



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:42 AM UTC

PDB ID : 3OQ1 / pdb_00003oq1
Title : Crystal Structure of 11beta-Hydroxysteroid Dehydrogenase-1 (11b-HSD1) in Complex with Diarylsulfone Inhibitor
Authors : Wang, Z.; Sudom, A.; Walker, N.P.
Deposited on : 2010-09-02
Resolution : 2.60 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

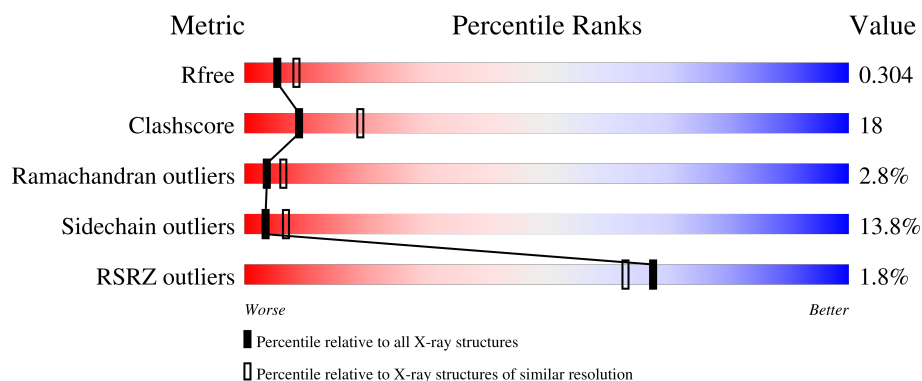
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	286	2% 47% 36% 7% 9%
1	B	286	% 54% 34% 6% 7%
1	C	286	2% 52% 34% 7% 6%
1	D	286	% 55% 32% • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8469 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2001	1277	339	370	15			
1	B	267	Total	C	N	O	S	0	1	0
			2057	1311	348	382	16			
1	C	269	Total	C	N	O	S	0	0	0
			2072	1321	351	384	16			
1	D	261	Total	C	N	O	S	0	1	0
			2008	1282	341	370	15			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	expression tag	UNP P28845
A	8	LYS	-	expression tag	UNP P28845
A	9	HIS	-	expression tag	UNP P28845
A	10	GLN	-	expression tag	UNP P28845
A	11	HIS	-	expression tag	UNP P28845
A	12	GLN	-	expression tag	UNP P28845
A	13	HIS	-	expression tag	UNP P28845
A	14	GLN	-	expression tag	UNP P28845
A	15	HIS	-	expression tag	UNP P28845
A	16	GLN	-	expression tag	UNP P28845
A	17	HIS	-	expression tag	UNP P28845
A	18	GLN	-	expression tag	UNP P28845
A	19	HIS	-	expression tag	UNP P28845
A	20	GLN	-	expression tag	UNP P28845
A	21	GLN	-	expression tag	UNP P28845
A	22	PRO	-	expression tag	UNP P28845
A	23	LEU	-	expression tag	UNP P28845
A	272	SER	CYS	engineered mutation	UNP P28845
B	7	MET	-	expression tag	UNP P28845
B	8	LYS	-	expression tag	UNP P28845
B	9	HIS	-	expression tag	UNP P28845

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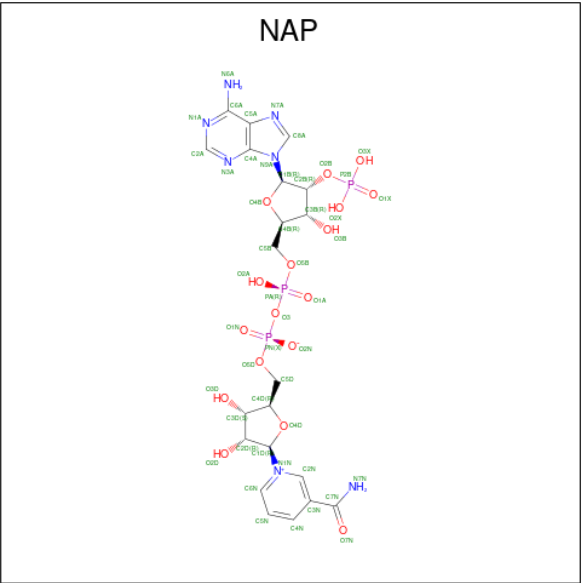
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	expression tag	UNP P28845
B	11	HIS	-	expression tag	UNP P28845
B	12	GLN	-	expression tag	UNP P28845
B	13	HIS	-	expression tag	UNP P28845
B	14	GLN	-	expression tag	UNP P28845
B	15	HIS	-	expression tag	UNP P28845
B	16	GLN	-	expression tag	UNP P28845
B	17	HIS	-	expression tag	UNP P28845
B	18	GLN	-	expression tag	UNP P28845
B	19	HIS	-	expression tag	UNP P28845
B	20	GLN	-	expression tag	UNP P28845
B	21	GLN	-	expression tag	UNP P28845
B	22	PRO	-	expression tag	UNP P28845
B	23	LEU	-	expression tag	UNP P28845
B	272	SER	CYS	engineered mutation	UNP P28845
C	7	MET	-	expression tag	UNP P28845
C	8	LYS	-	expression tag	UNP P28845
C	9	HIS	-	expression tag	UNP P28845
C	10	GLN	-	expression tag	UNP P28845
C	11	HIS	-	expression tag	UNP P28845
C	12	GLN	-	expression tag	UNP P28845
C	13	HIS	-	expression tag	UNP P28845
C	14	GLN	-	expression tag	UNP P28845
C	15	HIS	-	expression tag	UNP P28845
C	16	GLN	-	expression tag	UNP P28845
C	17	HIS	-	expression tag	UNP P28845
C	18	GLN	-	expression tag	UNP P28845
C	19	HIS	-	expression tag	UNP P28845
C	20	GLN	-	expression tag	UNP P28845
C	21	GLN	-	expression tag	UNP P28845
C	22	PRO	-	expression tag	UNP P28845
C	23	LEU	-	expression tag	UNP P28845
C	272	SER	CYS	engineered mutation	UNP P28845
D	7	MET	-	expression tag	UNP P28845
D	8	LYS	-	expression tag	UNP P28845
D	9	HIS	-	expression tag	UNP P28845
D	10	GLN	-	expression tag	UNP P28845
D	11	HIS	-	expression tag	UNP P28845
D	12	GLN	-	expression tag	UNP P28845
D	13	HIS	-	expression tag	UNP P28845
D	14	GLN	-	expression tag	UNP P28845
D	15	HIS	-	expression tag	UNP P28845

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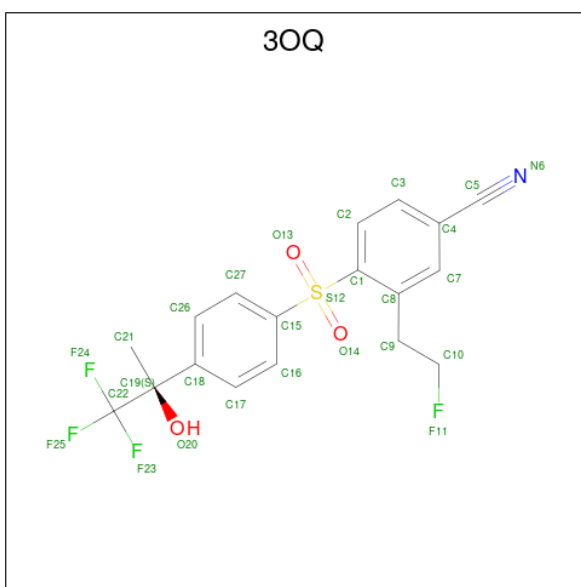
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	expression tag	UNP P28845
D	17	HIS	-	expression tag	UNP P28845
D	18	GLN	-	expression tag	UNP P28845
D	19	HIS	-	expression tag	UNP P28845
D	20	GLN	-	expression tag	UNP P28845
D	21	GLN	-	expression tag	UNP P28845
D	22	PRO	-	expression tag	UNP P28845
D	23	LEU	-	expression tag	UNP P28845
D	272	SER	CYS	engineered mutation	UNP P28845

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

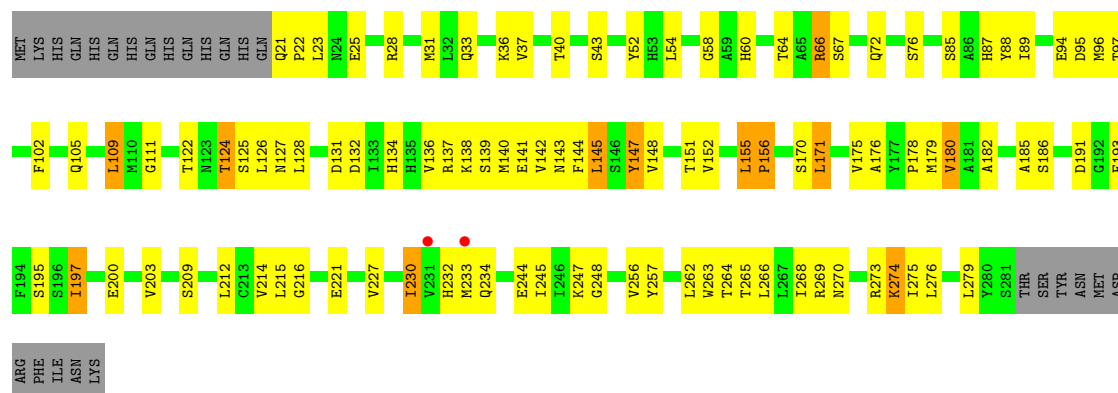
- Molecule 3 is 3-(2-fluoroethyl)-4-({4-[(2S)-1,1,1-trifluoro-2-hydroxypropan-2-yl]phenyl}sulfonyl)benzonitrile (CCD ID: 3OQ) (formula: $C_{18}H_{15}F_4NO_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			27	18	4	1	3	1		
3	B	1	Total	C	F	N	O	S	0	0
			27	18	4	1	3	1		
3	C	1	Total	C	F	N	O	S	0	0
			27	18	4	1	3	1		
3	D	1	Total	C	F	N	O	S	0	0
			27	18	4	1	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	10	Total	O	0	0
			10	10		
4	C	10	Total	O	0	0
			10	10		
4	D	9	Total	O	0	0
			9	9		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.30Å 153.40Å 73.59Å 90.00° 92.40° 90.00°	Depositor
Resolution (Å)	38.00 – 2.60 38.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.2 (38.00-2.60) 96.2 (38.00-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.220 , 0.308 0.221 , 0.304	Depositor DCC
R_{free} test set	1843 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8469	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3OQ, NAP

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	0.83	0/2035	1.07	5/2748 (0.2%)
1	B	0.90	1/2096 (0.0%)	1.14	7/2831 (0.2%)
1	C	0.88	0/2108	1.09	7/2846 (0.2%)
1	D	0.95	0/2046	1.17	7/2763 (0.3%)
All	All	0.89	1/8285 (0.0%)	1.12	26/11188 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	149	VAL	CA-CB	5.48	1.60	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	ASP	N-CA-C	8.02	122.50	112.24
1	B	37	VAL	N-CA-C	7.65	118.83	108.11
1	C	27	PHE	N-CA-C	7.40	121.12	110.24
1	C	61	VAL	N-CA-C	6.90	118.06	108.12
1	C	131	ASP	N-CA-C	6.86	120.97	112.47
1	D	132	ASP	N-CA-C	6.38	118.69	110.65
1	C	132	ASP	N-CA-C	6.26	119.38	110.68
1	D	147	TYR	N-CA-C	-5.99	104.83	111.71
1	D	145	LEU	N-CA-C	5.96	118.54	111.33
1	D	23	LEU	N-CA-C	5.87	118.11	110.43
1	D	25	GLU	N-CA-C	5.84	119.46	108.65
1	B	28	ARG	CA-C-N	5.71	126.98	119.84
1	B	28	ARG	C-N-CA	5.71	126.98	119.84
1	D	67	SER	N-CA-C	5.50	118.23	107.57
1	A	236	ALA	CA-C-N	5.42	125.34	119.76
1	A	236	ALA	C-N-CA	5.42	125.34	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	HIS	N-CA-C	5.26	117.32	110.43
1	B	228	SER	N-CA-C	5.24	119.42	113.19
1	C	177	TYR	CB-CA-C	-5.21	101.38	109.20
1	C	68	LYS	N-CA-C	-5.20	105.69	111.36
1	A	57	MET	N-CA-C	-5.20	106.86	114.39
1	A	61	VAL	N-CA-C	5.19	115.85	106.61
1	A	37	VAL	N-CA-C	5.18	115.50	107.78
1	D	212	LEU	N-CA-C	5.13	117.30	107.75
1	C	267	LEU	N-CA-C	-5.04	106.91	113.16
1	B	113	LEU	N-CA-C	5.02	117.58	108.69

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	2001	0	2051	103	0
1	B	2057	0	2098	83	0
1	C	2072	0	2113	83	0
1	D	2008	0	2058	63	0
2	A	48	0	25	5	0
2	B	48	0	25	5	0
2	C	48	0	25	4	0
2	D	48	0	25	3	0
3	A	27	0	15	0	0
3	B	27	0	15	0	0
3	C	27	0	15	3	0
3	D	27	0	15	3	0
4	A	2	0	0	0	0
4	B	10	0	0	1	0
4	C	10	0	0	2	0
4	D	9	0	0	1	0
All	All	8469	0	8480	312	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 18.

All (312) 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:A:62:VAL:HG23	1:A:110:MET:HE3	1.21	1.17
1:D:140:MET:HE1	1:D:186:SER:HA	1.42	1.01
1:B:179:MET:HE1	1:C:286:MET:HB3	1.39	1.00
1:C:44:LYS:O	1:C:48:ARG:HB3	1.63	0.99
1:B:126:LEU:O	1:B:127:ASN:ND2	2.00	0.94
1:C:60:HIS:HD1	1:C:85:SER:HG	1.24	0.84
1:A:206:VAL:HG12	1:A:208:VAL:HG23	1.61	0.82
1:A:32:LEU:O	1:A:35:LYS:HG2	1.79	0.82
1:C:43:SER:HB3	2:C:3:NAP:O3B	1.80	0.80
1:B:248:GLY:HA2	1:B:253:GLN:HE21	1.47	0.79
1:C:203:VAL:HG11	1:C:286:MET:HE3	1.65	0.79
1:A:271:PRO:O	1:A:275:ILE:HD12	1.82	0.78
1:A:273:ARG:HG3	1:D:175:VAL:HG12	1.67	0.77
1:B:259:ASP:OD1	1:B:264:THR:HG21	1.84	0.76
1:A:129:PHE:CD2	1:D:197:ILE:HD11	2.21	0.75
1:B:219:ASP:HA	1:B:224:MET:HE2	1.67	0.75
1:B:46:ILE:HG22	1:B:50:MET:HE2	1.67	0.75
1:C:60:HIS:ND1	1:C:85:SER:OG	2.20	0.75
1:C:179:MET:O	1:C:180:VAL:HG23	1.86	0.74
1:A:269:ARG:HH21	1:A:269:ARG:HB2	1.51	0.74
1:D:233:MET:HG3	3:D:293:3OQ:N6	2.01	0.73
1:B:44:LYS:HG3	2:B:2:NAP:H3B	1.70	0.72
1:B:216:GLY:HA3	1:B:259:ASP:OD2	1.90	0.72
1:B:40:THR:HA	1:B:64:THR:HG22	1.71	0.71
1:B:276:LEU:HD13	1:C:267:LEU:HD12	1.70	0.71
1:D:140:MET:CE	1:D:186:SER:HA	2.20	0.69
1:A:185:ALA:HB2	1:D:193:PHE:HB2	1.73	0.69
1:B:27:PHE:CD2	1:B:247:LYS:HE2	2.27	0.69
1:D:171:LEU:HD12	1:D:216:GLY:HA2	1.74	0.69
1:C:203:VAL:CG1	1:C:286:MET:HE3	2.22	0.68
1:A:62:VAL:HG23	1:A:110:MET:CE	2.13	0.68
1:B:126:LEU:C	1:B:127:ASN:HD22	2.00	0.68
1:C:239:GLU:CD	1:C:239:GLU:H	2.00	0.68
1:B:66:ARG:HB2	2:B:2:NAP:O2X	1.93	0.68
1:B:92:THR:OG1	1:B:94:GLU:HB2	1.93	0.68
1:C:279:LEU:HD13	1:D:263:TRP:CZ2	2.29	0.68
1:D:275:ILE:O	1:D:279:LEU:HG	1.94	0.67
1:D:137:ARG:O	1:D:141:GLU:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:ASN:ND2	1:D:273:ARG:H	1.93	0.67
1:B:200:GLU:O	1:B:204:SER:HB2	1.95	0.66
1:A:200:GLU:O	1:A:204:SER:HB2	1.97	0.65
1:A:57:MET:HE1	1:A:243:LEU:HD11	1.78	0.64
1:B:270:ASN:C	1:B:270:ASN:HD22	2.05	0.64
1:D:178:PRO:O	1:D:179:MET:HB2	1.96	0.64
1:D:248:GLY:HA3	1:D:256:VAL:HG21	1.80	0.64
1:D:37:VAL:HG11	1:D:54:LEU:HD13	1.79	0.64
1:A:35:LYS:O	1:A:59:ALA:HB1	1.98	0.63
1:D:136:VAL:HG22	1:D:182:ALA:HB2	1.79	0.63
1:B:148:VAL:HG22	1:B:193:PHE:CE1	2.33	0.63
2:D:4:NAP:N7N	2:D:4:NAP:O2N	2.32	0.63
1:B:270:ASN:C	1:B:270:ASN:ND2	2.57	0.63
1:A:263:TRP:C	1:A:263:TRP:HE3	2.07	0.63
1:C:94:GLU:OE2	1:C:138:LYS:HE3	1.99	0.63
1:A:121:ILE:HG13	1:A:143:ASN:ND2	2.14	0.62
3:C:293:3OQ:H15	3:C:293:3OQ:C16	2.29	0.62
3:C:293:3OQ:H15	3:C:293:3OQ:H11	1.82	0.62
1:C:113:LEU:CD2	1:C:158:LEU:HD21	2.30	0.62
1:D:124:THR:HG22	3:D:293:3OQ:F23	1.91	0.61
1:B:262:LEU:H	1:B:263:TRP:HE3	1.47	0.61
1:A:128:LEU:HG	1:A:179:MET:HE3	1.82	0.60
1:A:202:SER:O	1:A:204:SER:N	2.33	0.60
1:C:139:SER:O	1:C:143:ASN:HB2	2.00	0.60
1:D:28:ARG:O	1:D:31:MET:HG3	2.02	0.60
1:B:151:THR:HG23	1:B:165:ILE:HD12	1.83	0.59
1:D:60:HIS:ND1	1:D:85:SER:HB2	2.17	0.59
1:A:243:LEU:O	1:A:247:LYS:HG3	2.03	0.59
1:A:272:SER:O	1:A:276:LEU:HD23	2.03	0.59
1:C:215:LEU:O	2:C:3:NAP:H5N	2.03	0.59
1:B:193:PHE:HB2	1:C:185:ALA:HB2	1.85	0.59
1:D:66:ARG:HD3	2:D:4:NAP:C6A	2.33	0.59
1:A:170:SER:OG	2:A:1:NAP:H6N	2.04	0.58
1:A:62:VAL:CG2	1:A:110:MET:HE3	2.14	0.58
1:B:268:ILE:HG23	1:C:276:LEU:HD21	1.84	0.58
1:B:133:ILE:HD13	1:C:149:VAL:HG22	1.84	0.58
1:B:261:SER:OG	1:B:264:THR:HG22	2.04	0.58
1:B:27:PHE:CE2	1:B:247:LYS:HE2	2.39	0.58
1:D:264:THR:O	1:D:268:ILE:HG13	2.02	0.58
1:A:176:ALA:HB2	1:D:195:SER:HB3	1.84	0.57
1:B:179:MET:CE	1:C:286:MET:HB3	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:LEU:HD11	1:C:245:ILE:HD11	1.86	0.57
1:C:220:THR:O	1:C:224:MET:HG2	2.04	0.57
1:A:262:LEU:HA	1:A:265:THR:OG1	2.04	0.56
1:C:227:VAL:CG1	1:C:231:VAL:HG22	2.34	0.56
1:B:223:ALA:O	1:B:227:VAL:HG22	2.05	0.56
1:C:25:GLU:HG2	1:C:26:GLU:H	1.71	0.56
1:C:33:GLN:HB2	1:C:57:MET:O	2.05	0.56
1:A:263:TRP:C	1:A:263:TRP:CE3	2.83	0.56
1:D:139:SER:O	1:D:143:ASN:HB2	2.06	0.56
1:C:35:LYS:HD2	1:C:114:ASP:OD1	2.05	0.56
1:D:151:THR:O	1:D:152:VAL:C	2.48	0.56
1:D:274:LYS:NZ	4:D:300:HOH:O	2.38	0.55
1:B:280:TYR:OH	1:C:233:MET:HE3	2.06	0.55
1:D:95:ASP:OD1	1:D:97:THR:HB	2.07	0.55
1:A:37:VAL:HG22	1:A:115:MET:HB3	1.88	0.55
1:C:28:ARG:O	1:C:31:MET:HG3	2.05	0.55
1:B:94:GLU:OE2	1:B:138:LYS:HE2	2.07	0.55
1:B:262:LEU:HA	1:B:265:THR:OG1	2.06	0.55
1:A:197:ILE:HA	1:A:200:GLU:HG3	1.88	0.55
1:B:261:SER:HG	1:B:263:TRP:HE3	1.55	0.55
1:C:216:GLY:HA3	1:C:259:ASP:OD2	2.07	0.55
1:A:39:VAL:HB	1:A:63:VAL:HG12	1.87	0.55
1:B:96:MET:HE3	1:B:141:GLU:HG3	1.89	0.55
1:C:227:VAL:HG13	1:C:231:VAL:HG22	1.89	0.55
1:A:276:LEU:O	1:A:280:TYR:HD1	1.90	0.55
1:D:180:VAL:O	1:D:180:VAL:HG13	2.07	0.55
1:B:162:ASN:OD1	1:B:207:ASN:ND2	2.39	0.54
1:A:58:GLY:HA2	1:A:83:ALA:HA	1.89	0.54
1:A:124:THR:HG23	1:A:135:HIS:NE2	2.22	0.54
1:C:248:GLY:HA3	1:C:256:VAL:HG21	1.89	0.54
1:C:33:GLN:HA	1:C:58:GLY:O	2.07	0.54
1:D:33:GLN:HA	1:D:58:GLY:O	2.08	0.54
1:A:198:ARG:NE	1:A:254:GLU:HG2	2.22	0.54
1:A:244:GLU:HG3	1:A:258:TYR:CD2	2.43	0.54
1:A:218:ILE:C	1:A:235:ALA:HB1	2.33	0.54
1:C:38:ILE:HD12	1:C:113:LEU:HD11	1.90	0.54
1:D:87:HIS:CG	1:D:109:LEU:HD22	2.43	0.54
1:B:126:LEU:HD13	1:B:179:MET:HG3	1.90	0.54
1:D:214:VAL:HG11	1:D:268:ILE:HG21	1.90	0.54
1:A:240:GLU:O	1:A:244:GLU:HG2	2.08	0.53
1:B:131:ASP:CG	1:B:131:ASP:O	2.50	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:PHE:CD2	1:A:247:LYS:HG2	2.44	0.53
1:C:178:PRO:O	1:C:179:MET:HB2	2.09	0.53
1:D:40:THR:HA	1:D:64:THR:HG22	1.90	0.53
1:A:276:LEU:O	1:A:280:TYR:CD1	2.62	0.53
1:D:145:LEU:O	1:D:148:VAL:HB	2.08	0.53
1:B:140:MET:HE2	1:C:140:MET:SD	2.48	0.52
1:D:270:ASN:HD22	1:D:273:ARG:CB	2.21	0.52
1:B:141:GLU:OE1	1:B:145:LEU:HD23	2.10	0.52
1:D:215:LEU:HD11	1:D:245:ILE:HD11	1.90	0.52
1:A:144:PHE:O	1:A:148:VAL:HG23	2.10	0.52
1:A:180:VAL:O	1:A:183:TYR:HB3	2.09	0.52
1:A:198:ARG:HA	1:A:210:ILE:HD12	1.92	0.52
1:D:64:THR:HB	1:D:102:PHE:CE1	2.45	0.51
1:B:264:THR:HG23	1:B:265:THR:N	2.25	0.51
1:B:247:LYS:NZ	4:B:300:HOH:O	2.34	0.51
1:D:244:GLU:OE1	1:D:247:LYS:HE2	2.10	0.51
1:A:88:TYR:CD1	1:A:88:TYR:C	2.88	0.51
1:A:192:GLY:O	1:A:196:SER:HB3	2.11	0.51
1:A:212:LEU:HB3	1:A:255:GLU:HG3	1.93	0.51
1:D:88:TYR:C	1:D:89:ILE:HG13	2.35	0.51
1:A:223:ALA:CB	2:A:1:NAP:H72N	2.24	0.51
1:A:193:PHE:HB2	1:D:185:ALA:HB2	1.93	0.50
1:C:113:LEU:HD23	1:C:158:LEU:HD21	1.92	0.50
1:A:62:VAL:HG11	1:A:106:ALA:HB2	1.93	0.50
1:C:36:LYS:HG2	1:C:110:MET:HB3	1.93	0.50
1:C:73:LYS:HE3	4:C:5:HOH:O	2.11	0.50
1:B:219:ASP:O	1:B:219:ASP:OD2	2.30	0.50
1:C:279:LEU:HD12	1:C:279:LEU:C	2.36	0.50
1:B:63:VAL:HG23	1:B:71:LEU:HD22	1.94	0.50
1:A:95:ASP:HB3	1:A:98:PHE:HB3	1.94	0.50
1:A:128:LEU:HA	1:D:200:GLU:OE2	2.11	0.50
1:B:199:LYS:O	1:B:200:GLU:C	2.54	0.49
1:D:215:LEU:O	2:D:4:NAP:H5N	2.12	0.49
1:B:220:THR:O	1:B:221:GLU:C	2.54	0.49
1:C:49:GLU:HG3	1:C:238:LYS:HG3	1.95	0.49
1:C:171:LEU:HD23	1:C:268:ILE:HD11	1.94	0.49
1:D:88:TYR:C	1:D:88:TYR:CD1	2.90	0.49
1:D:88:TYR:O	1:D:89:ILE:HG13	2.12	0.49
1:B:185:ALA:HB2	1:C:193:PHE:HB2	1.94	0.49
1:C:96:MET:HE3	1:C:141:GLU:OE2	2.12	0.49
1:A:64:THR:O	1:A:65:ALA:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ASP:O	1:A:192:GLY:C	2.55	0.49
1:D:227:VAL:HB	1:D:230:ILE:HG21	1.94	0.49
1:A:201:TYR:O	1:A:202:SER:C	2.54	0.49
1:A:257:TYR:O	1:A:258:TYR:HB2	2.12	0.49
1:A:29:PRO:HB3	1:A:57:MET:HG2	1.95	0.49
1:B:259:ASP:CG	1:B:264:THR:HG21	2.39	0.48
1:C:95:ASP:C	1:C:95:ASP:OD1	2.56	0.48
1:C:227:VAL:HG12	1:C:228:SER:N	2.28	0.48
1:B:39:VAL:HG22	1:B:117:ILE:HD12	1.94	0.48
1:C:180:VAL:O	1:C:180:VAL:CG1	2.60	0.48
1:C:259:ASP:HB3	1:C:265:THR:HG23	1.95	0.48
1:A:201:TYR:O	1:A:204:SER:CB	2.62	0.48
1:B:261:SER:OG	1:B:263:TRP:HE3	1.97	0.48
1:D:140:MET:HE3	1:D:140:MET:HA	1.96	0.48
1:A:61:VAL:HG23	1:A:61:VAL:O	2.13	0.48
1:A:64:THR:HG22	1:A:65:ALA:H	1.79	0.48
1:C:43:SER:HB2	1:C:65:ALA:CB	2.44	0.48
1:B:62:VAL:HG23	1:B:110:MET:SD	2.53	0.48
1:A:220:THR:OG1	1:A:223:ALA:HB3	2.14	0.48
1:A:121:ILE:HG23	1:A:122:THR:N	2.29	0.47
1:C:264:THR:C	1:C:266:LEU:H	2.22	0.47
1:A:219:ASP:OD2	1:A:237:PRO:HA	2.14	0.47
1:B:44:LYS:HD2	2:B:2:NAP:H51A	1.95	0.47
1:A:72:GLN:O	1:A:73:LYS:C	2.58	0.47
1:A:248:GLY:HA2	1:A:251:LEU:HB2	1.96	0.47
1:D:37:VAL:HG11	1:D:54:LEU:CD1	2.43	0.47
1:B:126:LEU:HD22	1:B:180:VAL:HG13	1.96	0.47
1:C:217:LEU:HD23	1:C:235:ALA:HB2	1.96	0.47
1:A:75:VAL:HG21	1:A:88:TYR:HB3	1.96	0.47
1:C:230:ILE:HG22	1:C:231:VAL:HG12	1.97	0.47
1:A:275:ILE:O	1:A:279:LEU:HG	2.15	0.47
1:B:263:TRP:HE3	1:B:263:TRP:H	1.57	0.47
1:B:192:GLY:O	1:B:196:SER:HB3	2.15	0.47
1:A:37:VAL:HG11	1:A:54:LEU:HD13	1.97	0.47
1:A:83:ALA:C	1:A:85:SER:H	2.23	0.46
1:A:27:PHE:HB2	1:A:251:LEU:HD21	1.97	0.46
1:A:70:THR:O	1:A:73:LYS:HB2	2.15	0.46
1:B:157:MET:O	1:B:160:GLN:HG2	2.15	0.46
1:A:89:ILE:HD12	1:A:102:PHE:HD1	1.81	0.46
1:D:178:PRO:O	1:D:179:MET:CB	2.62	0.46
1:A:197:ILE:O	1:A:198:ARG:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:HD13	1:B:275:ILE:CD1	2.46	0.46
1:C:26:GLU:HG2	1:C:27:PHE:N	2.31	0.45
1:C:155:LEU:HB3	1:C:156:PRO:HD3	1.98	0.45
1:C:38:ILE:CD1	1:C:113:LEU:HD11	2.46	0.45
1:D:36:LYS:HE3	1:D:111:GLY:O	2.16	0.45
1:B:37:VAL:HG22	1:B:115:MET:HB3	1.97	0.45
1:A:264:THR:O	1:A:266:LEU:N	2.49	0.45
1:C:66:ARG:HB2	2:C:3:NAP:O2X	2.16	0.45
1:A:243:LEU:HD12	1:A:243:LEU:HA	1.76	0.45
1:B:45:GLY:HA2	1:B:220:THR:HG23	1.99	0.45
1:D:94:GLU:HG3	1:D:142:VAL:HG22	1.99	0.45
1:A:40:THR:O	1:A:41:GLY:C	2.60	0.45
1:C:223:ALA:HB2	2:C:3:NAP:H72N	1.82	0.45
1:D:270:ASN:ND2	1:D:273:ARG:HB2	2.32	0.45
1:A:175:VAL:HG12	1:D:273:ARG:HG3	1.96	0.45
1:A:118:LEU:HB3	1:A:147:TYR:CD2	2.52	0.45
1:A:196:SER:O	1:A:200:GLU:HG3	2.17	0.45
1:B:66:ARG:N	2:B:2:NAP:O2X	2.48	0.45
1:C:27:PHE:HB2	1:C:251:LEU:HD11	1.97	0.45
1:D:21:GLN:N	1:D:22:PRO:HD3	2.32	0.45
1:A:212:LEU:HD23	1:A:255:GLU:OE1	2.18	0.44
1:B:197:ILE:HD11	1:C:129:PHE:HB3	1.99	0.44
1:D:227:VAL:O	1:D:230:ILE:HG22	2.16	0.44
1:B:220:THR:HG22	1:B:222:THR:H	1.83	0.44
1:C:77:HIS:ND1	1:C:81:LEU:HD11	2.33	0.44
1:B:219:ASP:CA	1:B:224:MET:HE2	2.41	0.44
1:C:92:THR:C	1:C:94:GLU:H	2.25	0.44
1:A:200:GLU:HB3	1:D:128:LEU:HD22	1.98	0.44
1:C:203:VAL:HG11	1:C:286:MET:CE	2.41	0.44
1:A:130:HIS:HD2	1:A:131:ASP:CG	2.26	0.44
1:A:198:ARG:NH2	1:A:254:GLU:O	2.50	0.44
1:B:270:ASN:HA	1:B:271:PRO:HD3	1.79	0.44
1:C:25:GLU:HG2	1:C:26:GLU:N	2.32	0.44
1:C:41:GLY:O	1:C:47:GLY:HA3	2.18	0.44
1:A:89:ILE:HD12	1:A:102:PHE:CD1	2.53	0.44
1:A:267:LEU:HD13	1:B:275:ILE:HD11	1.99	0.44
1:B:268:ILE:H	1:B:268:ILE:HG12	1.57	0.44
1:B:96:MET:HG3	1:C:137:ARG:HH22	1.83	0.43
1:D:193:PHE:CZ	1:D:197:ILE:HD12	2.53	0.43
1:A:49:GLU:HG3	1:A:238:LYS:HB2	1.99	0.43
1:B:106:ALA:HA	1:B:109:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:TYR:O	1:A:204:SER:HB2	2.18	0.43
1:C:26:GLU:HG2	1:C:27:PHE:H	1.83	0.43
1:A:264:THR:C	1:A:266:LEU:N	2.76	0.43
1:C:197:ILE:O	1:C:200:GLU:HB2	2.19	0.43
1:B:190:LEU:CD2	1:B:194:PHE:HE1	2.31	0.43
3:C:293:3OQ:H4	3:C:293:3OQ:F25	2.08	0.43
1:A:129:PHE:CD2	1:D:197:ILE:CD1	2.98	0.43
1:A:273:ARG:HH21	1:D:176:ALA:HB2	1.83	0.43
1:A:32:LEU:O	1:A:35:LYS:CG	2.58	0.42
1:A:53:HIS:CG	1:A:243:LEU:HD13	2.53	0.42
1:C:243:LEU:O	1:C:247:LYS:HG3	2.20	0.42
1:B:158:LEU:O	1:B:159:LYS:C	2.61	0.42
1:C:197:ILE:HD13	1:C:197:ILE:HA	1.83	0.42
1:D:257:TYR:CE1	1:D:269:ARG:HG2	2.54	0.42
1:B:95:ASP:OD1	1:B:95:ASP:C	2.63	0.42
1:C:42:ALA:HA	1:C:47:GLY:HA3	2.02	0.42
1:C:180:VAL:HG12	1:C:184:SER:HB2	2.02	0.42
1:A:79:LEU:C	1:A:81:LEU:H	2.27	0.42
1:C:74:VAL:O	1:C:78:CYS:SG	2.71	0.42
1:B:44:LYS:CG	2:B:2:NAP:H3B	2.44	0.42
1:C:77:HIS:CE1	1:C:81:LEU:HD11	2.54	0.42
1:A:217:LEU:HG	1:A:235:ALA:HB2	2.01	0.42
1:C:273:ARG:O	1:C:274:LYS:C	2.61	0.42
1:D:191:ASP:O	1:D:195:SER:HB2	2.19	0.42
1:B:261:SER:CB	1:B:264:THR:HG22	2.50	0.42
1:D:144:PHE:O	1:D:147:TYR:HB2	2.20	0.42
1:C:28:ARG:HA	1:C:29:PRO:HD2	1.83	0.42
1:C:73:LYS:CE	4:C:5:HOH:O	2.66	0.42
1:C:133:ILE:H	1:C:133:ILE:HG13	1.60	0.42
1:C:217:LEU:O	1:C:218:ILE:HD13	2.20	0.42
1:C:252:ARG:NH1	1:C:252:ARG:HG2	2.35	0.42
1:A:264:THR:C	1:A:266:LEU:H	2.28	0.41
1:D:40:THR:HA	1:D:64:THR:CG2	2.50	0.41
1:B:264:THR:HG23	1:B:265:THR:H	1.85	0.41
1:C:92:THR:C	1:C:94:GLU:N	2.77	0.41
1:C:220:THR:O	1:C:221:GLU:C	2.64	0.41
1:C:169:SER:N	1:C:213:CYS:O	2.51	0.41
1:A:46:ILE:HD12	2:A:1:NAP:PN	2.61	0.41
1:A:121:ILE:HG23	1:A:122:THR:H	1.86	0.41
1:B:21:GLN:N	1:B:22:PRO:HD3	2.36	0.41
1:B:142:VAL:O	1:B:146:SER:OG	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ASP:HA	1:A:224:MET:HE3	2.01	0.41
1:A:272:SER:O	1:A:276:LEU:CD2	2.67	0.41
1:D:233:MET:CG	3:D:293:3OQ:N6	2.79	0.41
1:B:53:HIS:HD2	1:B:243:LEU:HD13	1.86	0.41
1:A:217:LEU:HD22	1:A:232:HIS:HB2	2.02	0.41
1:A:223:ALA:HB2	2:A:1:NAP:H72N	1.86	0.41
1:A:239:GLU:CD	1:A:239:GLU:H	2.28	0.41
1:B:91:GLY:HA3	1:B:98:PHE:CZ	2.56	0.41
1:B:134:HIS:O	1:B:138:LYS:HB2	2.21	0.41
1:B:261:SER:OG	1:B:262:LEU:N	2.53	0.41
1:C:252:ARG:HG2	1:C:252:ARG:HH11	1.86	0.41
1:C:285:ASN:O	1:C:285:ASN:ND2	2.54	0.41
1:D:96:MET:HE3	1:D:145:LEU:HB3	2.03	0.41
1:A:171:LEU:HD23	1:A:268:ILE:HD13	2.03	0.41
1:B:75:VAL:HG21	1:B:88:TYR:HD2	1.85	0.41
1:A:44:LYS:HB2	2:A:1:NAP:H3B	2.03	0.40
1:A:119:ASN:HD22	1:A:168:VAL:HG21	1.86	0.40
1:A:202:SER:OG	1:A:203:VAL:N	2.54	0.40
1:D:155:LEU:O	1:D:156:PRO:C	2.64	0.40
1:B:105:GLN:HE21	1:B:105:GLN:HB2	1.64	0.40
1:B:221:GLU:H	1:B:221:GLU:HG3	1.63	0.40
1:A:84:ALA:O	1:A:85:SER:CB	2.68	0.40
1:B:121:ILE:O	1:B:121:ILE:HG13	2.21	0.40
1:B:124:THR:HG23	1:B:135:HIS:CE1	2.57	0.40
1:C:168:VAL:O	1:C:187:LYS:NZ	2.55	0.40
1:A:37:VAL:HA	1:A:115:MET:O	2.21	0.40

There are no symmetry-related clashes.

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	259/286 (91%)	205 (79%)	40 (15%)	14 (5%)	1	1
1	B	266/286 (93%)	232 (87%)	29 (11%)	5 (2%)	6	13
1	C	267/286 (93%)	229 (86%)	31 (12%)	7 (3%)	4	7
1	D	260/286 (91%)	225 (86%)	32 (12%)	3 (1%)	10	23
All	All	1052/1144 (92%)	891 (85%)	132 (12%)	29 (3%)	4	6

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	SER
1	A	228	SER
1	A	265	THR
1	C	180	VAL
1	A	33	GLN
1	A	45	GLY
1	A	65	ALA
1	A	203	VAL
1	A	204	SER
1	A	258	TYR
1	B	69	GLU
1	C	45	GLY
1	D	52	TYR
1	D	180	VAL
1	A	109	LEU
1	A	263	TRP
1	C	65	ALA
1	C	279	LEU
1	B	22	PRO
1	B	65	ALA
1	B	70	THR
1	C	29	PRO
1	A	80	GLU
1	C	280	TYR
1	A	202	SER
1	B	279	LEU
1	C	265	THR
1	D	156	PRO
1	A	121	ILE

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	218/243 (90%)	190 (87%)	28 (13%)	4	8
1	B	225/243 (93%)	195 (87%)	30 (13%)	4	8
1	C	226/243 (93%)	190 (84%)	36 (16%)	2	4
1	D	219/243 (90%)	191 (87%)	28 (13%)	4	8
All	All	888/972 (91%)	766 (86%)	122 (14%)	3	7

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	33	GLN
1	A	53	HIS
1	A	64	THR
1	A	67	SER
1	A	70	THR
1	A	80	GLU
1	A	121	ILE
1	A	124	THR
1	A	126	LEU
1	A	145	LEU
1	A	152	VAL
1	A	160	GLN
1	A	180	VAL
1	A	203	VAL
1	A	204	SER
1	A	208	VAL
1	A	221	GLU
1	A	231	VAL
1	A	238	LYS
1	A	251	LEU
1	A	262	LEU
1	A	263	TRP
1	A	265	THR

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Mol	Chain	Res	Type
1	A	269	ARG
1	A	270	ASN
1	A	277	GLU
1	A	279	LEU
1	B	25	GLU
1	B	26	GLU
1	B	32	LEU
1	B	35	LYS
1	B	36	LYS
1	B	44	LYS
1	B	68	LYS
1	B	73	LYS
1	B	80	GLU
1	B	94	GLU
1	B	126	LEU
1	B	131	ASP
1	B	145	LEU
1	B	165	ILE
1	B	171	LEU
1	B	180	VAL
1	B	184	SER
1	B	203	VAL
1	B	204	SER
1	B	215	LEU
1	B	221	GLU
1	B	222	THR
1	B	228	SER
1	B	263	TRP
1	B	268	ILE
1	B	270	ASN
1	B	272	SER
1	B	276	LEU
1	B	283	SER
1	B	285	ASN
1	C	21	GLN
1	C	26	GLU
1	C	28	ARG
1	C	32	LEU
1	C	36	LYS
1	C	48	ARG
1	C	56	LYS
1	C	57	MET

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Mol	Chain	Res	Type
1	C	68	LYS
1	C	73	LYS
1	C	85	SER
1	C	109	LEU
1	C	119	ASN
1	C	126	LEU
1	C	127	ASN
1	C	132	ASP
1	C	157	MET
1	C	170	SER
1	C	179	MET
1	C	180	VAL
1	C	196	SER
1	C	205	ARG
1	C	221	GLU
1	C	231	VAL
1	C	233	MET
1	C	239	GLU
1	C	240	GLU
1	C	244	GLU
1	C	262	LEU
1	C	266	LEU
1	C	267	LEU
1	C	269	ARG
1	C	272	SER
1	C	279	LEU
1	C	281	SER
1	C	286	MET
1	D	43	SER
1	D	66	ARG
1	D	72	GLN
1	D	76	SER
1	D	105	GLN
1	D	109	LEU
1	D	122	THR
1	D	124	THR
1	D	125	SER
1	D	126	LEU
1	D	127	ASN
1	D	134	HIS
1	D	138	LYS
1	D	155	LEU

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Mol	Chain	Res	Type
1	D	170	SER
1	D	171	LEU
1	D	197	ILE
1	D	203	VAL
1	D	209	SER
1	D	221	GLU
1	D	230	ILE
1	D	232	HIS
1	D	234	GLN
1	D	262	LEU
1	D	265	THR
1	D	266	LEU
1	D	274	LYS
1	D	276	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	119	ASN
1	A	130	HIS
1	A	160	GLN
1	A	162	ASN
1	A	253	GLN
1	B	33	GLN
1	B	105	GLN
1	B	134	HIS
1	B	135	HIS
1	B	207	ASN
1	B	253	GLN
1	B	270	ASN
1	C	53	HIS
1	C	119	ASN
1	C	127	ASN
1	C	232	HIS
1	D	72	GLN
1	D	101	GLN
1	D	105	GLN
1	D	160	GLN
1	D	207	ASN
1	D	232	HIS
1	D	270	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](#)

8 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$
3	3OQ	D	293	-	28,28,28	2.25	5 (17%)	43,43,43	2.17	10 (23%)
3	3OQ	B	293	-	28,28,28	1.53	6 (21%)	43,43,43	1.79	8 (18%)
2	NAP	D	4	-	50,52,52	1.78	6 (12%)	71,80,80	1.83	16 (22%)
2	NAP	B	2	-	50,52,52	1.66	5 (10%)	71,80,80	1.84	12 (16%)
2	NAP	A	1	-	50,52,52	1.72	6 (12%)	71,80,80	1.66	11 (15%)
2	NAP	C	3	-	50,52,52	1.77	4 (8%)	71,80,80	1.65	14 (19%)
3	3OQ	A	293	-	28,28,28	1.53	4 (14%)	43,43,43	1.81	9 (20%)
3	3OQ	C	293	-	28,28,28	1.14	3 (10%)	43,43,43	2.04	12 (27%)

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	3OQ	D	293	-	-	15/32/32/32	0/2/2/2
3	3OQ	B	293	-	-	2/32/32/32	0/2/2/2
2	NAP	D	4	-	-	6/35/67/67	0/5/5/5
2	NAP	B	2	-	-	10/35/67/67	0/5/5/5
2	NAP	A	1	-	-	4/35/67/67	0/5/5/5
2	NAP	C	3	-	-	3/35/67/67	0/5/5/5
3	3OQ	A	293	-	-	4/32/32/32	0/2/2/2
3	3OQ	C	293	-	-	6/32/32/32	0/2/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	NAP	O7N-C7N	9.54	1.41	1.24
2	A	1	NAP	O7N-C7N	9.23	1.41	1.24
2	B	2	NAP	O7N-C7N	9.07	1.41	1.24
2	D	4	NAP	O7N-C7N	8.79	1.40	1.24
3	D	293	3OQ	C1-S12	-8.63	1.66	1.78
3	D	293	3OQ	C15-S12	-4.95	1.69	1.77
2	D	4	NAP	C2N-N1N	4.81	1.40	1.35
3	A	293	3OQ	C1-S12	-4.50	1.72	1.78
2	C	3	NAP	C2N-N1N	4.07	1.39	1.35
3	B	293	3OQ	O14-S12	3.94	1.51	1.44
3	A	293	3OQ	O14-S12	3.89	1.51	1.44
3	D	293	3OQ	O13-S12	3.85	1.51	1.44
3	B	293	3OQ	C10-C9	3.68	1.55	1.49
3	D	293	3OQ	O14-S12	3.59	1.50	1.44
3	B	293	3OQ	O13-S12	3.58	1.50	1.44
2	A	1	NAP	PA-O3	3.10	1.62	1.59
3	C	293	3OQ	O14-S12	3.07	1.49	1.44
3	A	293	3OQ	C15-S12	-3.02	1.72	1.77
3	A	293	3OQ	O13-S12	2.96	1.49	1.44
2	B	2	NAP	C8A-N7A	2.84	1.37	1.31
2	D	4	NAP	C5A-N7A	-2.80	1.34	1.39
3	C	293	3OQ	C1-S12	-2.78	1.74	1.78
3	C	293	3OQ	O13-S12	2.77	1.49	1.44
3	B	293	3OQ	C1-S12	-2.74	1.74	1.78
2	B	2	NAP	C2N-N1N	2.63	1.37	1.35
2	D	4	NAP	C8A-N7A	2.59	1.36	1.31
2	C	3	NAP	C2A-N1A	2.59	1.38	1.33
2	C	3	NAP	C2A-N3A	2.56	1.38	1.33
2	B	2	NAP	C2A-N1A	2.48	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NAP	C8A-N7A	2.45	1.36	1.31
2	A	1	NAP	PN-O3	2.45	1.62	1.59
2	A	1	NAP	C2A-N3A	2.42	1.38	1.33
2	D	4	NAP	C3N-C7N	2.41	1.54	1.50
2	B	2	NAP	C2A-N3A	2.36	1.38	1.33
3	B	293	3OQ	O20-C19	-2.34	1.39	1.43
2	D	4	NAP	C2A-N1A	2.30	1.38	1.33
2	A	1	NAP	C2A-N1A	2.28	1.38	1.33
3	D	293	3OQ	C10-C9	2.14	1.52	1.49
3	B	293	3OQ	C15-S12	-2.06	1.73	1.77

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	293	3OQ	C15-S12-C1	7.61	117.06	105.33
2	B	2	NAP	N3A-C2A-N1A	-7.09	117.84	128.58
3	C	293	3OQ	O14-S12-O13	-6.63	105.84	119.25
3	B	293	3OQ	O14-S12-O13	-6.50	106.10	119.25
2	A	1	NAP	N3A-C2A-N1A	-6.06	119.41	128.58
3	A	293	3OQ	O14-S12-O13	-5.89	107.35	119.25
3	D	293	3OQ	O14-S12-O13	-5.60	107.93	119.25
2	D	4	NAP	C3N-C7N-N7N	5.42	124.42	117.74
2	B	2	NAP	C5A-C4A-N3A	-5.16	119.62	126.72
2	C	3	NAP	N3A-C2A-N1A	-5.15	120.78	128.58
2	A	1	NAP	N9A-C8A-N7A	-4.90	106.99	113.94
3	D	293	3OQ	O13-S12-C15	4.79	113.85	107.96
2	B	2	NAP	C2A-N3A-C4A	4.71	123.34	111.83
3	C	293	3OQ	C22-C19-C18	4.66	115.28	109.25
2	B	2	NAP	N9A-C8A-N7A	-4.63	107.37	113.94
2	D	4	NAP	C5A-C4A-N3A	-4.59	120.40	126.72
3	A	293	3OQ	F24-C22-C19	-4.36	106.24	112.40
2	D	4	NAP	C5A-N7A-C8A	4.13	109.94	103.45
2	D	4	NAP	N3A-C2A-N1A	-4.09	122.38	128.58
3	B	293	3OQ	F24-C22-C19	-4.06	106.66	112.40
3	C	293	3OQ	C26-C18-C19	-4.03	117.00	121.43
3	D	293	3OQ	C22-C19-C18	4.01	114.43	109.25
2	D	4	NAP	O7N-C7N-N7N	-3.93	116.94	122.62
2	D	4	NAP	C4A-C5A-N7A	-3.92	106.10	110.58
2	B	2	NAP	C5A-N7A-C8A	3.90	109.58	103.45
2	A	1	NAP	C5A-N7A-C8A	3.83	109.47	103.45
2	A	1	NAP	C5A-C4A-N3A	-3.72	121.59	126.72
2	A	1	NAP	O2A-PA-O3	3.70	117.27	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	NAP	N9A-C8A-N7A	-3.57	108.87	113.94
2	B	2	NAP	C4A-C5A-N7A	-3.55	106.52	110.58
3	C	293	3OQ	F23-C22-C19	-3.50	107.45	112.40
3	D	293	3OQ	F23-C22-C19	-3.47	107.50	112.40
3	B	293	3OQ	O13-S12-C15	3.43	112.18	107.96
2	C	3	NAP	C5A-C4A-N3A	-3.41	122.02	126.72
2	A	1	NAP	C2A-N3A-C4A	3.38	120.08	111.83
2	B	2	NAP	O4B-C1B-N9A	3.36	114.54	108.09
2	C	3	NAP	O4B-C1B-N9A	3.28	114.38	108.09
2	C	3	NAP	C2B-C1B-N9A	-3.27	108.37	113.75
2	D	4	NAP	N9A-C8A-N7A	-3.26	109.31	113.94
2	A	1	NAP	C4A-N9A-C8A	3.24	109.14	105.74
2	D	4	NAP	C4D-O4D-C1D	3.19	112.84	109.92
3	C	293	3OQ	F24-C22-C19	-3.13	107.97	112.40
3	A	293	3OQ	C15-S12-C1	3.10	110.10	105.33
2	C	3	NAP	C3N-C7N-N7N	3.03	121.47	117.74
2	C	3	NAP	C2A-N3A-C4A	3.02	119.22	111.83
2	C	3	NAP	C4D-O4D-C1D	2.99	112.66	109.92
2	D	4	NAP	C2A-N3A-C4A	2.98	119.11	111.83
3	A	293	3OQ	C3-C4-C5	-2.97	115.13	119.97
3	C	293	3OQ	C16-C15-S12	2.92	123.30	119.49
3	C	293	3OQ	C17-C18-C19	2.92	124.64	121.43
3	D	293	3OQ	O14-S12-C15	-2.89	104.41	107.96
3	A	293	3OQ	C17-C18-C19	-2.87	118.28	121.43
3	D	293	3OQ	C3-C4-C5	-2.83	115.36	119.97
3	A	293	3OQ	O13-S12-C15	2.80	111.40	107.96
3	C	293	3OQ	C15-S12-C1	2.79	109.62	105.33
2	B	2	NAP	C5A-C4A-N9A	2.77	108.83	105.81
2	C	3	NAP	C5A-N7A-C8A	2.76	107.79	103.45
3	D	293	3OQ	C7-C4-C5	2.76	123.28	119.55
2	C	3	NAP	O2A-PA-O3	2.72	114.63	107.27
3	A	293	3OQ	C7-C4-C5	2.67	123.16	119.55
2	D	4	NAP	C5A-C4A-N9A	2.65	108.70	105.81
3	B	293	3OQ	C21-C19-C22	2.63	112.53	109.04
2	A	1	NAP	C4A-C5A-N7A	-2.62	107.59	110.58
2	A	1	NAP	N3A-C4A-N9A	2.61	131.60	127.17
2	B	2	NAP	N3A-C4A-N9A	2.57	131.54	127.17
3	C	293	3OQ	O13-S12-C15	2.56	111.11	107.96
2	D	4	NAP	O2B-C2B-C1B	2.51	118.86	110.05
3	C	293	3OQ	C7-C8-C1	2.50	118.83	117.21
2	C	3	NAP	N3A-C4A-N9A	2.49	131.40	127.17
2	A	1	NAP	O7N-C7N-C3N	-2.46	116.59	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	293	3OQ	C9-C8-C7	-2.37	114.70	119.38
2	B	2	NAP	C3N-C7N-N7N	2.36	120.65	117.74
3	B	293	3OQ	O14-S12-C15	2.36	110.86	107.96
2	D	4	NAP	C5B-C4B-C3B	-2.34	106.78	115.21
2	D	4	NAP	C2B-C1B-N9A	-2.33	109.92	113.75
3	B	293	3OQ	O20-C19-C18	-2.32	103.17	107.91
3	C	293	3OQ	C2-C1-S12	2.29	119.44	116.38
2	C	3	NAP	C4A-N9A-C8A	2.28	108.13	105.74
2	C	3	NAP	O4B-C4B-C3B	2.26	109.63	105.15
2	C	3	NAP	C6N-N1N-C1D	-2.23	115.35	119.73
3	D	293	3OQ	C2-C1-S12	-2.23	113.41	116.38
2	D	4	NAP	O2A-PA-O3	2.22	113.27	107.27
3	A	293	3OQ	F23-C22-C19	-2.21	109.27	112.40
2	D	4	NAP	N3A-C4A-N9A	2.19	130.90	127.17
2	B	2	NAP	O2N-PN-O1N	2.18	122.57	112.44
3	B	293	3OQ	O20-C19-C22	2.15	109.22	105.94
2	B	2	NAP	C5B-C4B-C3B	-2.13	107.56	115.21
3	A	293	3OQ	C27-C15-S12	2.10	122.22	119.49
2	D	4	NAP	C6A-C5A-C4A	2.09	120.03	117.18
3	D	293	3OQ	C2-C1-C8	2.09	123.23	121.40
3	C	293	3OQ	C8-C1-S12	-2.04	119.52	123.94
2	A	1	NAP	C4A-N9A-C1B	-2.02	121.91	126.63

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NAP	C5D-O5D-PN-O1N
2	B	2	NAP	C5B-O5B-PA-O2A
2	B	2	NAP	C5B-O5B-PA-O3
2	B	2	NAP	O4B-C4B-C5B-O5B
2	B	2	NAP	C5D-O5D-PN-O3
2	B	2	NAP	C5D-O5D-PN-O1N
2	D	4	NAP	O4D-C4D-C5D-O5D
3	A	293	3OQ	F11-C10-C9-C8
3	C	293	3OQ	C7-C8-C9-C10
3	C	293	3OQ	C17-C18-C19-C21
3	C	293	3OQ	C26-C18-C19-C21
3	C	293	3OQ	C26-C18-C19-C22
3	D	293	3OQ	F11-C10-C9-C8
3	D	293	3OQ	C21-C19-C22-F23
3	D	293	3OQ	O20-C19-C22-F23

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Mol	Chain	Res	Type	Atoms
3	D	293	3OQ	C18-C19-C22-F23
3	D	293	3OQ	C21-C19-C22-F24
3	D	293	3OQ	O20-C19-C22-F24
3	D	293	3OQ	C18-C19-C22-F24
3	D	293	3OQ	C21-C19-C22-F25
3	D	293	3OQ	O20-C19-C22-F25
3	D	293	3OQ	C18-C19-C22-F25
2	B	2	NAP	C3B-C4B-C5B-O5B
2	D	4	NAP	C3D-C4D-C5D-O5D
3	D	293	3OQ	C1-C8-C9-C10
2	B	2	NAP	C2B-O2B-P2B-O1X
3	A	293	3OQ	C27-C15-S12-O14
3	D	293	3OQ	C16-C15-S12-O14
3	D	293	3OQ	C27-C15-S12-O14
3	A	293	3OQ	C16-C15-S12-O14
3	C	293	3OQ	C21-C19-C22-F25
2	A	1	NAP	C5D-O5D-PN-O3
2	B	2	NAP	C5B-O5B-PA-O1A
2	B	2	NAP	C5D-O5D-PN-O2N
2	D	4	NAP	C5D-O5D-PN-O1N
2	A	1	NAP	C2B-O2B-P2B-O2X
2	C	3	NAP	O4D-C1D-N1N-C6N
2	C	3	NAP	C2B-O2B-P2B-O1X
2	C	3	NAP	PN-O3-PA-O1A
3	D	293	3OQ	C16-C15-S12-C1
2	D	4	NAP	PN-O3-PA-O1A
2	D	4	NAP	PN-O3-PA-O2A
2	D	4	NAP	O4B-C4B-C5B-O5B
3	C	293	3OQ	C17-C18-C19-C22
3	B	293	3OQ	C16-C15-S12-O14
3	D	293	3OQ	C27-C15-S12-C1
3	A	293	3OQ	C27-C15-S12-C1
3	B	293	3OQ	C27-C15-S12-O14
2	A	1	NAP	PN-O3-PA-O2A
2	B	2	NAP	PA-O3-PN-O2N

There are no ring outliers.

6 monomers are involved in 23 short contacts:

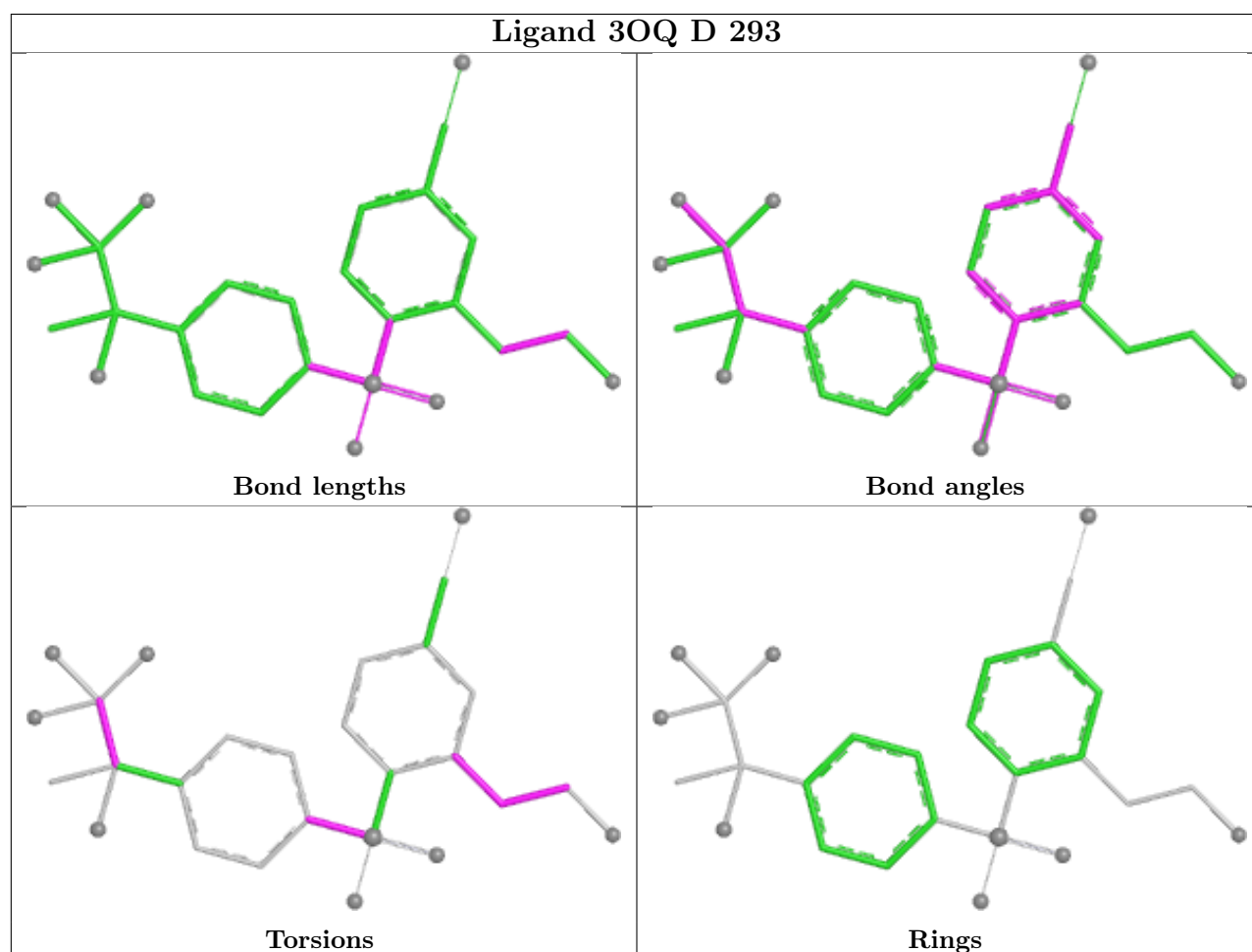
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	293	3OQ	3	0
2	D	4	NAP	3	0

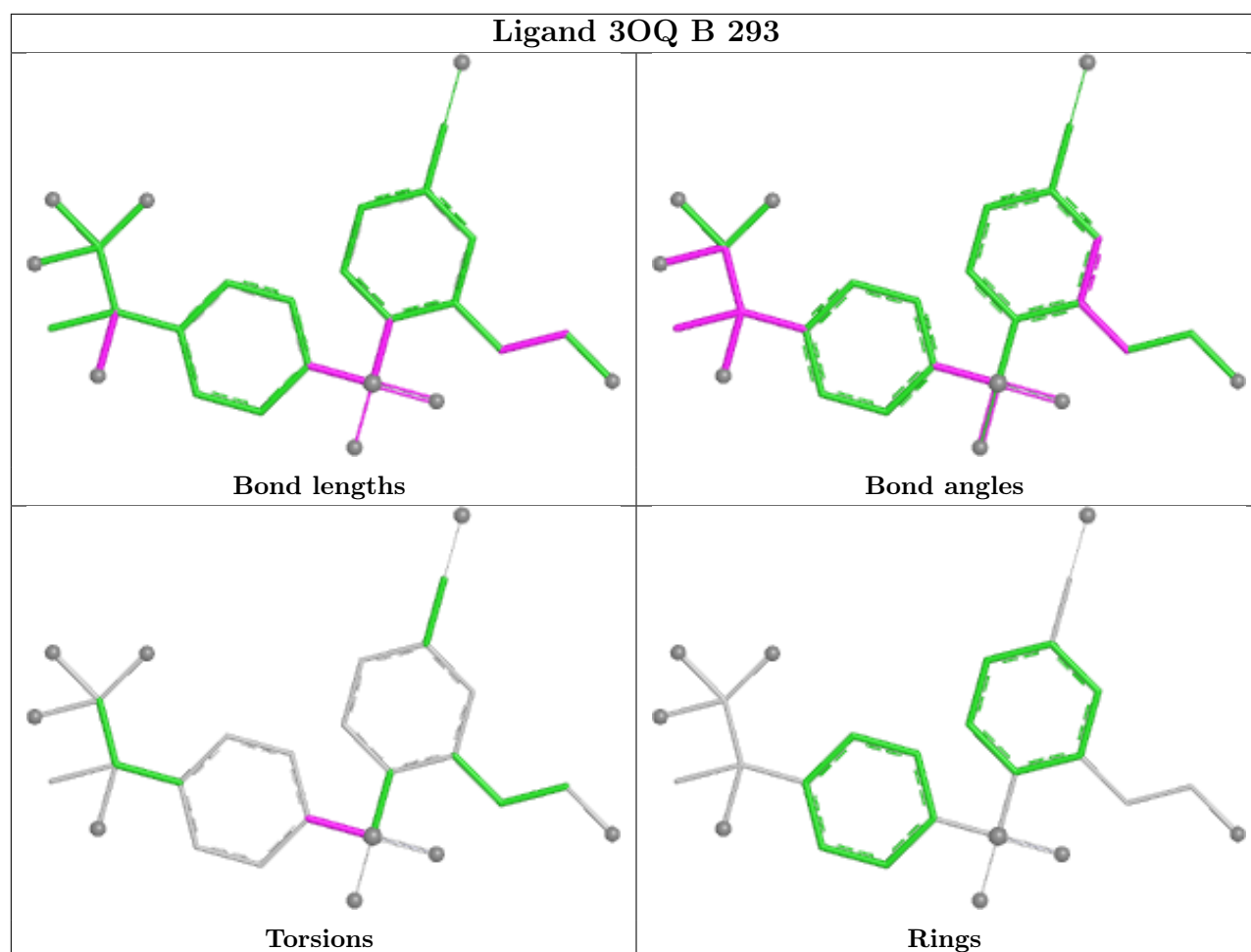
Continued on next page...

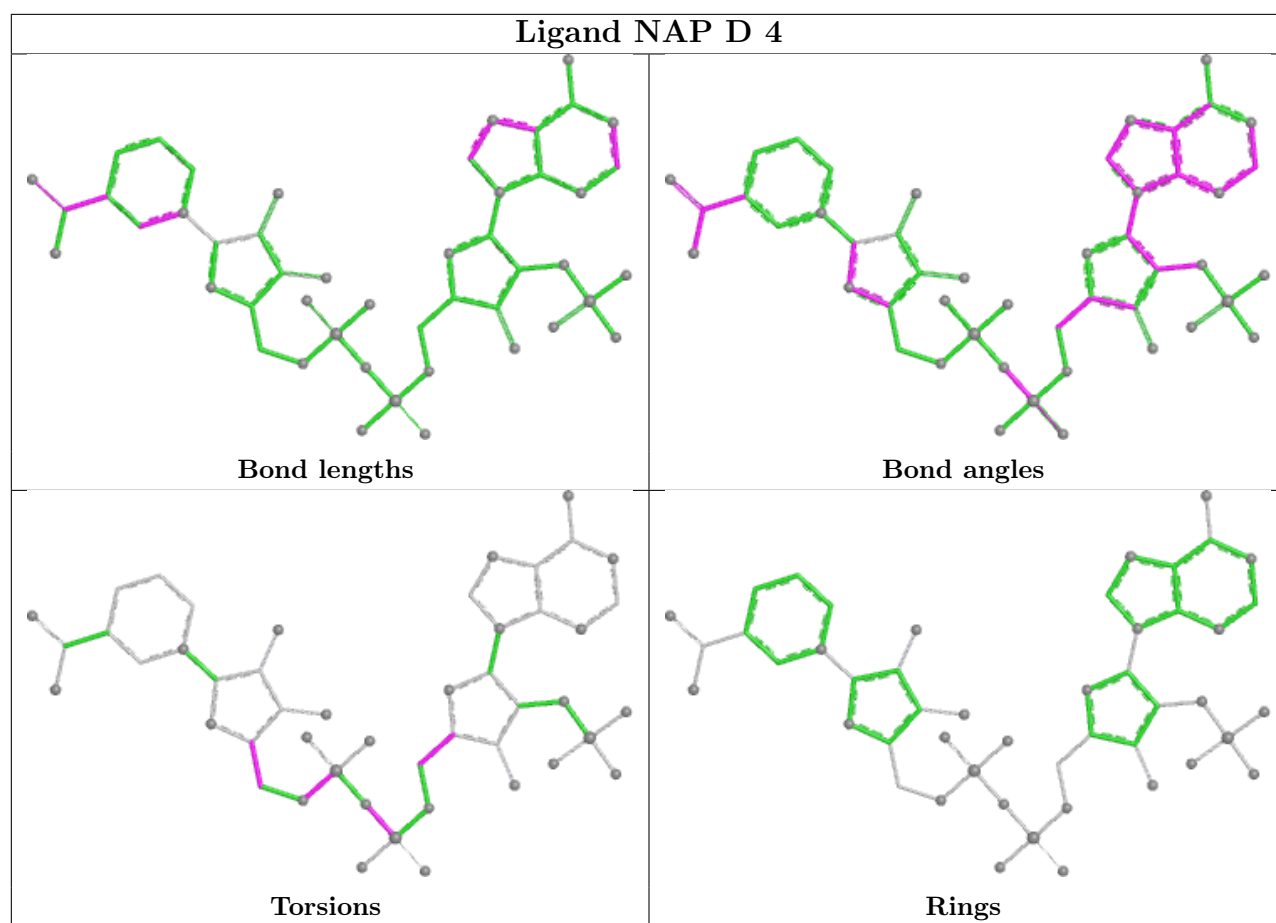
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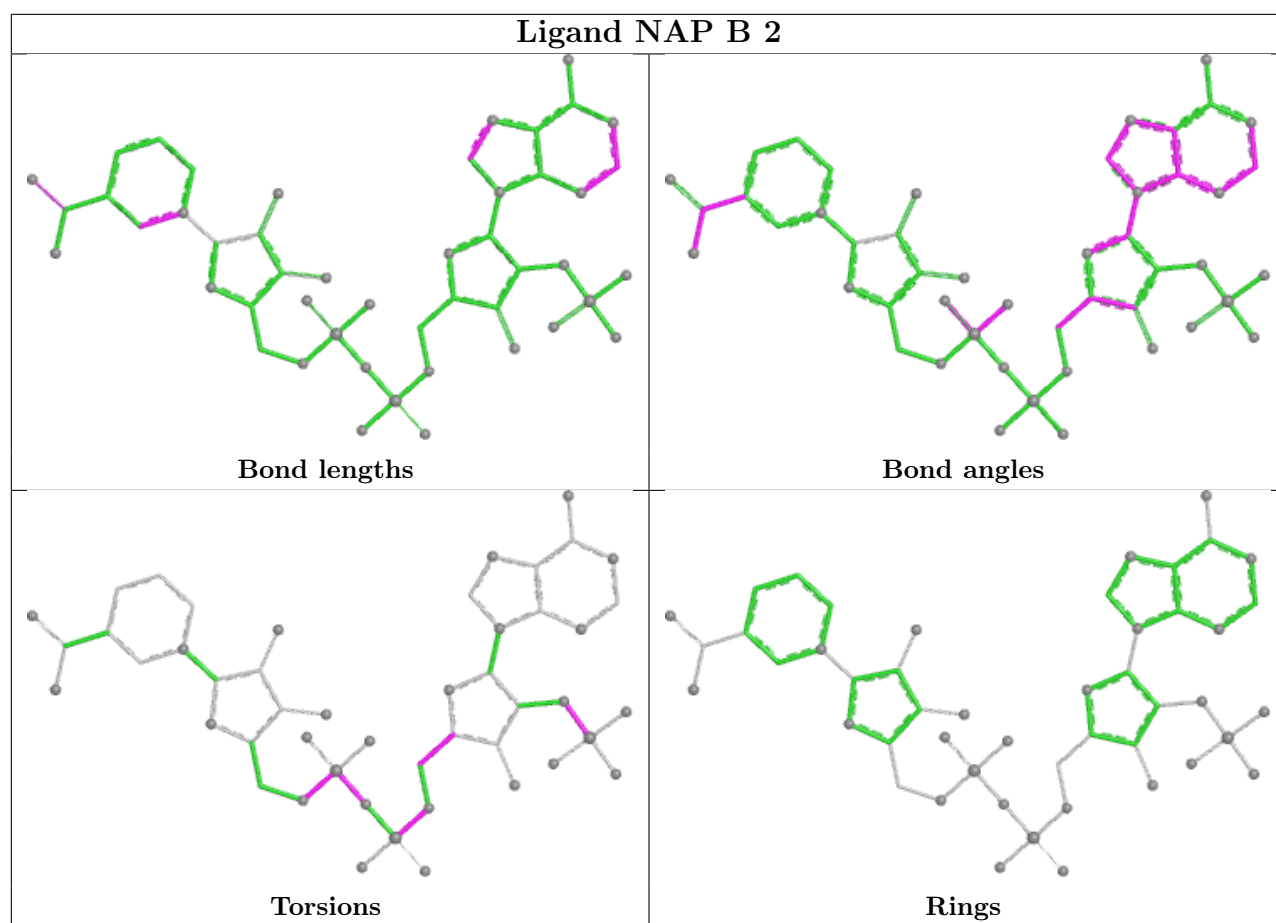
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAP	5	0
2	A	1	NAP	5	0
2	C	3	NAP	4	0
3	C	293	3OQ	3	0

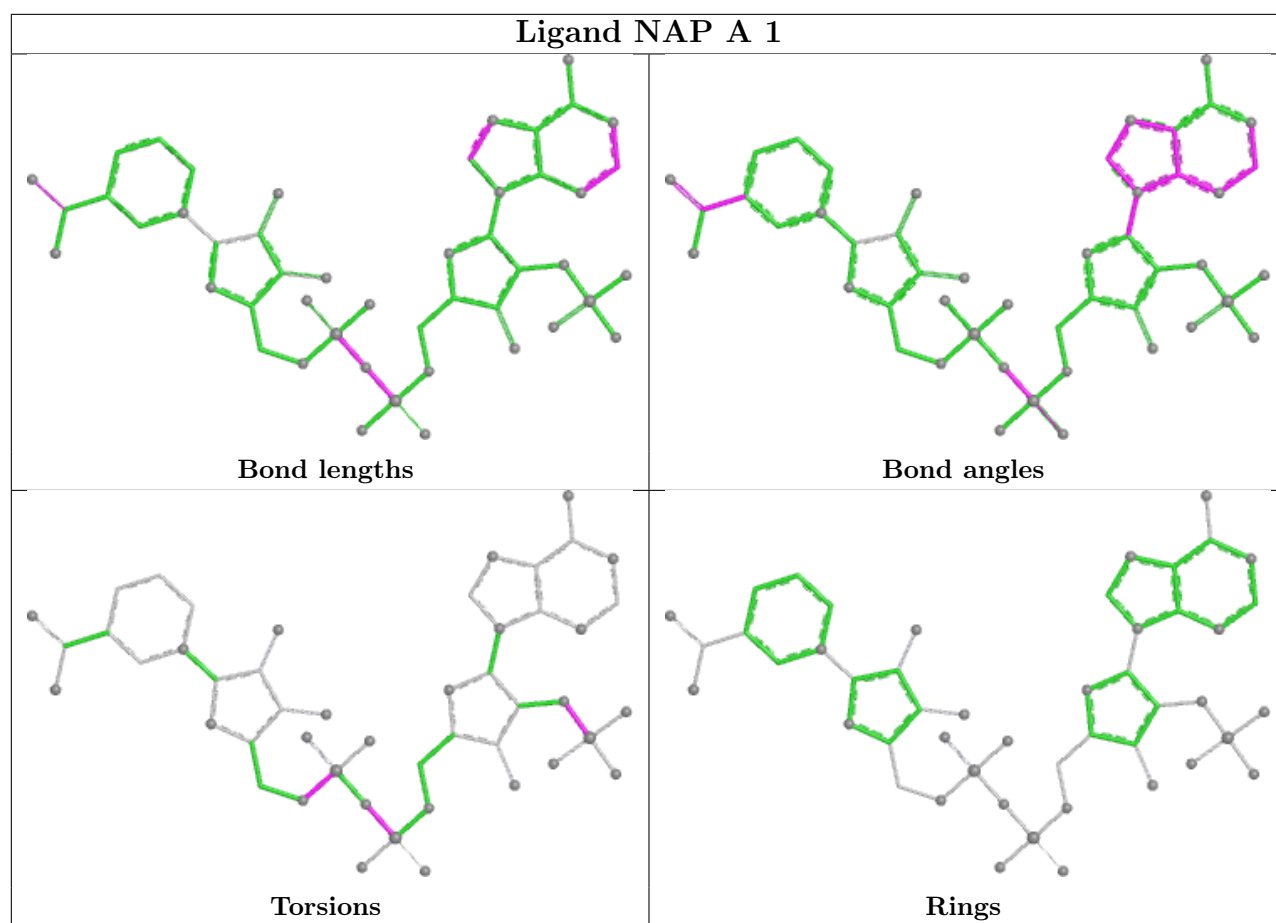
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

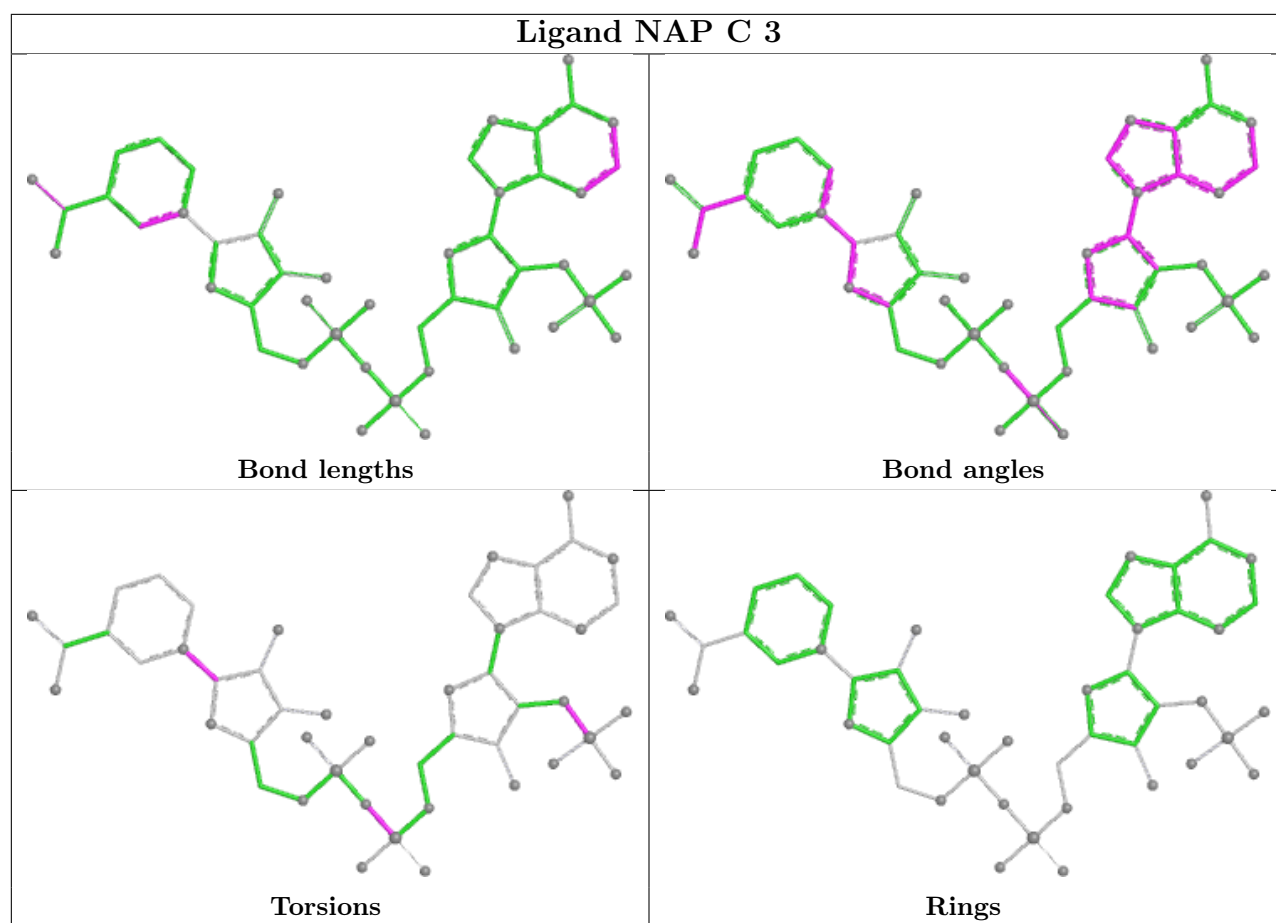




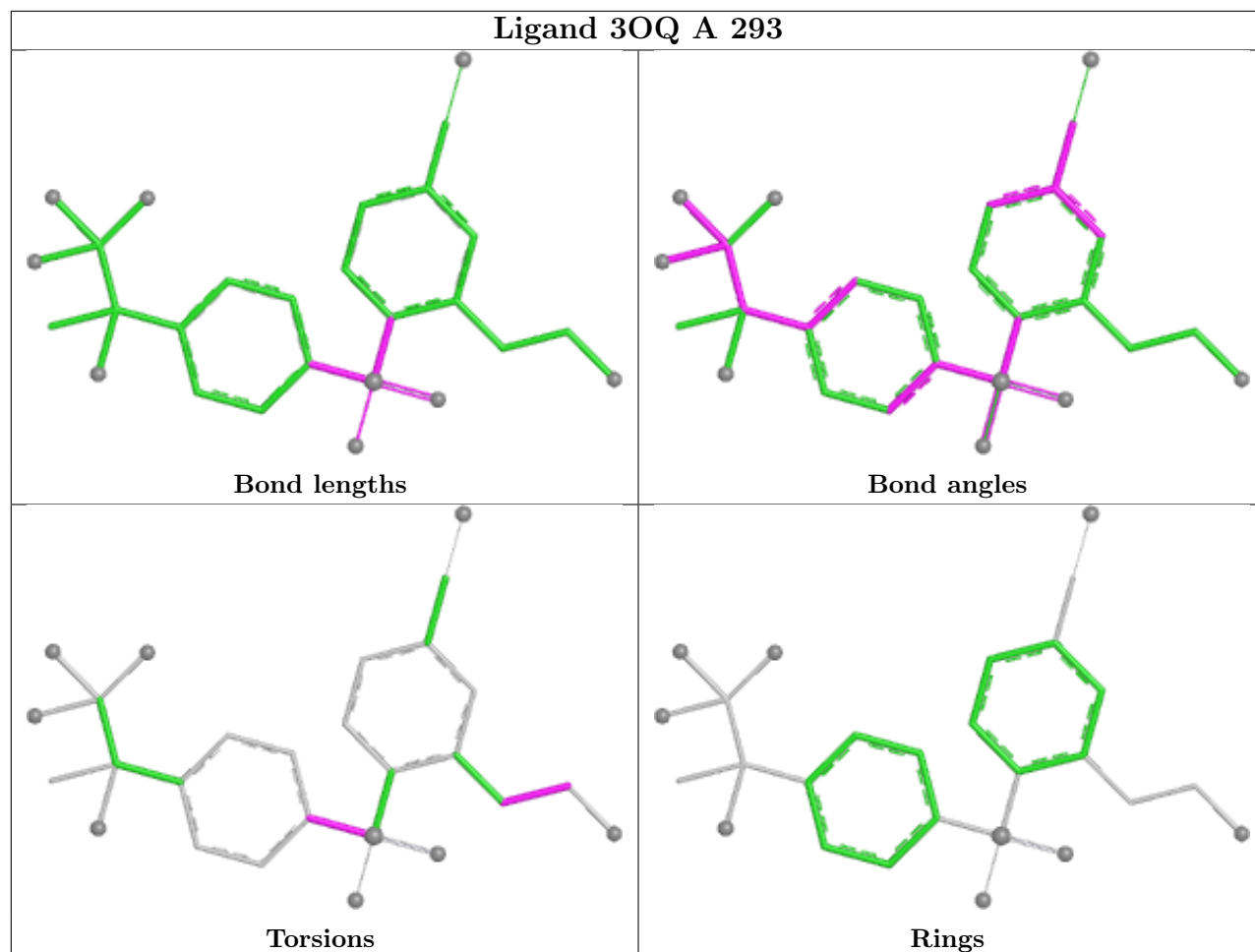


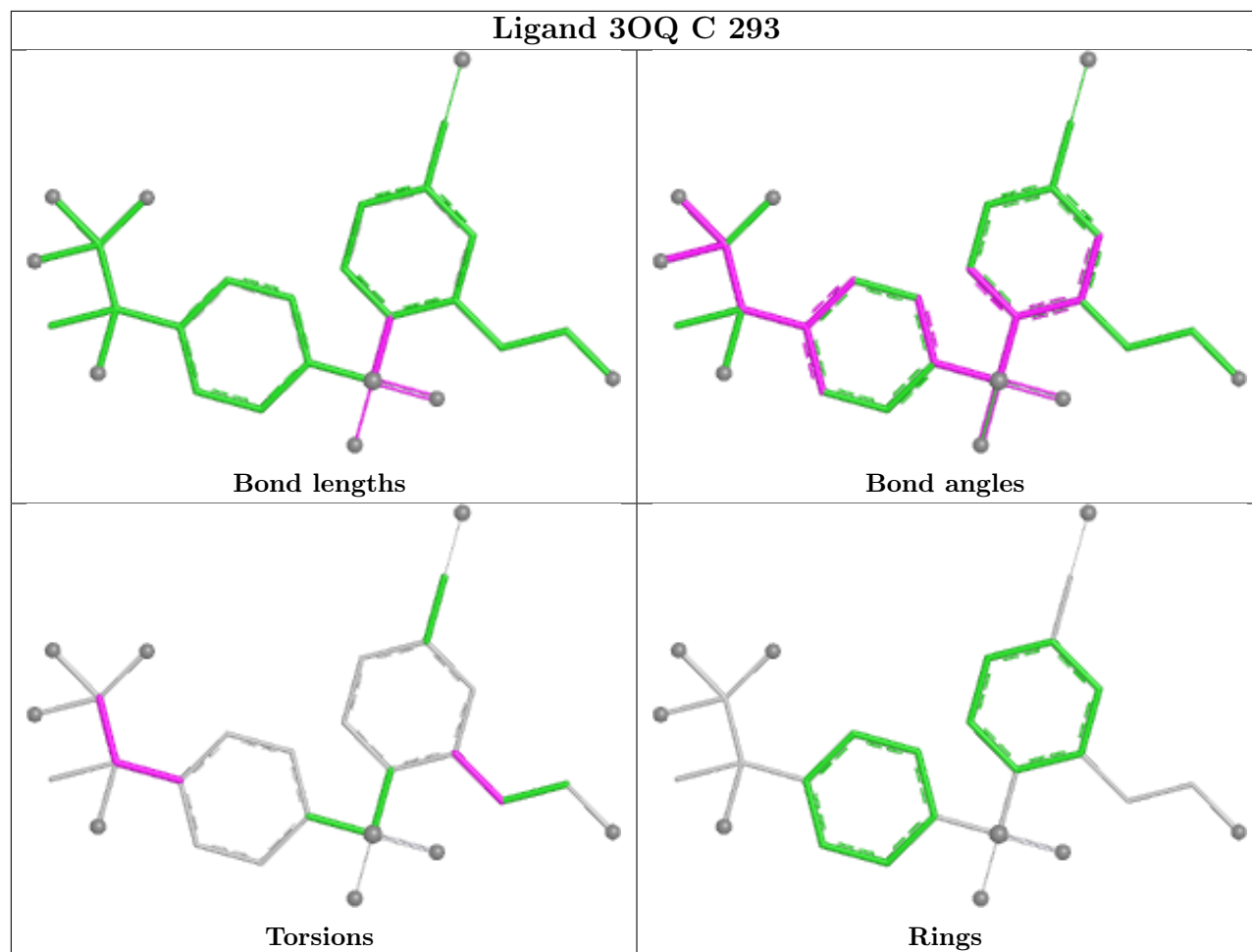






Ligand 3OQ A 293





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	261/286 (91%)	0.41	6 (2%) 61 55	33, 74, 100, 115	0
1	B	267/286 (93%)	0.08	4 (1%) 72 68	37, 58, 91, 109	1 (0%)
1	C	269/286 (94%)	0.20	7 (2%) 57 51	42, 63, 96, 112	0
1	D	261/286 (91%)	0.05	2 (0%) 82 80	34, 56, 89, 103	1 (0%)
All	All	1058/1144 (92%)	0.19	19 (1%) 67 63	33, 62, 97, 115	2 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	231	VAL	4.2
1	A	231	VAL	3.3
1	A	23	LEU	3.2
1	C	22	PRO	2.7
1	C	262	LEU	2.4
1	B	177	TYR	2.4
1	C	289	PHE	2.4
1	A	22	PRO	2.3
1	D	233	MET	2.3
1	C	130	HIS	2.3
1	C	229	GLY	2.2
1	A	203	VAL	2.1
1	A	226	ALA	2.1
1	C	76	SER	2.1
1	B	77	HIS	2.1
1	A	75	VAL	2.1
1	B	263	TRP	2.0
1	B	23	LEU	2.0
1	C	132	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

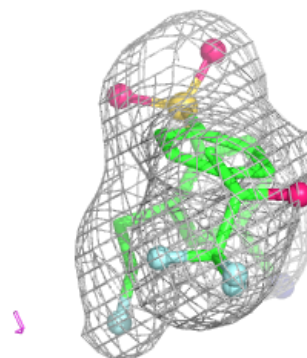
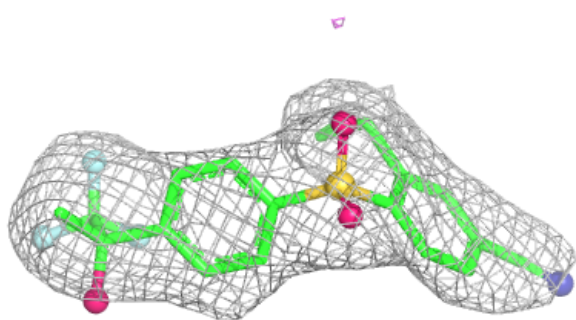
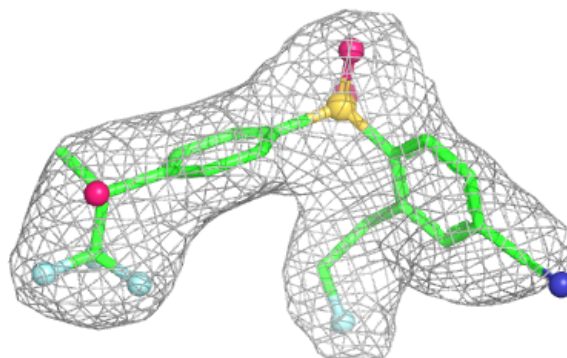
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	3OQ	A	293	27/27	0.92	0.10	69,72,75,78	0
3	3OQ	C	293	27/27	0.92	0.11	63,66,72,74	0
3	3OQ	D	293	27/27	0.92	0.12	80,84,91,95	0
2	NAP	A	1	48/48	0.94	0.08	64,70,74,76	0
3	3OQ	B	293	27/27	0.94	0.10	62,70,78,83	0
2	NAP	C	3	48/48	0.95	0.08	44,53,63,65	0
2	NAP	B	2	48/48	0.96	0.07	40,52,59,60	0
2	NAP	D	4	48/48	0.96	0.06	36,47,51,55	0

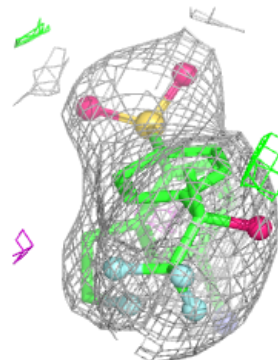
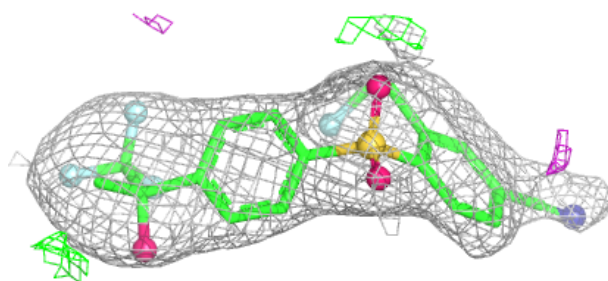
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3OQ A 293:

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

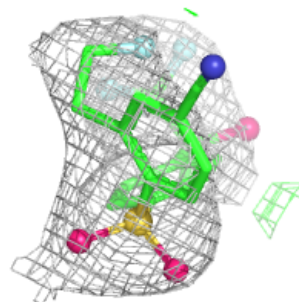
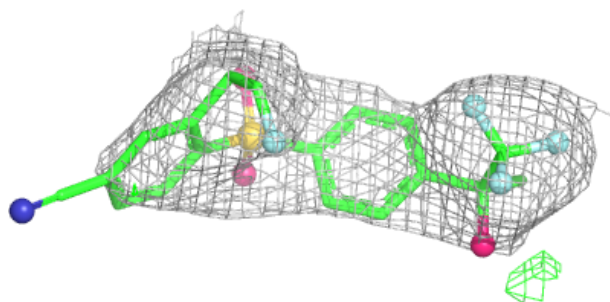
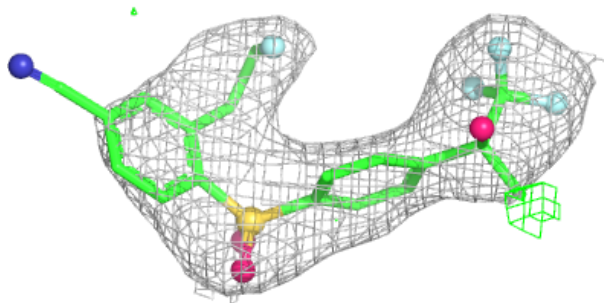
**Electron density around 3OQ C 293:**

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

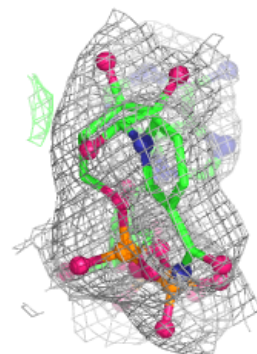
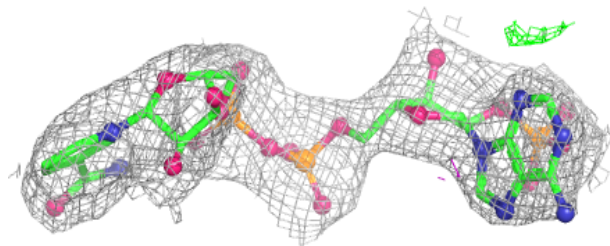
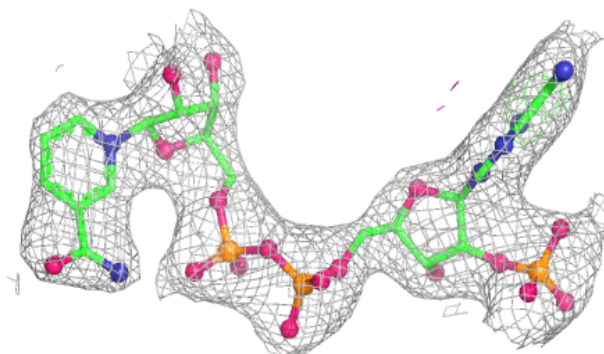


Electron density around 3OQ D 293:

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

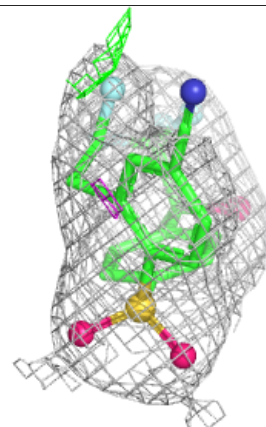
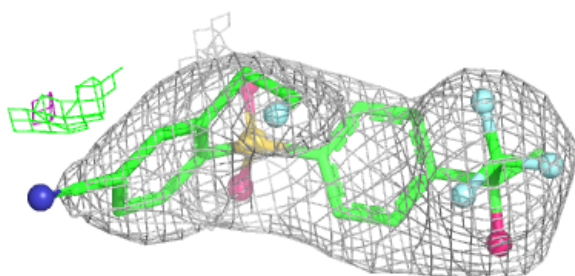
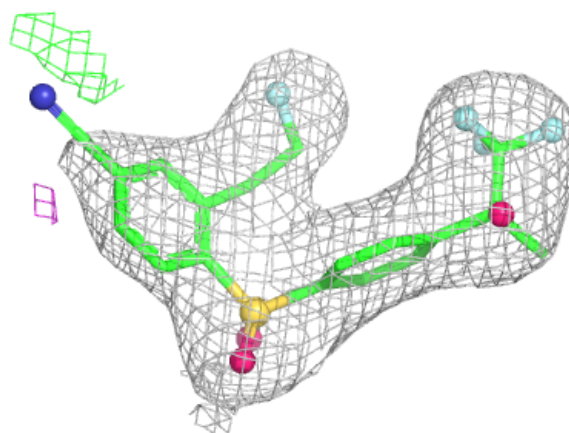
**Electron density around NAP A 1:**

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

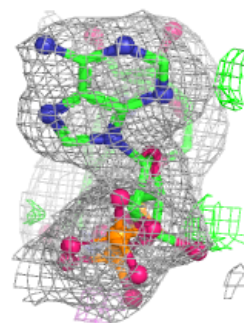
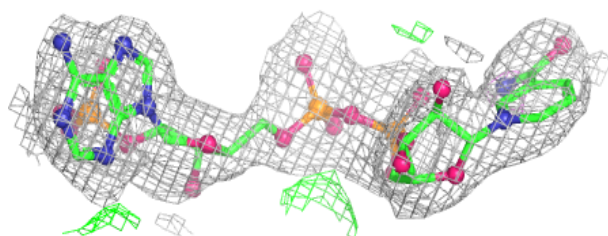
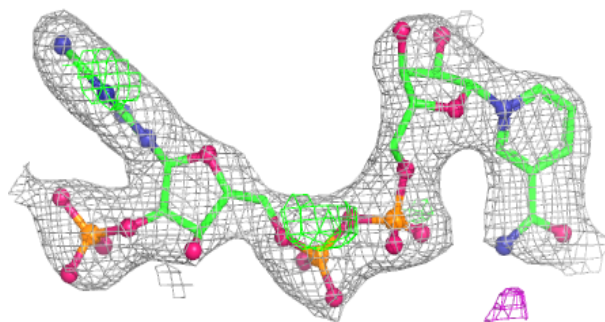


Electron density around 3OQ B 293:

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

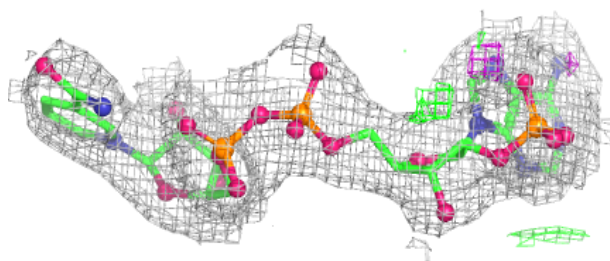
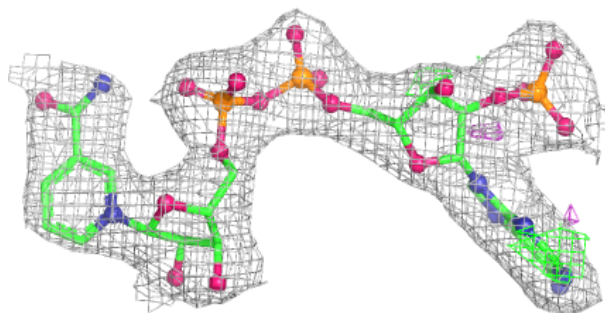
**Electron density around NAP C 3:**

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

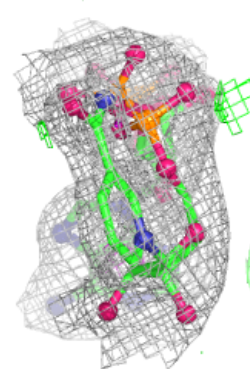
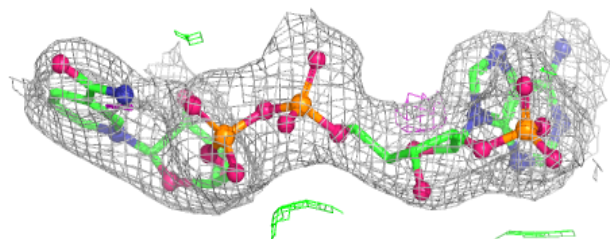
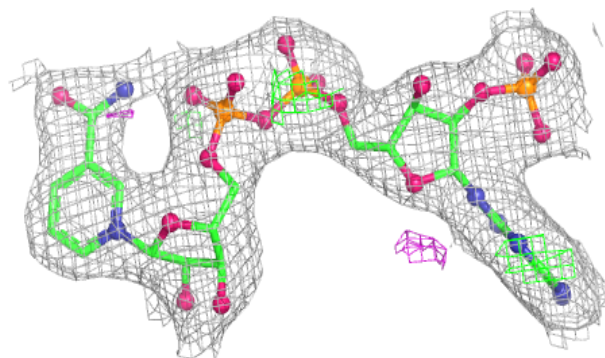


Electron density around NAP B 2:

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

**Electron density around NAP D 4:**

$2mF_o-DF_c$ (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.