



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:20 AM UTC

PDB ID : 3RAS / pdb_00003ras
Title : Crystal structure of 1-deoxy-D-xylulose 5-phosphate reductoisomerase (DXR) complexed with a lipophilic phosphonate inhibitor
Authors : Diao, J.; Deng, L.; Prasad, B.V.V.; Song, Y.
Deposited on : 2011-03-28
Resolution : 2.55 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

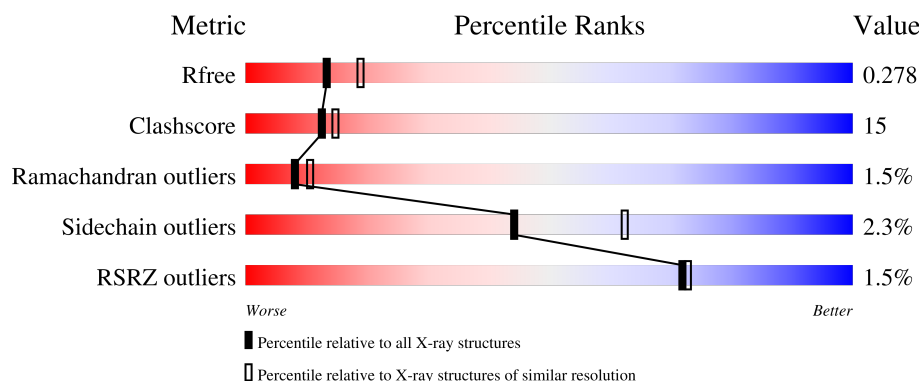
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

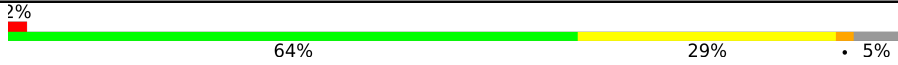
The reported resolution of this entry is 2.55 Å.

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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	398	
1	B	398	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5864 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 1-deoxy-D-xylulose 5-phosphate reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2781	1742	502	528	9			
1	B	379	Total	C	N	O	S	0	0	0
			2781	1742	502	528	9			

There are 20 discrepancies between the modelled and reference sequences:

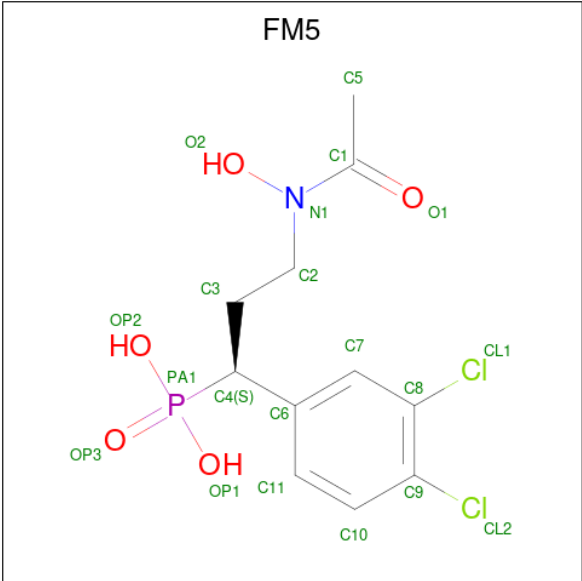
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	THR	-	expression tag	UNP P64012
A	-7	MET	-	expression tag	UNP P64012
A	-6	ALA	-	expression tag	UNP P64012
A	-5	HIS	-	expression tag	UNP P64012
A	-4	HIS	-	expression tag	UNP P64012
A	-3	HIS	-	expression tag	UNP P64012
A	-2	HIS	-	expression tag	UNP P64012
A	-1	HIS	-	expression tag	UNP P64012
A	0	HIS	-	expression tag	UNP P64012
A	1	VAL	-	expression tag	UNP P64012
B	-8	THR	-	expression tag	UNP P64012
B	-7	MET	-	expression tag	UNP P64012
B	-6	ALA	-	expression tag	UNP P64012
B	-5	HIS	-	expression tag	UNP P64012
B	-4	HIS	-	expression tag	UNP P64012
B	-3	HIS	-	expression tag	UNP P64012
B	-2	HIS	-	expression tag	UNP P64012
B	-1	HIS	-	expression tag	UNP P64012
B	0	HIS	-	expression tag	UNP P64012
B	1	VAL	-	expression tag	UNP P64012

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



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

- Molecule 3 is 3-(N-HYDROXYACETAMIDO)-1-(3,4-DICHLOROPHENYL)PROPYLPHOSPHONIC ACID (CCD ID: FM5) (formula: C₁₁H₁₄Cl₂NO₅P).



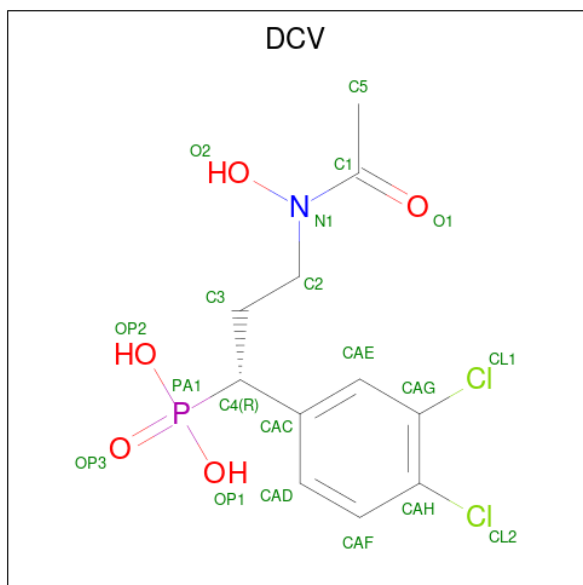
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	Cl	N	O	P	0	0
			20	11	2	1	5	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	O	P	
			20	11	2	1	5	1	
								0	0

- Molecule 4 is [(1R)-3-[acetyl(hydroxy)amino]-1-(3,4-dichlorophenyl)propyl]phosphonic acid (CCD ID: DCV) (formula: C₁₁H₁₄Cl₂NO₅P).

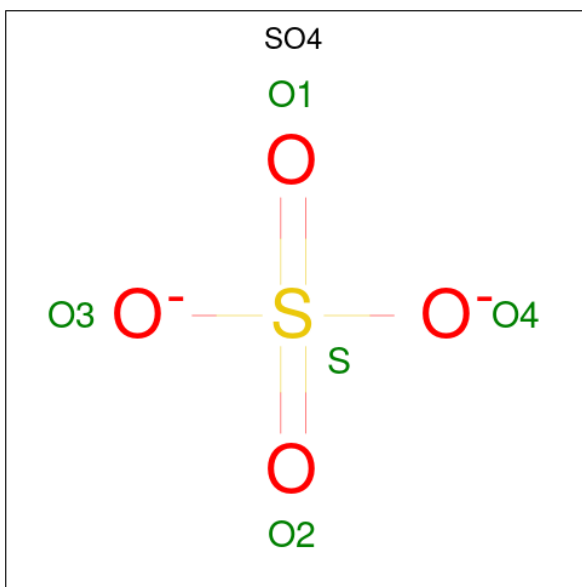


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	P	
			20	11	2	1	5	1	
								0	0
4	B	1	Total	C	Cl	N	O	P	
			20	11	2	1	5	1	
								0	0

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mn		
			1	1	0	0
5	B	1	Total	Mn		
			1	1	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		

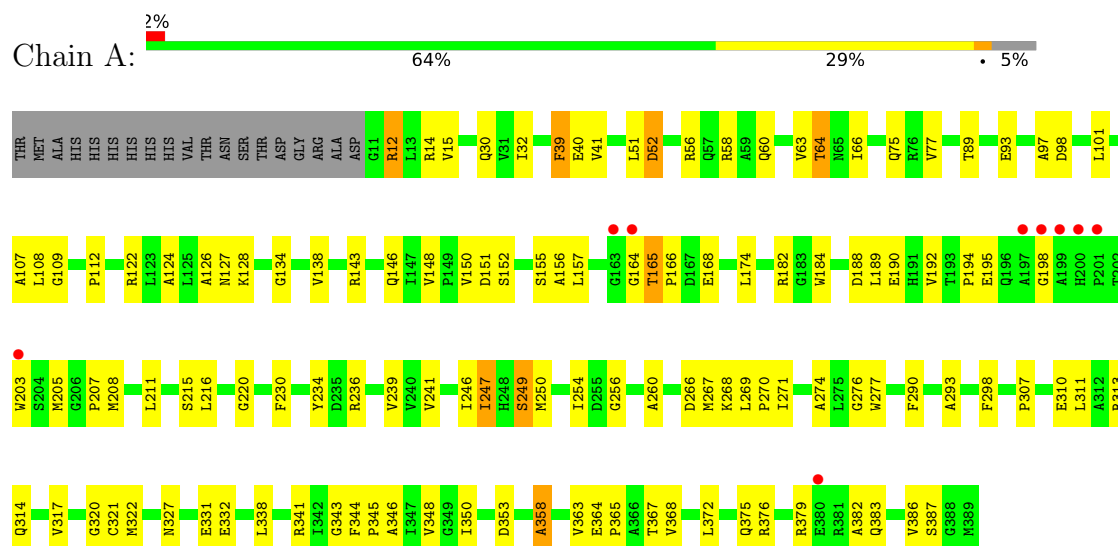
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	51	Total	O	0	0
			51	51		
7	B	68	Total	O	0	0
			68	68		

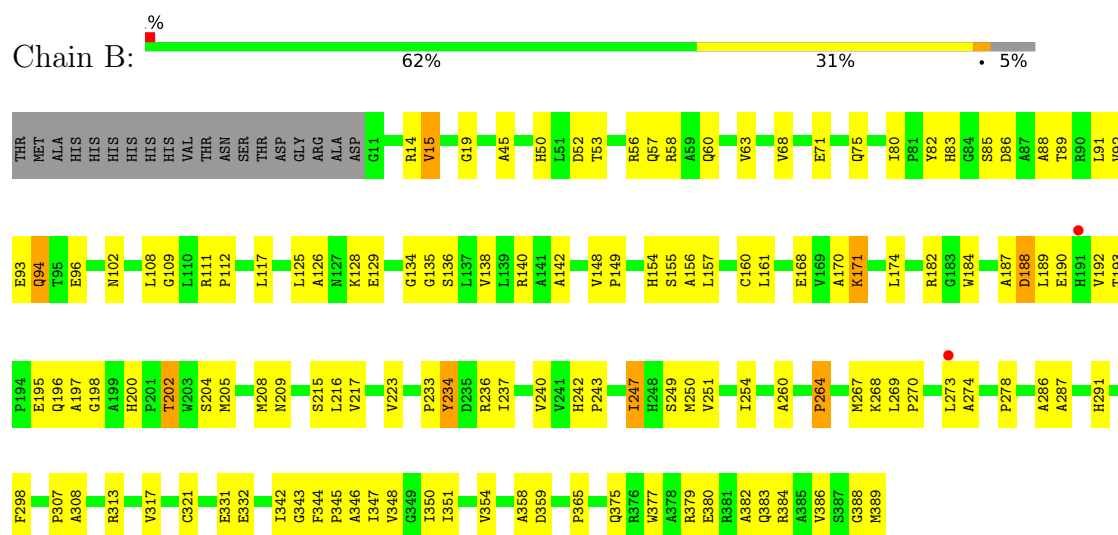
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.25Å 65.18Å 85.41Å 90.00° 101.28° 90.00°	Depositor
Resolution (Å)	33.45 – 2.55 33.45 – 2.55	Depositor EDS
% Data completeness (in resolution range)	93.5 (33.45-2.55) 93.5 (33.45-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.54Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.208 , 0.278 0.208 , 0.278	Depositor DCC
R_{free} test set	1111 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5864	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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: SO4, FM5, DCV, NDP, MN

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	0.51	0/2835	1.03	13/3873 (0.3%)
1	B	0.50	0/2835	0.98	10/3873 (0.3%)
All	All	0.50	0/5670	1.01	23/7746 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ALA	N-CA-C	-8.97	102.12	113.43
1	A	246	ILE	N-CA-C	-8.38	103.71	111.67
1	A	98	ASP	N-CA-C	-6.75	105.58	113.88
1	B	291	HIS	N-CA-C	-6.70	104.59	112.89
1	A	15	VAL	N-CA-C	6.53	117.88	108.48
1	B	15	VAL	N-CA-C	6.10	117.80	108.71
1	B	193	THR	CA-C-N	6.10	125.58	119.24
1	B	193	THR	C-N-CA	6.10	125.58	119.24
1	B	247	ILE	N-CA-C	-6.05	100.99	109.21
1	A	155	SER	N-CA-C	-5.96	104.78	111.28
1	A	152	SER	N-CA-C	5.81	118.39	111.71
1	A	234	TYR	N-CA-C	5.73	119.08	111.75
1	B	264	PRO	N-CA-C	-5.69	105.01	110.47
1	A	39	PHE	N-CA-C	5.69	118.33	109.52
1	B	125	LEU	N-CA-C	5.49	117.69	108.96
1	A	247	ILE	N-CA-C	-5.41	102.53	109.30
1	B	234	TYR	N-CA-C	5.40	117.87	111.33
1	B	242	HIS	CA-C-N	5.32	126.49	119.84
1	B	242	HIS	C-N-CA	5.32	126.49	119.84
1	A	220	GLY	N-CA-C	-5.28	106.38	112.50
1	A	230	PHE	N-CA-C	5.22	119.80	113.38
1	A	164	GLY	N-CA-C	5.01	118.30	110.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	VAL	N-CA-C	-5.01	107.95	112.96

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	2781	0	2768	78	0
1	B	2781	0	2768	98	0
2	A	48	0	26	0	0
2	B	48	0	26	2	0
3	A	20	0	7	1	0
3	B	20	0	6	1	0
4	A	20	0	5	0	0
4	B	20	0	7	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	5	0	0	0	0
7	A	51	0	0	3	0
7	B	68	0	0	7	0
All	All	5864	0	5613	174	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 15.

All (174) 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:307:PRO:HG2	1:A:348:VAL:HG11	1.50	0.92
1:A:75:GLN:HE21	1:A:75:GLN:HA	1.46	0.80
1:B:273:LEU:HB2	7:B:399:HOH:O	1.84	0.78
1:B:379:ARG:O	1:B:383:GLN:HG3	1.84	0.77
1:A:58:ARG:HG3	1:A:63:VAL:O	1.88	0.74
1:A:313:ARG:O	1:A:317:VAL:HG23	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:O	1:A:60:GLN:HG3	1.88	0.73
1:A:310:GLU:O	1:A:314:GLN:HG3	1.89	0.72
1:A:75:GLN:HA	1:A:75:GLN:NE2	2.05	0.71
1:B:234:TYR:HB3	1:B:313:ARG:HG2	1.73	0.69
1:B:148:VAL:HG11	1:B:274:ALA:HA	1.74	0.69
1:B:267:MET:HE2	2:B:1392:NDP:H42N	1.73	0.68
1:B:53:THR:O	1:B:57:GLN:HG3	1.95	0.67
1:A:190:GLU:HG3	1:A:345:PRO:HG2	1.76	0.66
1:A:108:LEU:HD12	1:A:109:GLY:N	2.12	0.65
1:A:379:ARG:O	1:A:383:GLN:HG2	1.97	0.65
1:B:14:ARG:HH12	1:B:96:GLU:HG2	1.62	0.65
1:A:211:LEU:HD22	1:A:338:LEU:HD21	1.80	0.64
1:B:313:ARG:O	1:B:317:VAL:HG23	1.98	0.64
1:B:195:GLU:HG3	1:B:200:HIS:NE2	2.13	0.63
1:B:71:GLU:O	1:B:75:GLN:HG2	1.98	0.63
1:B:85:SER:O	1:B:86:ASP:HB2	1.97	0.63
1:A:189:LEU:O	1:A:192:VAL:HG23	1.99	0.62
1:B:168:GLU:O	1:B:254:ILE:HG23	1.99	0.62
1:A:89:THR:O	1:A:93:GLU:HG3	1.99	0.62
1:B:344:PHE:HB3	1:B:345:PRO:HD3	1.82	0.62
1:B:184:TRP:CE3	1:B:188:ASP:HB3	2.35	0.62
1:B:307:PRO:HG2	1:B:348:VAL:HG11	1.81	0.61
1:B:202:THR:HG22	1:B:204:SER:H	1.66	0.61
1:B:56:ARG:O	1:B:60:GLN:HG3	2.01	0.60
1:A:332:GLU:HG3	1:A:379:ARG:HA	1.84	0.60
1:A:344:PHE:HB3	1:A:345:PRO:HD3	1.83	0.60
1:A:341:ARG:NH2	1:A:387:SER:HA	2.17	0.60
1:A:108:LEU:HD12	1:A:108:LEU:C	2.25	0.60
1:B:148:VAL:CG1	1:B:274:ALA:HA	2.32	0.60
1:B:247:ILE:HD12	1:B:298:PHE:HZ	1.66	0.60
1:B:189:LEU:HA	1:B:192:VAL:CG2	2.32	0.60
1:B:14:ARG:HH12	1:B:96:GLU:CG	2.16	0.59
1:B:52:ASP:HB3	1:B:56:ARG:HH12	1.68	0.58
1:B:82:TYR:OH	1:B:94:GLN:HG2	2.03	0.58
1:A:266:ASP:OD1	1:A:268:LYS:HG3	2.03	0.58
1:B:182:ARG:NE	1:B:243:PRO:HG3	2.19	0.58
1:B:205:MET:HE2	1:B:209:ASN:HB2	1.85	0.58
1:A:327:ASN:O	1:A:331:GLU:HG3	2.04	0.57
1:B:196:GLN:C	1:B:198:GLY:H	2.11	0.57
1:B:343:GLY:O	1:B:346:ALA:HB3	2.05	0.57
1:A:327:ASN:HB3	7:A:437:HOH:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ALA:O	1:A:386:VAL:HG23	2.06	0.56
1:A:269:LEU:HB3	1:A:270:PRO:CD	2.36	0.55
1:A:311:LEU:HD12	1:A:348:VAL:HG13	1.87	0.55
1:B:128:LYS:HD2	7:B:434:HOH:O	2.07	0.55
1:B:157:LEU:CD2	1:B:249:SER:HB3	2.37	0.55
1:B:205:MET:CE	1:B:209:ASN:HB2	2.36	0.55
1:A:12:ARG:HH21	1:A:40:GLU:CG	2.20	0.54
1:B:155:SER:OG	1:B:273:LEU:HD12	2.07	0.54
1:A:58:ARG:HD3	1:A:66:ILE:HD12	1.90	0.54
1:B:380:GLU:HG3	7:B:398:HOH:O	2.07	0.54
1:A:168:GLU:HA	1:A:254:ILE:HD13	1.89	0.53
1:B:321:CYS:SG	1:B:365:PRO:HB3	2.48	0.53
1:A:109:GLY:C	1:A:112:PRO:HD2	2.33	0.53
1:B:182:ARG:HE	1:B:243:PRO:HG3	1.73	0.53
1:B:187:ALA:O	1:B:190:GLU:HG2	2.08	0.53
1:B:189:LEU:HA	1:B:192:VAL:HG23	1.92	0.52
1:B:250:MET:HG2	1:B:260:ALA:HB2	1.91	0.52
1:B:269:LEU:HB3	1:B:270:PRO:CD	2.40	0.52
1:A:143:ARG:NH1	1:A:146:GLN:HG3	2.24	0.52
1:B:171:LYS:NZ	1:B:171:LYS:HB3	2.24	0.52
1:B:89:THR:O	1:B:93:GLU:HG3	2.10	0.51
1:B:215:SER:O	1:B:216:LEU:HB2	2.11	0.51
1:A:156:ALA:HB3	1:A:249:SER:HB2	1.93	0.51
1:B:170:ALA:O	1:B:171:LYS:HB3	2.12	0.50
1:A:311:LEU:CD1	1:A:348:VAL:HG13	2.40	0.50
1:B:382:ALA:O	1:B:386:VAL:HG23	2.11	0.50
1:A:75:GLN:HE21	1:A:75:GLN:CA	2.11	0.49
1:A:290:PHE:HB3	1:B:240:VAL:HG21	1.94	0.49
1:A:247:ILE:HD12	1:A:298:PHE:HZ	1.76	0.49
1:B:88:ALA:HB3	7:B:416:HOH:O	2.12	0.49
1:A:250:MET:HG2	1:A:260:ALA:HB2	1.94	0.49
1:A:128:LYS:HE2	1:A:151:ASP:OD2	2.13	0.49
1:B:117:LEU:HD13	1:B:142:ALA:HB2	1.94	0.49
1:A:350:ILE:HD13	1:A:386:VAL:HG22	1.95	0.49
1:A:332:GLU:OE2	1:A:383:GLN:NE2	2.45	0.49
1:B:75:GLN:HE21	1:B:75:GLN:HA	1.78	0.49
1:A:143:ARG:HG2	1:A:146:GLN:HB2	1.95	0.48
1:B:129:GLU:N	1:B:129:GLU:OE1	2.47	0.48
1:B:268:LYS:HE3	7:B:433:HOH:O	2.12	0.48
1:B:75:GLN:HA	1:B:75:GLN:NE2	2.29	0.48
1:B:160:CYS:HB2	1:B:251:VAL:HG23	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ARG:HD2	1:A:148:VAL:HG21	1.94	0.48
1:B:134:GLY:O	1:B:138:VAL:HG23	2.14	0.48
1:A:148:VAL:HG11	1:A:274:ALA:HA	1.96	0.48
1:B:58:ARG:HG3	1:B:63:VAL:O	2.14	0.48
1:B:250:MET:HG2	1:B:260:ALA:CB	2.43	0.48
1:B:50:HIS:HD2	3:B:390:FM5:OP1	1.97	0.47
1:B:136:SER:O	1:B:140:ARG:HG3	2.13	0.47
1:B:52:ASP:HB3	1:B:56:ARG:NH1	2.28	0.47
1:A:12:ARG:HH21	1:A:40:GLU:HG3	1.80	0.47
1:B:190:GLU:OE2	1:B:345:PRO:HG2	2.14	0.47
1:A:51:LEU:HD22	1:A:77:VAL:HG21	1.96	0.47
1:A:184:TRP:CD1	1:A:184:TRP:N	2.83	0.47
1:B:384:ARG:HD2	1:B:389:MET:O	2.15	0.46
1:A:75:GLN:NE2	1:A:75:GLN:CA	2.74	0.46
1:A:32:ILE:HG21	1:A:41:VAL:HG23	1.96	0.46
1:A:107:ALA:HB1	1:A:375:GLN:HE22	1.80	0.46
1:A:250:MET:HG2	1:A:260:ALA:CB	2.46	0.46
1:A:372:LEU:O	1:A:376:ARG:HB2	2.16	0.46
1:A:14:ARG:NH1	1:A:97:ALA:HA	2.31	0.46
1:A:269:LEU:HG	7:A:409:HOH:O	2.16	0.46
1:A:174:LEU:O	1:A:239:VAL:HA	2.16	0.45
1:B:157:LEU:HD21	1:B:249:SER:HB3	1.96	0.45
1:A:165:THR:HG22	1:A:166:PRO:HD2	1.97	0.45
1:A:343:GLY:O	1:A:346:ALA:HB3	2.17	0.45
1:B:160:CYS:CB	1:B:251:VAL:HG23	2.46	0.45
1:B:68:VAL:CG2	1:B:80:ILE:HD13	2.47	0.45
1:A:363:VAL:HG12	1:A:364:GLU:O	2.17	0.45
1:B:111:ARG:HB2	1:B:112:PRO:HD3	1.99	0.45
1:B:68:VAL:HG21	1:B:80:ILE:HD13	1.97	0.45
1:B:215:SER:OG	1:B:217:VAL:HG23	2.17	0.45
1:A:101:LEU:HA	1:A:124:ALA:HB3	1.99	0.44
1:A:208:MET:O	1:A:208:MET:HE3	2.17	0.44
1:A:134:GLY:HA3	1:A:138:VAL:HG23	1.99	0.44
1:A:182:ARG:HD2	1:A:241:VAL:HG11	1.99	0.44
1:A:322:MET:HE1	1:A:358:ALA:O	2.17	0.44
1:B:237:ILE:O	1:B:313:ARG:NH1	2.51	0.44
1:A:32:ILE:HG23	1:A:39:PHE:HB2	2.00	0.44
1:A:207:PRO:HG2	1:A:208:MET:H	1.83	0.44
1:B:233:PRO:HG2	1:B:236:ARG:HE	1.83	0.44
1:A:58:ARG:HD3	1:A:66:ILE:CD1	2.47	0.43
1:B:156:ALA:HB3	1:B:249:SER:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LEU:HD11	1:B:174:LEU:HD11	2.01	0.43
1:B:196:GLN:C	1:B:198:GLY:N	2.76	0.43
1:A:52:ASP:OD2	1:A:52:ASP:N	2.50	0.43
1:A:269:LEU:HB3	1:A:270:PRO:HD3	2.01	0.43
1:B:205:MET:HE2	1:B:209:ASN:HD22	1.84	0.43
1:A:30:GLN:OE1	1:A:268:LYS:NZ	2.47	0.43
1:A:157:LEU:CD2	1:A:249:SER:HB3	2.49	0.42
1:A:236:ARG:HD3	7:A:401:HOH:O	2.18	0.42
1:B:19:GLY:N	1:B:45:ALA:O	2.42	0.42
1:A:320:GLY:HA2	1:A:364:GLU:HA	2.02	0.42
1:B:149:PRO:HB2	1:B:154:HIS:HB2	2.01	0.42
1:B:88:ALA:O	1:B:92:VAL:HG23	2.19	0.42
1:B:157:LEU:O	1:B:161:LEU:HG	2.20	0.42
1:A:58:ARG:HD2	1:A:64:THR:HG22	2.01	0.42
1:A:321:CYS:SG	1:A:365:PRO:HB3	2.59	0.42
1:B:269:LEU:O	1:B:273:LEU:HG	2.20	0.42
1:B:386:VAL:C	1:B:388:GLY:H	2.27	0.42
1:B:182:ARG:HD3	7:B:440:HOH:O	2.20	0.42
1:B:347:ILE:O	1:B:351:ILE:HG13	2.20	0.42
1:A:215:SER:O	1:A:216:LEU:HB2	2.20	0.42
1:B:109:GLY:C	1:B:112:PRO:HD2	2.44	0.42
1:B:208:MET:HE2	1:B:331:GLU:OE1	2.20	0.42
1:B:375:GLN:O	1:B:379:ARG:HG3	2.20	0.42
1:A:267:MET:O	1:A:271:ILE:HG13	2.20	0.41
1:A:375:GLN:O	1:A:379:ARG:HG3	2.19	0.41
1:A:109:GLY:O	1:A:112:PRO:HD2	2.19	0.41
1:A:205:MET:SD	3:A:390:FM5:H22C	2.60	0.41
1:B:171:LYS:HB3	1:B:171:LYS:HZ3	1.84	0.41
1:B:264:PRO:HD2	1:B:286:ALA:O	2.20	0.41
1:B:379:ARG:HG2	1:B:379:ARG:HH11	1.85	0.41
1:B:308:ALA:HB2	7:B:427:HOH:O	2.21	0.41
1:A:276:GLY:O	1:A:277:TRP:C	2.61	0.41
1:B:354:VAL:HG21	1:B:382:ALA:HB2	2.03	0.41
1:B:358:ALA:HB2	1:B:377:TRP:CZ3	2.55	0.41
1:B:189:LEU:HA	1:B:192:VAL:HG21	2.03	0.41
1:B:91:LEU:HD23	1:B:91:LEU:C	2.46	0.41
1:B:189:LEU:C	1:B:192:VAL:HG23	2.46	0.41
1:A:367:THR:O	1:A:368:VAL:C	2.63	0.41
1:B:71:GLU:OE2	1:B:83:HIS:ND1	2.53	0.41
1:B:332:GLU:HG2	1:B:383:GLN:HG2	2.02	0.41
1:B:331:GLU:OE1	1:B:331:GLU:HA	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ILE:HD13	1:B:350:ILE:HD12	2.03	0.40
1:B:102:ASN:O	1:B:126:ALA:HB3	2.22	0.40
1:B:108:LEU:HD22	2:B:1392:NDP:H61A	1.86	0.40
1:A:256:GLY:HA2	1:B:287:ALA:HB2	2.04	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	377/398 (95%)	353 (94%)	17 (4%)	7 (2%)	6	7
1	B	377/398 (95%)	358 (95%)	15 (4%)	4 (1%)	11	15
All	All	754/796 (95%)	711 (94%)	32 (4%)	11 (2%)	8	10

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	SER
1	B	135	GLY
1	B	188	ASP
1	A	12	ARG
1	B	197	ALA
1	A	127	ASN
1	A	293	ALA
1	A	358	ALA
1	B	359	ASP
1	A	194	PRO
1	A	198	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/298 (95%)	275 (98%)	7 (2%)	42	60
1	B	282/298 (95%)	276 (98%)	6 (2%)	47	66
All	All	564/596 (95%)	551 (98%)	13 (2%)	44	62

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	64	THR
1	A	165	THR
1	A	188	ASP
1	A	195	GLU
1	A	203	TRP
1	A	353	ASP
1	B	15	VAL
1	B	94	GLN
1	B	171	LYS
1	B	202	THR
1	B	223	VAL
1	B	278	PRO

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	57	GLN
1	A	65	ASN
1	A	75	GLN
1	A	83	HIS
1	A	330	ASN
1	A	375	GLN
1	A	383	GLN
1	B	50	HIS
1	B	60	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	75	GLN
1	B	209	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	FM5	A	390	5	18,20,20	3.52	8 (44%)	20,29,29	1.44	4 (20%)
4	DCV	A	391	5	18,20,20	4.35	11 (61%)	20,29,29	2.53	2 (10%)
2	NDP	A	1391	-	51,52,52	1.64	8 (15%)	71,80,80	1.62	11 (15%)
2	NDP	B	1392	-	51,52,52	1.61	6 (11%)	71,80,80	1.63	12 (16%)
4	DCV	B	391	-	18,20,20	3.31	8 (44%)	20,29,29	1.56	3 (15%)
3	FM5	B	390	-	18,20,20	3.41	9 (50%)	20,29,29	1.49	3 (15%)
6	SO4	B	393	-	4,4,4	0.44	0	6,6,6	0.25	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
3	FM5	A	390	5	-	5/19/19/19	0/1/1/1
4	DCV	A	391	5	-	3/19/19/19	0/1/1/1
2	NDP	A	1391	-	-	4/34/77/77	0/5/5/5
2	NDP	B	1392	-	-	4/34/77/77	0/5/5/5
4	DCV	B	391	-	-	8/19/19/19	0/1/1/1
3	FM5	B	390	-	-	7/19/19/19	0/1/1/1

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	391	DCV	PA1-C4	-14.81	1.61	1.81
3	A	390	FM5	PA1-C4	-11.87	1.65	1.81
3	B	390	FM5	PA1-C4	-10.94	1.67	1.81
4	B	391	DCV	PA1-C4	-10.51	1.67	1.81
2	A	1391	NDP	PA-O3	5.91	1.65	1.59
2	A	1391	NDP	PN-O3	5.84	1.65	1.59
4	A	391	DCV	CAE-CAC	5.83	1.47	1.39
2	B	1392	NDP	PA-O3	5.66	1.65	1.59
3	B	390	FM5	O2-N1	5.23	1.44	1.40
2	B	1392	NDP	PN-O3	5.15	1.65	1.59
4	B	391	DCV	O2-N1	4.88	1.43	1.40
4	A	391	DCV	O2-N1	4.45	1.43	1.40
4	A	391	DCV	CAD-CAC	4.41	1.46	1.39
3	A	390	FM5	C11-C6	4.16	1.45	1.39
3	A	390	FM5	O2-N1	3.75	1.42	1.40
4	B	391	DCV	CAE-CAC	3.74	1.44	1.39
4	B	391	DCV	CAE-CAG	3.66	1.44	1.38
3	B	390	FM5	C7-C8	3.17	1.43	1.38
4	A	391	DCV	CAE-CAG	3.16	1.43	1.38
3	B	390	FM5	C11-C6	3.16	1.44	1.39
3	A	390	FM5	C11-C10	3.11	1.43	1.38
3	A	390	FM5	C10-C9	3.08	1.45	1.38
2	B	1392	NDP	O4D-C1D	3.01	1.49	1.42
4	A	391	DCV	CAF-CAH	2.96	1.44	1.38
3	B	390	FM5	C7-C6	2.92	1.43	1.39
3	A	390	FM5	C7-C6	2.81	1.43	1.39
2	A	1391	NDP	O4D-C1D	2.80	1.48	1.42
3	B	390	FM5	C11-C10	2.75	1.43	1.38
4	B	391	DCV	CAD-CAC	2.63	1.43	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1392	NDP	C5A-C4A	2.59	1.43	1.39
2	A	1391	NDP	O4B-C1B	2.57	1.48	1.42
2	A	1391	NDP	C5A-C4A	2.50	1.43	1.39
4	B	391	DCV	CAF-CAD	2.49	1.42	1.38
4	A	391	DCV	CAF-CAD	2.47	1.42	1.38
4	B	391	DCV	CAH-CAG	2.41	1.44	1.39
3	B	390	FM5	C8-C9	2.36	1.44	1.39
3	A	390	FM5	O1-C1	-2.32	1.13	1.23
4	A	391	DCV	CAH-CAG	2.26	1.44	1.39
3	B	390	FM5	C10-C9	2.26	1.43	1.38
3	A	390	FM5	C8-C9	2.25	1.44	1.39
2	A	1391	NDP	C5B-C4B	2.25	1.58	1.51
4	A	391	DCV	O1-C1	-2.22	1.13	1.23
2	B	1392	NDP	P2B-O2B	2.22	1.63	1.59
2	A	1391	NDP	C5A-N7A	-2.19	1.35	1.39
2	B	1392	NDP	C6A-N6A	2.14	1.39	1.34
4	A	391	DCV	PA1-OP2	-2.12	1.51	1.54
2	A	1391	NDP	C6A-N6A	2.05	1.39	1.34
3	B	390	FM5	O1-C1	-2.04	1.14	1.23
4	B	391	DCV	O1-C1	-2.02	1.14	1.23
4	A	391	DCV	CAC-C4	2.00	1.55	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	391	DCV	C3-C2-N1	-10.35	96.81	111.36
2	A	1391	NDP	N3A-C4A-N9A	5.16	135.94	127.17
2	B	1392	NDP	N3A-C2A-N1A	-5.01	121.00	128.58
2	B	1392	NDP	N3A-C4A-N9A	4.90	135.50	127.17
2	A	1391	NDP	N3A-C2A-N1A	-4.86	121.22	128.58
2	B	1392	NDP	C5A-C4A-N3A	-4.73	120.20	126.72
2	A	1391	NDP	C5A-C4A-N3A	-4.70	120.24	126.72
4	B	391	DCV	C3-C2-N1	-4.11	105.58	111.36
3	B	390	FM5	C3-C4-C6	-3.74	107.43	113.44
4	B	391	DCV	C3-C4-CAC	-3.55	107.74	113.44
2	B	1392	NDP	C2A-N3A-C4A	3.54	120.47	111.83
3	B	390	FM5	C3-C2-N1	-3.34	106.67	111.36
2	B	1392	NDP	P2B-O2B-C2B	-3.33	114.55	123.43
2	A	1391	NDP	C2A-N3A-C4A	3.28	119.84	111.83
2	A	1391	NDP	P2B-O2B-C2B	-3.19	114.91	123.43
3	A	390	FM5	C3-C4-C6	-3.17	108.35	113.44
3	A	390	FM5	C3-C2-N1	-3.03	107.10	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1391	NDP	C5A-N7A-C8A	2.81	107.87	103.45
2	B	1392	NDP	C4A-N9A-C1B	-2.76	120.18	126.63
2	B	1392	NDP	C5A-N7A-C8A	2.74	107.75	103.45
2	B	1392	NDP	C1D-N1N-C6N	-2.54	115.40	120.77
2	A	1391	NDP	C1D-N1N-C6N	-2.49	115.50	120.77
2	A	1391	NDP	C6N-N1N-C2N	2.49	121.99	119.32
3	B	390	FM5	O2-N1-C2	2.44	119.47	113.76
2	A	1391	NDP	C4A-N9A-C1B	-2.38	121.06	126.63
4	A	391	DCV	OP2-PA1-OP3	-2.35	107.57	113.45
2	A	1391	NDP	C4A-N9A-C8A	2.31	108.16	105.74
2	B	1392	NDP	C6N-N1N-C2N	2.30	121.78	119.32
2	B	1392	NDP	C1B-N9A-C8A	2.14	131.85	127.09
2	B	1392	NDP	C4A-N9A-C8A	2.12	107.97	105.74
2	A	1391	NDP	N9A-C8A-N7A	-2.12	110.93	113.94
4	B	391	DCV	OP2-PA1-OP3	-2.12	108.14	113.45
2	B	1392	NDP	N9A-C8A-N7A	-2.11	110.95	113.94
3	A	390	FM5	OP2-PA1-OP3	-2.04	108.32	113.45
3	A	390	FM5	C7-C6-C4	-2.02	117.68	120.62

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	390	FM5	C3-C2-N1-O2
3	B	390	FM5	C2-C3-C4-C6
3	B	390	FM5	C3-C2-N1-O2
3	B	390	FM5	C3-C2-N1-C1
4	B	391	DCV	C2-C3-C4-PA1
4	B	391	DCV	CAC-C4-PA1-OP1
4	B	391	DCV	CAC-C4-PA1-OP2
4	A	391	DCV	N1-C2-C3-C4
4	B	391	DCV	N1-C2-C3-C4
3	A	390	FM5	C3-C2-N1-C1
2	A	1391	NDP	O4D-C1D-N1N-C6N
4	B	391	DCV	CAC-C4-PA1-OP3
3	B	390	FM5	C3-C4-C6-C11
2	B	1392	NDP	O4D-C1D-N1N-C6N
2	A	1391	NDP	C2N-C3N-C7N-N7N
2	B	1392	NDP	C2N-C3N-C7N-N7N
3	B	390	FM5	C3-C4-C6-C7
3	A	390	FM5	C5-C1-N1-O2
3	B	390	FM5	C5-C1-N1-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	391	DCV	C5-C1-N1-O2
4	B	391	DCV	C5-C1-N1-O2
4	B	391	DCV	C3-C2-N1-C1
2	B	1392	NDP	O4B-C4B-C5B-O5B
2	A	1391	NDP	O4B-C4B-C5B-O5B
2	B	1392	NDP	C2B-O2B-P2B-O3X
3	A	390	FM5	C3-C4-C6-C7
2	A	1391	NDP	C2B-O2B-P2B-O1X
3	A	390	FM5	O1-C1-N1-O2
3	B	390	FM5	O1-C1-N1-O2
4	A	391	DCV	O1-C1-N1-O2
4	B	391	DCV	O1-C1-N1-O2

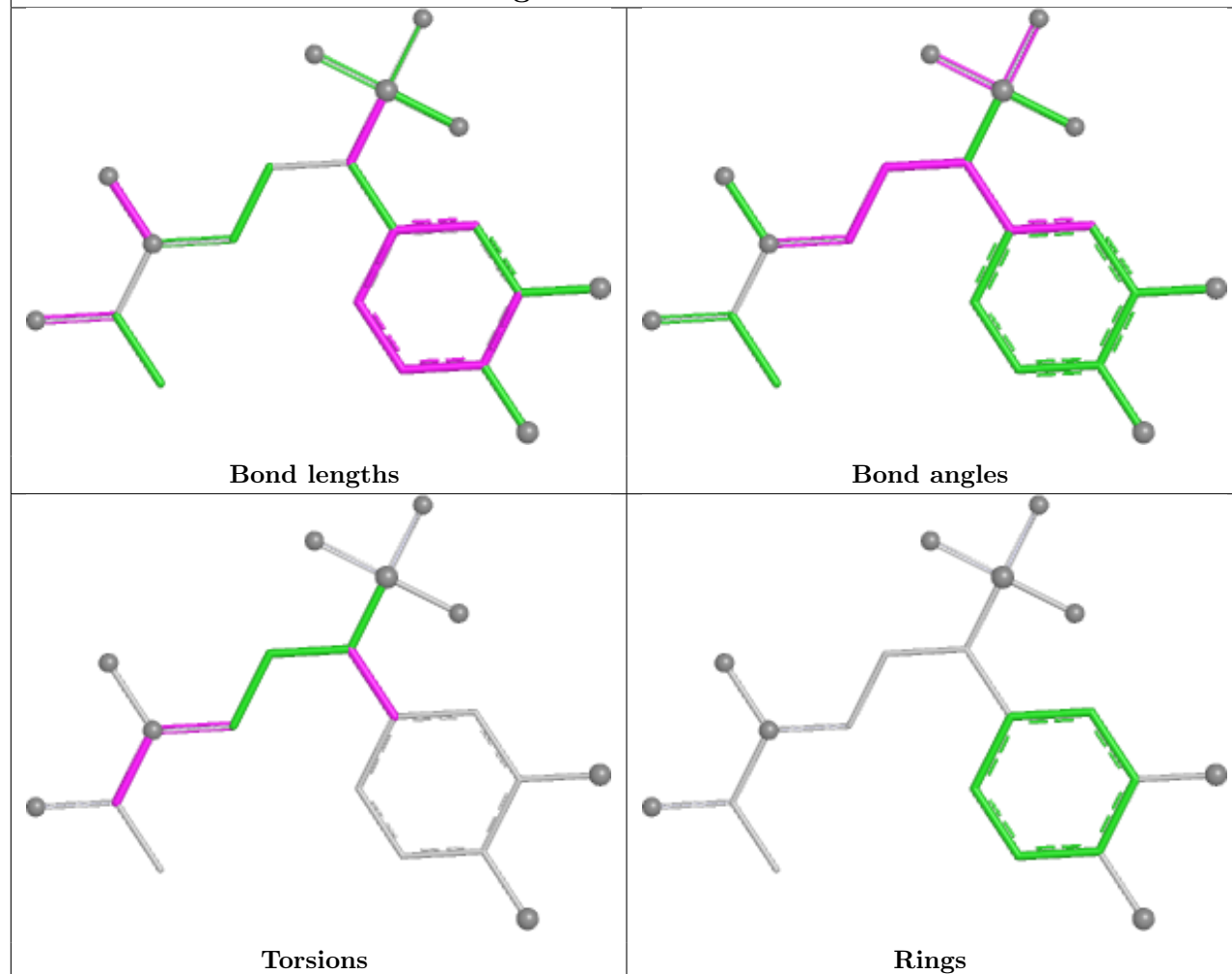
There are no ring outliers.

3 monomers are involved in 4 short contacts:

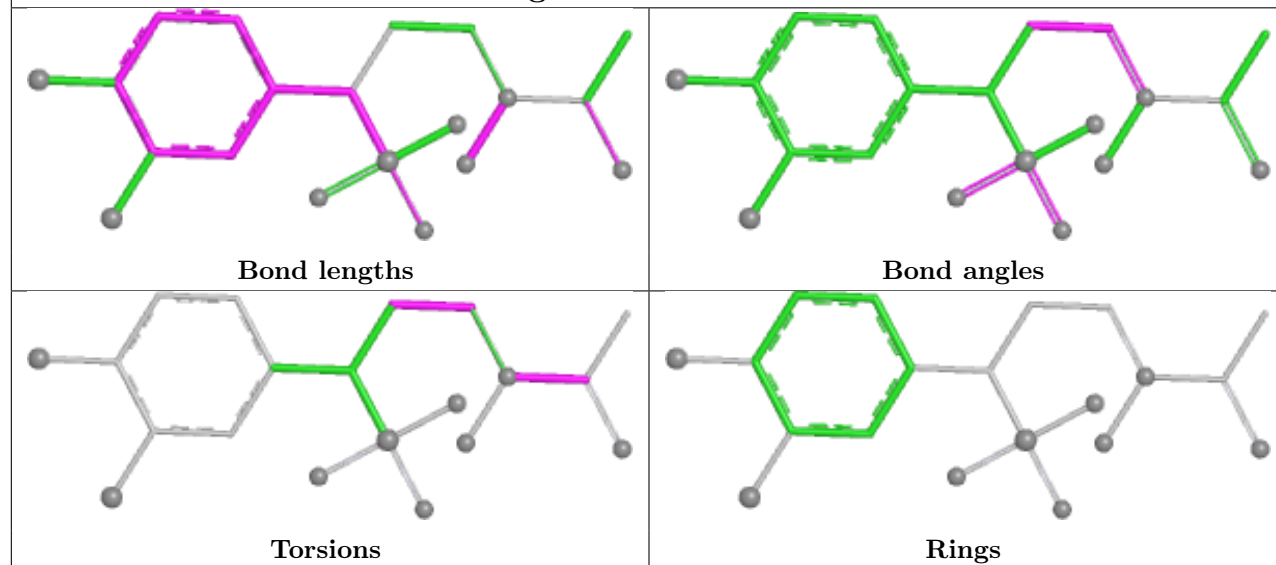
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	390	FM5	1	0
2	B	1392	NDP	2	0
3	B	390	FM5	1	0

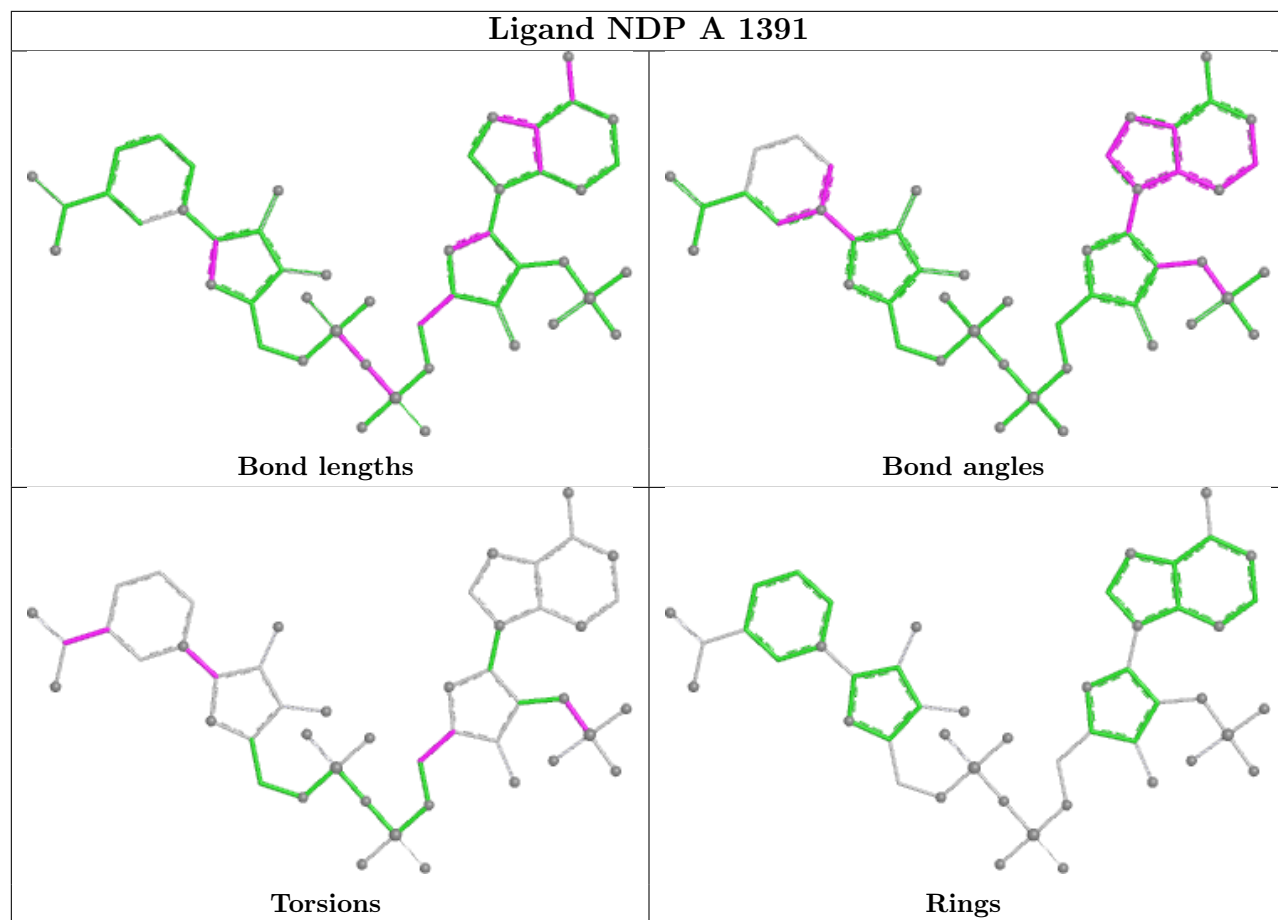
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand FM5 A 390

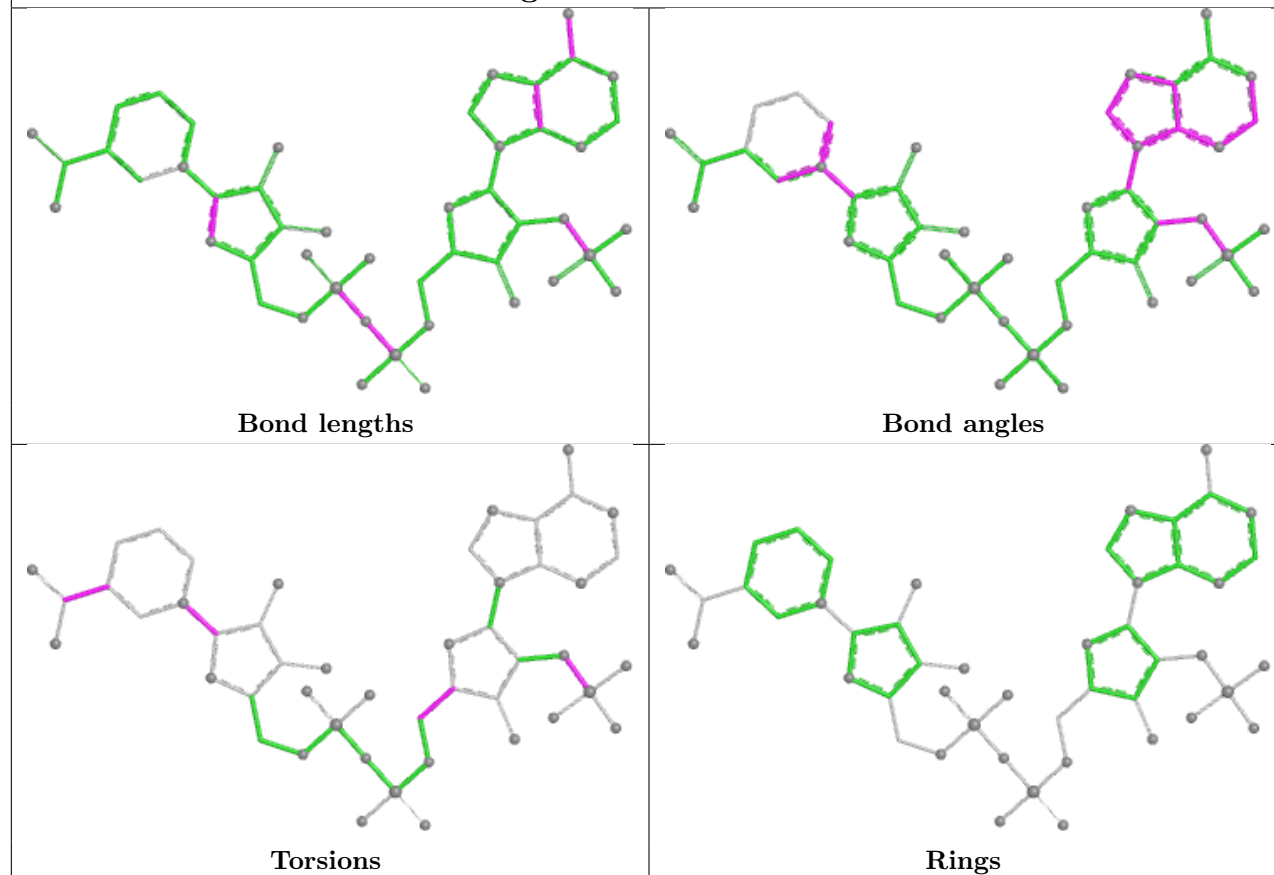


Ligand DCV A 391

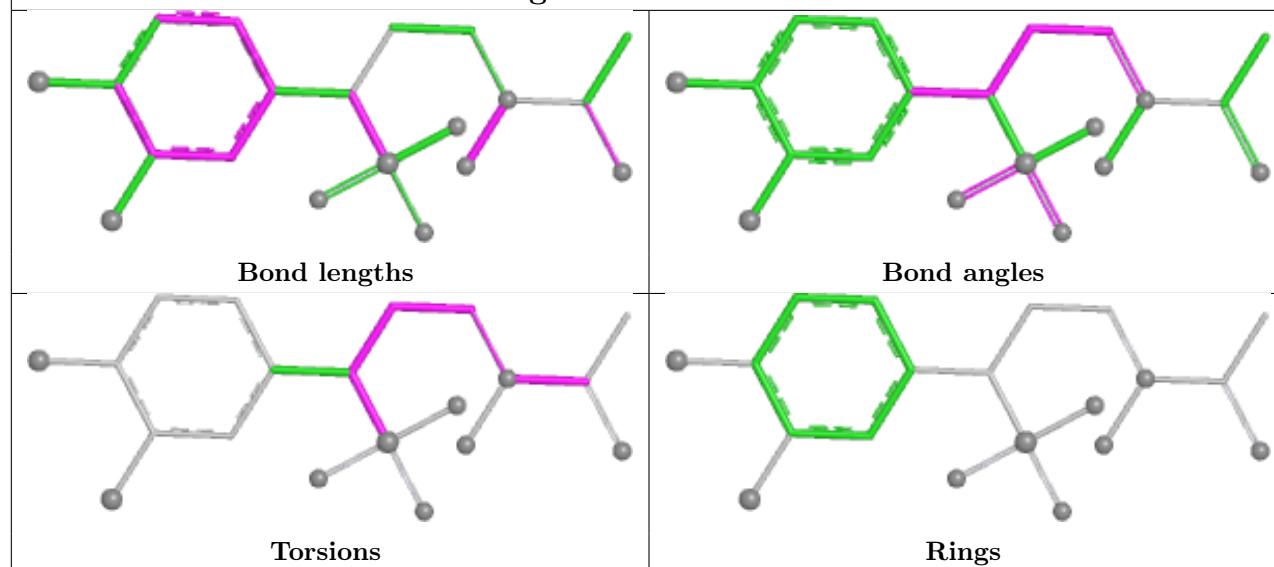


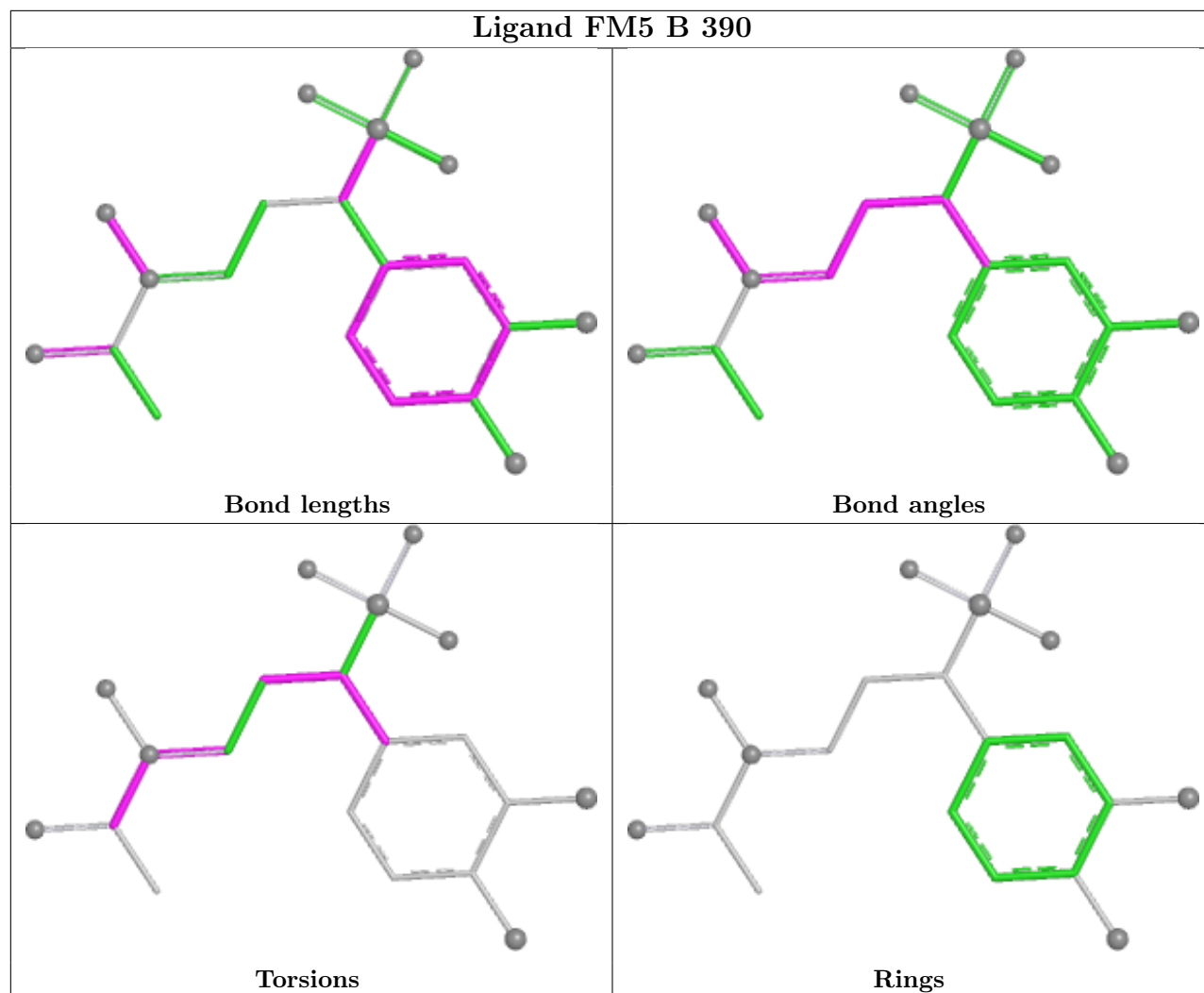


Ligand NDP B 1392



Ligand DCV B 391





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	379/398 (95%)	0.03	9 (2%) 59 61	36, 50, 72, 123	0
1	B	379/398 (95%)	-0.00	2 (0%) 87 89	33, 48, 77, 98	0
All	All	758/796 (95%)	0.01	11 (1%) 72 73	33, 49, 77, 123	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	ALA	4.9
1	A	163	GLY	3.8
1	A	198	GLY	3.4
1	A	201	PRO	3.3
1	A	203	TRP	2.7
1	A	200	HIS	2.5
1	B	191	HIS	2.5
1	A	197	ALA	2.4
1	A	380	GLU	2.3
1	B	273	LEU	2.2
1	A	164	GLY	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](#)

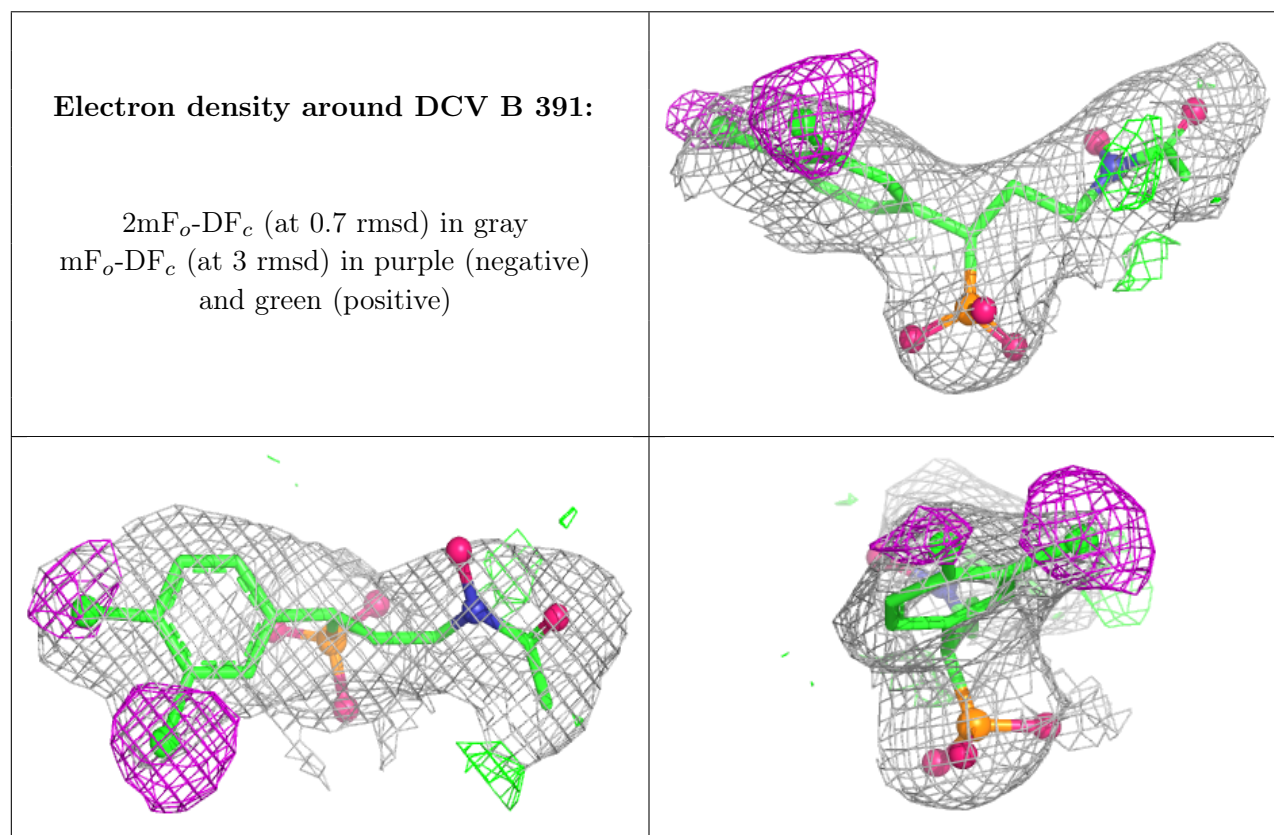
There are no oligosaccharides in this entry.

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.

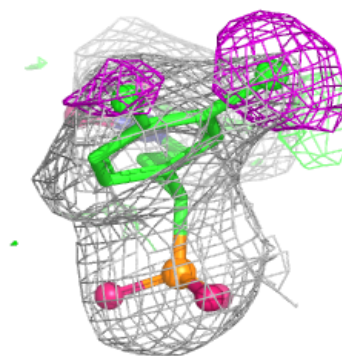
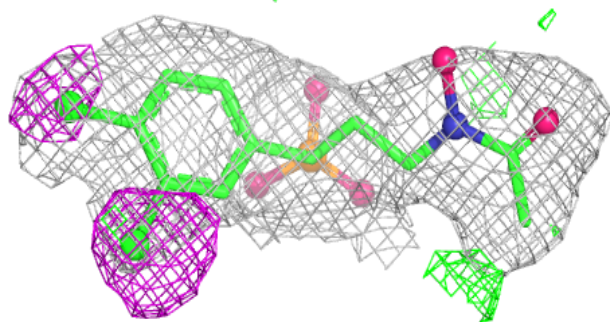
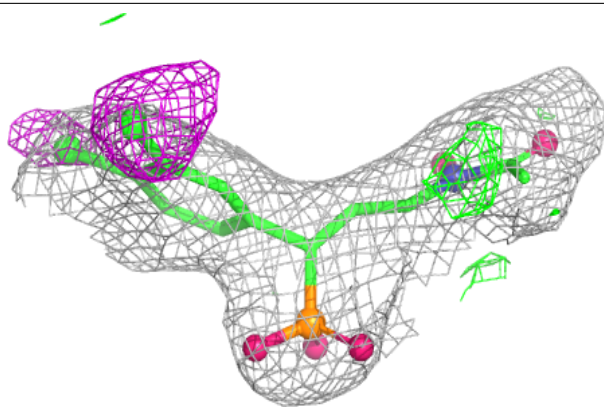
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	DCV	B	391	20/20	0.73	0.13	61,69,75,76	20
3	FM5	B	390	20/20	0.78	0.13	60,69,75,76	20
4	DCV	A	391	20/20	0.80	0.14	44,48,52,52	20
3	FM5	A	390	20/20	0.82	0.12	45,48,51,51	20
6	SO4	B	393	5/5	0.91	0.10	54,56,57,57	0
2	NDP	B	1392	48/48	0.95	0.08	49,56,63,65	0
2	NDP	A	1391	48/48	0.96	0.06	39,45,51,54	0
5	MN	A	392	1/1	0.97	0.05	51,51,51,51	0
5	MN	B	392	1/1	0.98	0.04	66,66,66,66	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.



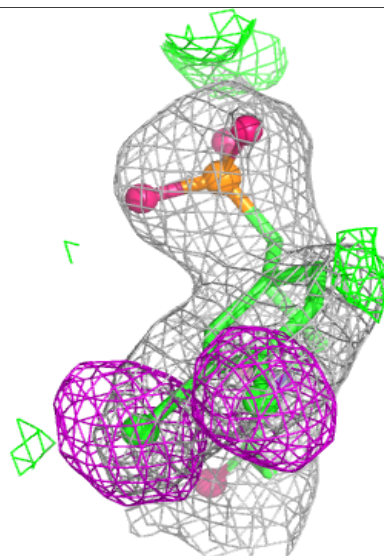
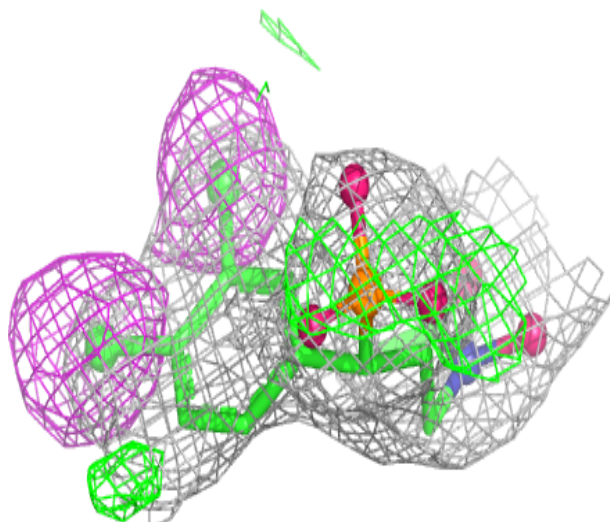
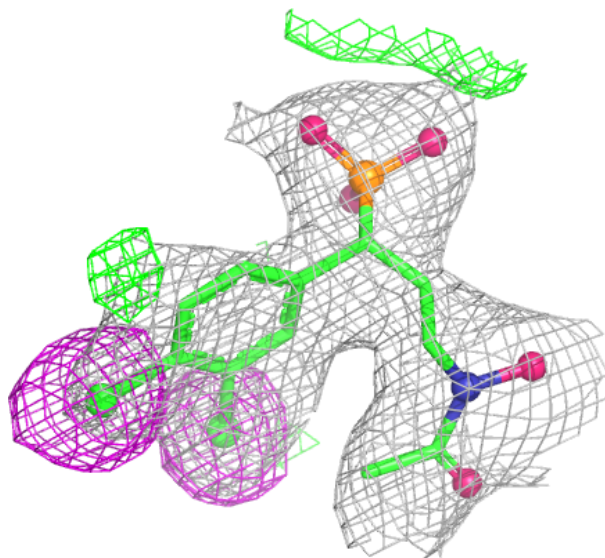
Electron density around FM5 B 390:

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



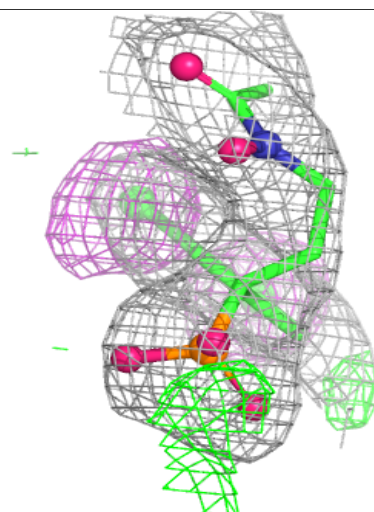
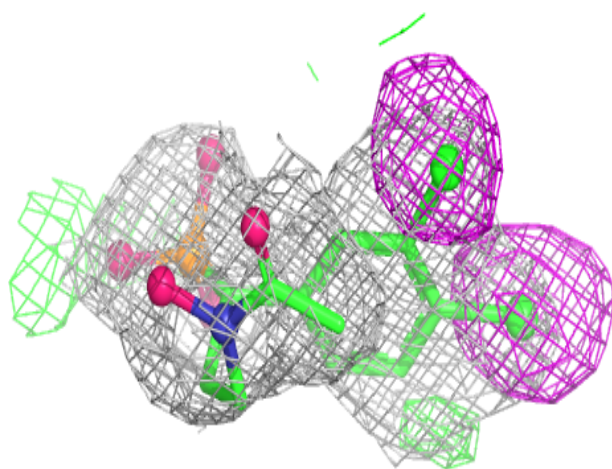
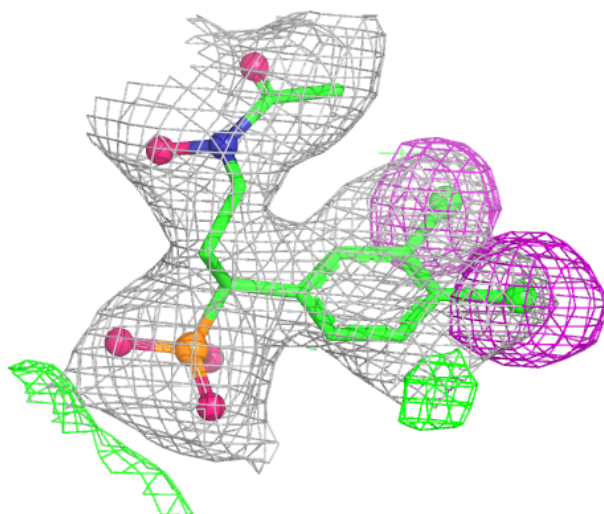
Electron density around DCV A 391:

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



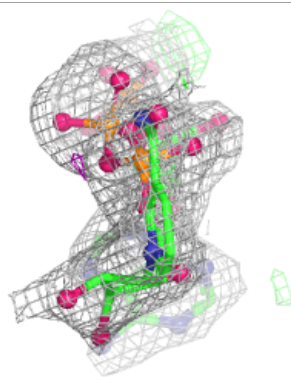
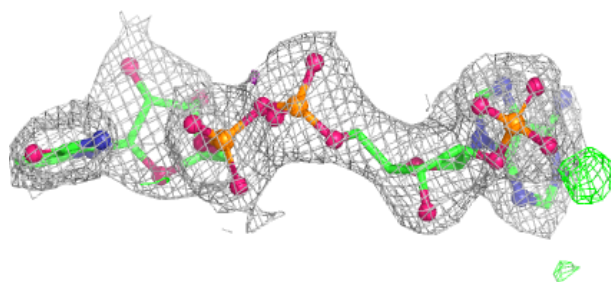
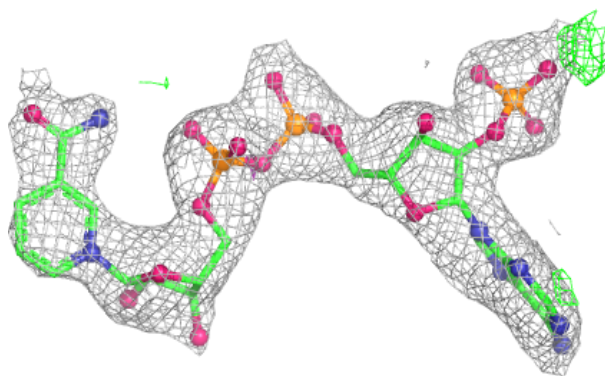
Electron density around FM5 A 390:

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

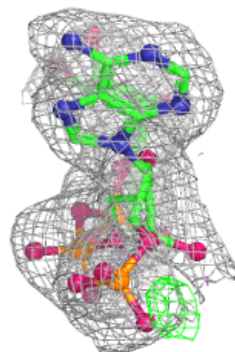
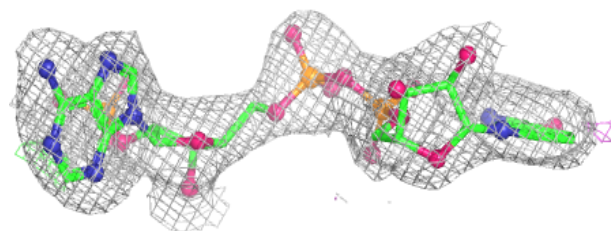
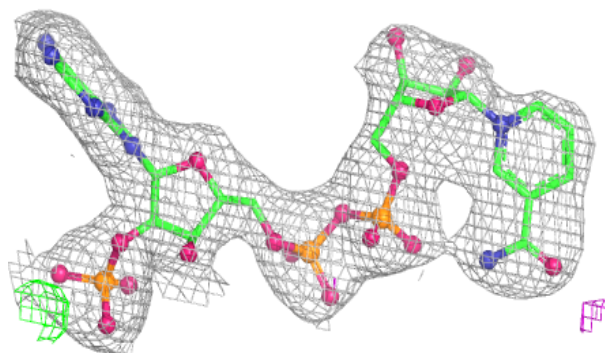


Electron density around NDP B 1392:

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

**Electron density around NDP A 1391:**

$2mF_o-DF_c$ (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.