



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:05 AM UTC

PDB ID : 3LUT / pdb_00003lut
Title : A Structural Model for the Full-length Shaker Potassium Channel Kv1.2
Authors : Chen, X.; Ni, F.; Wang, Q.; Ma, J.
Deposited on : 2010-02-18
Resolution : 2.90 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

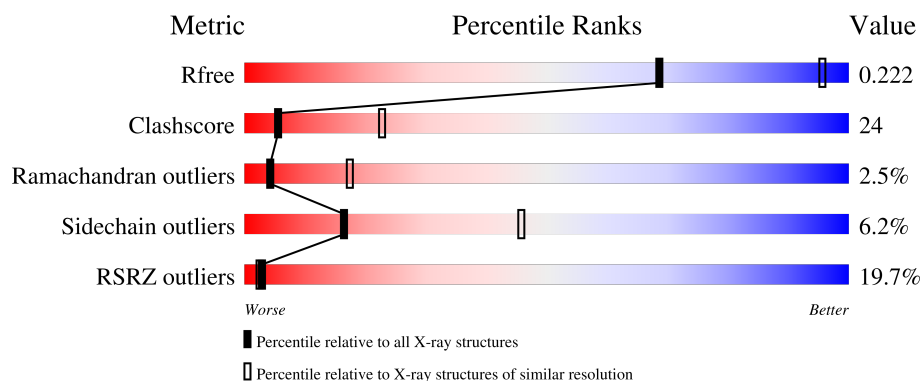
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	367	74% 13% 11%
2	B	499	27% 41% 29% 7% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	K	B	504	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5848 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 Voltage-gated potassium channel subunit beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2556	1627	443	470	16			

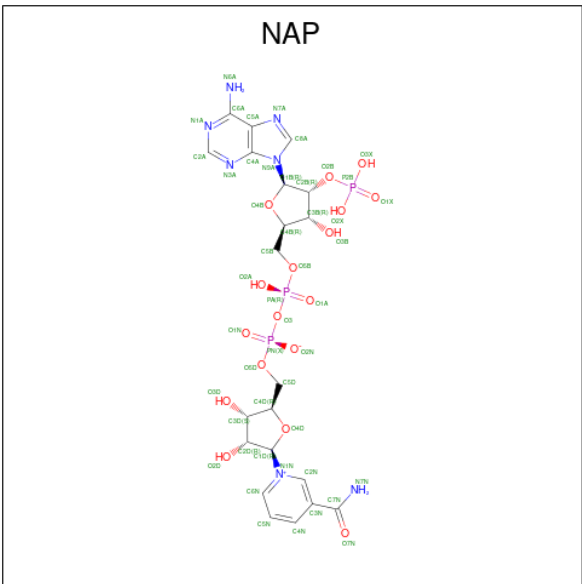
- Molecule 2 is a protein called Potassium voltage-gated channel subfamily A member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	390	Total	C	N	O	S	0	0	0
			3152	2060	509	568	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	207	GLN	ASN	engineered mutation	UNP P63142

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	6	Total	K	0	0
			6	6		

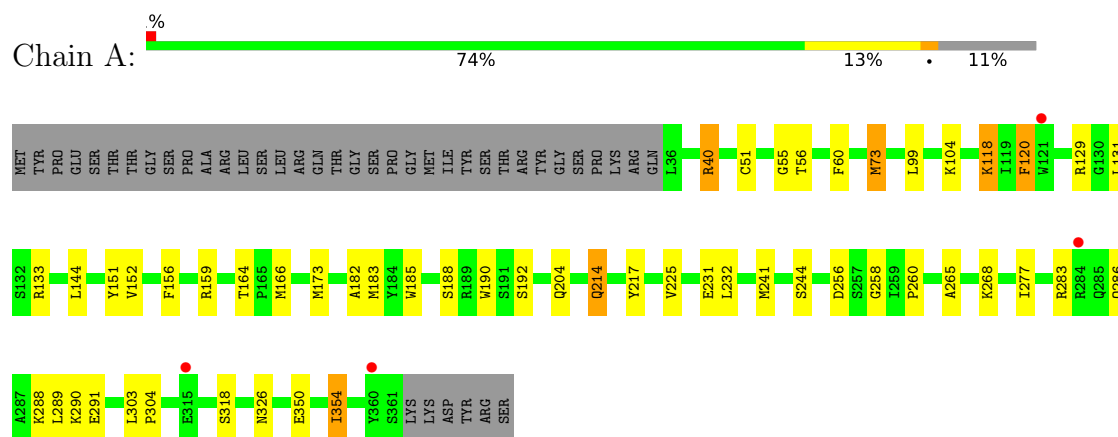
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	72	Total	O	0	0
			72	72		
5	B	14	Total	O	0	0
			14	14		

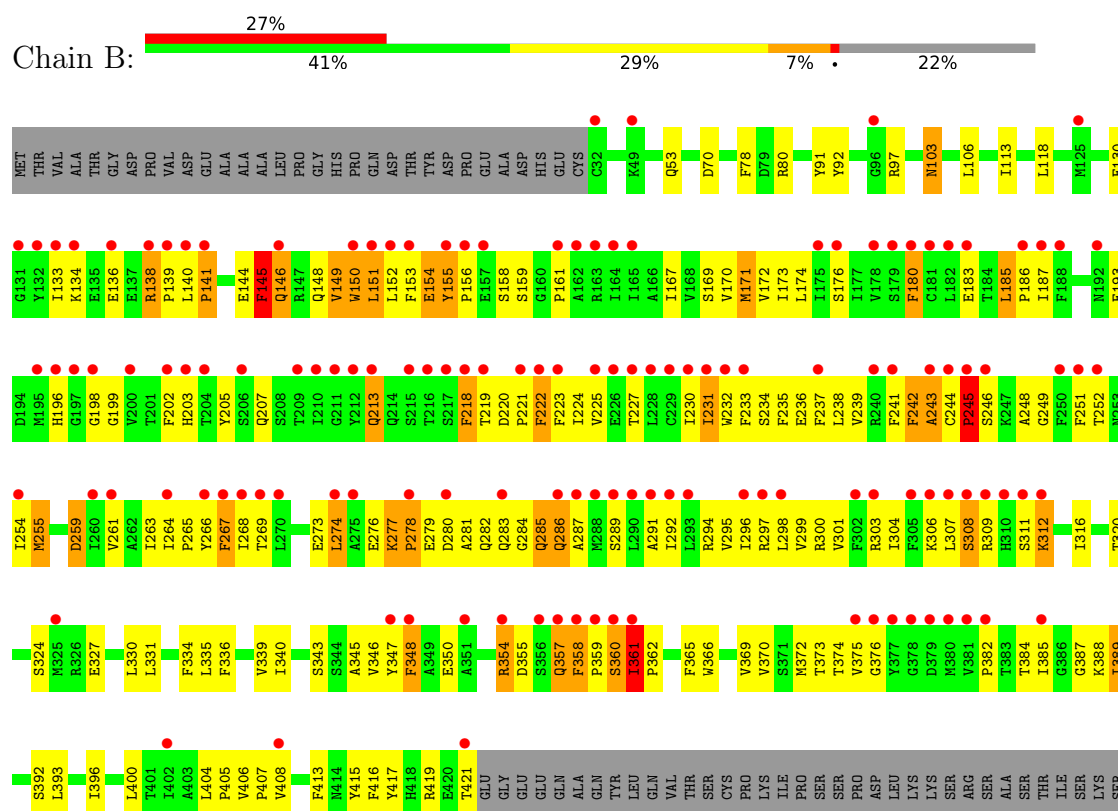
3 Residue-property plots

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: Voltage-gated potassium channel subunit beta-2



- Molecule 2: Potassium voltage-gated channel subfamily A member 2



ASP	TYR	MET	GLU	ILE	GLN	GLU	GLY	VAL	ASN	ASN	SER	ASN	GLU	ASP	PHE	ARG	GLU	GLU	ASN	LEU	LYS	THR	ALA	ASN	CYS	THR	LEU	ALA	ASN	THR	ASN	TYR	VAL	ASN	ILE	THR	LYS	MET	LEU	THR	ASP	VAL
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4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	113.61Å 113.61Å 260.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 – 2.90 29.48 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.48-2.90) 91.5 (29.48-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.221 0.209 , 0.222	Depositor DCC
R_{free} test set	1952 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 92.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5848	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: NAP, K

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	0.47	0/2608	0.80	0/3524
2	B	0.62	3/3234 (0.1%)	1.03	17/4385 (0.4%)
All	All	0.56	3/5842 (0.1%)	0.93	17/7909 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	245	PRO	N-CD	8.49	1.59	1.47
2	B	243	ALA	CA-C	5.74	1.55	1.52
2	B	171	MET	SD-CE	5.56	1.93	1.79

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	138	ARG	N-CA-C	-6.75	101.28	109.72
2	B	138	ARG	CA-C-N	6.57	126.81	119.32
2	B	138	ARG	C-N-CA	6.57	126.81	119.32
2	B	145	PHE	CB-CA-C	-6.38	107.46	115.89
2	B	361	ILE	N-CA-C	6.25	122.39	108.88
2	B	145	PHE	N-CA-C	6.14	119.34	109.02
2	B	136	GLU	N-CA-C	-5.95	103.15	110.65
2	B	146	GLN	N-CA-C	5.75	118.40	110.35
2	B	358	PHE	CA-C-N	5.64	126.89	119.84
2	B	358	PHE	C-N-CA	5.64	126.89	119.84
2	B	354	ARG	N-CA-C	5.49	117.95	110.55
2	B	145	PHE	CA-C-N	5.42	129.38	121.31
2	B	145	PHE	C-N-CA	5.42	129.38	121.31
2	B	308	SER	N-CA-C	5.28	119.20	112.87
2	B	218	PHE	N-CA-C	5.22	117.67	108.75
2	B	285	GLN	N-CA-C	-5.15	106.69	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	289	SER	N-CA-C	-5.02	105.63	112.26

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	2556	0	2582	32	0
2	B	3152	0	3116	239	1
3	A	48	0	25	2	0
4	B	6	0	0	0	0
5	A	72	0	0	2	0
5	B	14	0	0	0	0
All	All	5848	0	5723	271	1

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 24.

All (271) 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)
2:B:199:GLY:O	2:B:205:TYR:HB2	1.52	1.10
2:B:277:LYS:HB2	2:B:278:PRO:HD3	1.31	1.06
2:B:145:PHE:CZ	2:B:155:TYR:HE1	1.75	1.05
2:B:185:LEU:HB2	2:B:186:PRO:CD	1.89	1.01
2:B:278:PRO:HG2	2:B:281:ALA:HB3	1.42	1.00
2:B:185:LEU:HB2	2:B:186:PRO:HD3	1.03	0.99
2:B:266:TYR:CE2	2:B:300:ARG:HG2	2.01	0.96
1:A:129:ARG:HD3	5:A:438:HOH:O	1.66	0.94
2:B:153:PHE:C	2:B:156:PRO:HD2	1.94	0.92
1:A:40:ARG:HD2	1:A:318:SER:O	1.70	0.91
2:B:415:TYR:OH	2:B:419:ARG:NH2	2.04	0.91
2:B:219:THR:HB	2:B:222:PHE:CE2	2.06	0.91
2:B:221:PRO:HA	2:B:224:ILE:HD12	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:PRO:HB2	2:B:299:VAL:HG11	1.51	0.90
2:B:199:GLY:O	2:B:205:TYR:CB	2.18	0.90
2:B:185:LEU:CB	2:B:186:PRO:HD3	1.97	0.90
2:B:277:LYS:HB2	2:B:278:PRO:CD	2.00	0.90
2:B:198:GLY:HA2	2:B:205:TYR:CE1	2.06	0.90
2:B:277:LYS:CB	2:B:278:PRO:HD3	2.03	0.89
2:B:286:GLN:HG3	2:B:287:ALA:H	1.39	0.87
2:B:140:LEU:H	2:B:141:PRO:HD2	1.39	0.86
2:B:266:TYR:HE2	2:B:300:ARG:HG2	1.36	0.86
2:B:278:PRO:HG2	2:B:281:ALA:CB	2.05	0.86
2:B:138:ARG:HB3	2:B:141:PRO:CG	2.07	0.84
2:B:155:TYR:HA	2:B:158:SER:HB2	1.60	0.83
2:B:259:ASP:OD2	2:B:309:ARG:NH2	2.10	0.83
2:B:265:PRO:CB	2:B:299:VAL:HG11	2.09	0.83
2:B:219:THR:HB	2:B:222:PHE:CD2	2.14	0.83
2:B:146:GLN:HG2	2:B:151:LEU:HB3	1.61	0.82
2:B:140:LEU:N	2:B:141:PRO:HD2	1.93	0.82
2:B:278:PRO:CG	2:B:281:ALA:HB3	2.10	0.81
1:A:118:LYS:HG3	1:A:156:PHE:HB2	1.63	0.80
2:B:234:SER:O	2:B:238:LEU:HB2	1.81	0.80
2:B:145:PHE:CZ	2:B:155:TYR:CE1	2.67	0.79
2:B:277:LYS:HE2	2:B:291:ALA:HB2	1.65	0.79
2:B:292:ILE:HG23	2:B:296:ILE:HG21	1.63	0.78
2:B:263:ILE:HG13	2:B:264:ILE:N	1.99	0.78
2:B:372:MET:C	2:B:374:THR:H	1.87	0.77
2:B:220:ASP:O	2:B:224:ILE:HG13	1.85	0.77
2:B:320:THR:HG22	2:B:416:PHE:HD1	1.49	0.77
2:B:144:GLU:HA	2:B:144:GLU:OE1	1.85	0.76
2:B:153:PHE:HA	2:B:156:PRO:HG2	1.67	0.76
2:B:266:TYR:O	2:B:269:THR:HG22	1.86	0.75
2:B:308:SER:HA	2:B:311:SER:HB3	1.67	0.75
2:B:372:MET:C	2:B:374:THR:N	2.44	0.75
2:B:292:ILE:O	2:B:296:ILE:HG12	1.87	0.74
2:B:146:GLN:HE21	2:B:151:LEU:HD13	1.52	0.74
2:B:146:GLN:HG2	2:B:151:LEU:CB	2.18	0.74
2:B:138:ARG:HB3	2:B:141:PRO:HG3	1.69	0.73
2:B:286:GLN:HG3	2:B:287:ALA:N	2.02	0.73
2:B:404:LEU:HB2	2:B:405:PRO:HD3	1.68	0.73
2:B:241:PHE:C	2:B:243:ALA:H	1.97	0.72
2:B:138:ARG:HB3	2:B:141:PRO:HG2	1.70	0.72
2:B:266:TYR:HE2	2:B:300:ARG:CG	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:370:VAL:HG12	2:B:376:GLY:H	1.55	0.72
2:B:331:LEU:HB2	2:B:405:PRO:HG2	1.72	0.71
1:A:133:ARG:HD2	5:A:372:HOH:O	1.89	0.71
2:B:156:PRO:HA	2:B:161:PRO:HG2	1.73	0.71
2:B:330:LEU:HG	2:B:334:PHE:HE1	1.55	0.69
2:B:366:TRP:O	2:B:370:VAL:HG23	1.91	0.69
1:A:291:GLU:HB2	1:A:354:ILE:HD13	1.73	0.69
2:B:297:ARG:O	2:B:301:VAL:HG23	1.93	0.69
2:B:202:PHE:CE2	2:B:203:HIS:HD2	2.11	0.68
2:B:330:LEU:HG	2:B:334:PHE:CE1	2.28	0.68
2:B:265:PRO:HG2	2:B:299:VAL:CG1	2.24	0.68
2:B:219:THR:HB	2:B:222:PHE:HE2	1.57	0.68
2:B:223:PHE:CZ	2:B:227:THR:HG21	2.30	0.67
2:B:286:GLN:CG	2:B:287:ALA:N	2.58	0.66
2:B:213:GLN:O	2:B:213:GLN:HG2	1.95	0.66
2:B:170:VAL:O	2:B:174:LEU:HG	1.94	0.66
2:B:372:MET:O	2:B:374:THR:HG23	1.94	0.66
2:B:148:GLN:HB3	2:B:151:LEU:HB2	1.77	0.65
2:B:149:VAL:C	2:B:150:TRP:HE3	2.05	0.65
2:B:346:VAL:O	2:B:350:GLU:HG2	1.96	0.65
1:A:40:ARG:HE	1:A:51:CYS:HB3	1.62	0.65
2:B:149:VAL:HG23	2:B:150:TRP:CE3	2.32	0.65
2:B:274:LEU:O	2:B:274:LEU:HG	1.96	0.64
2:B:320:THR:HG22	2:B:416:PHE:CD1	2.32	0.64
2:B:205:TYR:O	2:B:205:TYR:CD1	2.51	0.64
2:B:169:SER:O	2:B:172:VAL:HG22	1.98	0.64
2:B:276:GLU:HB3	2:B:282:GLN:OE1	1.98	0.64
2:B:361:ILE:HD13	2:B:361:ILE:H	1.62	0.63
2:B:279:GLU:HG3	2:B:280:ASP:H	1.63	0.63
2:B:304:ILE:O	2:B:307:LEU:HG	1.98	0.63
2:B:278:PRO:CD	2:B:281:ALA:HB3	2.29	0.62
1:A:166:MET:HE1	1:A:190:TRP:HH2	1.65	0.62
2:B:284:GLY:C	2:B:286:GLN:H	2.06	0.62
2:B:264:ILE:O	2:B:268:ILE:HG13	1.99	0.62
2:B:279:GLU:HG3	2:B:280:ASP:N	2.15	0.61
2:B:266:TYR:CZ	2:B:300:ARG:HG2	2.35	0.61
2:B:370:VAL:HG12	2:B:376:GLY:N	2.15	0.61
2:B:202:PHE:CE2	2:B:203:HIS:CD2	2.88	0.61
2:B:284:GLY:C	2:B:286:GLN:N	2.58	0.60
2:B:146:GLN:NE2	2:B:151:LEU:HD13	2.17	0.59
2:B:336:PHE:O	2:B:340:ILE:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:PHE:CE2	2:B:155:TYR:HE1	2.19	0.59
2:B:140:LEU:N	2:B:141:PRO:CD	2.66	0.59
2:B:155:TYR:CD2	2:B:158:SER:HB2	2.37	0.59
2:B:198:GLY:CA	2:B:205:TYR:CE1	2.85	0.58
2:B:389:ILE:HG12	2:B:393:LEU:HD23	1.84	0.58
2:B:106:LEU:HD11	2:B:130:GLU:HG2	1.86	0.58
2:B:223:PHE:O	2:B:227:THR:HG23	2.04	0.58
2:B:221:PRO:O	2:B:224:ILE:HB	2.04	0.58
2:B:267:PHE:HD2	2:B:267:PHE:C	2.12	0.58
2:B:180:PHE:CD1	2:B:180:PHE:C	2.81	0.57
2:B:155:TYR:CE2	2:B:159:SER:HB3	2.40	0.57
2:B:113:ILE:HG23	2:B:118:LEU:HD12	1.87	0.57
2:B:171:MET:CE	2:B:174:LEU:HD12	2.34	0.57
1:A:166:MET:HE1	1:A:190:TRP:CH2	2.40	0.57
2:B:296:ILE:O	2:B:300:ARG:HG3	2.03	0.56
2:B:384:THR:O	2:B:388:LYS:HE2	2.06	0.56
2:B:278:PRO:HD2	2:B:281:ALA:HB3	1.86	0.56
2:B:276:GLU:HB3	2:B:282:GLN:CD	2.31	0.56
2:B:78:PHE:HB3	2:B:80:ARG:HG3	1.86	0.56
2:B:155:TYR:HD2	2:B:158:SER:HB2	1.70	0.56
2:B:267:PHE:C	2:B:267:PHE:CD2	2.84	0.56
2:B:357:GLN:O	2:B:357:GLN:HG3	2.05	0.55
2:B:198:GLY:HA2	2:B:205:TYR:CD1	2.41	0.55
2:B:350:GLU:OE2	2:B:387:GLY:HA3	2.05	0.55
2:B:167:ILE:O	2:B:171:MET:HG2	2.06	0.54
2:B:276:GLU:HA	2:B:276:GLU:OE1	2.07	0.54
2:B:254:ILE:HG13	2:B:255:MET:HE3	1.89	0.54
2:B:171:MET:HE1	2:B:174:LEU:HD12	1.89	0.54
2:B:286:GLN:HE21	2:B:287:ALA:HB2	1.73	0.54
2:B:155:TYR:HE2	2:B:159:SER:HB3	1.72	0.53
2:B:232:TRP:CE3	2:B:232:TRP:HA	2.43	0.53
2:B:265:PRO:CG	2:B:299:VAL:HG11	2.39	0.53
2:B:263:ILE:HG13	2:B:264:ILE:H	1.72	0.53
2:B:343:SER:O	2:B:346:VAL:HG12	2.09	0.53
2:B:279:GLU:CG	2:B:280:ASP:H	2.21	0.52
2:B:316:ILE:O	2:B:320:THR:HG23	2.10	0.52
2:B:286:GLN:NE2	2:B:287:ALA:HB2	2.24	0.52
2:B:372:MET:O	2:B:374:THR:N	2.43	0.52
2:B:148:GLN:O	2:B:151:LEU:N	2.42	0.52
2:B:392:SER:O	2:B:396:ILE:HG12	2.10	0.52
2:B:176:SER:HB3	2:B:303:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:PHE:HA	2:B:183:GLU:CG	2.40	0.52
2:B:265:PRO:HG2	2:B:299:VAL:HG13	1.92	0.52
2:B:292:ILE:HG23	2:B:296:ILE:CG2	2.39	0.51
2:B:145:PHE:HD2	2:B:146:GLN:H	1.58	0.51
2:B:232:TRP:CZ3	2:B:235:PHE:CD2	2.98	0.51
2:B:327:GLU:HG2	2:B:408:VAL:HG11	1.92	0.51
2:B:400:LEU:O	2:B:404:LEU:HG	2.10	0.51
2:B:233:PHE:O	2:B:237:PHE:HB3	2.11	0.51
2:B:345:ALA:HA	2:B:348:PHE:HD2	1.74	0.51
2:B:180:PHE:O	2:B:183:GLU:HG3	2.11	0.51
2:B:265:PRO:CG	2:B:299:VAL:HG21	2.41	0.51
2:B:359:PRO:O	2:B:360:SER:C	2.53	0.51
1:A:56:THR:HB	1:A:60:PHE:HB2	1.93	0.51
2:B:346:VAL:HG22	2:B:350:GLU:HG3	1.93	0.50
1:A:214:GLN:HA	1:A:241:MET:O	2.12	0.50
1:A:288:LYS:HG2	1:A:354:ILE:HD12	1.94	0.50
2:B:339:VAL:HG21	2:B:369:VAL:HG22	1.94	0.50
2:B:417:TYR:CD1	2:B:417:TYR:C	2.90	0.50
2:B:148:GLN:C	2:B:150:TRP:N	2.69	0.49
2:B:171:MET:HE2	2:B:171:MET:HA	1.94	0.49
2:B:241:PHE:C	2:B:243:ALA:N	2.66	0.49
2:B:220:ASP:HB2	2:B:221:PRO:HD3	1.94	0.49
2:B:155:TYR:N	2:B:156:PRO:CD	2.75	0.49
1:A:256:ASP:OD2	1:A:290:LYS:HD3	2.11	0.49
2:B:185:LEU:CB	2:B:186:PRO:CD	2.71	0.49
2:B:279:GLU:CG	2:B:280:ASP:N	2.75	0.49
2:B:180:PHE:HA	2:B:183:GLU:HG3	1.94	0.49
1:A:217:TYR:HB2	1:A:225:VAL:HG21	1.94	0.48
2:B:154:GLU:OE2	2:B:239:VAL:CG1	2.60	0.48
2:B:265:PRO:HG2	2:B:299:VAL:CG2	2.42	0.48
2:B:219:THR:HB	2:B:222:PHE:HD2	1.75	0.48
2:B:264:ILE:HG13	2:B:265:PRO:HD3	1.96	0.48
2:B:266:TYR:OH	2:B:300:ARG:HG2	2.12	0.48
2:B:264:ILE:N	2:B:265:PRO:CD	2.76	0.48
2:B:145:PHE:CD2	2:B:146:GLN:N	2.81	0.48
2:B:357:GLN:O	2:B:357:GLN:CG	2.61	0.48
2:B:264:ILE:CG1	2:B:265:PRO:HD3	2.44	0.48
2:B:360:SER:C	2:B:362:PRO:HD2	2.38	0.47
2:B:406:VAL:HB	2:B:407:PRO:HD3	1.96	0.47
2:B:358:PHE:N	2:B:358:PHE:CD1	2.82	0.47
2:B:230:ILE:HA	2:B:233:PHE:HD2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:PHE:CD1	2:B:237:PHE:C	2.91	0.47
2:B:145:PHE:HD2	2:B:146:GLN:N	2.12	0.47
2:B:282:GLN:O	2:B:283:GLN:C	2.58	0.47
2:B:385:ILE:O	2:B:388:LYS:HG2	2.15	0.47
2:B:267:PHE:HD2	2:B:267:PHE:O	1.97	0.47
2:B:103:ASN:H	2:B:103:ASN:HD22	1.63	0.47
2:B:148:GLN:C	2:B:150:TRP:H	2.23	0.47
1:A:244:SER:OG	3:A:368:NAP:O2N	2.25	0.46
2:B:180:PHE:HB2	2:B:300:ARG:NH2	2.30	0.46
2:B:296:ILE:HG13	2:B:297:ARG:N	2.29	0.46
2:B:350:GLU:OE2	2:B:387:GLY:CA	2.62	0.46
2:B:372:MET:O	2:B:374:THR:CG2	2.63	0.46
2:B:222:PHE:HA	2:B:225:VAL:HG23	1.98	0.46
2:B:295:VAL:HG13	2:B:299:VAL:CG2	2.45	0.46
2:B:320:THR:CG2	2:B:416:PHE:HD1	2.24	0.46
2:B:134:LYS:O	2:B:134:LYS:HG3	2.15	0.46
2:B:265:PRO:HB3	2:B:299:VAL:HG21	1.98	0.46
2:B:236:GLU:HA	2:B:236:GLU:OE1	2.15	0.46
2:B:320:THR:O	2:B:324:SER:N	2.49	0.46
2:B:237:PHE:CD1	2:B:237:PHE:O	2.69	0.46
1:A:159:ARG:HA	1:A:188:SER:O	2.16	0.45
2:B:241:PHE:O	2:B:243:ALA:N	2.50	0.45
2:B:148:GLN:CB	2:B:151:LEU:HD12	2.47	0.45
2:B:106:LEU:CD1	2:B:130:GLU:HG2	2.46	0.45
2:B:294:ARG:O	2:B:298:LEU:HG	2.17	0.45
1:A:258:GLY:O	1:A:260:PRO:HD3	2.17	0.45
2:B:348:PHE:CD1	2:B:348:PHE:C	2.95	0.45
2:B:173:ILE:HG21	2:B:307:LEU:CD2	2.47	0.45
2:B:173:ILE:HG21	2:B:307:LEU:HD21	1.98	0.45
2:B:230:ILE:HG13	2:B:231:ILE:N	2.32	0.45
2:B:419:ARG:C	2:B:421:THR:H	2.24	0.45
2:B:145:PHE:CE2	2:B:155:TYR:CE1	3.01	0.45
2:B:242:PHE:CD1	2:B:242:PHE:N	2.85	0.44
2:B:148:GLN:HG2	2:B:151:LEU:HD12	1.98	0.44
2:B:350:GLU:OE1	2:B:350:GLU:HA	2.18	0.44
2:B:343:SER:OG	2:B:365:PHE:HD2	2.01	0.44
2:B:265:PRO:CG	2:B:299:VAL:CG1	2.94	0.44
2:B:297:ARG:HD2	2:B:297:ARG:HA	1.78	0.44
1:A:256:ASP:HA	1:A:286:GLN:HG2	1.99	0.44
2:B:145:PHE:CE1	2:B:155:TYR:HE1	2.30	0.44
2:B:148:GLN:O	2:B:150:TRP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:ILE:O	2:B:296:ILE:HG23	2.18	0.44
2:B:139:PRO:HB2	2:B:140:LEU:HD23	2.00	0.44
2:B:295:VAL:HG13	2:B:299:VAL:HG21	2.00	0.44
2:B:370:VAL:HG13	2:B:375:VAL:HB	2.00	0.44
1:A:350:GLU:O	1:A:354:ILE:HG23	2.18	0.43
2:B:207:GLN:O	2:B:207:GLN:HG3	2.18	0.43
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.85	0.43
2:B:278:PRO:O	2:B:282:GLN:N	2.34	0.43
1:A:192:SER:HA	1:A:232:LEU:HD11	2.01	0.43
2:B:154:GLU:N	2:B:156:PRO:HD2	2.32	0.43
2:B:316:ILE:HG21	2:B:417:TYR:HB2	2.00	0.43
2:B:171:MET:HE2	2:B:174:LEU:HD12	2.01	0.43
1:A:73:MET:SD	1:A:99:LEU:HD12	2.59	0.43
2:B:223:PHE:CE1	2:B:227:THR:CG2	3.02	0.43
1:A:55:GLY:HA3	3:A:368:NAP:O3D	2.19	0.42
1:A:289:LEU:HD22	1:A:303:LEU:HD21	2.00	0.42
2:B:70:ASP:OD1	2:B:70:ASP:C	2.62	0.42
2:B:259:ASP:OD2	2:B:306:LYS:NZ	2.49	0.42
2:B:259:ASP:CG	2:B:309:ARG:NH2	2.77	0.42
2:B:91:TYR:HA	2:B:97:ARG:O	2.19	0.42
2:B:242:PHE:N	2:B:242:PHE:HD1	2.17	0.42
2:B:296:ILE:HG13	2:B:297:ARG:HD3	2.00	0.42
1:A:131:LEU:O	1:A:164:THR:HG21	2.20	0.42
2:B:264:ILE:HG13	2:B:265:PRO:CD	2.50	0.42
2:B:336:PHE:CE1	2:B:340:ILE:HD11	2.55	0.42
2:B:354:ARG:HG2	2:B:355:ASP:N	2.35	0.42
1:A:151:TYR:CE1	1:A:183:MET:HE2	2.54	0.42
2:B:264:ILE:O	2:B:268:ILE:CG1	2.67	0.42
2:B:265:PRO:CB	2:B:299:VAL:HG21	2.50	0.42
2:B:419:ARG:C	2:B:421:THR:N	2.78	0.42
2:B:146:GLN:HG2	2:B:151:LEU:HB2	2.00	0.42
1:A:144:LEU:HD21	1:A:152:VAL:HG13	2.02	0.41
2:B:316:ILE:HG22	2:B:413:PHE:CD1	2.55	0.41
2:B:198:GLY:HA2	2:B:205:TYR:HE1	1.73	0.41
1:A:265:ALA:HB2	1:A:277:ILE:HD12	2.01	0.41
2:B:138:ARG:O	2:B:141:PRO:HG2	2.20	0.41
2:B:312:LYS:H	2:B:312:LYS:HG2	1.58	0.41
2:B:261:VAL:O	2:B:261:VAL:CG1	2.69	0.41
1:A:120:PHE:O	1:A:129:ARG:HA	2.21	0.41
2:B:265:PRO:CG	2:B:299:VAL:CG2	2.97	0.41
1:A:152:VAL:O	1:A:182:ALA:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LEU:HB3	1:A:304:PRO:HD3	2.02	0.41
2:B:53:GLN:NE2	2:B:92:TYR:O	2.53	0.41
2:B:155:TYR:N	2:B:156:PRO:HD2	2.35	0.41
1:A:173:MET:HG3	1:A:185:TRP:CE3	2.56	0.40
2:B:154:GLU:O	2:B:158:SER:N	2.53	0.40
2:B:172:VAL:O	2:B:176:SER:CB	2.69	0.40
2:B:176:SER:HB3	2:B:303:ARG:CZ	2.51	0.40
2:B:244:CYS:HA	2:B:245:PRO:HD3	1.92	0.40
2:B:276:GLU:OE1	2:B:282:GLN:HG3	2.21	0.40
1:A:166:MET:HA	1:A:166:MET:HE3	2.04	0.40
2:B:139:PRO:C	2:B:140:LEU:HD23	2.46	0.40
2:B:278:PRO:HG2	2:B:281:ALA:HB2	1.97	0.40

All (1) 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)
2:B:297:ARG:NH2	2:B:347:TYR:OH[3_755]	2.18	0.02

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	324/367 (88%)	316 (98%)	7 (2%)	1 (0%)	36	65
2	B	388/499 (78%)	325 (84%)	46 (12%)	17 (4%)	2	8
All	All	712/866 (82%)	641 (90%)	53 (7%)	18 (2%)	4	17

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	193	GLU

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Mol	Chain	Res	Type
2	B	252	THR
2	B	286	GLN
1	A	120	PHE
2	B	242	PHE
2	B	245	PRO
2	B	248	ALA
2	B	373	THR
2	B	278	PRO
2	B	360	SER
2	B	141	PRO
2	B	149	VAL
2	B	249	GLY
2	B	357	GLN
2	B	274	LEU
2	B	277	LYS
2	B	185	LEU
2	B	382	PRO

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	273/309 (88%)	262 (96%)	11 (4%)	28	62
2	B	342/441 (78%)	315 (92%)	27 (8%)	11	34
All	All	615/750 (82%)	577 (94%)	38 (6%)	16	46

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	73	MET
1	A	104	LYS
1	A	118	LYS
1	A	204	GLN
1	A	214	GLN

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Mol	Chain	Res	Type
1	A	231	GLU
1	A	268	LYS
1	A	283	ARG
1	A	326	ASN
1	A	354	ILE
2	B	103	ASN
2	B	133	ILE
2	B	145	PHE
2	B	150	TRP
2	B	151	LEU
2	B	152	LEU
2	B	154	GLU
2	B	155	TYR
2	B	180	PHE
2	B	187	ILE
2	B	196	HIS
2	B	213	GLN
2	B	218	PHE
2	B	222	PHE
2	B	231	ILE
2	B	246	SER
2	B	251	PHE
2	B	255	MET
2	B	259	ASP
2	B	267	PHE
2	B	273	GLU
2	B	285	GLN
2	B	312	LYS
2	B	335	LEU
2	B	348	PHE
2	B	361	ILE
2	B	389	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	71	HIS
1	A	163	ASN
1	A	333	ASN
1	A	338	GLN
2	B	103	ASN

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Mol	Chain	Res	Type
2	B	146	GLN
2	B	203	HIS
2	B	286	GLN
2	B	357	GLN
2	B	414	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAP	A	368	-	50,52,52	1.73	5 (10%)	71,80,80	1.73	13 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	A	368	-	-	5/35/67/67	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	368	NAP	O7N-C7N	9.42	1.41	1.24
3	A	368	NAP	C2A-N1A	2.74	1.38	1.33
3	A	368	NAP	C2A-N3A	2.66	1.38	1.33
3	A	368	NAP	C5A-N7A	-2.24	1.35	1.39
3	A	368	NAP	C8A-N7A	2.08	1.35	1.31

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	368	NAP	N3A-C2A-N1A	-5.48	120.29	128.58
3	A	368	NAP	C5A-C4A-N3A	-5.44	119.23	126.72
3	A	368	NAP	C2B-C1B-N9A	-5.40	104.86	113.75
3	A	368	NAP	C2A-N3A-C4A	3.72	120.91	111.83
3	A	368	NAP	P2B-O2B-C2B	3.66	133.21	123.43
3	A	368	NAP	N3A-C4A-N9A	3.31	132.81	127.17
3	A	368	NAP	C5A-N7A-C8A	3.04	108.22	103.45
3	A	368	NAP	O2B-C2B-C1B	2.80	119.91	110.05
3	A	368	NAP	N9A-C8A-N7A	-2.50	110.39	113.94
3	A	368	NAP	C4A-C5A-N7A	-2.35	107.89	110.58
3	A	368	NAP	C6A-C5A-C4A	2.31	120.33	117.18
3	A	368	NAP	O4B-C1B-N9A	2.24	112.39	108.09
3	A	368	NAP	C4D-O4D-C1D	2.18	111.92	109.92

There are no chirality outliers.

All (5) torsion outliers are listed below:

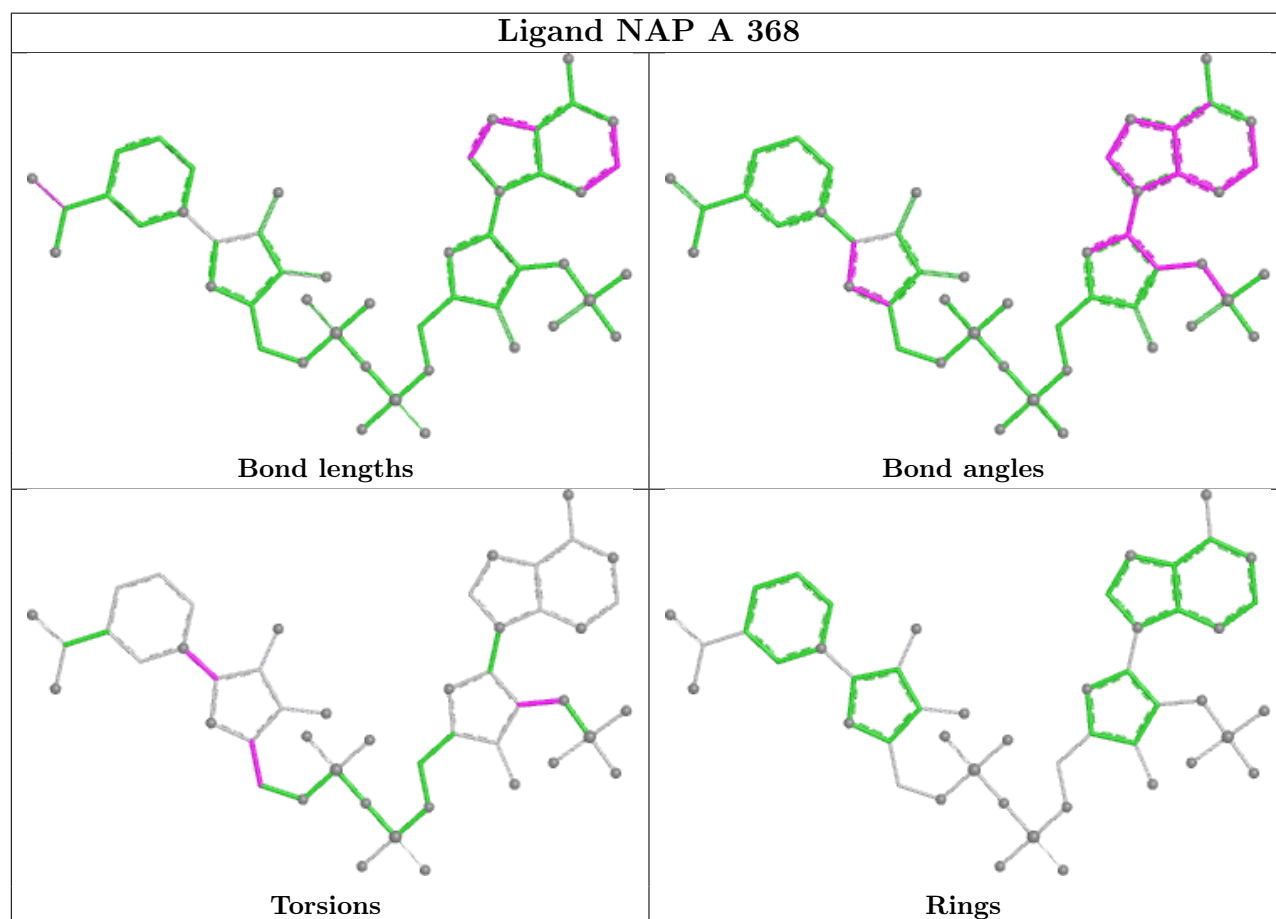
Mol	Chain	Res	Type	Atoms
3	A	368	NAP	C1B-C2B-O2B-P2B
3	A	368	NAP	O4D-C1D-N1N-C6N
3	A	368	NAP	O4D-C4D-C5D-O5D
3	A	368	NAP	C3D-C4D-C5D-O5D
3	A	368	NAP	O4D-C1D-N1N-C2N

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	368	NAP	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	326/367 (88%)	-0.04	4 (1%) 76 69	34, 56, 98, 117	0
2	B	390/499 (78%)	1.68	137 (35%) 1 1	49, 187, 273, 349	0
All	All	716/866 (82%)	0.89	141 (19%) 3 2	34, 89, 262, 349	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	245	PRO	8.9
2	B	182	LEU	7.8
2	B	381	VAL	7.5
2	B	179	SER	6.4
2	B	274	LEU	5.8
2	B	196	HIS	5.6
2	B	303	ARG	5.5
2	B	382	PRO	5.4
2	B	231	ILE	5.3
2	B	212	TYR	5.0
2	B	187	ILE	5.0
2	B	140	LEU	4.9
2	B	379	ASP	4.9
2	B	211	GLY	4.7
2	B	213	GLN	4.7
2	B	293	LEU	4.6
2	B	219	THR	4.6
2	B	186	PRO	4.5
2	B	267	PHE	4.5
2	B	252	THR	4.4
1	A	315	GLU	4.4
2	B	200	VAL	4.3
2	B	204	THR	4.2
2	B	348	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	180	PHE	4.1
2	B	188	PHE	4.1
2	B	162	ALA	4.0
2	B	152	LEU	4.0
2	B	153	PHE	4.0
2	B	292	ILE	3.9
2	B	246	SER	3.9
2	B	178	VAL	3.9
2	B	210	ILE	3.9
2	B	150	TRP	3.9
2	B	378	GLY	3.9
2	B	164	ILE	3.8
2	B	287	ALA	3.8
2	B	203	HIS	3.8
2	B	359	PRO	3.8
2	B	216	THR	3.8
2	B	32	CYS	3.8
2	B	221	PRO	3.7
2	B	175	ILE	3.7
2	B	250	PHE	3.7
2	B	308	SER	3.7
2	B	244	CYS	3.5
2	B	218	PHE	3.5
2	B	96	GLY	3.5
2	B	347	TYR	3.5
2	B	151	LEU	3.5
2	B	354	ARG	3.4
2	B	266	TYR	3.4
2	B	181	CYS	3.4
2	B	377	TYR	3.4
2	B	296	ILE	3.4
2	B	298	LEU	3.4
2	B	139	PRO	3.4
2	B	357	GLN	3.4
2	B	241	PHE	3.3
2	B	202	PHE	3.2
2	B	132	TYR	3.2
2	B	222	PHE	3.2
2	B	251	PHE	3.2
2	B	217	SER	3.2
2	B	254	ILE	3.2
2	B	283	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	356	SER	3.1
2	B	134	LYS	3.1
2	B	311	SER	3.1
2	B	228	LEU	3.1
2	B	288	MET	3.1
2	B	358	PHE	3.0
1	A	284	ARG	3.0
2	B	260	ILE	3.0
2	B	125	MET	3.0
2	B	161	PRO	3.0
2	B	310	HIS	3.0
2	B	275	ALA	2.9
2	B	361	ILE	2.9
2	B	131	GLY	2.9
2	B	305	PHE	2.9
2	B	312	LYS	2.9
2	B	380	MET	2.8
2	B	269	THR	2.8
2	B	229	CYS	2.8
2	B	289	SER	2.8
2	B	360	SER	2.8
2	B	183	GLU	2.7
2	B	197	GLY	2.7
2	B	291	ALA	2.7
2	B	307	LEU	2.7
2	B	375	VAL	2.7
2	B	243	ALA	2.7
2	B	264	ILE	2.6
2	B	351	ALA	2.6
2	B	192	ASN	2.6
2	B	225	VAL	2.6
2	B	290	LEU	2.6
2	B	402	ILE	2.6
2	B	237	PHE	2.6
2	B	325	MET	2.6
2	B	136	GLU	2.6
2	B	240	ARG	2.6
2	B	176	SER	2.5
2	B	230	ILE	2.5
2	B	223	PHE	2.5
2	B	302	PHE	2.5
2	B	421	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	198	GLY	2.4
2	B	227	THR	2.4
2	B	297	ARG	2.4
2	B	232	TRP	2.4
2	B	133	ILE	2.4
2	B	157	GLU	2.4
2	B	49	LYS	2.3
2	B	306	LYS	2.3
2	B	195	MET	2.3
2	B	270	LEU	2.3
2	B	206	SER	2.3
2	B	385	ILE	2.3
2	B	155	TYR	2.3
2	B	141	PRO	2.3
2	B	309	ARG	2.3
1	A	360	TYR	2.3
2	B	376	GLY	2.3
2	B	286	GLN	2.2
2	B	163	ARG	2.2
2	B	146	GLN	2.2
2	B	226	GLU	2.2
1	A	121	TRP	2.2
2	B	261	VAL	2.1
2	B	209	THR	2.1
2	B	278	PRO	2.1
2	B	280	ASP	2.1
2	B	268	ILE	2.1
2	B	156	PRO	2.1
2	B	138	ARG	2.1
2	B	215	SER	2.0
2	B	408	VAL	2.0
2	B	233	PHE	2.0
2	B	165	ILE	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](#)

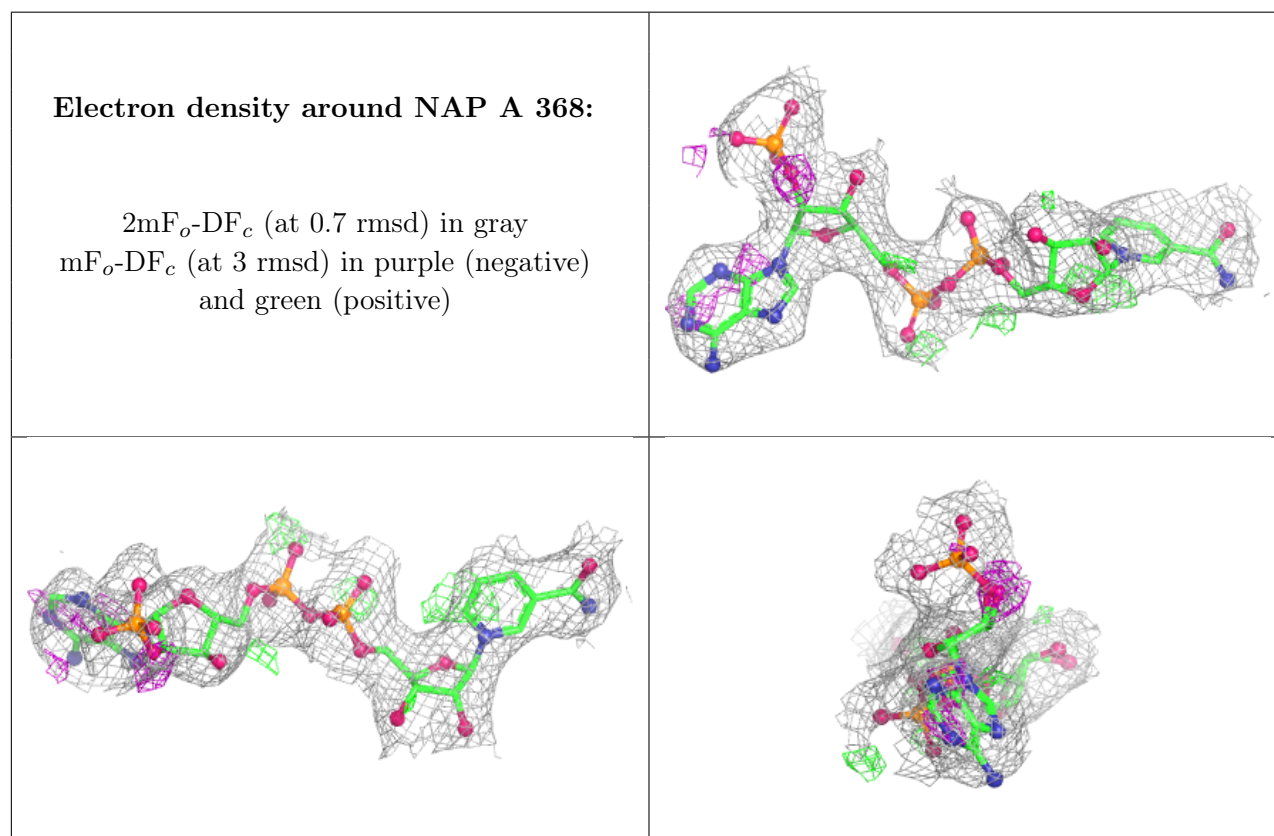
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	K	B	504	1/1	-0.09	0.42	258,258,258,258	1
4	K	B	500	1/1	0.84	0.15	173,173,173,173	1
4	K	B	505	1/1	0.85	0.24	165,165,165,165	1
4	K	B	503	1/1	0.87	0.23	226,226,226,226	1
4	K	B	501	1/1	0.90	0.16	192,192,192,192	1
4	K	B	502	1/1	0.93	0.14	209,209,209,209	1
3	NAP	A	368	48/48	0.96	0.08	37,42,50,51	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.