B	233	LEU	3.7
1	D	16	ILE	3.7
1	D	367	ASP	3.7
1	A	207	LYS	3.7
1	B	46	ALA	3.7
1	C	81	ALA	3.7
1	C	62	PRO	3.7
1	C	126	GLU	3.7
1	C	110	THR	3.6
1	A	31	TYR	3.6
1	A	370	ALA	3.6
1	C	83	ALA	3.6
1	D	54	ALA	3.6
1	D	138	ALA	3.6
1	D	305	PHE	3.6
1	A	198	GLN	3.6
1	C	162	HIS	3.6
1	A	284	ALA	3.6
1	A	9	VAL	3.6
1	A	58	VAL	3.6
1	B	70	GLU	3.6
1	C	111	LEU	3.6
1	B	16	ILE	3.6
1	A	109	ALA	3.6
1	C	225	ALA	3.6
1	A	366	GLU	3.6
1	C	87	VAL	3.6
1	A	30	ARG	3.6
1	A	29	ASP	3.6
1	A	67	ASP	3.6
1	A	206	ALA	3.6
1	D	311	ALA	3.6
1	D	369	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	19	SER	3.6
1	D	118	LYS	3.6
1	D	125	LYS	3.6
1	A	24	ILE	3.5
1	A	20	THR	3.5
1	A	92	MET	3.5
1	A	178	GLY	3.5
1	A	351	GLU	3.5
1	A	33	VAL	3.5
1	C	197	VAL	3.5
1	C	114	ILE	3.5
1	C	383	MET	3.5
1	D	74	GLY	3.5
1	B	127	SER	3.5
1	B	293	ARG	3.5
1	C	261	ILE	3.5
1	A	372	ASP	3.5
1	A	311	ALA	3.5
1	B	335	ALA	3.5
1	D	319	GLY	3.5
1	A	363	SER	3.5
1	D	173	ILE	3.5
1	A	192	THR	3.5
1	C	339	LYS	3.5
1	C	17	GLY	3.5
1	C	35	ALA	3.5
1	C	381	ALA	3.5
1	D	219	GLY	3.5
1	D	323	ALA	3.5
1	D	379	ALA	3.5
1	A	187	GLU	3.5
1	A	32	GLN	3.5
1	A	222	LEU	3.5
1	A	18	HIS	3.5
1	C	229	PHE	3.5
1	C	129	VAL	3.5
1	C	270	ILE	3.4
1	A	254	ASP	3.4
1	A	338	ASP	3.4
1	C	94	ALA	3.4
1	D	49	ALA	3.4
1	A	162	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	369	PHE	3.4
1	D	149	VAL	3.4
1	A	346	ILE	3.4
1	D	114	ILE	3.4
1	D	385	SER	3.4
1	B	362	PRO	3.4
1	A	265	ASP	3.4
1	B	44	ASP	3.4
1	D	164	ASN	3.4
1	C	36	LEU	3.4
1	D	382	LEU	3.4
1	D	226	PHE	3.4
1	A	42	VAL	3.4
1	A	339	LYS	3.4
1	A	159	CYS	3.4
1	A	28	LEU	3.4
1	B	80	ALA	3.4
1	B	196	ALA	3.4
1	D	375	ALA	3.4
1	C	22	ASP	3.4
1	C	59	ILE	3.4
1	C	371	ILE	3.4
1	B	286	SER	3.4
1	C	75	SER	3.4
1	C	353	THR	3.4
1	A	71	ALA	3.4
1	B	230	GLN	3.4
1	C	259	ALA	3.4
1	C	360	ALA	3.4
1	D	33	VAL	3.4
1	D	349	ILE	3.3
1	A	8	THR	3.3
1	B	165	ARG	3.3
1	C	26	ARG	3.3
1	D	5	ARG	3.3
1	D	161	PRO	3.3
1	D	46	ALA	3.3
1	B	383	MET	3.3
1	A	333	VAL	3.3
1	D	65	TYR	3.3
1	D	309	THR	3.3
1	B	194	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	359	PRO	3.3
1	C	322	PRO	3.3
1	D	123	ALA	3.3
1	D	189	ALA	3.3
1	A	53	ASN	3.3
1	A	326	ASN	3.3
1	A	47	ASP	3.3
1	B	207	LYS	3.3
1	B	367	ASP	3.3
1	A	151	SER	3.3
1	D	68	LEU	3.3
1	D	215	MET	3.3
1	D	186	ALA	3.3
1	D	301	ASP	3.3
1	C	30	ARG	3.3
1	A	290	THR	3.3
1	B	62	PRO	3.3
1	C	31	TYR	3.3
1	C	135	MET	3.3
1	A	106	GLY	3.3
1	C	318	GLY	3.3
1	A	289	PHE	3.3
1	A	321	ARG	3.2
1	A	383	MET	3.2
1	C	69	LYS	3.2
1	D	18	HIS	3.2
1	D	20	THR	3.2
1	B	76	SER	3.2
1	C	186	ALA	3.2
1	C	335	ALA	3.2
1	A	77	VAL	3.2
1	B	59	ILE	3.2
1	D	7	VAL	3.2
1	D	102	ILE	3.2
1	D	336	PHE	3.2
1	C	84	ASP	3.2
1	D	195	ARG	3.2
1	C	264	PRO	3.2
1	C	330	GLU	3.2
1	D	148	PRO	3.2
1	A	119	THR	3.2
1	B	378	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	219	GLY	3.2
1	A	335	ALA	3.2
1	C	332	ALA	3.2
1	A	136	ILE	3.2
1	A	297	PHE	3.2
1	D	157	PHE	3.2
1	C	154	ASN	3.2
1	D	51	ARG	3.2
1	C	21	LEU	3.2
1	C	28	LEU	3.2
1	D	276	TRP	3.2
1	D	282	THR	3.2
1	D	358	THR	3.2
1	A	143	GLY	3.2
1	B	73	ALA	3.2
1	D	167	TYR	3.2
1	A	210	ILE	3.2
1	C	331	ILE	3.2
1	D	341	ILE	3.2
1	C	137	ASP	3.2
1	C	376	ARG	3.2
1	A	128	LEU	3.2
1	D	285	GLU	3.2
1	C	119	THR	3.2
1	B	60	ALA	3.2
1	A	310	LEU	3.1
1	B	68	LEU	3.1
1	D	194	GLU	3.1
1	D	362	PRO	3.1
1	B	6	THR	3.1
1	B	186	ALA	3.1
1	D	71	ALA	3.1
1	D	380	ALA	3.1
1	A	367	ASP	3.1
1	C	47	ASP	3.1
1	A	224	GLU	3.1
1	C	18	HIS	3.1
1	A	174	THR	3.1
1	C	282	THR	3.1
1	A	74	GLY	3.1
1	C	226	PHE	3.1
1	D	256	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	50	LYS	3.1
1	C	372	ASP	3.1
1	A	78	GLU	3.1
1	A	374	GLU	3.1
1	C	179	PRO	3.1
1	D	174	THR	3.1
1	A	213	ALA	3.1
1	C	80	ALA	3.1
1	C	377	ILE	3.1
1	D	175	ALA	3.1
1	A	336	PHE	3.1
1	D	291	LYS	3.1
1	B	385	SER	3.1
1	A	233	LEU	3.1
1	B	23	LEU	3.1
1	B	53	ASN	3.1
1	B	163	HIS	3.1
1	D	47	ASP	3.1
1	A	214	THR	3.1
1	D	183	THR	3.1
1	B	118	LYS	3.1
1	C	102	ILE	3.1
1	D	24	ILE	3.1
1	D	34	ILE	3.1
1	D	38	ALA	3.1
1	D	335	ALA	3.1
1	B	276	TRP	3.1
1	D	304	ARG	3.1
1	C	245	VAL	3.1
1	D	42	VAL	3.1
1	D	236	PHE	3.1
1	D	343	PHE	3.1
1	A	39	ASN	3.0
1	A	70	GLU	3.0
1	C	224	GLU	3.0
1	D	230	GLN	3.0
1	D	190	THR	3.0
1	D	235	LYS	3.0
1	A	54	ALA	3.0
1	A	328	ALA	3.0
1	B	151	SER	3.0
1	C	147	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	366	GLU	3.0
1	B	161	PRO	3.0
1	A	3	GLN	3.0
1	A	270	ILE	3.0
1	B	195	ARG	3.0
1	C	349	ILE	3.0
1	A	320	ALA	3.0
1	B	48	ALA	3.0
1	C	113	ALA	3.0
1	D	96	TRP	3.0
1	A	21	LEU	3.0
1	B	184	SER	3.0
1	D	354	LEU	3.0
1	C	164	ASN	3.0
1	B	150	ASP	3.0
1	C	5	ARG	3.0
1	C	267	ARG	3.0
1	A	14	GLY	3.0
1	C	97	THR	3.0
1	C	262	GLY	3.0
1	C	46	ALA	3.0
1	C	123	ALA	3.0
1	C	15	SER	3.0
1	D	263	SER	3.0
1	D	302	TYR	3.0
1	A	135	MET	3.0
1	D	231	ILE	3.0
1	C	74	GLY	3.0
1	C	132	GLY	3.0
1	A	229	PHE	3.0
1	A	276	TRP	2.9
1	A	4	PRO	2.9
1	C	118	LYS	2.9
1	B	65	TYR	2.9
1	B	29	ASP	2.9
1	C	40	ARG	2.9
1	B	189	ALA	2.9
1	B	320	ALA	2.9
1	C	9	VAL	2.9
1	A	147	LEU	2.9
1	B	162	HIS	2.9
1	C	269	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	266	MET	2.9
1	A	373	ASN	2.9
1	C	16	ILE	2.9
1	D	342	GLY	2.9
1	D	73	ALA	2.9
1	C	227	HIS	2.9
1	D	278	LYS	2.9
1	C	3	GLN	2.9
1	B	61	ASP	2.9
1	C	61	ASP	2.9
1	C	73	ALA	2.9
1	C	370	ALA	2.9
1	D	381	ALA	2.9
1	C	352	LYS	2.9
1	D	78	GLU	2.9
1	C	91	MET	2.9
1	D	82	GLY	2.9
1	B	190	THR	2.9
1	D	119	THR	2.9
1	C	25	GLU	2.8
1	D	384	GLU	2.8
1	D	91	MET	2.8
1	D	242	PRO	2.8
1	C	167	TYR	2.8
1	A	48	ALA	2.8
1	A	57	ALA	2.8
1	A	344	LEU	2.8
1	B	175	ALA	2.8
1	C	258	LEU	2.8
1	D	337	LEU	2.8
1	D	360	ALA	2.8
1	A	168	VAL	2.8
1	A	226	PHE	2.8
1	C	152	GLU	2.8
1	A	148	PRO	2.8
1	D	326	ASN	2.8
1	A	133	GLY	2.8
1	A	219	GLY	2.8
1	A	72	LEU	2.8
1	D	72	LEU	2.8
1	A	94	ALA	2.8
1	B	356	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	129	VAL	2.8
1	A	235	LYS	2.8
1	D	262	GLY	2.8
1	D	166	ASP	2.8
1	D	372	ASP	2.8
1	A	38	ALA	2.8
1	A	183	THR	2.8
1	B	309	THR	2.8
1	D	6	THR	2.8
1	D	155	ALA	2.8
1	D	353	THR	2.8
1	C	187	GLU	2.8
1	C	250	VAL	2.8
1	C	384	GLU	2.8
1	D	191	VAL	2.8
1	A	98	MET	2.8
1	D	295	MET	2.8
1	B	5	ARG	2.8
1	D	207	LYS	2.8
1	B	72	LEU	2.8
1	B	177	GLY	2.8
1	D	17	GLY	2.8
1	D	134	LEU	2.8
1	D	287	LEU	2.8
1	B	67	ASP	2.8
1	A	307	ALA	2.8
1	B	250	VAL	2.8
1	C	120	VAL	2.8
1	C	361	THR	2.8
1	D	77	VAL	2.8
1	D	333	VAL	2.8
1	D	30	ARG	2.8
1	B	148	PRO	2.7
1	C	4	PRO	2.7
1	D	55	LYS	2.7
1	D	339	LYS	2.7
1	B	28	LEU	2.7
1	D	28	LEU	2.7
1	C	14	GLY	2.7
1	A	295	MET	2.7
1	C	92	MET	2.7
1	A	90	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	70	GLU	2.7
1	D	328	ALA	2.7
1	B	179	PRO	2.7
1	B	114	ILE	2.7
1	A	86	LEU	2.7
1	D	185	LEU	2.7
1	B	133	GLY	2.7
1	D	63	SER	2.7
1	D	355	ASP	2.7
1	C	243	GLN	2.7
1	C	348	LYS	2.7
1	D	331	ILE	2.7
1	C	82	GLY	2.7
1	C	56	ARG	2.7
1	C	212	SER	2.7
1	C	70	GLU	2.7
1	B	226	PHE	2.7
1	C	350	VAL	2.7
1	D	80	ALA	2.7
1	D	297	PHE	2.7
1	D	368	VAL	2.7
1	D	44	ASP	2.7
1	A	218	LYS	2.7
1	A	243	GLN	2.7
1	A	294	GLN	2.7
1	B	292	LEU	2.7
1	A	63	SER	2.7
1	D	39	ASN	2.7
1	A	100	ALA	2.7
1	B	7	VAL	2.7
1	B	311	ALA	2.7
1	D	137	ASP	2.7
1	A	173	ILE	2.6
1	B	377	ILE	2.6
1	D	171	ILE	2.6
1	C	280	MET	2.6
1	B	228	LEU	2.6
1	D	23	LEU	2.6
1	D	310	LEU	2.6
1	A	165	ARG	2.6
1	C	247	HIS	2.6
1	C	303	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	234	GLU	2.6
1	A	96	TRP	2.6
1	A	381	ALA	2.6
1	B	83	ALA	2.6
1	C	148	PRO	2.6
1	D	223	ILE	2.6
1	B	147	LEU	2.6
1	C	354	LEU	2.6
1	D	258	LEU	2.6
1	D	344	LEU	2.6
1	A	352	LYS	2.6
1	D	340	LYS	2.6
1	B	9	VAL	2.6
1	B	379	ALA	2.6
1	C	375	ALA	2.6
1	D	113	ALA	2.6
1	D	212	SER	2.6
1	B	361	THR	2.6
1	C	231	ILE	2.6
1	B	302	TYR	2.6
1	C	72	LEU	2.6
1	A	5	ARG	2.6
1	A	112	ALA	2.6
1	B	113	ALA	2.6
1	C	105	ALA	2.6
1	D	60	ALA	2.6
1	D	329	ASN	2.6
1	B	96	TRP	2.6
1	B	358	THR	2.6
1	D	97	THR	2.6
1	D	144	THR	2.6
1	B	315	ILE	2.6
1	B	252	TYR	2.6
1	D	116	LYS	2.6
1	C	121	ALA	2.6
1	C	328	ALA	2.6
1	B	75	SER	2.5
1	D	214	THR	2.5
1	B	338	ASP	2.5
1	B	102	ILE	2.5
1	B	21	LEU	2.5
1	C	86	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	252	TYR	2.5
1	A	303	GLU	2.5
1	B	303	GLU	2.5
1	C	133	GLY	2.5
1	A	80	ALA	2.5
1	B	81	ALA	2.5
1	C	131	ALA	2.5
1	C	213	ALA	2.5
1	C	144	THR	2.5
1	D	37	THR	2.5
1	D	53	ASN	2.5
1	D	317	SER	2.5
1	B	291	LYS	2.5
1	C	185	LEU	2.5
1	C	293	ARG	2.5
1	A	227	HIS	2.5
1	D	142	HIS	2.5
1	C	93	GLY	2.5
1	C	236	PHE	2.5
1	D	121	ALA	2.5
1	D	248	SER	2.5
1	A	16	ILE	2.5
1	D	26	ARG	2.5
1	A	25	GLU	2.5
1	A	62	PRO	2.5
1	A	85	ALA	2.5
1	A	131	ALA	2.5
1	B	71	ALA	2.5
1	B	85	ALA	2.5
1	C	336	PHE	2.5
1	D	259	ALA	2.5
1	B	27	ASN	2.5
1	C	268	THR	2.5
1	A	122	LEU	2.5
1	A	172	ILE	2.5
1	A	292	LEU	2.5
1	B	185	LEU	2.5
1	C	244	SER	2.5
1	D	122	LEU	2.5
1	D	247	HIS	2.5
1	B	283	PRO	2.5
1	D	3	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	240	VAL	2.5
1	A	327	ALA	2.5
1	C	90	ALA	2.5
1	D	94	ALA	2.5
1	B	316	LYS	2.4
1	B	119	THR	2.4
1	B	40	ARG	2.4
1	C	172	ILE	2.4
1	C	346	ILE	2.4
1	D	101	ILE	2.4
1	A	248	SER	2.4
1	B	63	SER	2.4
1	B	364	SER	2.4
1	C	314	SER	2.4
1	D	151	SER	2.4
1	D	163	HIS	2.4
1	C	255	GLY	2.4
1	C	295	MET	2.4
1	D	318	GLY	2.4
1	C	340	LYS	2.4
1	C	347	ALA	2.4
1	D	131	ALA	2.4
1	B	173	ILE	2.4
1	D	210	ILE	2.4
1	D	222	LEU	2.4
1	D	228	LEU	2.4
1	C	288	ASP	2.4
1	D	61	ASP	2.4
1	C	50	LYS	2.4
1	D	348	LYS	2.4
1	C	260	GLN	2.4
1	D	229	PHE	2.4
1	A	107	LEU	2.4
1	C	134	LEU	2.4
1	C	337	LEU	2.4
1	B	373	ASN	2.4
1	B	301	ASP	2.4
1	C	43	LYS	2.4
1	D	378	GLN	2.4
1	A	7	VAL	2.4
1	D	87	VAL	2.4
1	A	49	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	180	PHE	2.4
1	B	357	TYR	2.4
1	D	140	ARG	2.4
1	A	257	ILE	2.4
1	C	192	THR	2.4
1	D	238	ILE	2.4
1	D	253	LEU	2.4
1	C	217	ASN	2.4
1	D	162	HIS	2.4
1	A	61	ASP	2.4
1	A	280	MET	2.4
1	D	383	MET	2.4
1	C	321	ARG	2.4
1	C	122	LEU	2.3
1	A	41	ASN	2.3
1	C	66	ASN	2.3
1	D	27	ASN	2.3
1	B	25	GLU	2.3
1	B	78	GLU	2.3
1	D	115	ARG	2.3
1	D	158	GLN	2.3
1	B	168	VAL	2.3
1	B	324	VAL	2.3
1	B	112	ALA	2.3
1	B	155	ALA	2.3
1	C	320	ALA	2.3
1	D	225	ALA	2.3
1	D	370	ALA	2.3
1	B	371	ILE	2.3
1	D	227	HIS	2.3
1	A	164	ASN	2.3
1	A	285	GLU	2.3
1	C	116	LYS	2.3
1	A	296	ASP	2.3
1	C	363	SER	2.3
1	D	95	ASP	2.3
1	B	4	PRO	2.3
1	B	193	PRO	2.3
1	D	179	PRO	2.3
1	A	342	GLY	2.3
1	D	132	GLY	2.3
1	A	245	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	100	ALA	2.3
1	D	365	LEU	2.3
1	A	114	ILE	2.3
1	B	261	ILE	2.3
1	B	52	THR	2.3
1	C	145	THR	2.3
1	D	188	MET	2.3
1	D	330	GLU	2.3
1	D	374	GLU	2.3
1	C	283	PRO	2.3
1	C	345	ASP	2.3
1	B	178	GLY	2.3
1	B	191	VAL	2.3
1	D	245	VAL	2.3
1	B	336	PHE	2.3
1	A	118	LYS	2.3
1	A	188	MET	2.3
1	A	304	ARG	2.3
1	D	364	SER	2.3
1	B	77	VAL	2.3
1	B	160	PHE	2.3
1	B	236	PHE	2.3
1	A	121	ALA	2.2
1	A	175	ALA	2.2
1	A	259	ALA	2.2
1	B	210	ILE	2.2
1	B	360	ALA	2.2
1	C	136	ILE	2.2
1	C	275	ALA	2.2
1	D	156	ILE	2.2
1	A	43	LYS	2.2
1	B	192	THR	2.2
1	A	384	GLU	2.2
1	A	154	ASN	2.2
1	A	329	ASN	2.2
1	A	279	ARG	2.2
1	D	127	SER	2.2
1	D	265	ASP	2.2
1	B	255	GLY	2.2
1	A	324	VAL	2.2
1	B	134	LEU	2.2
1	B	310	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	274	LEU	2.2
1	C	324	VAL	2.2
1	A	69	LYS	2.2
1	D	208	ILE	2.2
1	A	216	MET	2.2
1	B	188	MET	2.2
1	D	266	MET	2.2
1	A	313	GLU	2.2
1	C	141	GLU	2.2
1	C	290	THR	2.2
1	B	66	ASN	2.2
1	A	132	GLY	2.2
1	D	338	ASP	2.2
1	B	365	LEU	2.2
1	A	348	LYS	2.2
1	A	246	ILE	2.2
1	B	266	MET	2.2
1	C	156	ILE	2.2
1	D	92	MET	2.2
1	A	155	ALA	2.2
1	C	60	ALA	2.2
1	A	145	THR	2.2
1	A	268	THR	2.2
1	B	20	THR	2.2
1	B	330	GLU	2.2
1	A	115	ARG	2.2
1	C	304	ARG	2.2
1	B	254	ASP	2.2
1	B	339	LYS	2.2
1	C	254	ASP	2.2
1	D	150	ASP	2.2
1	D	274	LEU	2.2
1	D	9	VAL	2.2
1	A	171	ILE	2.2
1	C	334	ALA	2.2
1	D	141	GLU	2.2
1	A	6	THR	2.2
1	A	97	THR	2.2
1	A	282	THR	2.2
1	A	309	THR	2.2
1	C	13	THR	2.2
1	B	279	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	300	PRO	2.2
1	A	260	GLN	2.2
1	C	230	GLN	2.2
1	C	108	LYS	2.2
1	A	228	LEU	2.2
1	A	271	GLY	2.2
1	D	11	GLY	2.2
1	D	86	LEU	2.2
1	D	220	LEU	2.2
1	C	211	ASP	2.2
1	C	296	ASP	2.2
1	D	324	VAL	2.2
1	A	99	ALA	2.1
1	B	375	ALA	2.1
1	D	100	ALA	2.1
1	B	224	GLU	2.1
1	B	384	GLU	2.1
1	A	283	PRO	2.1
1	D	36	LEU	2.1
1	C	103	GLY	2.1
1	A	305	PHE	2.1
1	C	189	ALA	2.1
1	D	48	ALA	2.1
1	A	56	ARG	2.1
1	C	169	ARG	2.1
1	A	182	THR	2.1
1	D	361	THR	2.1
1	C	125	LYS	2.1
1	C	158	GLN	2.1
1	A	239	LEU	2.1
1	C	373	ASN	2.1
1	A	156	ILE	2.1
1	C	142	HIS	2.1
1	C	153	HIS	2.1
1	D	139	VAL	2.1
1	D	261	ILE	2.1
1	D	176	SER	2.1
1	A	347	ALA	2.1
1	C	100	ALA	2.1
1	B	187	GLU	2.1
1	B	234	GLU	2.1
1	B	43	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	3	GLN	2.1
1	B	231	ILE	2.1
1	C	333	VAL	2.1
1	B	57	ALA	2.1
1	C	109	ALA	2.1
1	B	125	LYS	2.1
1	C	278	LYS	2.1
1	D	273	THR	2.1
1	A	167	TYR	2.1
1	C	7	VAL	2.1
1	C	139	VAL	2.1
1	A	166	ASP	2.0
1	A	267	ARG	2.0
1	B	296	ASP	2.0
1	B	49	ALA	2.0
1	B	323	ALA	2.0
1	D	352	LYS	2.0
1	D	322	PRO	2.0
1	B	103	GLY	2.0
1	B	238	ILE	2.0
1	C	319	GLY	2.0
1	C	104	CYS	2.0
1	A	160	PHE	2.0
1	D	165	ARG	2.0
1	B	285	GLU	2.0
1	A	105	ALA	2.0
1	C	112	ALA	2.0
1	D	296	ASP	2.0
1	B	340	LYS	2.0
1	D	232	PRO	2.0
1	D	243	GLN	2.0
1	B	18	HIS	2.0
1	B	24	ILE	2.0
1	C	257	ILE	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

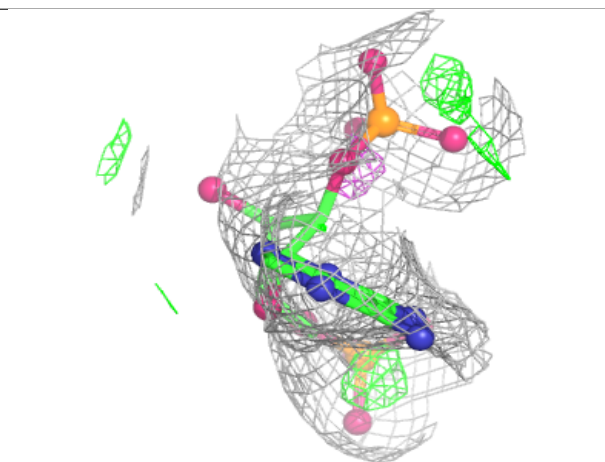
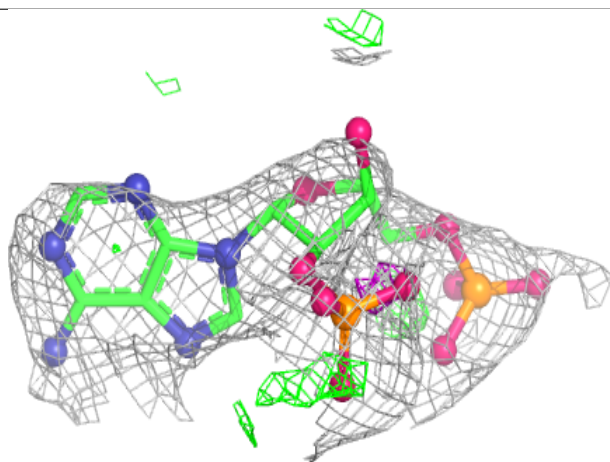
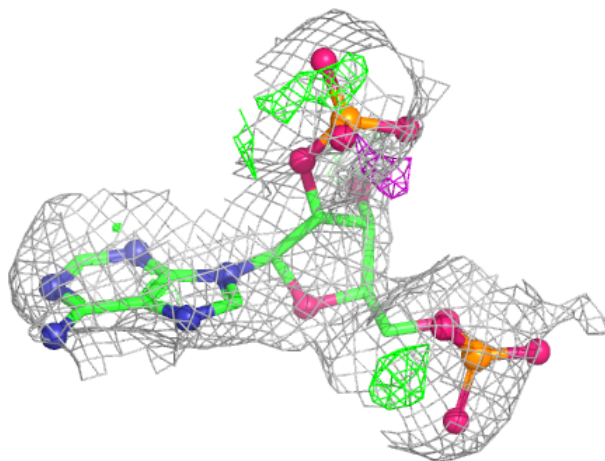
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NDP	C	402	27/48	0.60	0.24	74,76,99,101	0
2	NDP	A	400	27/48	0.68	0.22	61,63,89,95	0
2	NDP	B	401	27/48	0.75	0.21	41,53,88,96	0
2	NDP	D	403	27/48	0.79	0.19	51,55,75,78	0

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

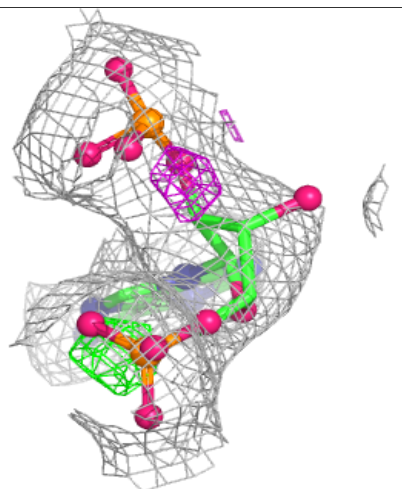
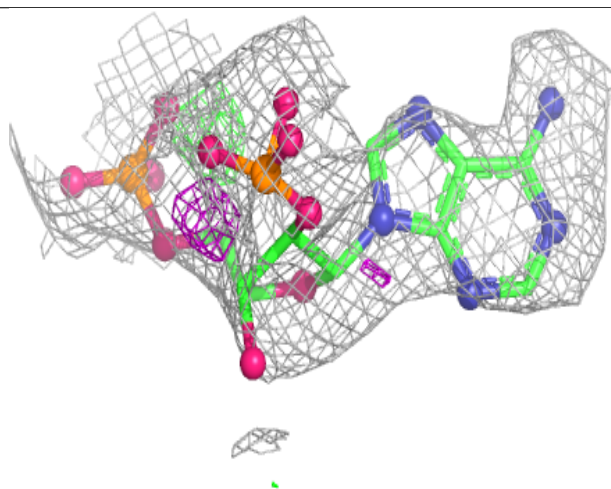
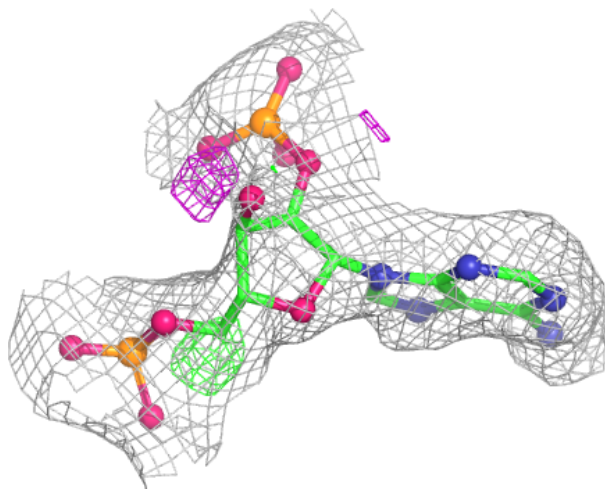
Electron density around NDP C 402:

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



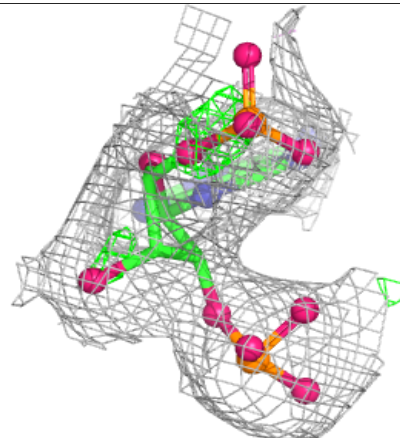
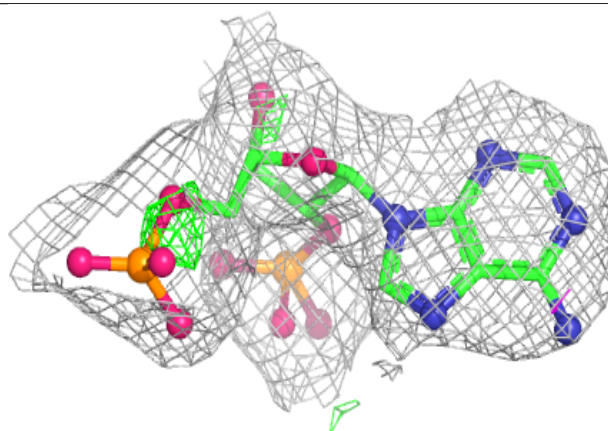
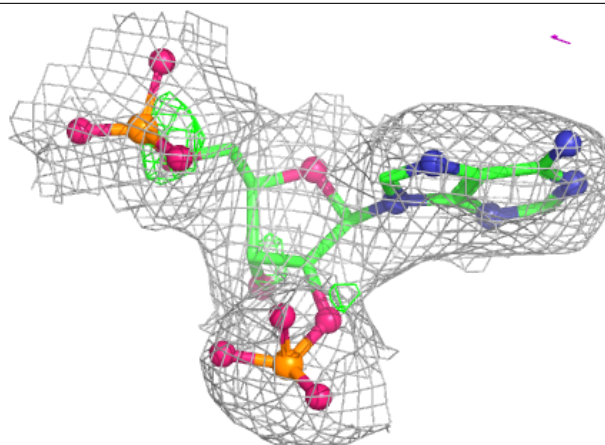
Electron density around NDP A 400:

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



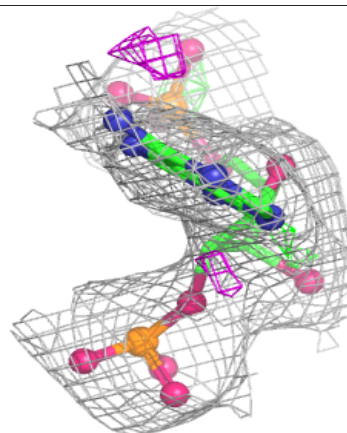
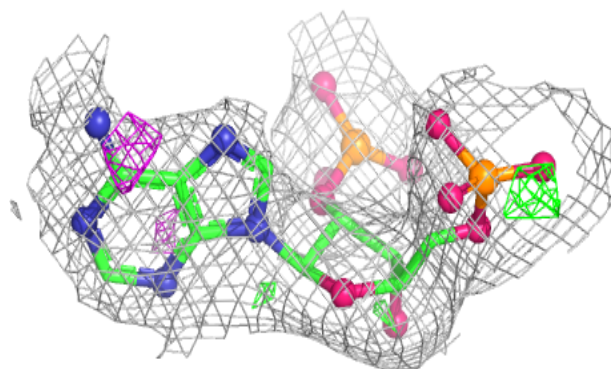
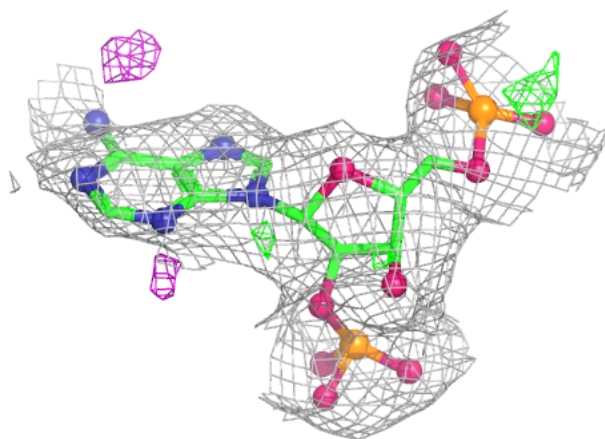
Electron density around NDP B 401:

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



Electron density around NDP D 403:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.