



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:54 PM UTC

PDB ID : 8TDB / pdb_00008tdb
Title : Structure of PYCR1 complexed with NADH and 1-hydroxyethane-1-sulfonate
Authors : Tanner, J.J.; Meeks, K.R.
Deposited on : 2023-07-02
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

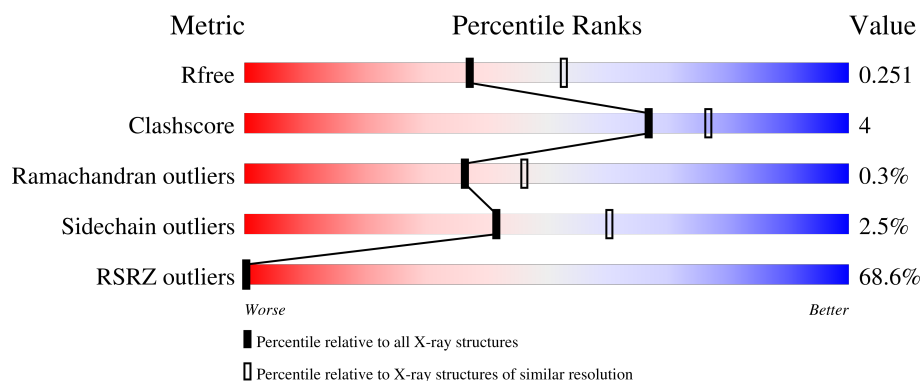
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	316	54% 77% 9% • 13%
1	B	316	58% 81% 7% • 11%
1	C	316	63% 78% 8% 13%
1	D	316	66% 80% 8% 11%
1	E	316	60% 78% 10% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10122 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 Pyrroline-5-carboxylate reductase 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	1	0
			1931	1214	345	360	12			
1	B	280	Total	C	N	O	S	0	1	0
			1939	1221	347	360	11			
1	C	275	Total	C	N	O	S	0	1	0
			1917	1203	342	361	11			
1	D	281	Total	C	N	O	S	0	1	0
			1940	1219	347	364	10			
1	E	278	Total	C	N	O	S	0	1	0
			1936	1217	343	365	11			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP P32322
A	-20	HIS	-	expression tag	UNP P32322
A	-19	HIS	-	expression tag	UNP P32322
A	-18	HIS	-	expression tag	UNP P32322
A	-17	HIS	-	expression tag	UNP P32322
A	-16	HIS	-	expression tag	UNP P32322
A	-15	HIS	-	expression tag	UNP P32322
A	-14	SER	-	expression tag	UNP P32322
A	-13	SER	-	expression tag	UNP P32322
A	-12	GLY	-	expression tag	UNP P32322
A	-11	VAL	-	expression tag	UNP P32322
A	-10	ASP	-	expression tag	UNP P32322
A	-9	LEU	-	expression tag	UNP P32322
A	-8	GLY	-	expression tag	UNP P32322
A	-7	THR	-	expression tag	UNP P32322
A	-6	GLU	-	expression tag	UNP P32322
A	-5	ASN	-	expression tag	UNP P32322
A	-4	LEU	-	expression tag	UNP P32322
A	-3	TYR	-	expression tag	UNP P32322

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PHE	-	expression tag	UNP P32322
A	-1	GLN	-	expression tag	UNP P32322
A	0	SER	-	expression tag	UNP P32322
B	-21	MET	-	initiating methionine	UNP P32322
B	-20	HIS	-	expression tag	UNP P32322
B	-19	HIS	-	expression tag	UNP P32322
B	-18	HIS	-	expression tag	UNP P32322
B	-17	HIS	-	expression tag	UNP P32322
B	-16	HIS	-	expression tag	UNP P32322
B	-15	HIS	-	expression tag	UNP P32322
B	-14	SER	-	expression tag	UNP P32322
B	-13	SER	-	expression tag	UNP P32322
B	-12	GLY	-	expression tag	UNP P32322
B	-11	VAL	-	expression tag	UNP P32322
B	-10	ASP	-	expression tag	UNP P32322
B	-9	LEU	-	expression tag	UNP P32322
B	-8	GLY	-	expression tag	UNP P32322
B	-7	THR	-	expression tag	UNP P32322
B	-6	GLU	-	expression tag	UNP P32322
B	-5	ASN	-	expression tag	UNP P32322
B	-4	LEU	-	expression tag	UNP P32322
B	-3	TYR	-	expression tag	UNP P32322
B	-2	PHE	-	expression tag	UNP P32322
B	-1	GLN	-	expression tag	UNP P32322
B	0	SER	-	expression tag	UNP P32322
C	-21	MET	-	initiating methionine	UNP P32322
C	-20	HIS	-	expression tag	UNP P32322
C	-19	HIS	-	expression tag	UNP P32322
C	-18	HIS	-	expression tag	UNP P32322
C	-17	HIS	-	expression tag	UNP P32322
C	-16	HIS	-	expression tag	UNP P32322
C	-15	HIS	-	expression tag	UNP P32322
C	-14	SER	-	expression tag	UNP P32322
C	-13	SER	-	expression tag	UNP P32322
C	-12	GLY	-	expression tag	UNP P32322
C	-11	VAL	-	expression tag	UNP P32322
C	-10	ASP	-	expression tag	UNP P32322
C	-9	LEU	-	expression tag	UNP P32322
C	-8	GLY	-	expression tag	UNP P32322
C	-7	THR	-	expression tag	UNP P32322
C	-6	GLU	-	expression tag	UNP P32322
C	-5	ASN	-	expression tag	UNP P32322

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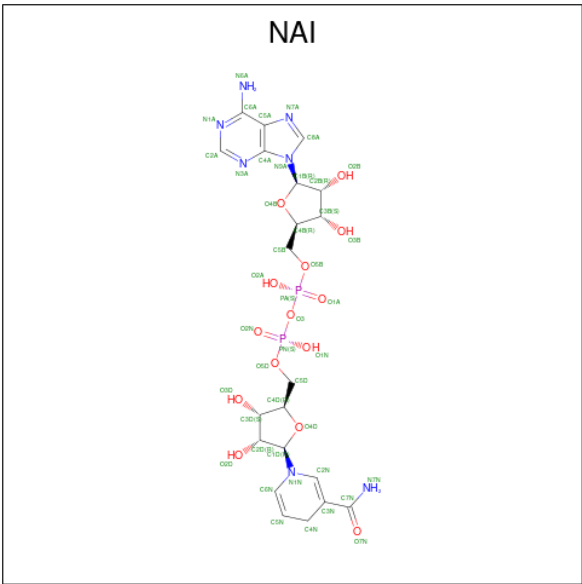
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	LEU	-	expression tag	UNP P32322
C	-3	TYR	-	expression tag	UNP P32322
C	-2	PHE	-	expression tag	UNP P32322
C	-1	GLN	-	expression tag	UNP P32322
C	0	SER	-	expression tag	UNP P32322
D	-21	MET	-	initiating methionine	UNP P32322
D	-20	HIS	-	expression tag	UNP P32322
D	-19	HIS	-	expression tag	UNP P32322
D	-18	HIS	-	expression tag	UNP P32322
D	-17	HIS	-	expression tag	UNP P32322
D	-16	HIS	-	expression tag	UNP P32322
D	-15	HIS	-	expression tag	UNP P32322
D	-14	SER	-	expression tag	UNP P32322
D	-13	SER	-	expression tag	UNP P32322
D	-12	GLY	-	expression tag	UNP P32322
D	-11	VAL	-	expression tag	UNP P32322
D	-10	ASP	-	expression tag	UNP P32322
D	-9	LEU	-	expression tag	UNP P32322
D	-8	GLY	-	expression tag	UNP P32322
D	-7	THR	-	expression tag	UNP P32322
D	-6	GLU	-	expression tag	UNP P32322
D	-5	ASN	-	expression tag	UNP P32322
D	-4	LEU	-	expression tag	UNP P32322
D	-3	TYR	-	expression tag	UNP P32322
D	-2	PHE	-	expression tag	UNP P32322
D	-1	GLN	-	expression tag	UNP P32322
D	0	SER	-	expression tag	UNP P32322
E	-21	MET	-	initiating methionine	UNP P32322
E	-20	HIS	-	expression tag	UNP P32322
E	-19	HIS	-	expression tag	UNP P32322
E	-18	HIS	-	expression tag	UNP P32322
E	-17	HIS	-	expression tag	UNP P32322
E	-16	HIS	-	expression tag	UNP P32322
E	-15	HIS	-	expression tag	UNP P32322
E	-14	SER	-	expression tag	UNP P32322
E	-13	SER	-	expression tag	UNP P32322
E	-12	GLY	-	expression tag	UNP P32322
E	-11	VAL	-	expression tag	UNP P32322
E	-10	ASP	-	expression tag	UNP P32322
E	-9	LEU	-	expression tag	UNP P32322
E	-8	GLY	-	expression tag	UNP P32322
E	-7	THR	-	expression tag	UNP P32322

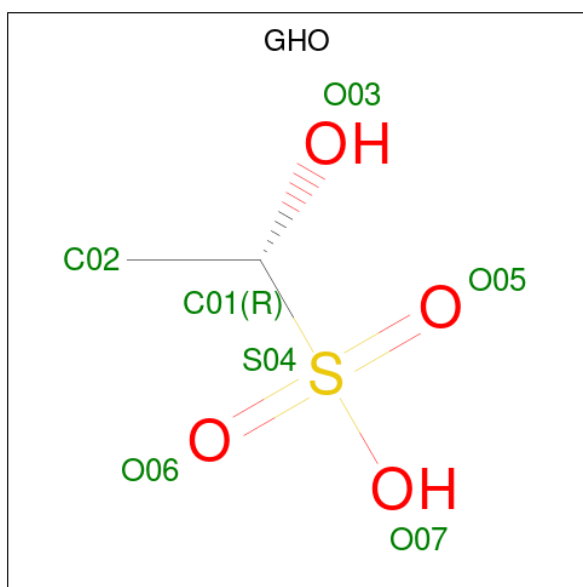
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	GLU	-	expression tag	UNP P32322
E	-5	ASN	-	expression tag	UNP P32322
E	-4	LEU	-	expression tag	UNP P32322
E	-3	TYR	-	expression tag	UNP P32322
E	-2	PHE	-	expression tag	UNP P32322
E	-1	GLN	-	expression tag	UNP P32322
E	0	SER	-	expression tag	UNP P32322

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			7	2	4	1		
3	B	1	Total	C	O	S	0	0
			7	2	4	1		
3	C	1	Total	C	O	S	0	0
			7	2	4	1		
3	D	1	Total	C	O	S	0	0
			7	2	4	1		
3	E	1	Total	C	O	S	0	0
			7	2	4	1		

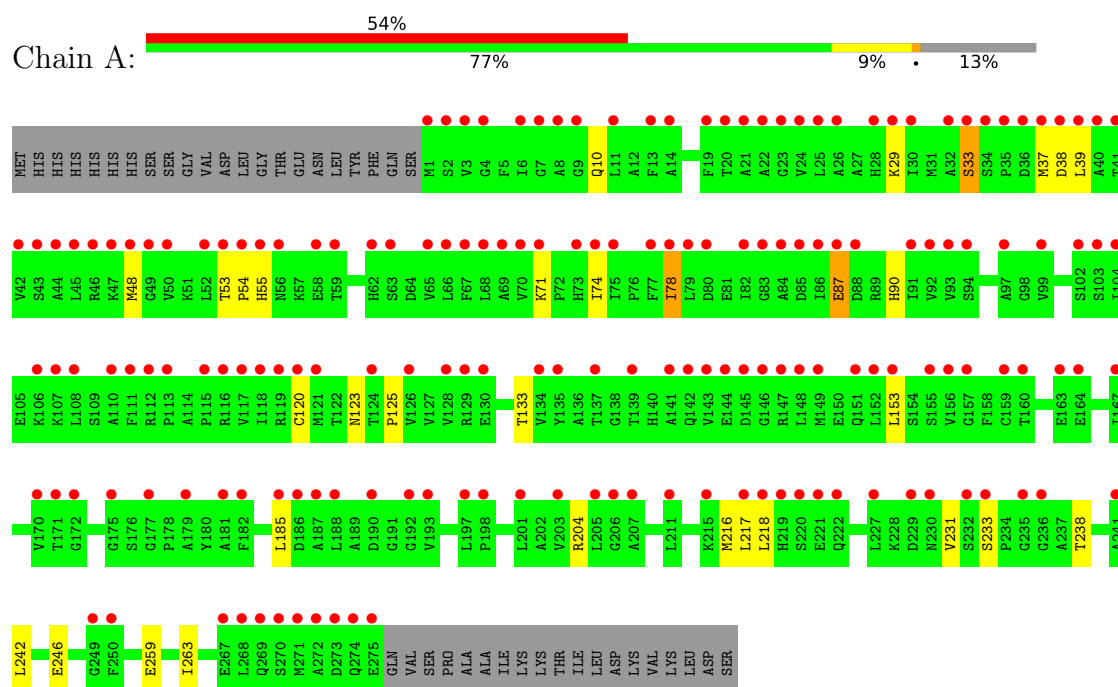
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	41	Total	O	0	0
			41	41		
4	C	28	Total	O	0	0
			28	28		
4	D	38	Total	O	0	0
			38	38		
4	E	54	Total	O	0	0
			54	54		

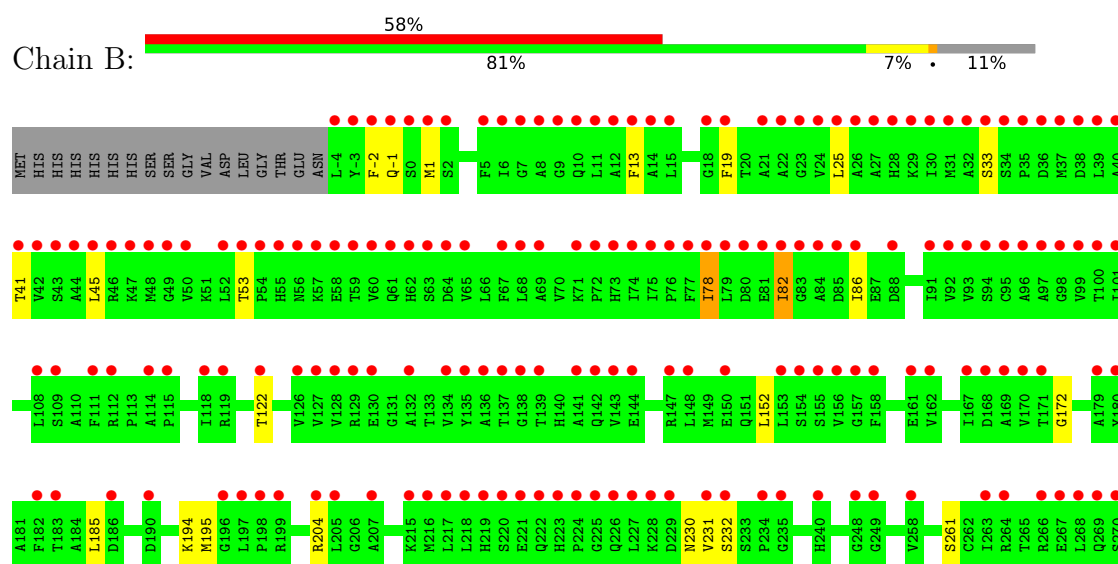
3 Residue-property plots

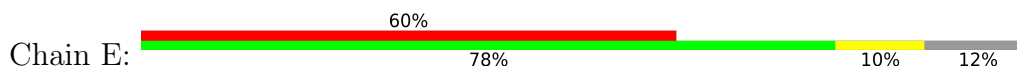
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

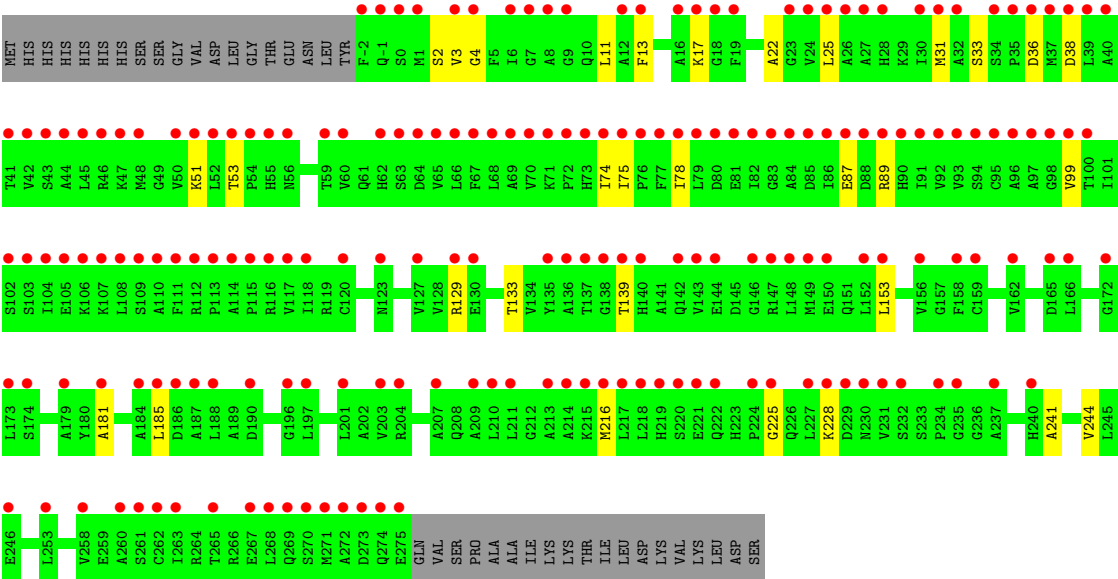
- Molecule 1: Pyrroline-5-carboxylate reductase 1, mitochondrial



- Molecule 1: Pyrroline-5-carboxylate reductase 1, mitochondrial







4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.73Å 180.68Å 88.01Å 90.00° 106.26° 90.00°	Depositor
Resolution (Å)	71.46 – 2.30 71.46 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.8 (71.46-2.30) 97.3 (71.46-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20.1_4887	Depositor
R, R_{free}	0.211 , 0.250 0.207 , 0.251	Depositor DCC
R_{free} test set	1442 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	10122	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, GH0

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	0.35	0/1965	0.55	0/2674
1	B	0.36	0/1973	0.52	0/2691
1	C	0.35	0/1950	0.54	0/2657
1	D	0.34	0/1974	0.50	0/2696
1	E	0.36	0/1969	0.53	0/2683
All	All	0.35	0/9831	0.53	0/13401

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1931	0	1888	17	0
1	B	1939	0	1873	13	0
1	C	1917	0	1865	16	0
1	D	1940	0	1857	16	0
1	E	1936	0	1890	15	0
2	A	44	0	26	1	0
2	B	44	0	27	2	0
2	C	44	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	44	0	27	2	0
2	E	44	0	27	0	0
3	A	7	0	0	1	0
3	B	7	0	0	0	0
3	C	7	0	0	1	0
3	D	7	0	0	0	0
3	E	7	0	0	0	0
4	A	43	0	0	0	0
4	B	41	0	0	0	0
4	C	28	0	0	0	0
4	D	38	0	0	0	0
4	E	54	0	0	0	0
All	All	10122	0	9507	72	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (72) 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:E:133:THR:HG21	1:E:153:LEU:HD13	1.76	0.66
1:A:217:LEU:HD23	1:B:185:LEU:HD13	1.82	0.62
1:B:13:PHE:HA	1:B:45:LEU:HD21	1.81	0.60
1:A:259:GLU:O	1:A:263:ILE:HG12	2.01	0.60
1:C:74:ILE:HG22	1:C:78:ILE:HG12	1.83	0.60
1:D:13:PHE:HA	1:D:45:LEU:HD21	1.84	0.58
1:E:225:GLY:HA2	1:E:228:LYS:HZ3	1.69	0.58
1:D:-2:PHE:HA	1:D:1:MET:HE2	1.85	0.58
1:C:233:SER:OG	3:C:402:GHO:O07	2.23	0.55
1:D:89:ARG:HH11	1:D:89:ARG:HG2	1.73	0.54
1:E:3:VAL:HG21	1:E:25:LEU:HD11	1.90	0.53
1:C:133:THR:HG21	1:C:153:LEU:HD13	1.91	0.52
1:D:22:ALA:HB2	1:D:129:ARG:HE	1.75	0.52
1:D:129:ARG:NH2	1:D:155:SER:O	2.43	0.52
1:B:194:LYS:HD3	1:B:195:MET:HE3	1.92	0.51
1:E:33:SER:HA	1:E:53:THR:O	2.10	0.51
1:C:36:ASP:C	1:C:38:ASP:H	2.18	0.50
1:C:130:GLU:HG3	1:D:215:LYS:HD3	1.92	0.50
1:D:37:MET:O	1:D:39:LEU:N	2.45	0.50
1:E:87:GLU:HG3	1:E:89:ARG:NH1	2.27	0.50
1:E:22:ALA:HB2	1:E:129:ARG:HE	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HE1	1:C:152:LEU:HD22	1.94	0.49
1:C:4:GLY:HA2	1:C:31:MET:O	2.12	0.49
1:A:71:LYS:NZ	2:A:401:NAI:O3	2.43	0.49
1:B:33:SER:HA	1:B:53:THR:O	2.13	0.48
1:E:75:ILE:HG21	1:E:99:VAL:HG11	1.96	0.48
1:C:133:THR:O	1:C:159:CYS:HA	2.15	0.47
1:A:74:ILE:HG22	1:A:78:ILE:HG12	1.96	0.47
1:B:19:PHE:HB3	1:B:25:LEU:HD12	1.96	0.47
1:B:122:THR:O	2:B:401:NAI:H5N	2.16	0.46
1:D:193:VAL:HG21	1:D:199[B]:ARG:NE	2.31	0.46
1:E:181:ALA:O	1:E:185:LEU:HG	2.15	0.46
1:D:71:LYS:HE3	2:D:401:NAI:O1A	2.17	0.45
1:A:218:LEU:CD2	1:B:204:ARG:HD3	2.47	0.45
1:E:36:ASP:C	1:E:38:ASP:H	2.24	0.44
1:A:33:SER:HA	1:A:53:THR:O	2.17	0.44
1:E:31:MET:HA	1:E:51:LYS:O	2.17	0.44
1:A:54:PRO:HG2	1:A:55:HIS:CD2	2.52	0.44
1:C:36:ASP:O	1:C:38:ASP:N	2.51	0.44
1:D:33:SER:HA	1:D:53:THR:O	2.18	0.44
1:B:1:MET:HE1	1:B:152:LEU:HD13	1.99	0.44
1:A:87:GLU:HG3	1:A:90:HIS:CE1	2.53	0.44
1:E:13:PHE:CZ	1:E:17:LYS:HD3	2.53	0.44
1:E:241:ALA:O	1:E:244:VAL:HG22	2.18	0.44
1:A:10:GLN:NE2	1:B:230:ASN:HB3	2.32	0.43
1:A:37:MET:C	1:A:39:LEU:H	2.26	0.43
1:C:16:ALA:HB1	1:C:48:MET:HE1	1.99	0.43
1:C:185:LEU:HA	1:C:185:LEU:HD23	1.79	0.43
1:E:74:ILE:HG22	1:E:78:ILE:HG12	2.00	0.43
1:D:122:THR:HB	1:D:133:THR:HG23	2.00	0.43
1:B:78:ILE:HA	1:B:78:ILE:HD13	1.72	0.43
1:B:78:ILE:HD11	2:B:401:NAI:N1A	2.33	0.43
1:C:185:LEU:HD13	1:D:217:LEU:HD23	2.01	0.42
1:D:78:ILE:HD11	2:D:401:NAI:N1A	2.35	0.42
1:A:48:MET:HE2	1:A:48:MET:HB3	1.89	0.42
1:A:242:LEU:O	1:A:246:GLU:HG2	2.19	0.42
1:E:78:ILE:HD13	1:E:78:ILE:HA	1.81	0.42
1:C:34:SER:O	1:C:54:PRO:HA	2.20	0.41
1:D:83:GLY:HA3	1:D:111:PHE:CE2	2.55	0.41
1:A:133:THR:HG21	1:A:153:LEU:HD13	2.02	0.41
1:C:33:SER:HA	1:C:53:THR:O	2.19	0.41
1:E:4:GLY:HA2	1:E:31:MET:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:VAL:HG12	1:A:238:THR:HG21	2.02	0.41
1:B:82:ILE:HD12	1:B:86:ILE:HD11	2.03	0.41
1:A:185:LEU:HD23	1:A:185:LEU:HA	1.90	0.41
1:D:11:LEU:HD12	1:D:11:LEU:HA	1.89	0.41
1:A:233:SER:OG	3:A:402:GHO:O07	2.32	0.41
1:B:172:GLY:HA2	1:B:261:SER:OG	2.21	0.41
1:C:193:VAL:HG21	1:C:199[A]:ARG:CZ	2.51	0.41
1:A:123:ASN:CG	1:A:125:PRO:HD2	2.45	0.41
1:C:15:LEU:HD23	1:C:15:LEU:HA	1.91	0.40
1:D:172:GLY:HA2	1:D:261:SER:OG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	274/316 (87%)	265 (97%)	8 (3%)	1 (0%)	30	38
1	B	279/316 (88%)	271 (97%)	7 (2%)	1 (0%)	30	38
1	C	274/316 (87%)	265 (97%)	8 (3%)	1 (0%)	30	38
1	D	280/316 (89%)	269 (96%)	10 (4%)	1 (0%)	30	38
1	E	277/316 (88%)	270 (98%)	7 (2%)	0	100	100
All	All	1384/1580 (88%)	1340 (97%)	40 (3%)	4 (0%)	36	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	37	MET
1	D	38	ASP
1	A	38	ASP
1	B	-1	GLN

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	187/251 (74%)	180 (96%)	7 (4%)	30	45
1	B	183/251 (73%)	177 (97%)	6 (3%)	33	50
1	C	185/251 (74%)	181 (98%)	4 (2%)	45	65
1	D	182/251 (72%)	180 (99%)	2 (1%)	65	81
1	E	188/251 (75%)	184 (98%)	4 (2%)	47	66
All	All	925/1255 (74%)	902 (98%)	23 (2%)	42	60

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	33	SER
1	A	78	ILE
1	A	87	GLU
1	A	120	CYS
1	A	204	ARG
1	A	216	MET
1	B	-2	PHE
1	B	41	THR
1	B	78	ILE
1	B	82	ILE
1	B	231	VAL
1	B	232	SER
1	C	11	LEU
1	C	139	THR
1	C	233	SER
1	C	244	VAL
1	D	89	ARG
1	D	226	GLN
1	E	2	SER
1	E	11	LEU
1	E	139	THR
1	E	216	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	28	HIS
1	A	140	HIS
1	B	55	HIS
1	C	62	HIS
1	D	62	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 ⓘ

10 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	NAI	B	401	-	47,48,48	1.59	8 (17%)	64,73,73	1.54	15 (23%)
3	GHO	A	402	-	5,6,6	3.90	1 (20%)	4,9,9	0.65	0
2	NAI	E	401	-	47,48,48	1.84	10 (21%)	64,73,73	1.63	13 (20%)
2	NAI	C	401	-	47,48,48	1.40	7 (14%)	64,73,73	1.61	13 (20%)
2	NAI	A	401	-	47,48,48	1.47	8 (17%)	64,73,73	1.55	14 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAI	D	401	-	47,48,48	1.58	10 (21%)	64,73,73	1.67	15 (23%)
3	GHO	B	402	-	5,6,6	3.94	1 (20%)	4,9,9	1.12	0
3	GHO	E	402	-	5,6,6	4.02	1 (20%)	4,9,9	1.12	0
3	GHO	D	402	-	5,6,6	3.71	1 (20%)	4,9,9	0.91	0
3	GHO	C	402	-	5,6,6	4.15	1 (20%)	4,9,9	0.93	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	B	401	-	-	3/29/72/72	0/5/5/5
3	GHO	A	402	-	-	0/2/6/6	-
2	NAI	E	401	-	-	6/29/72/72	0/5/5/5
2	NAI	C	401	-	-	14/29/72/72	0/5/5/5
2	NAI	A	401	-	-	8/29/72/72	0/5/5/5
2	NAI	D	401	-	-	9/29/72/72	0/5/5/5
3	GHO	B	402	-	-	1/2/6/6	-
3	GHO	E	402	-	-	2/2/6/6	-
3	GHO	D	402	-	-	0/2/6/6	-
3	GHO	C	402	-	-	0/2/6/6	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	GHO	C01-S04	9.14	2.01	1.81
3	E	402	GHO	C01-S04	8.90	2.00	1.81
3	B	402	GHO	C01-S04	8.70	2.00	1.81
3	A	402	GHO	C01-S04	8.64	2.00	1.81
3	D	402	GHO	C01-S04	8.19	1.99	1.81
2	E	401	NAI	PA-O3	5.37	1.65	1.59
2	E	401	NAI	PA-O5B	4.32	1.76	1.59
2	E	401	NAI	PN-O3	4.27	1.64	1.59
2	B	401	NAI	PN-O5D	4.24	1.76	1.59
2	D	401	NAI	PN-O3	3.81	1.63	1.59
2	B	401	NAI	PN-O3	3.76	1.63	1.59
2	B	401	NAI	PA-O5B	3.66	1.73	1.59
2	C	401	NAI	PA-O5B	3.62	1.73	1.59
2	A	401	NAI	PN-O5D	3.44	1.72	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NAI	PA-O3	3.42	1.63	1.59
2	D	401	NAI	PA-O5B	3.39	1.72	1.59
2	E	401	NAI	PN-O5D	3.35	1.72	1.59
2	D	401	NAI	C8A-N9A	3.16	1.42	1.37
2	E	401	NAI	C8A-N9A	3.07	1.42	1.37
2	A	401	NAI	PA-O5B	3.02	1.71	1.59
2	B	401	NAI	C8A-N9A	2.85	1.42	1.37
2	C	401	NAI	PN-O3	2.81	1.62	1.59
2	C	401	NAI	C4A-N3A	2.76	1.39	1.34
2	A	401	NAI	PA-O3	2.75	1.62	1.59
2	D	401	NAI	PN-O5D	2.66	1.69	1.59
2	E	401	NAI	C4A-N3A	2.64	1.39	1.34
2	A	401	NAI	C8A-N9A	2.64	1.42	1.37
2	E	401	NAI	C3D-C4D	2.58	1.59	1.53
2	A	401	NAI	O2D-C2D	-2.51	1.36	1.43
2	D	401	NAI	C4A-N3A	2.49	1.39	1.34
2	B	401	NAI	C6N-N1N	2.47	1.43	1.37
2	B	401	NAI	C4A-N3A	2.45	1.39	1.34
2	A	401	NAI	C7N-C3N	2.39	1.53	1.48
2	E	401	NAI	C7N-N7N	2.31	1.40	1.33
2	C	401	NAI	C7N-N7N	2.31	1.40	1.33
2	C	401	NAI	PN-O5D	2.31	1.68	1.59
2	B	401	NAI	C7N-N7N	2.29	1.40	1.33
2	A	401	NAI	C5A-C4A	2.27	1.43	1.39
2	B	401	NAI	C2A-N1A	2.22	1.37	1.33
2	A	401	NAI	C7N-N7N	2.22	1.39	1.33
2	D	401	NAI	C5A-C4A	2.19	1.43	1.39
2	E	401	NAI	C3B-C4B	2.19	1.58	1.53
2	D	401	NAI	C7N-N7N	2.11	1.39	1.33
2	D	401	NAI	C8A-N7A	2.08	1.35	1.31
2	C	401	NAI	C3B-C4B	2.08	1.58	1.53
2	E	401	NAI	C2A-N1A	2.08	1.37	1.33
2	D	401	NAI	O2B-C2B	-2.05	1.37	1.43
2	C	401	NAI	C2A-N1A	2.02	1.37	1.33

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	NAI	O2A-PA-O3	4.63	119.78	107.27
2	D	401	NAI	O2A-PA-O3	4.29	118.87	107.27
2	E	401	NAI	O3-PA-O1A	-4.22	98.00	110.70
2	C	401	NAI	O1N-PN-O3	3.86	117.69	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAI	O1N-PN-O3	3.78	117.49	107.27
2	D	401	NAI	O3-PA-O1A	-3.70	99.57	110.70
2	D	401	NAI	O1N-PN-O2N	3.67	129.50	112.44
2	B	401	NAI	O2A-PA-O3	3.60	117.01	107.27
2	C	401	NAI	O1N-PN-O2N	3.54	128.91	112.44
2	A	401	NAI	O2A-PA-O3	3.46	116.63	107.27
2	C	401	NAI	O2A-PA-O3	3.44	116.58	107.27
2	B	401	NAI	O3-PA-O1A	-3.43	100.38	110.70
2	C	401	NAI	O3-PA-O1A	-3.40	100.48	110.70
2	C	401	NAI	O3-PN-O2N	-3.31	100.76	110.70
2	E	401	NAI	O1N-PN-O2N	3.29	127.75	112.44
2	D	401	NAI	O2A-PA-O1A	3.23	127.46	112.44
2	D	401	NAI	O1N-PN-O3	3.22	115.98	107.27
2	A	401	NAI	O2A-PA-O1A	3.21	127.39	112.44
2	E	401	NAI	O1N-PN-O3	3.21	115.96	107.27
2	E	401	NAI	O5B-PA-O1A	-3.16	96.40	108.94
2	A	401	NAI	O1N-PN-O2N	3.09	126.81	112.44
2	C	401	NAI	O2A-PA-O1A	3.08	126.77	112.44
2	E	401	NAI	O2A-PA-O1A	3.07	126.75	112.44
2	C	401	NAI	O5D-PN-O2N	-2.98	97.14	108.94
2	A	401	NAI	O7N-C7N-N7N	-2.95	116.29	122.89
2	B	401	NAI	O2A-PA-O1A	2.95	126.15	112.44
2	E	401	NAI	O5D-PN-O2N	-2.92	97.37	108.94
2	B	401	NAI	O1N-PN-O2N	2.92	126.01	112.44
2	A	401	NAI	O5D-PN-O2N	-2.90	97.44	108.94
2	D	401	NAI	O5D-PN-O2N	-2.88	97.50	108.94
2	A	401	NAI	O3-PA-O1A	-2.84	102.17	110.70
2	A	401	NAI	O1N-PN-O3	2.81	114.87	107.27
2	E	401	NAI	O7N-C7N-N7N	-2.58	117.10	122.89
2	D	401	NAI	O3-PN-O2N	-2.58	102.96	110.70
2	D	401	NAI	C5B-C4B-C3B	-2.52	106.13	115.21
2	A	401	NAI	O3-PN-O2N	-2.51	103.14	110.70
2	E	401	NAI	C4B-O4B-C1B	-2.50	103.94	109.47
2	A	401	NAI	O5B-PA-O1A	-2.50	99.03	108.94
2	C	401	NAI	PN-O5D-C5D	-2.50	107.04	121.35
2	D	401	NAI	PA-O5B-C5B	-2.48	107.11	121.35
2	D	401	NAI	O7N-C7N-N7N	-2.47	117.36	122.89
2	D	401	NAI	O3B-C3B-C4B	-2.46	104.02	111.08
2	B	401	NAI	O5B-PA-O1A	-2.44	99.25	108.94
2	E	401	NAI	PA-O5B-C5B	-2.43	107.41	121.35
2	B	401	NAI	C5B-C4B-C3B	-2.37	106.67	115.21
2	B	401	NAI	O5D-PN-O2N	-2.36	99.59	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAI	C5B-C4B-C3B	-2.35	106.77	115.21
2	D	401	NAI	O4B-C1B-C2B	-2.31	101.67	106.62
2	B	401	NAI	PA-O5B-C5B	-2.30	108.14	121.35
2	A	401	NAI	PA-O5B-C5B	-2.30	108.16	121.35
2	B	401	NAI	C4B-O4B-C1B	-2.29	104.42	109.47
2	C	401	NAI	O5B-PA-O1A	-2.28	99.88	108.94
2	D	401	NAI	O5B-PA-O1A	-2.27	99.92	108.94
2	B	401	NAI	O7N-C7N-N7N	-2.27	117.81	122.89
2	B	401	NAI	O3-PN-O2N	-2.22	104.03	110.70
2	A	401	NAI	O3B-C3B-C4B	-2.21	104.72	111.08
2	C	401	NAI	O4B-C1B-C2B	-2.19	101.92	106.62
2	D	401	NAI	C4B-O4B-C1B	-2.18	104.65	109.47
2	D	401	NAI	C5D-C4D-C3D	-2.17	107.40	115.21
2	E	401	NAI	O3-PN-O2N	-2.16	104.22	110.70
2	C	401	NAI	C3N-C2N-N1N	-2.14	120.06	123.20
2	C	401	NAI	PA-O5B-C5B	-2.14	109.11	121.35
2	B	401	NAI	C5D-C4D-C3D	-2.13	107.55	115.21
2	E	401	NAI	C3N-C2N-N1N	-2.11	120.11	123.20
2	E	401	NAI	O4B-C1B-C2B	-2.06	102.21	106.62
2	B	401	NAI	PN-O5D-C5D	-2.05	109.58	121.35
2	A	401	NAI	C4B-O4B-C1B	-2.05	104.94	109.47
2	B	401	NAI	O3B-C3B-C4B	-2.03	105.24	111.08
2	A	401	NAI	N3A-C4A-N9A	2.00	130.57	127.17
2	C	401	NAI	C4B-O4B-C1B	-2.00	105.05	109.47

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAI	C5D-O5D-PN-O3
2	C	401	NAI	C5D-O5D-PN-O2N
2	D	401	NAI	C5D-O5D-PN-O2N
3	B	402	GHO	O03-C01-S04-O05
3	E	402	GHO	O03-C01-S04-O05
3	E	402	GHO	O03-C01-S04-O06
2	C	401	NAI	O4D-C4D-C5D-O5D
2	D	401	NAI	O4D-C4D-C5D-O5D
2	A	401	NAI	O4D-C4D-C5D-O5D
2	C	401	NAI	O4B-C4B-C5B-O5B
2	D	401	NAI	C3D-C4D-C5D-O5D
2	E	401	NAI	O4B-C4B-C5B-O5B
2	B	401	NAI	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	C	401	NAI	C3D-C4D-C5D-O5D
2	E	401	NAI	C3B-C4B-C5B-O5B
2	C	401	NAI	C2B-C1B-N9A-C8A
2	A	401	NAI	O4D-C1D-N1N-C6N
2	A	401	NAI	C5D-O5D-PN-O2N
2	C	401	NAI	C5B-O5B-PA-O1A
2	C	401	NAI	C5B-O5B-PA-O2A
2	C	401	NAI	C5B-O5B-PA-O3
2	C	401	NAI	C5D-O5D-PN-O3
2	C	401	NAI	C5D-O5D-PN-O1N
2	D	401	NAI	C5D-O5D-PN-O3
2	D	401	NAI	O4B-C4B-C5B-O5B
2	D	401	NAI	C3B-C4B-C5B-O5B
2	E	401	NAI	PN-O3-PA-O2A
2	E	401	NAI	O4D-C1D-N1N-C6N
2	D	401	NAI	O4D-C1D-N1N-C6N
2	C	401	NAI	O4D-C1D-N1N-C6N
2	A	401	NAI	C3D-C4D-C5D-O5D
2	B	401	NAI	O4D-C4D-C5D-O5D
2	C	401	NAI	C3B-C4B-C5B-O5B
2	C	401	NAI	C2N-C3N-C7N-N7N
2	B	401	NAI	PN-O3-PA-O2A
2	C	401	NAI	PN-O3-PA-O2A
2	D	401	NAI	C2B-C1B-N9A-C8A
2	E	401	NAI	PN-O3-PA-O1A
2	D	401	NAI	C2D-C1D-N1N-C6N
2	A	401	NAI	C2B-C1B-N9A-C8A
2	A	401	NAI	PN-O3-PA-O2A
2	A	401	NAI	O4B-C4B-C5B-O5B
2	E	401	NAI	O4D-C4D-C5D-O5D

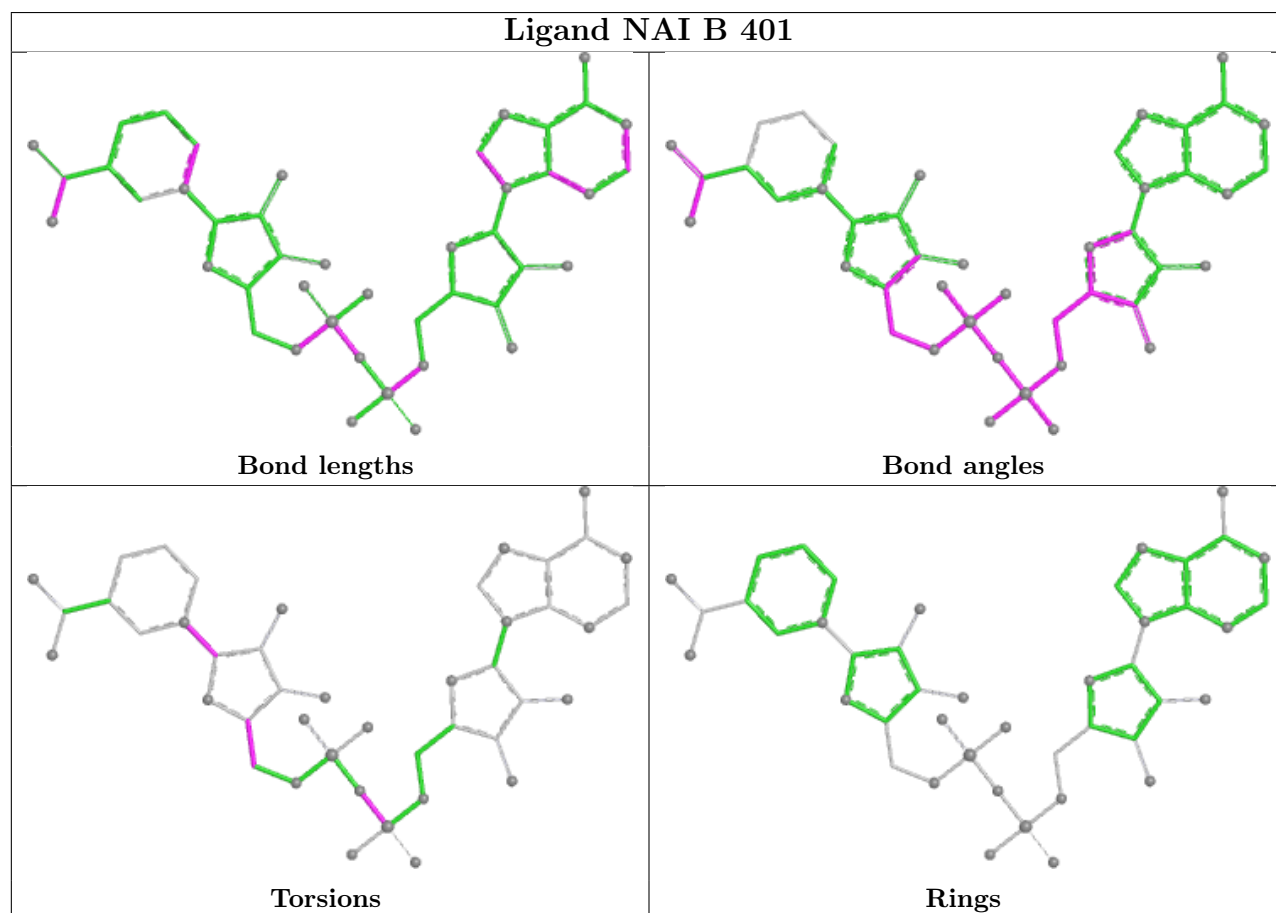
There are no ring outliers.

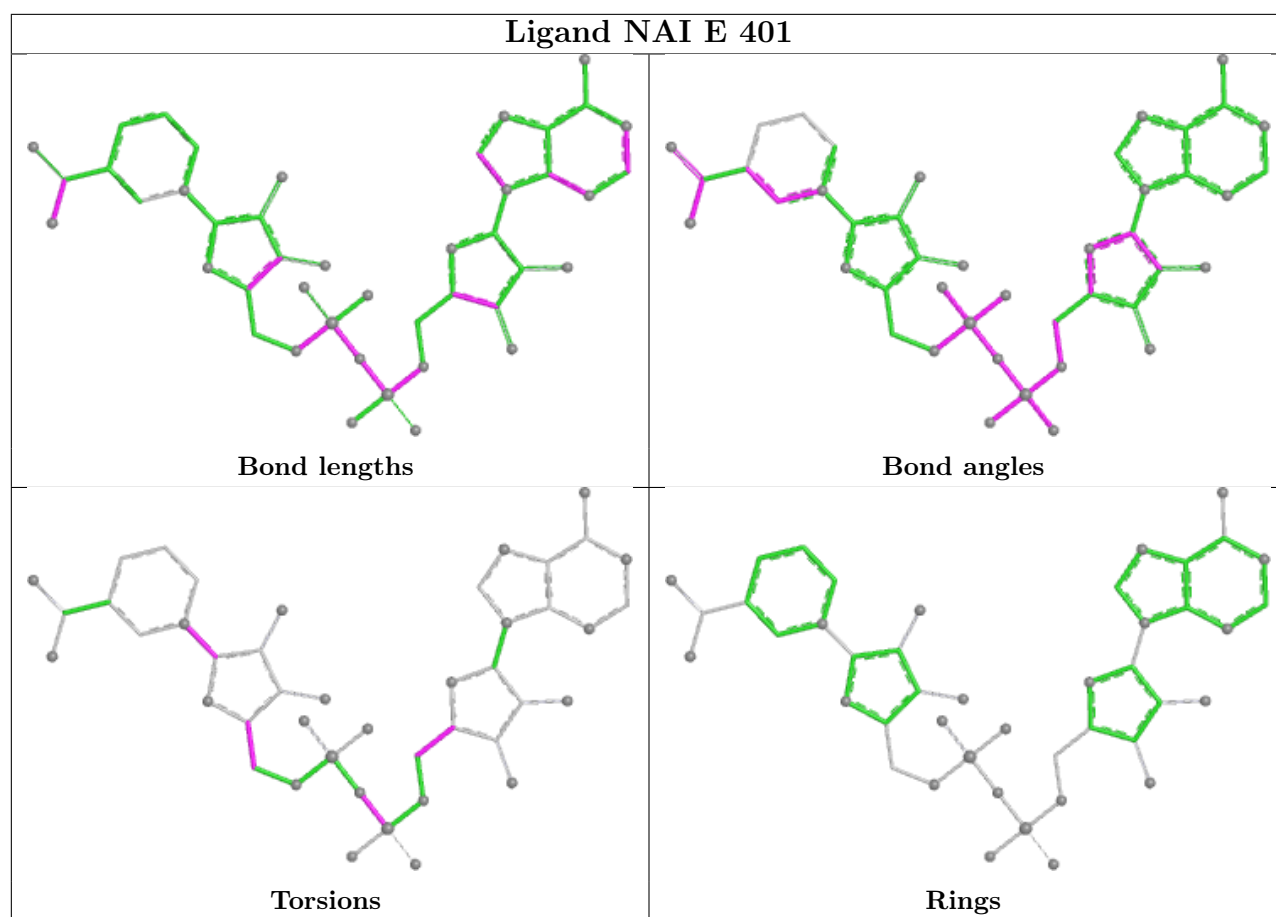
5 monomers are involved in 7 short contacts:

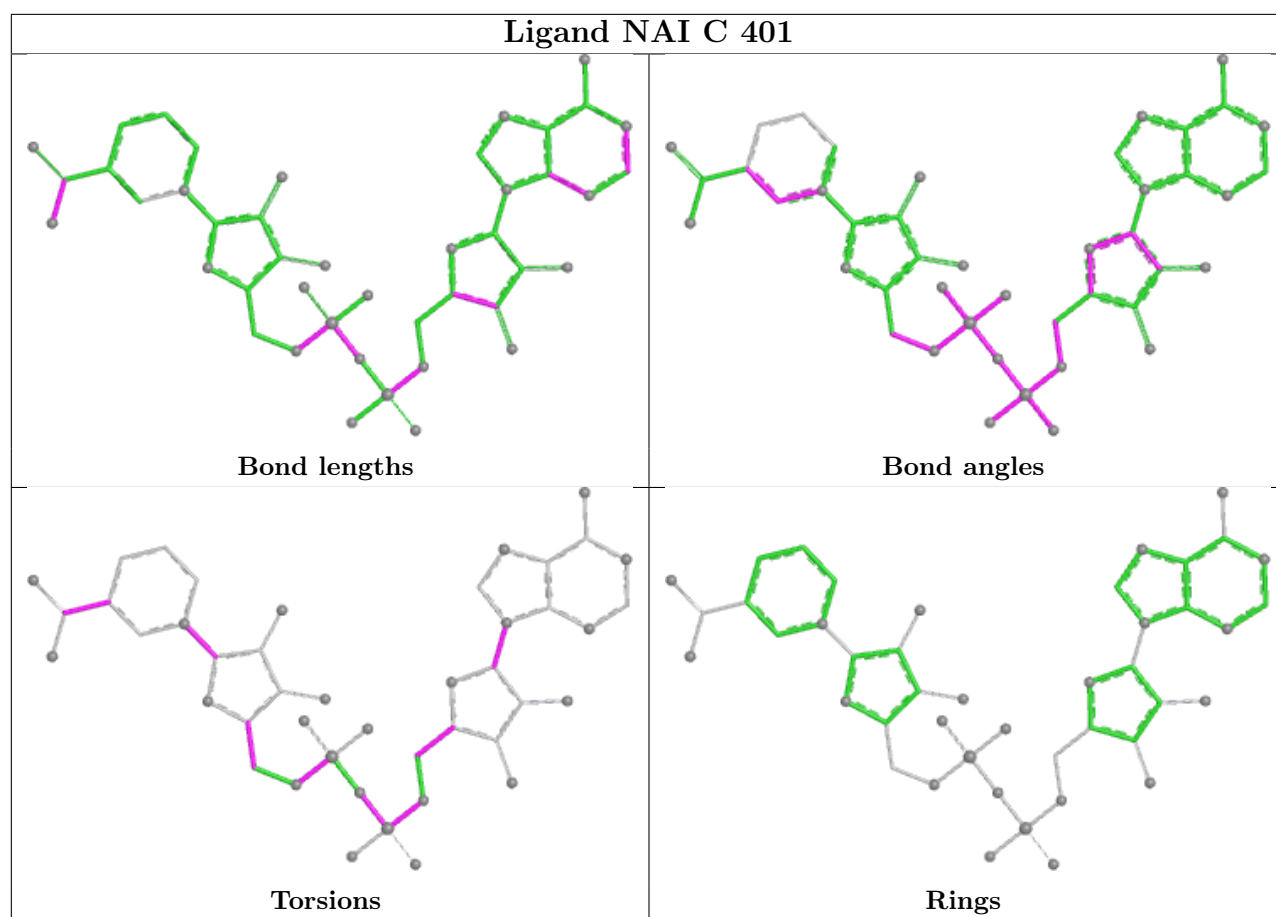
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	NAI	2	0
3	A	402	GHO	1	0
2	A	401	NAI	1	0
2	D	401	NAI	2	0
3	C	402	GHO	1	0

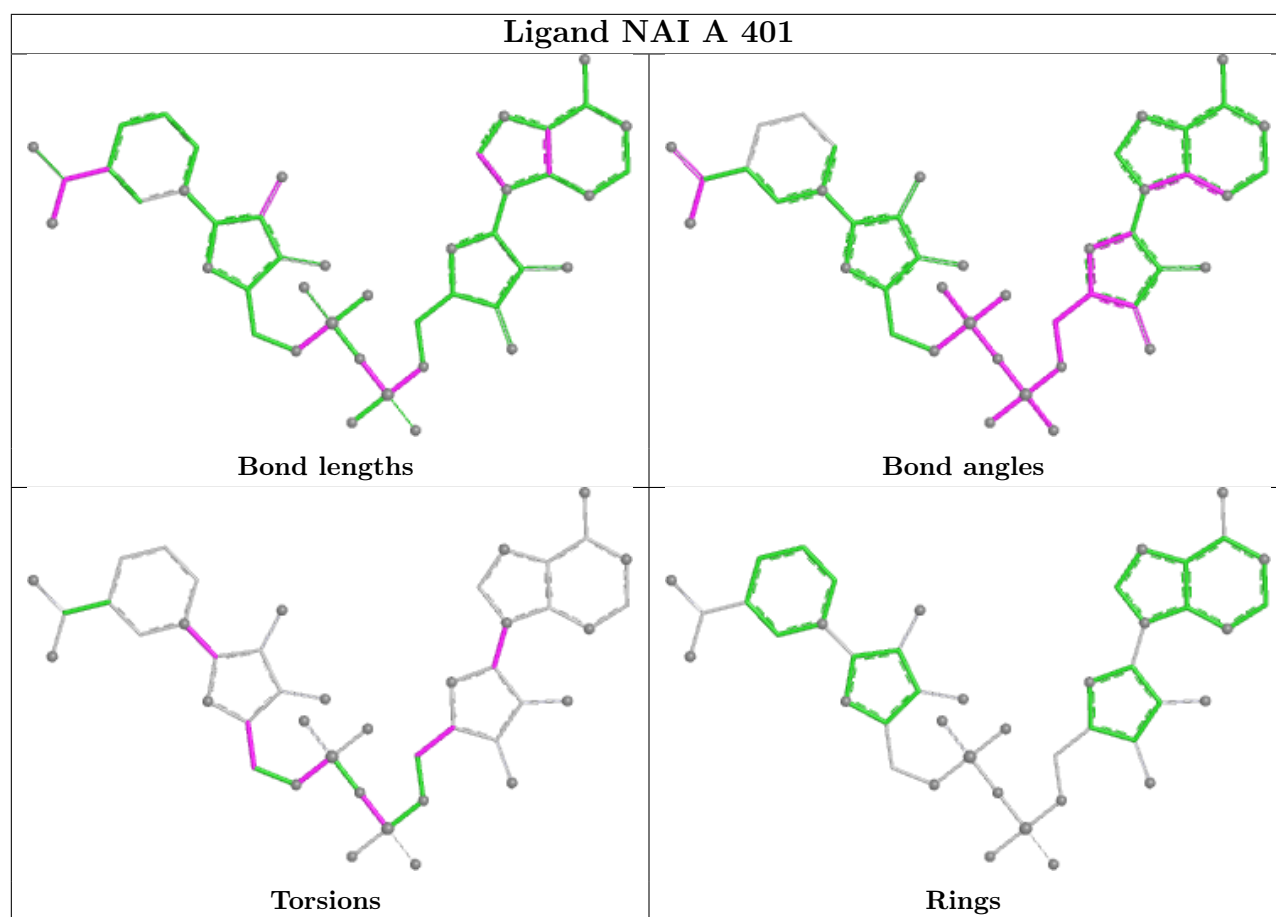
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

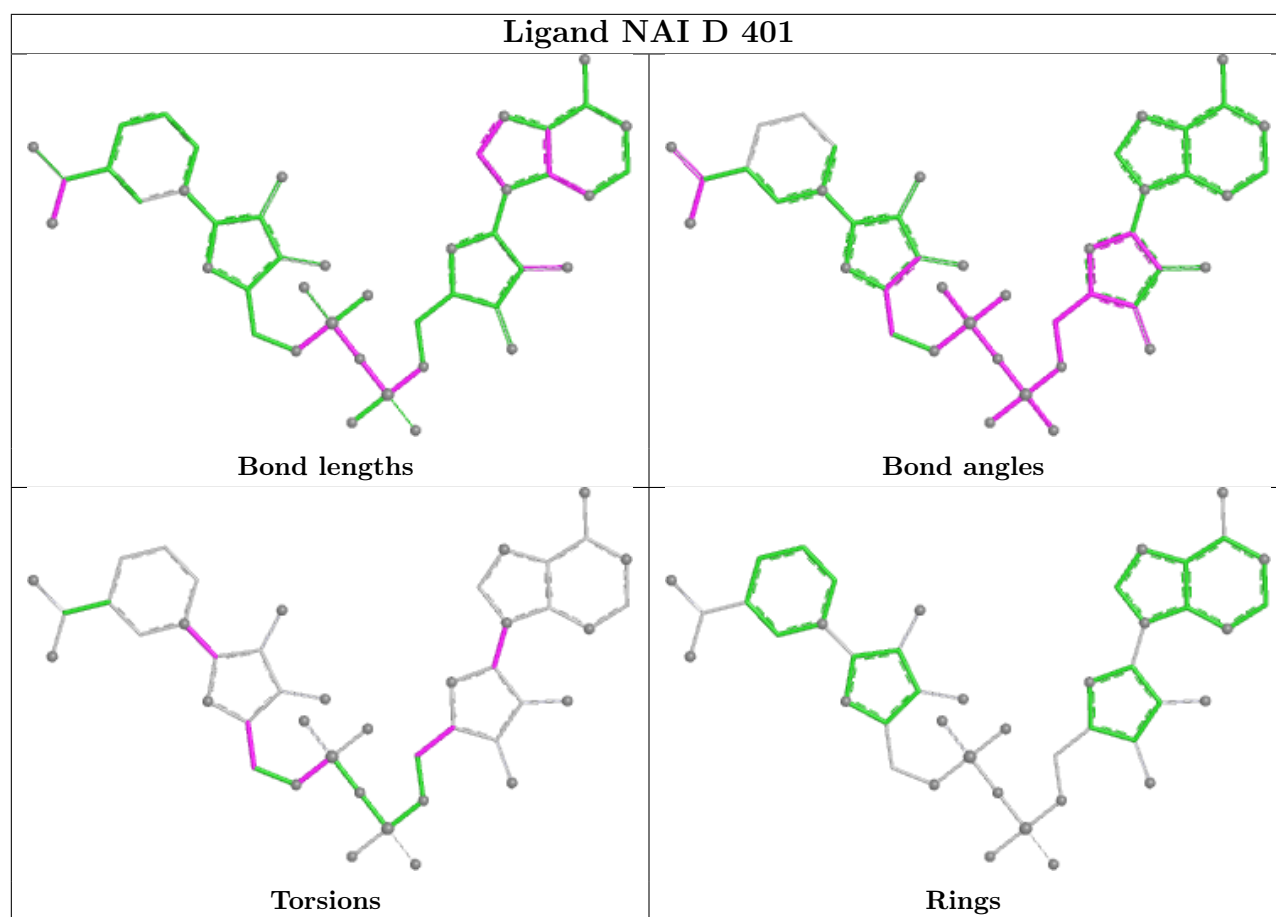
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	275/316 (87%)	2.34	172 (62%) 0 0	23, 44, 70, 108	1 (0%)
1	B	280/316 (88%)	2.70	184 (65%) 0 0	21, 46, 76, 93	1 (0%)
1	C	275/316 (87%)	2.74	198 (72%) 0 0	24, 50, 74, 101	1 (0%)
1	D	281/316 (88%)	3.05	208 (74%) 0 0	23, 49, 76, 95	1 (0%)
1	E	278/316 (87%)	2.70	191 (68%) 0 0	21, 44, 69, 97	1 (0%)
All	All	1389/1580 (87%)	2.71	953 (68%) 0 0	21, 46, 74, 108	5 (0%)

All (953) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	36	ASP	8.0
1	B	-4	LEU	7.7
1	B	0	SER	7.6
1	B	39	LEU	7.6
1	B	26	ALA	7.3
1	B	38	ASP	7.3
1	A	38	ASP	7.1
1	B	36	ASP	7.0
1	D	37	MET	7.0
1	B	274	GLN	6.9
1	D	143	VAL	6.9
1	E	-2	PHE	6.8
1	D	23	GLY	6.7
1	D	221	GLU	6.7
1	D	25	LEU	6.6
1	D	24	VAL	6.6
1	D	40	ALA	6.5
1	C	36	ASP	6.5
1	B	24	VAL	6.5
1	B	275	GLU	6.5

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Mol	Chain	Res	Type	RSRZ
1	D	-5	ASN	6.4
1	D	146	GLY	6.3
1	D	-3	TYR	6.2
1	E	97	ALA	6.2
1	B	-2	PHE	6.1
1	C	35	PRO	6.1
1	E	75	ILE	6.0
1	E	83	GLY	5.9
1	B	40	ALA	5.9
1	D	16	ALA	5.9
1	A	36	ASP	5.8
1	E	-1	GLN	5.8
1	E	82	ILE	5.8
1	D	42	VAL	5.7
1	D	38	ASP	5.7
1	D	-4	LEU	5.7
1	B	50	VAL	5.7
1	E	39	LEU	5.7
1	D	26	ALA	5.6
1	C	271	MET	5.6
1	B	271	MET	5.5
1	C	82	ILE	5.5
1	D	28	HIS	5.5
1	E	143	VAL	5.5
1	B	37	MET	5.5
1	B	228	LYS	5.5
1	C	37	MET	5.4
1	B	45	LEU	5.4
1	C	275	GLU	5.4
1	C	273	ASP	5.4
1	E	65	VAL	5.4
1	D	273	ASP	5.3
1	E	25	LEU	5.3
1	B	8	ALA	5.3
1	D	274	GLN	5.3
1	D	45	LEU	5.3
1	B	-3	TYR	5.3
1	B	60	VAL	5.2
1	D	-1	GLN	5.2
1	E	211	LEU	5.2
1	D	96	ALA	5.2
1	E	8	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	42	VAL	5.2
1	E	36	ASP	5.1
1	E	42	VAL	5.1
1	C	25	LEU	5.1
1	D	8	ALA	5.1
1	C	5	PHE	5.1
1	C	38	ASP	5.1
1	B	75	ILE	5.0
1	B	25	LEU	5.0
1	C	108	LEU	5.0
1	E	52	LEU	5.0
1	B	-1	GLN	5.0
1	D	27	ALA	5.0
1	C	40	ALA	5.0
1	E	96	ALA	5.0
1	D	43	SER	4.9
1	B	96	ALA	4.9
1	C	225	GLY	4.9
1	D	88	ASP	4.9
1	B	143	VAL	4.9
1	D	11	LEU	4.9
1	E	270	SER	4.9
1	C	60	VAL	4.9
1	E	78	ILE	4.9
1	E	274	GLN	4.8
1	D	13	PHE	4.8
1	B	144	GLU	4.8
1	E	93	VAL	4.8
1	D	144	GLU	4.8
1	D	63	SER	4.8
1	C	42	VAL	4.8
1	A	77	PHE	4.8
1	D	22	ALA	4.8
1	D	55	HIS	4.8
1	B	1	MET	4.8
1	B	42	VAL	4.8
1	D	39	LEU	4.7
1	E	86	ILE	4.7
1	D	158	PHE	4.7
1	A	84	ALA	4.7
1	D	176	SER	4.7
1	E	43	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	59	THR	4.7
1	B	11	LEU	4.7
1	B	249	GLY	4.6
1	B	48	MET	4.6
1	D	35	PRO	4.6
1	D	149	MET	4.6
1	E	38	ASP	4.6
1	E	59	THR	4.6
1	E	1	MET	4.6
1	C	177	GLY	4.6
1	C	96	ALA	4.6
1	E	273	ASP	4.6
1	B	128	VAL	4.6
1	E	275	GLU	4.5
1	D	212	GLY	4.5
1	E	67	PHE	4.5
1	C	28	HIS	4.5
1	D	272	ALA	4.5
1	D	222	GLN	4.5
1	B	52	LEU	4.5
1	C	86	ILE	4.5
1	C	143	VAL	4.5
1	D	77	PHE	4.5
1	C	32	ALA	4.5
1	B	78	ILE	4.4
1	B	98	GLY	4.4
1	E	70	VAL	4.4
1	C	219	HIS	4.4
1	C	44	ALA	4.4
1	D	229	ASP	4.4
1	D	71	LYS	4.4
1	B	43	SER	4.4
1	D	132	ALA	4.4
1	D	129	ARG	4.4
1	C	78	ILE	4.4
1	C	83	GLY	4.4
1	E	9	GLY	4.4
1	A	270	SER	4.4
1	D	47	LYS	4.3
1	A	93	VAL	4.3
1	B	127	VAL	4.3
1	C	1	MET	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	224	PRO	4.3
1	E	185	LEU	4.3
1	A	78	ILE	4.3
1	D	60	VAL	4.3
1	D	142	GLN	4.3
1	C	85	ASP	4.3
1	E	88	ASP	4.3
1	E	44	ALA	4.3
1	A	74	ILE	4.3
1	E	91	ILE	4.3
1	C	231	VAL	4.3
1	E	24	VAL	4.3
1	B	34	SER	4.3
1	B	273	ASP	4.3
1	D	136	ALA	4.3
1	D	214	ALA	4.3
1	E	181	ALA	4.3
1	C	15	LEU	4.3
1	C	39	LEU	4.3
1	A	8	ALA	4.2
1	A	111	PHE	4.2
1	E	158	PHE	4.2
1	E	37	MET	4.2
1	D	41	THR	4.2
1	E	79	LEU	4.2
1	D	98	GLY	4.2
1	B	47	LYS	4.2
1	C	6	ILE	4.2
1	D	81	GLU	4.2
1	D	2	SER	4.2
1	C	41	THR	4.2
1	C	49	GLY	4.2
1	D	6	ILE	4.2
1	D	118	ILE	4.2
1	B	190	ASP	4.2
1	A	68	LEU	4.2
1	C	79	LEU	4.2
1	A	94	SER	4.2
1	D	271	MET	4.2
1	A	274	GLN	4.2
1	E	77	PHE	4.2
1	E	68	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	221	GLU	4.2
1	D	7	GLY	4.1
1	C	30	ILE	4.1
1	B	88	ASP	4.1
1	B	270	SER	4.1
1	D	70	VAL	4.1
1	D	1	MET	4.1
1	D	56	ASN	4.1
1	E	6	ILE	4.1
1	C	3	VAL	4.1
1	C	65	VAL	4.1
1	C	70	VAL	4.1
1	E	111	PHE	4.1
1	D	51	LYS	4.1
1	C	80	ASP	4.1
1	E	263	ILE	4.1
1	A	181	ALA	4.0
1	E	114	ALA	4.0
1	E	227	LEU	4.0
1	C	222	GLN	4.0
1	A	273	ASP	4.0
1	D	270	SER	4.0
1	E	0	SER	4.0
1	C	238	THR	4.0
1	D	-2	PHE	4.0
1	A	229	ASP	4.0
1	C	163	GLU	4.0
1	D	78	ILE	4.0
1	A	39	LEU	4.0
1	D	84	ALA	4.0
1	B	13	PHE	4.0
1	A	86	ILE	4.0
1	B	95	CYS	4.0
1	C	69	ALA	4.0
1	E	213	ALA	4.0
1	D	111	PHE	4.0
1	E	135	TYR	4.0
1	B	2	SER	4.0
1	B	62	HIS	3.9
1	D	50	VAL	3.9
1	E	60	VAL	3.9
1	D	268	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	19	PHE	3.9
1	D	223	HIS	3.9
1	E	62	HIS	3.9
1	E	118	ILE	3.9
1	A	143	VAL	3.9
1	D	233	SER	3.9
1	D	211	LEU	3.9
1	D	49	GLY	3.9
1	E	190	ASP	3.9
1	C	111	PHE	3.9
1	A	6	ILE	3.9
1	B	35	PRO	3.9
1	C	126	VAL	3.9
1	B	71	LYS	3.9
1	B	44	ALA	3.9
1	E	272	ALA	3.9
1	C	145	ASP	3.8
1	D	30	ILE	3.8
1	A	163	GLU	3.8
1	E	271	MET	3.8
1	C	127	VAL	3.8
1	E	152	LEU	3.8
1	E	262	CYS	3.8
1	A	271	MET	3.8
1	E	217	LEU	3.8
1	E	84	ALA	3.8
1	C	56	ASN	3.8
1	E	222	GLN	3.8
1	A	275	GLU	3.8
1	E	117	VAL	3.8
1	D	139	THR	3.8
1	D	48	MET	3.8
1	A	40	ALA	3.7
1	B	12	ALA	3.7
1	C	190	ASP	3.7
1	D	209	ALA	3.7
1	E	80	ASP	3.7
1	B	74	ILE	3.7
1	B	28	HIS	3.7
1	D	52	LEU	3.7
1	C	144	GLU	3.7
1	E	41	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	64	ASP	3.7
1	A	69	ALA	3.7
1	D	66	LEU	3.7
1	C	50	VAL	3.7
1	C	26	ALA	3.7
1	C	189	ALA	3.7
1	D	174	SER	3.7
1	D	175	GLY	3.7
1	D	275	GLU	3.7
1	A	134	VAL	3.7
1	C	31	MET	3.7
1	A	41	THR	3.7
1	B	229	ASP	3.7
1	D	122	THR	3.7
1	D	46	ARG	3.7
1	C	141	ALA	3.7
1	B	224	PRO	3.7
1	A	43	SER	3.7
1	B	77	PHE	3.6
1	D	153	LEU	3.6
1	B	231	VAL	3.6
1	B	53	THR	3.6
1	A	97	ALA	3.6
1	B	141	ALA	3.6
1	C	272	ALA	3.6
1	D	267	GLU	3.6
1	B	142	GLN	3.6
1	E	149	MET	3.6
1	B	79	LEU	3.6
1	E	66	LEU	3.6
1	E	129	ARG	3.6
1	E	165	ASP	3.6
1	A	70	VAL	3.6
1	D	127	VAL	3.6
1	E	156	VAL	3.6
1	C	12	ALA	3.6
1	D	110	ALA	3.6
1	E	140	HIS	3.6
1	D	10	GLN	3.6
1	B	5	PHE	3.6
1	A	108	LEU	3.6
1	D	145	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	92	VAL	3.6
1	E	219	HIS	3.6
1	D	135	TYR	3.6
1	A	37	MET	3.6
1	A	9	GLY	3.6
1	C	4	GLY	3.6
1	C	234	PRO	3.6
1	B	27	ALA	3.6
1	C	233	SER	3.5
1	D	15	LEU	3.5
1	E	210	LEU	3.5
1	E	73	HIS	3.5
1	B	41	THR	3.5
1	C	72	PRO	3.5
1	E	102	SER	3.5
1	A	11	LEU	3.5
1	A	218	LEU	3.5
1	A	80	ASP	3.5
1	D	62	HIS	3.5
1	E	139	THR	3.5
1	B	198	PRO	3.5
1	D	224	PRO	3.5
1	C	24	VAL	3.5
1	D	44	ALA	3.5
1	D	75	ILE	3.5
1	A	201	LEU	3.5
1	C	68	LEU	3.5
1	C	230	ASN	3.5
1	E	99	VAL	3.5
1	B	136	ALA	3.5
1	C	232	SER	3.5
1	B	221	GLU	3.5
1	D	87	GLU	3.5
1	D	123	ASN	3.5
1	E	72	PRO	3.4
1	A	24	VAL	3.4
1	A	58	GLU	3.4
1	B	197	LEU	3.4
1	C	11	LEU	3.4
1	D	204	ARG	3.4
1	C	274	GLN	3.4
1	C	158	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	54	PRO	3.4
1	C	117	VAL	3.4
1	A	272	ALA	3.4
1	D	0	SER	3.4
1	B	49	GLY	3.4
1	E	186	ASP	3.4
1	C	67	PHE	3.4
1	C	92	VAL	3.4
1	D	231	VAL	3.4
1	B	46	ARG	3.4
1	D	147	ARG	3.4
1	B	226	GLN	3.4
1	C	75	ILE	3.4
1	C	173	LEU	3.4
1	C	201	LEU	3.4
1	D	91	ILE	3.4
1	D	19	PHE	3.4
1	A	139	THR	3.4
1	B	112	ARG	3.4
1	B	130	GLU	3.4
1	C	202	ALA	3.4
1	D	97	ALA	3.4
1	E	94	SER	3.4
1	E	209	ALA	3.4
1	E	85	ASP	3.4
1	E	173	LEU	3.3
1	B	139	THR	3.3
1	D	133	THR	3.3
1	C	62	HIS	3.3
1	A	170	VAL	3.3
1	E	26	ALA	3.3
1	B	23	GLY	3.3
1	A	85	ASP	3.3
1	C	45	LEU	3.3
1	C	217	LEU	3.3
1	D	68	LEU	3.3
1	C	115	PRO	3.3
1	B	100	THR	3.3
1	C	84	ALA	3.3
1	E	136	ALA	3.3
1	E	196	GLY	3.3
1	A	88	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	229	ASP	3.3
1	B	217	LEU	3.3
1	E	45	LEU	3.3
1	E	87	GLU	3.3
1	D	53	THR	3.3
1	D	59	THR	3.3
1	B	222	GLN	3.3
1	B	132	ALA	3.3
1	D	213	ALA	3.3
1	E	229	ASP	3.3
1	B	108	LEU	3.3
1	E	148	LEU	3.3
1	C	125	PRO	3.3
1	C	239	ILE	3.3
1	D	74	ILE	3.3
1	E	95	CYS	3.3
1	A	106	LYS	3.3
1	A	124	THR	3.3
1	B	59	THR	3.3
1	B	92	VAL	3.3
1	C	27	ALA	3.2
1	D	134	VAL	3.3
1	E	214	ALA	3.2
1	D	83	GLY	3.2
1	A	75	ILE	3.2
1	C	63	SER	3.2
1	C	102	SER	3.2
1	B	97	ALA	3.2
1	E	12	ALA	3.2
1	C	9	GLY	3.2
1	C	52	LEU	3.2
1	D	100	THR	3.2
1	C	19	PHE	3.2
1	C	34	SER	3.2
1	A	141	ALA	3.2
1	A	83	GLY	3.2
1	D	225	GLY	3.2
1	A	54	PRO	3.2
1	A	82	ILE	3.2
1	D	34	SER	3.2
1	D	150	GLU	3.2
1	B	15	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	54	PRO	3.2
1	A	269	GLN	3.2
1	D	82	ILE	3.2
1	D	167	ILE	3.2
1	D	266	ARG	3.1
1	A	13	PHE	3.1
1	A	232	SER	3.1
1	A	44	ALA	3.1
1	E	40	ALA	3.1
1	E	110	ALA	3.1
1	E	146	GLY	3.1
1	E	172	GLY	3.1
1	C	256	ASN	3.1
1	E	203	VAL	3.1
1	A	197	LEU	3.1
1	A	268	LEU	3.1
1	D	148	LEU	3.1
1	B	64	ASP	3.1
1	D	117	VAL	3.1
1	C	253	LEU	3.1
1	C	221	GLU	3.1
1	B	155	SER	3.1
1	A	230	ASN	3.1
1	A	235	GLY	3.1
1	D	230	ASN	3.1
1	C	22	ALA	3.1
1	C	257	ALA	3.1
1	D	12	ALA	3.1
1	D	3	VAL	3.1
1	E	50	VAL	3.1
1	A	25	LEU	3.1
1	B	218	LEU	3.1
1	B	82	ILE	3.1
1	C	87	GLU	3.1
1	C	124	THR	3.1
1	C	223	HIS	3.1
1	D	61	GLN	3.1
1	C	16	ALA	3.1
1	D	207	ALA	3.1
1	C	129	ARG	3.1
1	B	29	LYS	3.1
1	D	162	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	108	LEU	3.1
1	B	101	ILE	3.0
1	E	232	SER	3.0
1	B	69	ALA	3.0
1	B	179	ALA	3.0
1	D	32	ALA	3.0
1	A	193	VAL	3.0
1	C	180	TYR	3.0
1	E	30	ILE	3.0
1	E	74	ILE	3.0
1	B	199[A]	ARG	3.0
1	C	236	GLY	3.0
1	B	111	PHE	3.0
1	A	113	PRO	3.0
1	E	27	ALA	3.0
1	C	148	LEU	3.0
1	C	267	GLU	3.0
1	B	219	HIS	3.0
1	C	55	HIS	3.0
1	D	86	ILE	3.0
1	A	103	SER	3.0
1	B	220	SER	3.0
1	C	88	ASP	3.0
1	A	67	PHE	3.0
1	E	224	PRO	3.0
1	E	207	ALA	3.0
1	A	45	LEU	3.0
1	C	263	ILE	3.0
1	A	112	ARG	3.0
1	C	220	SER	3.0
1	E	174	SER	3.0
1	B	138	GLY	3.0
1	D	248	GLY	3.0
1	D	249	GLY	3.0
1	B	268	LEU	2.9
1	C	203	VAL	2.9
1	A	71	LYS	2.9
1	E	100	THR	2.9
1	D	232	SER	2.9
1	B	168	ASP	2.9
1	D	58	GLU	2.9
1	D	246	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	115	PRO	2.9
1	A	19	PHE	2.9
1	D	227	LEU	2.9
1	A	128	VAL	2.9
1	B	65	VAL	2.9
1	E	106	LYS	2.9
1	B	86	ILE	2.9
1	A	33	SER	2.9
1	B	72	PRO	2.9
1	E	76	PRO	2.9
1	D	21	ALA	2.9
1	E	153	LEU	2.9
1	B	269	GLN	2.9
1	E	269	GLN	2.9
1	A	126	VAL	2.9
1	D	203	VAL	2.9
1	C	95	CYS	2.9
1	E	104	ILE	2.9
1	D	20	THR	2.9
1	C	33	SER	2.9
1	E	7	GLY	2.9
1	C	71	LYS	2.9
1	E	89	ARG	2.9
1	A	217	LEU	2.9
1	C	13	PHE	2.9
1	C	182	PHE	2.9
1	D	108	LEU	2.9
1	D	201	LEU	2.9
1	A	118	ILE	2.9
1	C	104	ILE	2.9
1	B	109	SER	2.8
1	E	98	GLY	2.8
1	A	35	PRO	2.8
1	A	73	HIS	2.8
1	B	180	TYR	2.8
1	D	151	GLN	2.8
1	B	227	LEU	2.8
1	C	97	ALA	2.8
1	D	67	PHE	2.8
1	C	48	MET	2.8
1	C	64	ASP	2.8
1	D	168	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	199[A]	ARG	2.8
1	A	115	PRO	2.8
1	C	178	PRO	2.8
1	D	216	MET	2.8
1	E	51	LYS	2.8
1	A	30	ILE	2.8
1	B	263	ILE	2.8
1	A	56	ASN	2.8
1	C	249	GLY	2.8
1	D	157	GLY	2.8
1	C	61	GLN	2.8
1	D	72	PRO	2.8
1	D	253	LEU	2.8
1	E	197	LEU	2.8
1	E	144	GLU	2.8
1	A	65	VAL	2.8
1	C	156	VAL	2.8
1	B	30	ILE	2.8
1	C	73	HIS	2.8
1	E	90	HIS	2.8
1	C	157	GLY	2.8
1	D	102	SER	2.8
1	B	234	PRO	2.8
1	B	267	GLU	2.8
1	C	150	GLU	2.8
1	C	268	LEU	2.8
1	C	107	LYS	2.8
1	A	14	ALA	2.8
1	B	22	ALA	2.8
1	B	32	ALA	2.8
1	E	116	ARG	2.8
1	A	167	ILE	2.7
1	B	80	ASP	2.7
1	A	146	GLY	2.7
1	D	76	PRO	2.7
1	C	81	GLU	2.7
1	D	215	LYS	2.7
1	D	152	LEU	2.7
1	A	46	ARG	2.7
1	B	14	ALA	2.7
1	B	207	ALA	2.7
1	C	89	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	219	HIS	2.7
1	B	122	THR	2.7
1	C	10	GLN	2.7
1	D	226	GLN	2.7
1	C	51	LYS	2.7
1	D	120	CYS	2.7
1	A	52	LEU	2.7
1	E	268	LEU	2.7
1	A	26	ALA	2.7
1	D	69	ALA	2.7
1	C	140	HIS	2.7
1	D	160	THR	2.7
1	E	265	THR	2.7
1	C	118	ILE	2.7
1	E	54	PRO	2.7
1	D	217	LEU	2.7
1	D	202	ALA	2.7
1	A	222	GLN	2.7
1	C	77	PHE	2.7
1	D	5	PHE	2.7
1	B	156	VAL	2.7
1	D	170	VAL	2.7
1	A	49	GLY	2.7
1	A	157	GLY	2.7
1	B	18	GLY	2.7
1	B	118	ILE	2.7
1	C	146	GLY	2.7
1	D	104	ILE	2.7
1	E	138	GLY	2.7
1	A	211	LEU	2.7
1	E	166	LEU	2.7
1	A	179	ALA	2.6
1	A	207	ALA	2.6
1	D	179	ALA	2.6
1	D	182	PHE	2.6
1	B	248	GLY	2.6
1	D	236	GLY	2.6
1	E	204	ARG	2.6
1	E	48	MET	2.6
1	D	95	CYS	2.6
1	D	197	LEU	2.6
1	D	218	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	55	HIS	2.6
1	D	269	GLN	2.6
1	C	106	LYS	2.6
1	B	169	ALA	2.6
1	E	81	GLU	2.6
1	C	123	ASN	2.6
1	A	171	THR	2.6
1	A	48	MET	2.6
1	A	149	MET	2.6
1	B	94	SER	2.6
1	C	91	ILE	2.6
1	D	94	SER	2.6
1	C	142	GLN	2.6
1	E	159	CYS	2.6
1	B	81	GLU	2.6
1	E	179	ALA	2.6
1	C	18	GLY	2.6
1	B	33	SER	2.6
1	E	63	SER	2.6
1	E	261	SER	2.6
1	D	57	LYS	2.6
1	A	227	LEU	2.6
1	C	185	LEU	2.6
1	E	218	LEU	2.6
1	A	221	GLU	2.6
1	B	204	ARG	2.6
1	C	214	ALA	2.6
1	D	181	ALA	2.6
1	E	16	ALA	2.6
1	E	184	ALA	2.6
1	A	186	ASP	2.6
1	B	183	THR	2.6
1	C	23	GLY	2.6
1	D	113	PRO	2.6
1	D	124	THR	2.6
1	E	18	GLY	2.6
1	A	92	VAL	2.6
1	B	170	VAL	2.6
1	D	156	VAL	2.6
1	E	115	PRO	2.6
1	A	104	ILE	2.6
1	B	154	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	174	SER	2.6
1	E	107	LYS	2.6
1	C	147	ARG	2.5
1	B	84	ALA	2.5
1	C	110	ALA	2.5
1	D	159	CYS	2.5
1	E	32	ALA	2.5
1	E	69	ALA	2.5
1	E	225	GLY	2.5
1	A	34	SER	2.5
1	A	156	VAL	2.5
1	E	71	LYS	2.5
1	B	6	ILE	2.5
1	B	167	ILE	2.5
1	E	220	SER	2.5
1	A	129	ARG	2.5
1	B	147	ARG	2.5
1	D	112	ARG	2.5
1	A	32	ALA	2.5
1	B	21	ALA	2.5
1	B	272	ALA	2.5
1	C	21	ALA	2.5
1	E	230	ASN	2.5
1	B	235	GLY	2.5
1	C	131	GLY	2.5
1	E	35	PRO	2.5
1	D	250	PHE	2.5
1	A	267	GLU	2.5
1	B	148	LEU	2.5
1	B	205	LEU	2.5
1	E	31	MET	2.5
1	E	216	MET	2.5
1	A	190	ASP	2.5
1	B	85	ASP	2.5
1	A	7	GLY	2.5
1	A	28	HIS	2.5
1	A	177	GLY	2.5
1	B	157	GLY	2.5
1	B	196	GLY	2.5
1	D	196	GLY	2.5
1	D	238	THR	2.5
1	E	53	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	87	GLU	2.5
1	E	112	ARG	2.5
1	A	66	LEU	2.5
1	C	205	LEU	2.5
1	B	73	HIS	2.5
1	B	223	HIS	2.5
1	B	76	PRO	2.5
1	B	83	GLY	2.5
1	B	225	GLY	2.5
1	A	147	ARG	2.4
1	E	105	GLU	2.4
1	A	182	PHE	2.4
1	A	220	SER	2.4
1	B	67	PHE	2.4
1	A	172	GLY	2.4
1	D	116	ARG	2.4
1	A	2	SER	2.4
1	C	270	SER	2.4
1	E	103	SER	2.4
1	A	3	VAL	2.4
1	B	93	VAL	2.4
1	B	134	VAL	2.4
1	B	158	PHE	2.4
1	B	162	VAL	2.4
1	E	92	VAL	2.4
1	C	149	MET	2.4
1	A	219	HIS	2.4
1	A	142	GLN	2.4
1	A	130	GLU	2.4
1	A	249	GLY	2.4
1	B	7	GLY	2.4
1	B	232	SER	2.4
1	D	109	SER	2.4
1	D	220	SER	2.4
1	A	203	VAL	2.4
1	C	74	ILE	2.4
1	C	255	ILE	2.4
1	D	101	ILE	2.4
1	C	66	LEU	2.4
1	C	152	LEU	2.4
1	C	218	LEU	2.4
1	D	210	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	201	LEU	2.4
1	E	56	ASN	2.4
1	A	4	GLY	2.4
1	A	22	ALA	2.4
1	A	236	GLY	2.4
1	D	9	GLY	2.4
1	E	237	ALA	2.4
1	D	252	SER	2.4
1	C	128	VAL	2.4
1	C	159	CYS	2.4
1	A	205	LEU	2.4
1	D	205	LEU	2.4
1	E	188	LEU	2.4
1	C	199[A]	ARG	2.4
1	A	135	TYR	2.3
1	A	145	ASP	2.3
1	C	186	ASP	2.3
1	D	192	GLY	2.3
1	A	21	ALA	2.3
1	C	183	THR	2.3
1	D	171	THR	2.3
1	A	102	SER	2.3
1	A	121	MET	2.3
1	C	162	VAL	2.3
1	D	65	VAL	2.3
1	D	263	ILE	2.3
1	A	55	HIS	2.3
1	B	129	ARG	2.3
1	C	211	LEU	2.3
1	A	29	LYS	2.3
1	A	47	LYS	2.3
1	B	135	TYR	2.3
1	C	29	LYS	2.3
1	C	54	PRO	2.3
1	E	215	LYS	2.3
1	B	114	ALA	2.3
1	C	187	ALA	2.3
1	E	260	ALA	2.3
1	C	137	THR	2.3
1	C	155	SER	2.3
1	B	55	HIS	2.3
1	B	61	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	120	CYS	2.3
1	A	148	LEU	2.3
1	A	206	GLY	2.3
1	E	23	GLY	2.3
1	A	241	ALA	2.3
1	C	213	ALA	2.3
1	C	139	THR	2.3
1	E	28	HIS	2.3
1	E	240	HIS	2.3
1	A	164	GLU	2.3
1	A	99	VAL	2.3
1	D	93	VAL	2.3
1	E	231	VAL	2.3
1	B	68	LEU	2.3
1	C	153	LEU	2.3
1	D	106	LYS	2.3
1	E	17	LYS	2.3
1	E	47	LYS	2.3
1	A	175	GLY	2.3
1	B	9	GLY	2.3
1	E	46	ARG	2.3
1	C	20	THR	2.3
1	B	150	GLU	2.3
1	C	90	HIS	2.3
1	E	34	SER	2.3
1	B	215	LYS	2.3
1	A	23	GLY	2.2
1	A	116	ARG	2.2
1	B	31	MET	2.2
1	B	216	MET	2.2
1	C	46	ARG	2.2
1	C	119	ARG	2.2
1	D	31	MET	2.2
1	A	110	ALA	2.2
1	B	137	THR	2.2
1	A	233	SER	2.2
1	C	2	SER	2.2
1	A	250	PHE	2.2
1	B	258	VAL	2.2
1	C	254	LEU	2.2
1	D	126	VAL	2.2
1	E	3	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	13	PHE	2.2
1	B	264	ARG	2.2
1	E	120	CYS	2.2
1	D	131	GLY	2.2
1	A	144	GLU	2.2
1	A	63	SER	2.2
1	A	155	SER	2.2
1	C	135	TYR	2.2
1	E	109	SER	2.2
1	A	153	LEU	2.2
1	A	50	VAL	2.2
1	E	127	VAL	2.2
1	E	258	VAL	2.2
1	E	19	PHE	2.2
1	B	266	ARG	2.2
1	C	138	GLY	2.2
1	C	235	GLY	2.2
1	D	161	GLU	2.2
1	E	150	GLU	2.2
1	A	107	LYS	2.2
1	E	137	THR	2.2
1	B	91	ILE	2.2
1	A	119	ARG	2.2
1	A	188	LEU	2.2
1	B	99	VAL	2.2
1	C	258	VAL	2.2
1	E	162	VAL	2.2
1	C	198	PRO	2.2
1	E	113	PRO	2.2
1	D	130	GLU	2.2
1	D	228	LYS	2.2
1	C	7	GLY	2.2
1	E	235	GLY	2.2
1	A	59	THR	2.2
1	A	187	ALA	2.2
1	B	171	THR	2.2
1	D	114	ALA	2.2
1	E	187	ALA	2.2
1	B	153	LEU	2.1
1	A	117	VAL	2.1
1	B	57	LYS	2.1
1	B	161	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	182	PHE	2.1
1	C	246	GLU	2.1
1	E	234	PRO	2.1
1	C	240	HIS	2.1
1	D	154	SER	2.1
1	C	167	ILE	2.1
1	C	242	LEU	2.1
1	E	123	ASN	2.1
1	B	126	VAL	2.1
1	D	244	VAL	2.1
1	A	159	CYS	2.1
1	A	53	THR	2.1
1	A	137	THR	2.1
1	C	215	LYS	2.1
1	A	91	ILE	2.1
1	C	210	LEU	2.1
1	D	18	GLY	2.1
1	A	1	MET	2.1
1	E	267	GLU	2.1
1	A	62	HIS	2.1
1	A	151	GLN	2.1
1	A	152	LEU	2.1
1	C	166	LEU	2.1
1	C	226	GLN	2.1
1	A	192	GLY	2.1
1	B	119	ARG	2.1
1	A	215	LYS	2.0
1	C	154	SER	2.0
1	B	58	GLU	2.0
1	C	184	ALA	2.0
1	E	130	GLU	2.0
1	B	240	HIS	2.0
1	E	142	GLN	2.0
1	A	79	LEU	2.0
1	A	185	LEU	2.0
1	B	56	ASN	2.0
1	B	186	ASP	2.0
1	C	227	LEU	2.0
1	E	147	ARG	2.0
1	E	4	GLY	2.0
1	A	20	THR	2.0
1	A	160	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	63	SER	2.0
1	C	43	SER	2.0
1	E	246	GLU	2.0
1	B	10	GLN	2.0
1	D	80	ASP	2.0
1	E	253	LEU	2.0
1	A	198	PRO	2.0
1	C	204	ARG	2.0
1	E	228	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

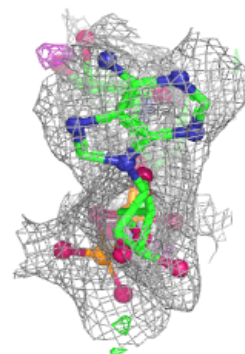
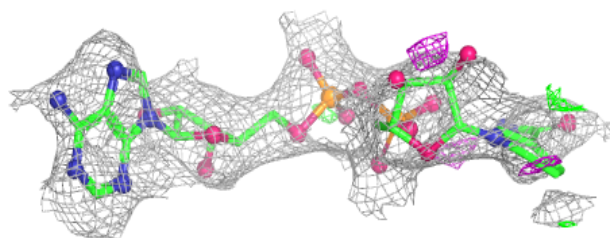
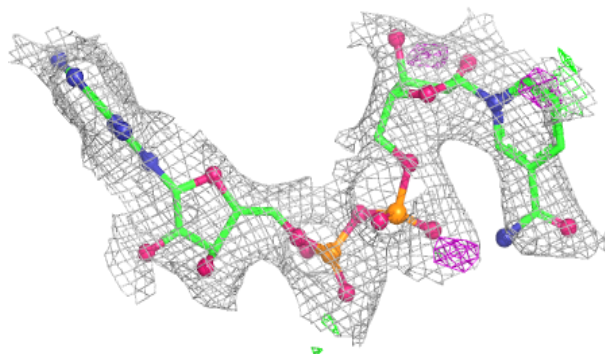
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GHO	A	402	7/7	0.73	0.21	39,44,47,50	7
2	NAI	D	401	44/44	0.74	0.20	45,54,61,61	0
3	GHO	C	402	7/7	0.74	0.25	46,48,49,53	7
3	GHO	B	402	7/7	0.76	0.24	40,45,49,52	7
3	GHO	D	402	7/7	0.78	0.22	40,46,48,49	7
2	NAI	B	401	44/44	0.80	0.17	44,50,54,56	0
3	GHO	E	402	7/7	0.80	0.21	42,45,49,50	7
2	NAI	C	401	44/44	0.82	0.18	50,56,62,63	0
2	NAI	E	401	44/44	0.83	0.15	43,50,55,60	0
2	NAI	A	401	44/44	0.84	0.16	43,50,54,56	0

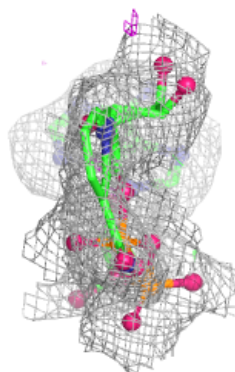
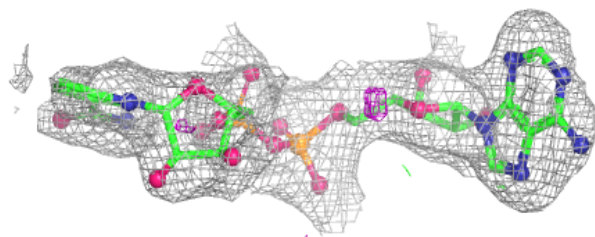
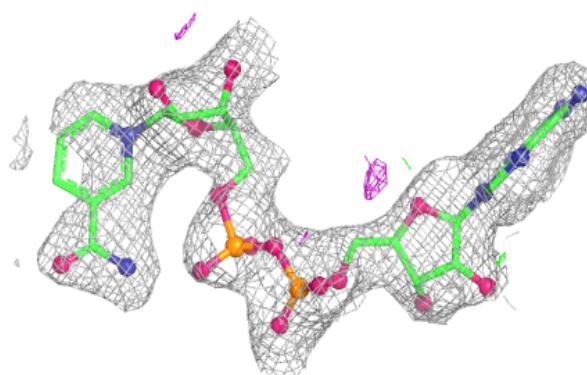
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAI D 401:

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

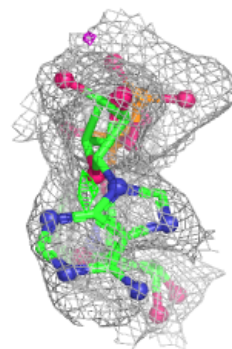
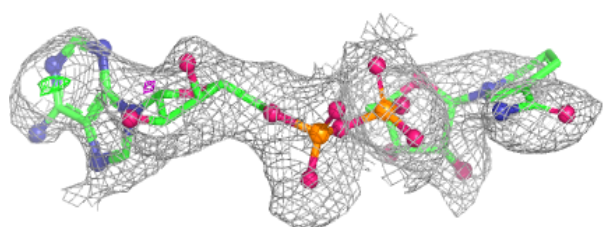
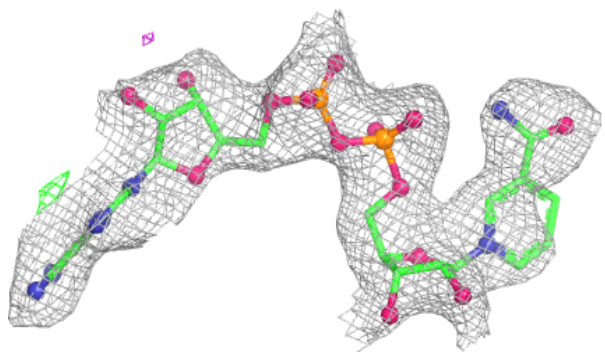
**Electron density around NAI B 401:**

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

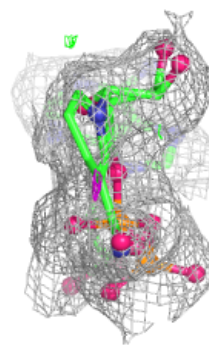
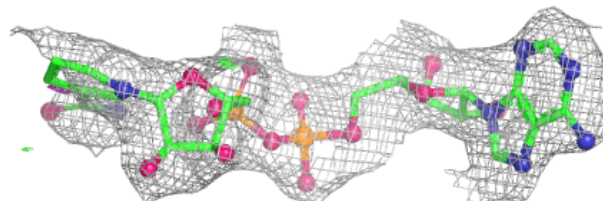
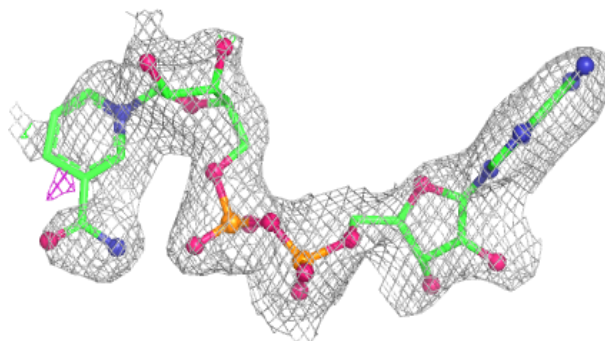


Electron density around NAI C 401:

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

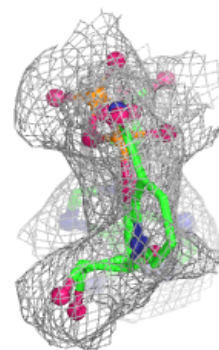
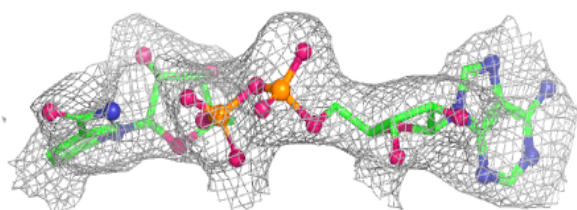
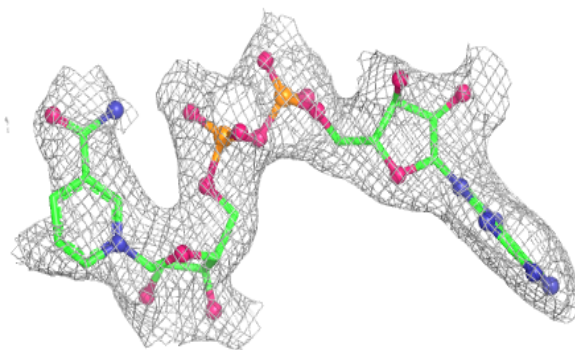
**Electron density around NAI E 401:**

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



Electron density around NAI A 401:

$2mF_o-DF_c$ (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.