



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:39 PM UTC

PDB ID : 2F29 / pdb\_00002f29  
Title : Crystal Structure of the Human Sialidase Neu2 Q116E Mutant in Complex with DANA Inhibitor  
Authors : Chavas, L.M.G.; Kato, R.; Fusi, P.; Tringali, C.; Venerando, B.; Tettamanti, G.; Monti, E.; Wakatsuki, S.  
Deposited on : 2005-11-15  
Resolution : 2.92 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](mailto: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>.

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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

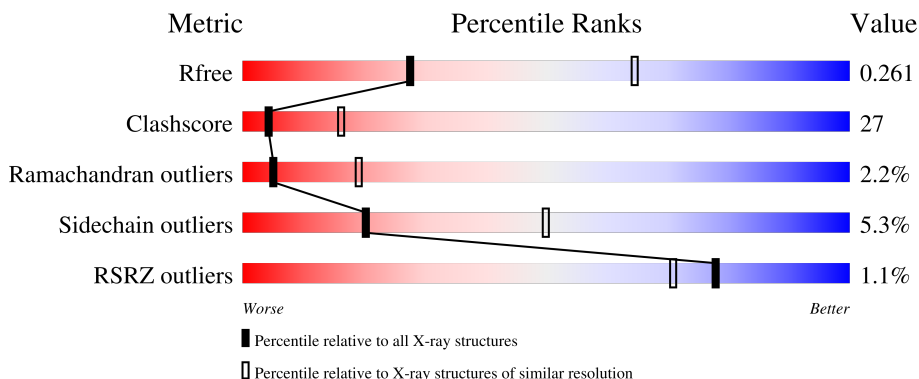
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.92 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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  $\geq 3$ , 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	382	 % 51% 41% 5% •
1	B	382	 % 48% 43% 5% ••

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6005 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.

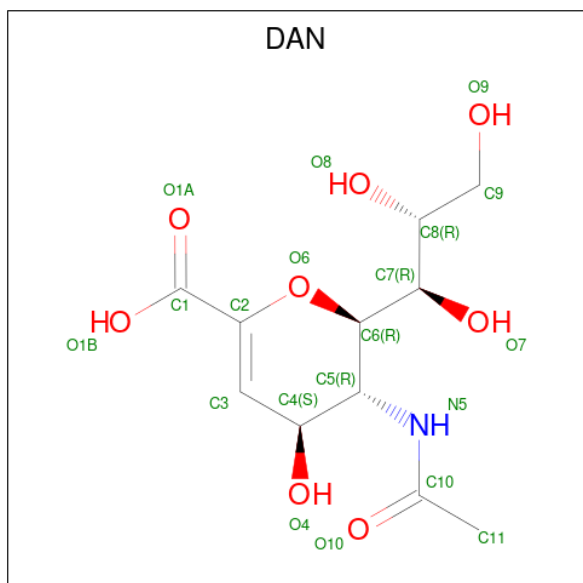
- Molecule 1 is a protein called Sialidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	370	Total 2915	C 1844	N 521	O 538	S 12	0	0	0
1	B	370	Total 2915	C 1844	N 521	O 538	S 12	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

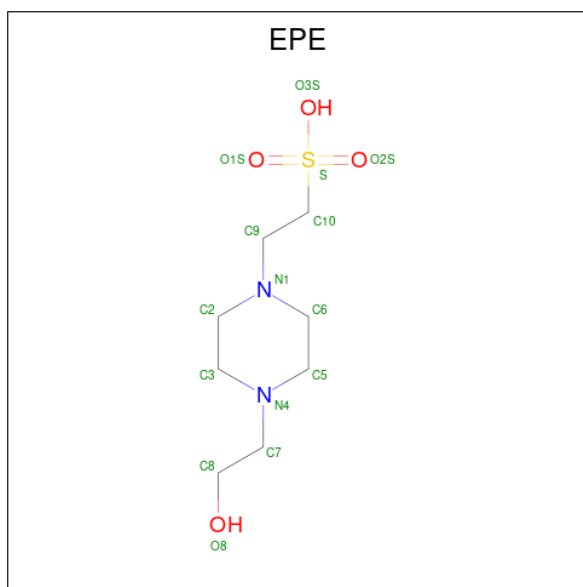
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP Q9Y3R4
A	0	SER	-	cloning artifact	UNP Q9Y3R4
A	116	GLU	GLN	engineered mutation	UNP Q9Y3R4
B	-1	GLY	-	cloning artifact	UNP Q9Y3R4
B	0	SER	-	cloning artifact	UNP Q9Y3R4
B	116	GLU	GLN	engineered mutation	UNP Q9Y3R4

- Molecule 2 is 2-DEOXY-2,3-DEHYDRO-N-ACETYL-NEURAMINIC ACID (CCD ID: DAN) (formula: C<sub>11</sub>H<sub>17</sub>NO<sub>8</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	11	1	8		
2	B	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

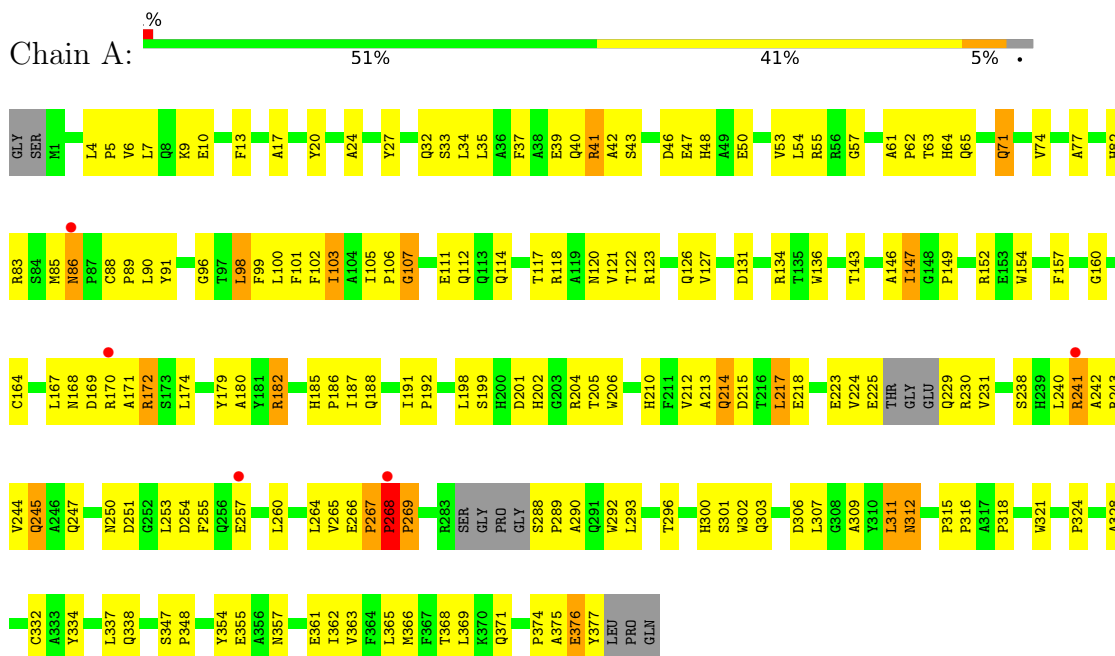
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total	O	0	0
			37	37		
4	B	38	Total	O	0	0
			38	38		

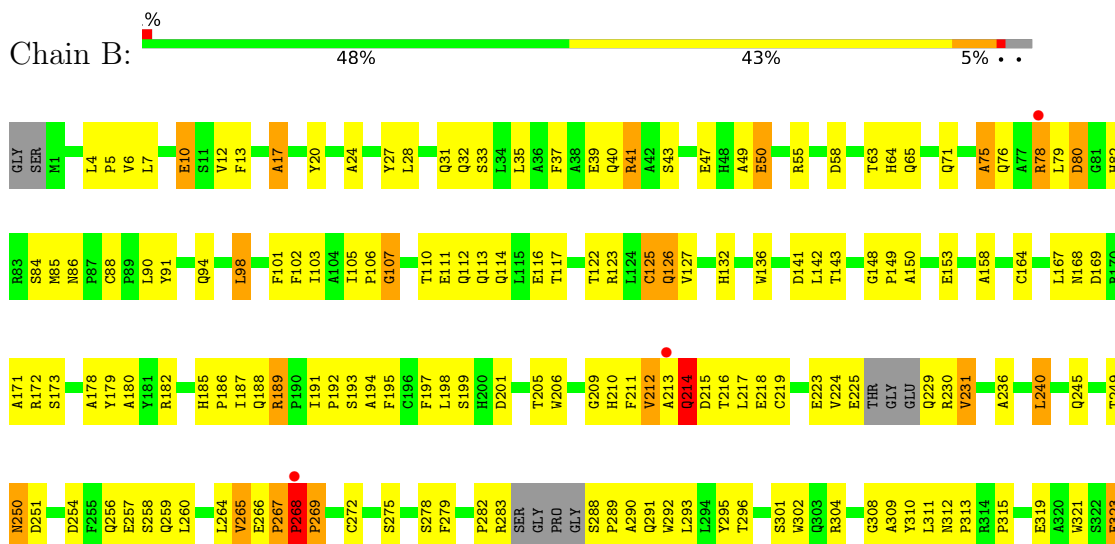
### 3 Residue-property plots [i](#)

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: Sialidase 2



#### • Molecule 1: Sialidase 2



P324	V325	A333	Y334	S335	D336	L337	Q338	D345	G346	S347	P348	L353	Y354	E355	A356	N357	D358	Y359	E360	E361	I362	V363	F364	L365	M366	L369	F373	E376	Y377	LEU	PRO	GLN
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.29Å 73.98Å 77.18Å 90.00° 93.14° 90.00°	Depositor
Resolution (Å)	79.06 – 2.92 78.53 – 2.92	Depositor EDS
% Data completeness (in resolution range)	96.3 (79.06-2.92) 98.3 (78.53-2.92)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.64 (at 2.91Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.188 , 0.265 0.188 , 0.261	Depositor DCC
$R_{free}$ test set	980 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.4	Xtrriage
Anisotropy	0.895	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 65.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6005	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EPE, DAN

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	0.49	0/2996	0.99	10/4084 (0.2%)
1	B	0.46	0/2996	1.05	17/4084 (0.4%)
All	All	0.47	0/5992	1.02	27/8168 (0.3%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	PRO	CA-C-N	12.62	133.38	120.38
1	B	267	PRO	C-N-CA	12.62	133.38	120.38
1	A	267	PRO	CA-C-N	9.90	130.58	120.38
1	A	267	PRO	C-N-CA	9.90	130.58	120.38
1	B	268	PRO	N-CA-C	9.88	122.75	110.70
1	B	76	GLN	OE1-CD-NE2	-9.46	113.14	122.60
1	A	268	PRO	N-CA-C	8.79	121.43	110.70
1	A	312	ASN	CA-C-N	7.46	127.63	119.87
1	A	312	ASN	C-N-CA	7.46	127.63	119.87
1	B	240	LEU	N-CA-C	-7.27	100.31	110.35
1	B	76	GLN	CG-CD-NE2	6.80	126.61	116.40
1	B	132	HIS	N-CA-C	6.62	120.68	112.47
1	B	209	GLY	N-CA-C	-6.32	103.78	112.25
1	B	17	ALA	N-CA-C	-5.99	105.94	113.18
1	A	363	VAL	N-CA-C	5.94	117.15	108.53
1	A	111	GLU	N-CA-C	-5.87	104.84	112.23
1	B	197	PHE	N-CA-C	-5.84	100.18	109.76
1	B	211	PHE	N-CA-C	5.72	118.28	110.55
1	B	111	GLU	N-CA-C	-5.72	105.41	112.90
1	B	236	ALA	N-CA-C	5.38	118.36	109.85
1	A	146	ALA	N-CA-C	-5.36	106.87	113.41
1	B	75	ALA	N-CA-C	5.30	117.74	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	GLU	N-CA-C	-5.23	103.48	110.07
1	A	251	ASP	N-CA-C	5.17	118.72	111.74
1	A	168	ASN	N-CA-C	-5.10	106.81	112.57
1	B	279	PHE	CA-C-N	5.00	126.09	119.84
1	B	279	PHE	C-N-CA	5.00	126.09	119.84

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2915	0	2825	148	0
1	B	2915	0	2825	168	0
2	A	20	0	16	1	0
2	B	20	0	16	1	0
3	A	30	0	36	3	0
3	B	30	0	36	2	0
4	A	37	0	0	2	0
4	B	38	0	0	0	0
All	All	6005	0	5754	315	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 27.

All (315) 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:B:27:TYR:H	1:B:338:GLN:NE2	1.59	1.00
1:B:245:GLN:HE22	1:B:321:TRP:HE1	1.08	0.98
1:B:27:TYR:N	1:B:338:GLN:HE21	1.66	0.93
1:A:268:PRO:HB2	1:A:269:PRO:HD3	1.48	0.92
1:B:27:TYR:H	1:B:338:GLN:HE21	0.94	0.91
1:B:345:ASP:OD1	1:B:347:SER:HB3	1.72	0.88
1:B:191:ILE:HG21	1:B:214:GLN:HB3	1.64	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:VAL:HG22	1:B:266:GLU:H	1.50	0.76
1:A:112:GLN:HE21	1:A:112:GLN:HA	1.51	0.75
1:A:212:VAL:HG12	1:A:255:PHE:HB2	1.67	0.75
1:A:191:ILE:HG23	1:A:215:ASP:OD2	1.86	0.75
1:B:245:GLN:NE2	1:B:321:TRP:HE1	1.85	0.74
1:A:250:ASN:ND2	1:A:253:LEU:HB3	2.02	0.73
1:B:224:VAL:HG22	1:B:231:VAL:HG22	1.70	0.73
1:A:354:TYR:HE2	1:A:365:LEU:HD22	1.54	0.73
1:B:185:HIS:HB3	1:B:188:GLN:HB2	1.71	0.72
1:A:6:VAL:O	3:B:382:EPE:H52	1.89	0.72
1:A:90:LEU:HB2	1:A:164:CYS:HB2	1.72	0.72
1:B:240:LEU:HD13	1:B:260:LEU:HD11	1.71	0.71
1:A:268:PRO:HD3	1:A:301:SER:O	1.90	0.71
1:A:42:ALA:HB2	1:A:50:GLU:OE2	1.90	0.71
1:B:191:ILE:HG21	1:B:214:GLN:CB	2.20	0.70
1:A:90:LEU:HD12	1:A:91:TYR:H	1.57	0.69
1:A:27:TYR:N	1:A:338:GLN:HE21	1.91	0.69
1:A:265:VAL:HG22	1:A:266:GLU:H	1.58	0.69
1:A:296:THR:HG23	1:A:337:LEU:HD11	1.74	0.68
1:A:27:TYR:H	1:A:338:GLN:HE21	1.41	0.68
1:B:40:GLN:O	1:B:50:GLU:HG3	1.93	0.67
1:B:354:TYR:HE2	1:B:365:LEU:HD13	1.58	0.67
1:B:103:ILE:HG23	1:B:122:THR:HG23	1.76	0.67
1:B:180:ALA:O	1:B:192:PRO:HA	1.94	0.67
1:A:112:GLN:HA	1:A:112:GLN:NE2	2.10	0.66
1:B:28:LEU:HB3	1:B:31:GLN:HG2	1.76	0.65
1:B:182:ARG:HG2	1:B:191:ILE:O	1.97	0.65
1:A:354:TYR:CE2	1:A:365:LEU:HD22	2.32	0.65
1:B:288:SER:N	1:B:289:PRO:HD2	2.11	0.64
1:B:193:SER:HA	1:B:216:THR:OG1	1.97	0.64
1:B:265:VAL:HG22	1:B:266:GLU:N	2.12	0.64
1:A:348:PRO:HD2	1:A:369:LEU:HB3	1.78	0.64
1:A:217:LEU:HD22	2:A:381:DAN:H92	1.79	0.64
1:B:7:LEU:HD22	1:B:64:HIS:HD2	1.63	0.64
1:B:250:ASN:HD21	1:B:254:ASP:H	1.45	0.64
1:A:265:VAL:HG22	1:A:266:GLU:N	2.13	0.63
1:B:126:GLN:HG2	1:B:142:LEU:HD21	1.80	0.63
1:B:290:ALA:HB1	1:B:291:GLN:HE22	1.63	0.63
1:A:24:ALA:HB3	1:A:37:PHE:HB2	1.81	0.63
1:B:79:LEU:O	1:B:80:ASP:C	2.41	0.62
1:B:4:LEU:HD12	1:B:5:PRO:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:GLN:O	1:B:116:GLU:HG2	1.99	0.62
1:B:268:PRO:HB2	1:B:269:PRO:HD3	1.82	0.61
1:A:86:ASN:O	1:A:102:PHE:HA	2.00	0.61
1:B:112:GLN:HA	1:B:112:GLN:NE2	2.16	0.61
1:A:7:LEU:HD22	1:A:64:HIS:HD2	1.66	0.61
1:B:334:TYR:HB2	1:B:355:GLU:OE1	2.01	0.61
1:B:127:VAL:CG1	1:B:136:TRP:HB3	2.30	0.60
1:B:240:LEU:HD12	1:B:260:LEU:HD21	1.82	0.60
1:A:27:TYR:H	1:A:338:GLN:NE2	2.00	0.60
3:A:382:EPE:H71	1:B:6:VAL:O	2.01	0.60
1:A:90:LEU:HD12	1:A:91:TYR:N	2.16	0.60
1:B:13:PHE:HB2	1:B:362:ILE:HB	1.84	0.60
1:A:4:LEU:HD12	1:A:5:PRO:HD2	1.85	0.59
1:B:333:ALA:HB3	1:B:355:GLU:HB2	1.82	0.59
1:B:357:ASN:ND2	1:B:361:GLU:OE1	2.34	0.59
1:A:180:ALA:O	1:A:192:PRO:HA	2.01	0.59
1:A:225:GLU:C	1:A:229:GLN:O	2.44	0.59
1:A:90:LEU:HD21	1:A:174:LEU:HD22	1.84	0.58
1:A:210:HIS:HD2	1:A:254:ASP:OD1	1.86	0.58
1:B:268:PRO:HD3	1:B:301:SER:O	2.03	0.58
1:A:191:ILE:HG21	1:A:214:GLN:HB2	1.84	0.58
1:A:224:VAL:HG12	1:A:225:GLU:N	2.18	0.58
1:B:113:GLN:O	1:B:117:THR:HG22	2.04	0.58
1:B:290:ALA:HB1	1:B:291:GLN:NE2	2.19	0.57
1:A:27:TYR:HD1	1:A:34:LEU:HD23	1.68	0.57
1:B:188:GLN:NE2	1:B:189:ARG:NH2	2.53	0.57
1:A:289:PRO:HG2	1:A:292:TRP:HE1	1.69	0.57
1:A:102:PHE:HE2	1:A:127:VAL:HG23	1.70	0.57
1:A:103:ILE:HD11	1:A:157:PHE:CE1	2.39	0.57
1:B:225:GLU:HA	1:B:229:GLN:O	2.05	0.57
1:A:375:ALA:C	1:A:377:TYR:H	2.13	0.56
1:A:238:SER:HB3	1:A:244:VAL:HG23	1.88	0.56
1:B:245:GLN:HE22	1:B:321:TRP:NE1	1.91	0.56
1:B:55:ARG:HG2	1:B:71:GLN:HA	1.87	0.56
1:B:189:ARG:HD2	1:B:189:ARG:H	1.69	0.56
1:B:249:THR:HG22	1:B:249:THR:O	2.06	0.55
1:A:268:PRO:HB2	1:A:269:PRO:CD	2.29	0.55
1:A:225:GLU:OE2	1:A:225:GLU:O	2.25	0.55
1:A:147:ILE:HD13	1:A:154:TRP:CZ3	2.42	0.55
1:B:123:ARG:HH11	1:B:143:THR:HG21	1.71	0.54
1:B:75:ALA:O	1:B:78:ARG:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ASP:OD2	1:B:141:ASP:C	2.49	0.54
1:A:41:ARG:HB2	1:A:43:SER:O	2.06	0.54
1:A:89:PRO:HA	1:A:99:PHE:O	2.07	0.54
1:B:189:ARG:H	1:B:189:ARG:CD	2.21	0.54
1:B:275:SER:O	1:B:295:TYR:HA	2.07	0.54
1:A:225:GLU:HB2	1:A:290:ALA:HB3	1.89	0.53
1:B:259:GLN:N	1:B:259:GLN:CD	2.66	0.53
1:B:7:LEU:HD22	1:B:64:HIS:CD2	2.43	0.53
1:B:103:ILE:CG2	1:B:122:THR:HG23	2.38	0.53
1:A:63:THR:O	1:A:65:GLN:HG2	2.08	0.53
1:A:88:CYS:HB2	1:A:101:PHE:HB2	1.89	0.53
1:B:94:GLN:HE21	1:B:172:ARG:HG3	1.74	0.53
1:B:27:TYR:N	1:B:338:GLN:NE2	2.40	0.52
1:B:217:LEU:HD22	2:B:381:DAN:O9	2.10	0.52
1:A:55:ARG:HG2	1:A:71:GLN:HA	1.91	0.52
1:A:312:ASN:HB2	1:A:321:TRP:CE3	2.44	0.52
1:B:194:ALA:O	1:B:195:PHE:HB3	2.08	0.52
1:A:33:SER:HB2	1:A:57:GLY:O	2.10	0.52
1:A:224:VAL:CG1	1:A:225:GLU:N	2.73	0.52
1:B:323:GLU:OE1	1:B:323:GLU:HA	2.10	0.52
1:A:306:ASP:HA	1:A:328:ALA:O	2.10	0.52
1:B:179:TYR:CE2	1:B:218:GLU:HG2	2.45	0.52
1:B:41:ARG:HB3	1:B:49:ALA:HA	1.92	0.51
1:B:90:LEU:HB2	1:B:164:CYS:HB2	1.91	0.51
1:B:288:SER:N	1:B:289:PRO:CD	2.72	0.51
1:B:41:ARG:HA	1:B:50:GLU:HG3	1.92	0.51
1:B:112:GLN:HA	1:B:112:GLN:HE21	1.74	0.51
1:B:158:ALA:HB3	1:B:179:TYR:CE2	2.45	0.51
1:A:123:ARG:NH1	1:A:143:THR:HG21	2.25	0.51
1:B:63:THR:O	1:B:65:GLN:HG2	2.09	0.51
1:B:78:ARG:HA	1:B:84:SER:OG	2.11	0.51
1:A:10:GLU:HB2	1:B:10:GLU:HB2	1.93	0.51
1:A:214:GLN:O	1:A:215:ASP:HB2	2.08	0.51
1:A:147:ILE:O	1:A:149:PRO:HD2	2.10	0.51
1:A:7:LEU:HB2	1:A:366:MET:O	2.11	0.51
1:B:210:HIS:HD2	1:B:254:ASP:OD1	1.93	0.51
1:A:46:ASP:C	1:A:48:HIS:H	2.19	0.51
1:A:212:VAL:HG12	1:A:255:PHE:CB	2.37	0.51
1:A:185:HIS:CE1	1:A:188:GLN:HG2	2.46	0.51
1:A:201:ASP:CG	1:A:205:THR:H	2.18	0.51
1:B:296:THR:HA	1:B:308:GLY:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:TYR:CE2	1:B:365:LEU:HD13	2.44	0.50
1:B:35:LEU:CD1	1:B:98:LEU:HD11	2.40	0.50
1:A:7:LEU:HD22	1:A:64:HIS:CD2	2.46	0.50
1:A:143:THR:O	1:A:147:ILE:N	2.37	0.50
1:A:167:LEU:O	1:A:172:ARG:HA	2.11	0.50
1:B:257:GLU:HG3	1:B:259:GLN:OE1	2.11	0.50
1:A:348:PRO:HD2	1:A:369:LEU:CB	2.41	0.50
1:A:127:VAL:CG1	1:A:136:TRP:HB3	2.42	0.50
1:B:309:ALA:HB3	1:B:325:VAL:CG1	2.42	0.49
1:A:103:ILE:HG13	1:A:122:THR:CG2	2.43	0.49
1:A:131:ASP:CG	1:A:134:ARG:HB3	2.37	0.49
1:B:47:GLU:HB3	1:B:110:THR:HG22	1.95	0.49
1:B:171:ALA:O	1:B:172:ARG:C	2.55	0.49
1:A:213:ALA:HA	4:A:416:HOH:O	2.12	0.49
1:A:185:HIS:HB3	1:A:188:GLN:HB2	1.95	0.48
1:B:334:TYR:HB2	1:B:355:GLU:CD	2.38	0.48
1:B:311:LEU:C	1:B:311:LEU:HD13	2.38	0.48
1:B:78:ARG:HH21	1:B:80:ASP:N	2.12	0.48
1:B:106:PRO:O	1:B:107:GLY:C	2.57	0.48
1:A:191:ILE:CG2	1:A:214:GLN:HB2	2.42	0.48
1:B:88:CYS:HB2	1:B:101:PHE:HB2	1.96	0.48
1:A:88:CYS:HB3	1:A:164:CYS:SG	2.54	0.48
1:A:371:GLN:O	1:A:374:PRO:HD3	2.13	0.48
1:B:188:GLN:HE22	1:B:189:ARG:NH2	2.12	0.48
1:B:78:ARG:HH21	1:B:80:ASP:CA	2.27	0.48
1:A:117:THR:O	1:A:117:THR:HG22	2.13	0.47
1:A:242:ALA:HB1	1:A:264:LEU:O	2.14	0.47
1:A:13:PHE:HB2	1:A:362:ILE:HB	1.96	0.47
1:B:191:ILE:CG2	1:B:215:ASP:H	2.27	0.47
1:A:182:ARG:HG2	1:A:191:ILE:O	2.14	0.47
1:A:300:HIS:HE1	1:A:302:TRP:HB2	1.79	0.47
1:A:91:TYR:OH	1:A:96:GLY:HA2	2.15	0.47
1:B:17:ALA:N	3:B:382:EPE:O1S	2.46	0.47
1:B:24:ALA:HB3	1:B:37:PHE:HB2	1.97	0.47
1:B:103:ILE:HG23	1:B:122:THR:CG2	2.44	0.47
1:A:114:GLN:HG2	1:A:121:VAL:HG22	1.96	0.47
1:A:83:ARG:NH2	1:A:85:MET:SD	2.88	0.47
1:A:265:VAL:CG2	1:A:266:GLU:H	2.28	0.47
1:B:194:ALA:HB1	1:B:219:CYS:SG	2.55	0.46
1:B:266:GLU:OE2	1:B:267:PRO:HD2	2.14	0.46
1:B:363:VAL:HG12	1:B:364:PHE:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:CD1	1:A:98:LEU:HD11	2.45	0.46
1:A:41:ARG:NH1	1:A:46:ASP:OD1	2.49	0.46
1:A:74:VAL:HG13	1:A:136:TRP:CD1	2.50	0.46
1:A:46:ASP:O	1:A:48:HIS:N	2.49	0.46
1:A:120:ASN:HD21	1:A:157:PHE:HD2	1.64	0.46
1:A:240:LEU:O	1:A:241:ARG:C	2.57	0.46
1:B:268:PRO:HG2	1:B:302:TRP:HA	1.96	0.46
1:A:106:PRO:O	1:A:107:GLY:C	2.58	0.46
1:A:169:ASP:C	1:A:171:ALA:H	2.24	0.46
1:A:199:SER:HB2	1:A:206:TRP:CE3	2.51	0.46
1:A:244:VAL:HG22	1:A:260:LEU:HD23	1.97	0.46
1:A:357:ASN:ND2	1:A:361:GLU:OE1	2.49	0.46
1:B:90:LEU:HD12	1:B:91:TYR:H	1.81	0.46
1:A:77:ALA:HA	1:A:127:VAL:HG21	1.96	0.46
1:A:288:SER:HB3	1:A:289:PRO:HD3	1.98	0.46
1:A:265:VAL:HG21	1:A:301:SER:HB3	1.96	0.46
1:B:41:ARG:HB2	1:B:43:SER:O	2.16	0.46
1:A:46:ASP:C	1:A:48:HIS:N	2.72	0.46
1:A:243:ARG:HD2	1:A:266:GLU:OE1	2.16	0.46
1:B:12:VAL:HG23	1:B:13:PHE:CD2	2.51	0.46
1:B:39:GLU:OE1	1:B:41:ARG:NH2	2.46	0.45
1:B:39:GLU:OE2	1:B:85:MET:HB2	2.16	0.45
1:A:37:PHE:CE1	1:A:54:LEU:HD13	2.51	0.45
1:B:31:GLN:HB2	1:B:33:SER:OG	2.16	0.45
1:A:257:GLU:OE1	1:A:257:GLU:HA	2.17	0.45
1:B:357:ASN:O	1:B:360:GLU:HB2	2.16	0.45
1:B:35:LEU:HD11	1:B:98:LEU:HD11	1.98	0.45
1:B:289:PRO:CG	1:B:292:TRP:HE1	2.29	0.45
1:A:312:ASN:HB2	1:A:321:TRP:CZ3	2.52	0.45
1:A:39:GLU:OE2	1:A:85:MET:HB2	2.17	0.45
1:A:88:CYS:SG	1:A:160:GLY:HA3	2.56	0.45
1:A:179:TYR:CE2	1:A:218:GLU:HG2	2.51	0.45
1:B:33:SER:HB3	1:B:58:ASP:OD1	2.17	0.45
1:B:283:ARG:HH12	1:B:376:GLU:HG3	1.82	0.45
1:A:224:VAL:HG21	1:A:293:LEU:HD21	1.98	0.45
1:B:189:ARG:HD2	1:B:189:ARG:N	2.32	0.45
1:B:258:SER:C	1:B:259:GLN:CD	2.85	0.45
1:A:131:ASP:OD1	1:A:134:ARG:HB3	2.17	0.44
1:A:171:ALA:O	1:A:172:ARG:C	2.60	0.44
1:A:201:ASP:O	1:A:202:HIS:HB2	2.17	0.44
1:A:300:HIS:CE1	1:A:303:GLN:HG2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:VAL:HG12	1:B:136:TRP:CE3	2.52	0.44
1:A:17:ALA:N	3:A:382:EPE:O1S	2.50	0.44
1:B:264:LEU:N	1:B:264:LEU:HD23	2.32	0.44
1:A:201:ASP:CG	1:A:204:ARG:HB3	2.43	0.44
1:B:88:CYS:HB3	1:B:164:CYS:SG	2.57	0.44
1:B:127:VAL:HG12	1:B:136:TRP:HE3	1.82	0.44
1:A:147:ILE:HD13	1:A:154:TRP:HZ3	1.82	0.44
1:B:310:TYR:CE2	1:B:324:PRO:HD3	2.53	0.44
1:B:311:LEU:HB2	1:B:373:PHE:CE2	2.52	0.44
1:B:169:ASP:HB3	1:B:230:ARG:NH2	2.32	0.44
1:B:265:VAL:CG2	1:B:266:GLU:H	2.25	0.44
1:A:229:GLN:N	4:A:389:HOH:O	2.50	0.44
1:B:86:ASN:N	1:B:86:ASN:HD22	2.15	0.44
1:B:250:ASN:C	1:B:250:ASN:HD22	2.24	0.44
1:A:100:LEU:O	1:A:126:GLN:HA	2.18	0.44
1:A:289:PRO:CG	1:A:292:TRP:HE1	2.31	0.43
1:B:105:ILE:HA	1:B:106:PRO:HD3	1.89	0.43
1:B:210:HIS:CD2	1:B:254:ASP:OD1	2.71	0.43
1:A:20:TYR:CE1	1:A:40:GLN:HG3	2.53	0.43
1:A:117:THR:O	1:A:118:ARG:HB2	2.18	0.43
1:A:245:GLN:OE1	1:A:318:PRO:HG3	2.18	0.43
1:A:267:PRO:HA	1:A:268:PRO:HD3	1.81	0.43
1:B:123:ARG:HH11	1:B:143:THR:CG2	2.31	0.43
1:A:347:SER:OG	1:A:368:THR:HB	2.18	0.43
1:B:272:CYS:HB2	1:B:304:ARG:HE	1.83	0.43
1:B:94:GLN:HE21	1:B:172:ARG:CG	2.30	0.43
1:A:185:HIS:CE1	1:A:187:ILE:HB	2.54	0.43
3:A:382:EPE:H52	1:B:6:VAL:O	2.18	0.43
1:B:245:GLN:O	1:B:258:SER:HA	2.18	0.43
1:A:123:ARG:HH11	1:A:143:THR:HG21	1.82	0.43
1:B:185:HIS:HA	1:B:186:PRO:HD3	1.86	0.43
1:B:90:LEU:HD12	1:B:91:TYR:N	2.33	0.43
1:B:102:PHE:CZ	1:B:125:CYS:HB2	2.54	0.43
1:A:185:HIS:CG	1:A:188:GLN:HG2	2.53	0.43
1:B:126:GLN:HG2	1:B:142:LEU:CD2	2.49	0.43
1:B:311:LEU:HD13	1:B:313:PRO:HD3	2.01	0.43
1:B:123:ARG:NH1	1:B:143:THR:HB	2.34	0.43
1:B:168:ASN:ND2	1:B:172:ARG:NH1	2.66	0.43
1:A:185:HIS:HA	1:A:186:PRO:HD3	1.92	0.43
1:B:230:ARG:HH11	1:B:230:ARG:HG2	1.84	0.42
1:B:267:PRO:HA	1:B:268:PRO:HD3	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLN:O	1:A:245:GLN:HG3	2.19	0.42
1:A:315:PRO:HA	1:A:316:PRO:HA	1.72	0.42
1:A:334:TYR:HB2	1:A:355:GLU:CD	2.44	0.42
1:B:20:TYR:HA	1:B:39:GLU:O	2.19	0.42
1:A:185:HIS:ND1	1:A:188:GLN:HG2	2.35	0.42
1:A:265:VAL:CG2	1:A:266:GLU:N	2.81	0.42
1:B:78:ARG:O	1:B:79:LEU:HD23	2.19	0.42
1:B:63:THR:C	1:B:64:HIS:ND1	2.78	0.42
1:B:218:GLU:H	1:B:218:GLU:HG3	1.54	0.42
1:B:256:GLN:CD	1:B:256:GLN:H	2.26	0.42
1:B:178:ALA:O	1:B:195:PHE:N	2.53	0.42
1:B:311:LEU:CD1	1:B:313:PRO:HD3	2.50	0.42
1:A:40:GLN:HB2	1:A:53:VAL:HG13	2.01	0.42
1:A:347:SER:HB2	1:A:348:PRO:CD	2.49	0.42
1:A:309:ALA:O	1:A:324:PRO:HA	2.20	0.42
1:A:311:LEU:CD2	1:A:312:ASN:N	2.83	0.42
1:B:148:GLY:HA3	1:B:149:PRO:HD3	1.95	0.42
1:A:218:GLU:H	1:A:218:GLU:HG3	1.65	0.42
1:A:293:LEU:HG	1:A:315:PRO:HB3	2.01	0.42
1:A:307:LEU:HB2	1:A:332:CYS:SG	2.60	0.42
1:B:31:GLN:O	1:B:32:GLN:C	2.63	0.42
1:B:245:GLN:O	1:B:259:GLN:NE2	2.53	0.41
1:B:348:PRO:HD2	1:B:369:LEU:HB3	2.02	0.41
1:B:278:SER:HA	1:B:292:TRP:O	2.20	0.41
1:A:105:ILE:HA	1:A:106:PRO:HD3	1.96	0.41
1:A:311:LEU:HD22	1:A:312:ASN:N	2.34	0.41
1:B:39:GLU:CD	1:B:85:MET:HB2	2.45	0.41
1:B:114:GLN:HA	1:B:117:THR:HG22	2.01	0.41
1:B:167:LEU:O	1:B:172:ARG:HA	2.20	0.41
1:B:282:PRO:HD2	1:B:292:TRP:CH2	2.55	0.41
1:B:335:SER:HA	1:B:353:LEU:O	2.21	0.41
1:B:185:HIS:ND1	1:B:186:PRO:HD2	2.35	0.41
1:B:199:SER:HB2	1:B:206:TRP:CE3	2.56	0.41
1:A:223:GLU:OE2	1:A:230:ARG:HD2	2.21	0.41
1:A:375:ALA:C	1:A:377:TYR:N	2.79	0.41
1:B:102:PHE:CE1	1:B:125:CYS:HB2	2.55	0.41
1:B:150:ALA:HA	1:B:153:GLU:CD	2.46	0.41
1:B:102:PHE:HE2	1:B:127:VAL:HG23	1.85	0.41
1:B:296:THR:HG23	1:B:337:LEU:HD11	2.02	0.41
1:A:214:GLN:H	1:A:214:GLN:HG2	1.70	0.41
1:B:312:ASN:O	1:B:315:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:CYS:N	1:A:101:PHE:O	2.51	0.41
1:A:126:GLN:O	1:A:126:GLN:HG3	2.21	0.41
1:B:126:GLN:CG	1:B:142:LEU:HD21	2.50	0.41
1:B:185:HIS:CE1	1:B:187:ILE:HB	2.56	0.41
1:B:223:GLU:HA	1:B:231:VAL:O	2.21	0.41
1:A:9:LYS:HG3	1:A:365:LEU:HD13	2.03	0.41
1:A:312:ASN:O	1:A:315:PRO:HD3	2.21	0.41
1:B:6:VAL:HB	1:B:366:MET:O	2.21	0.41
1:B:185:HIS:HE1	1:B:187:ILE:HG12	1.85	0.41
1:B:79:LEU:O	1:B:82:HIS:N	2.48	0.40
1:B:289:PRO:HG3	1:B:292:TRP:HE1	1.87	0.40
1:B:293:LEU:HB2	1:B:312:ASN:HB3	2.03	0.40
1:A:82:HIS:CD2	1:A:106:PRO:HG3	2.56	0.40
1:B:358:ASP:O	1:B:359:TYR:HB2	2.21	0.40
1:B:194:ALA:HB3	1:B:212:VAL:CG1	2.51	0.40
1:B:250:ASN:O	1:B:251:ASP:HB2	2.21	0.40
1:A:61:ALA:N	1:A:62:PRO:CD	2.85	0.40
1:A:212:VAL:HG23	1:A:213:ALA:N	2.37	0.40
1:A:300:HIS:CE1	1:A:302:TRP:HB2	2.56	0.40
1:B:78:ARG:HE	1:B:78:ARG:HB2	1.72	0.40
1:B:201:ASP:CG	1:B:205:THR:H	2.30	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	364/382 (95%)	327 (90%)	28 (8%)	9 (2%)	4	16
1	B	364/382 (95%)	326 (90%)	31 (8%)	7 (2%)	6	22
All	All	728/764 (95%)	653 (90%)	59 (8%)	16 (2%)	5	19

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	PRO
1	B	214	GLN
1	B	269	PRO
1	A	47	GLU
1	A	268	PRO
1	B	80	ASP
1	B	213	ALA
1	A	172	ARG
1	A	376	GLU
1	B	107	GLY
1	A	107	GLY
1	A	170	ARG
1	B	265	VAL
1	A	147	ILE
1	A	86	ASN
1	B	268	PRO

### 5.3.2 Protein sidechains [i](#)

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	310/318 (98%)	293 (94%)	17 (6%)	19	49
1	B	310/318 (98%)	294 (95%)	16 (5%)	21	50
All	All	620/636 (98%)	587 (95%)	33 (5%)	20	50

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	41	ARG
1	A	71	GLN
1	A	98	LEU
1	A	103	ILE
1	A	152	ARG
1	A	182	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	198	LEU
1	A	214	GLN
1	A	217	LEU
1	A	231	VAL
1	A	241	ARG
1	A	245	GLN
1	A	247	GLN
1	A	268	PRO
1	A	311	LEU
1	A	376	GLU
1	B	10	GLU
1	B	41	ARG
1	B	50	GLU
1	B	78	ARG
1	B	98	LEU
1	B	125	CYS
1	B	126	GLN
1	B	173	SER
1	B	189	ARG
1	B	198	LEU
1	B	212	VAL
1	B	214	GLN
1	B	231	VAL
1	B	250	ASN
1	B	319	GLU
1	B	376	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	64	HIS
1	A	69	GLN
1	A	94	GLN
1	A	108	GLN
1	A	112	GLN
1	A	113	GLN
1	A	126	GLN
1	A	163	HIS
1	A	168	ASN
1	A	210	HIS
1	A	214	GLN
1	A	270	GLN

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Mol	Chain	Res	Type
1	A	303	GLN
1	A	338	GLN
1	A	357	ASN
1	B	31	GLN
1	B	65	GLN
1	B	86	ASN
1	B	94	GLN
1	B	112	GLN
1	B	113	GLN
1	B	126	GLN
1	B	132	HIS
1	B	168	ASN
1	B	188	GLN
1	B	202	HIS
1	B	210	HIS
1	B	245	GLN
1	B	247	GLN
1	B	250	ASN
1	B	270	GLN
1	B	291	GLN
1	B	338	GLN
1	B	357	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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DAN	B	381	-	20,20,20	3.16	5 (25%)	24,28,28	1.97	6 (25%)
2	DAN	A	381	-	20,20,20	3.19	6 (30%)	24,28,28	1.94	5 (20%)
3	EPE	A	382	-	15,15,15	1.89	3 (20%)	19,20,20	1.34	3 (15%)
3	EPE	B	383	-	15,15,15	2.00	3 (20%)	19,20,20	1.12	2 (10%)
3	EPE	A	383	-	15,15,15	1.93	3 (20%)	19,20,20	1.09	2 (10%)
3	EPE	B	382	-	15,15,15	1.70	3 (20%)	19,20,20	1.28	2 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DAN	B	381	-	-	0/18/34/34	0/1/1/1
2	DAN	A	381	-	-	2/18/34/34	0/1/1/1
3	EPE	A	382	-	-	1/9/19/19	0/1/1/1
3	EPE	B	383	-	-	3/9/19/19	0/1/1/1
3	EPE	A	383	-	-	0/9/19/19	0/1/1/1
3	EPE	B	382	-	-	1/9/19/19	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	381	DAN	C3-C2	9.96	1.50	1.33
2	A	381	DAN	C3-C2	9.70	1.50	1.33
2	A	381	DAN	O10-C10	6.49	1.37	1.23
2	A	381	DAN	O1A-C1	6.14	1.37	1.22
2	B	381	DAN	O1A-C1	6.09	1.37	1.22
2	B	381	DAN	O10-C10	6.07	1.36	1.23
3	B	383	EPE	O3S-S	5.32	1.67	1.47
3	A	383	EPE	O3S-S	5.21	1.66	1.47
3	B	382	EPE	O3S-S	5.02	1.66	1.47
3	A	382	EPE	O3S-S	5.01	1.66	1.47
3	B	383	EPE	C10-S	3.86	1.83	1.77
3	A	383	EPE	C10-S	3.34	1.82	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	381	DAN	C4-C3	3.33	1.54	1.50
2	A	381	DAN	C4-C3	3.17	1.54	1.50
3	A	382	EPE	C10-S	3.04	1.81	1.77
3	A	382	EPE	C7-N4	2.91	1.54	1.47
3	B	383	EPE	C7-N4	2.65	1.53	1.47
3	A	383	EPE	C7-N4	2.64	1.53	1.47
2	B	381	DAN	C2-C1	-2.55	1.43	1.48
2	A	381	DAN	C2-C1	-2.55	1.43	1.48
3	B	382	EPE	C7-N4	2.39	1.52	1.47
2	A	381	DAN	C7-C6	2.13	1.55	1.52
3	B	382	EPE	C10-S	2.09	1.80	1.77

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	381	DAN	C4-C3-C2	-6.16	111.02	121.45
2	A	381	DAN	C4-C3-C2	-5.69	111.81	121.45
2	A	381	DAN	C4-C5-N5	-4.00	106.65	111.13
3	A	382	EPE	O3S-S-O1S	-3.93	101.57	111.40
3	B	382	EPE	O3S-S-O1S	-3.93	101.57	111.40
2	B	381	DAN	C4-C5-N5	-3.44	107.27	111.13
3	B	383	EPE	O3S-S-O1S	-2.82	104.34	111.40
3	A	383	EPE	O3S-S-O1S	-2.66	104.75	111.40
2	A	381	DAN	O1B-C1-C2	2.63	120.02	114.06
2	B	381	DAN	O10-C10-C11	-2.59	117.45	122.05
2	B	381	DAN	O1B-C1-O1A	-2.49	117.96	123.90
2	A	381	DAN	O1B-C1-O1A	-2.49	117.96	123.90
3	B	383	EPE	O1S-S-C10	2.38	110.33	106.73
3	A	382	EPE	O1S-S-C10	2.34	110.27	106.73
2	B	381	DAN	O1B-C1-C2	2.34	119.36	114.06
2	A	381	DAN	O10-C10-C11	-2.33	117.90	122.05
3	A	383	EPE	O1S-S-C10	2.29	110.19	106.73
3	B	382	EPE	C6-N1-C2	2.20	113.58	108.84
2	B	381	DAN	O6-C2-C1	2.11	116.23	112.02
3	A	382	EPE	C6-N1-C2	2.03	113.21	108.84

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	381	DAN	O8-C8-C9-O9
2	A	381	DAN	C7-C8-C9-O9

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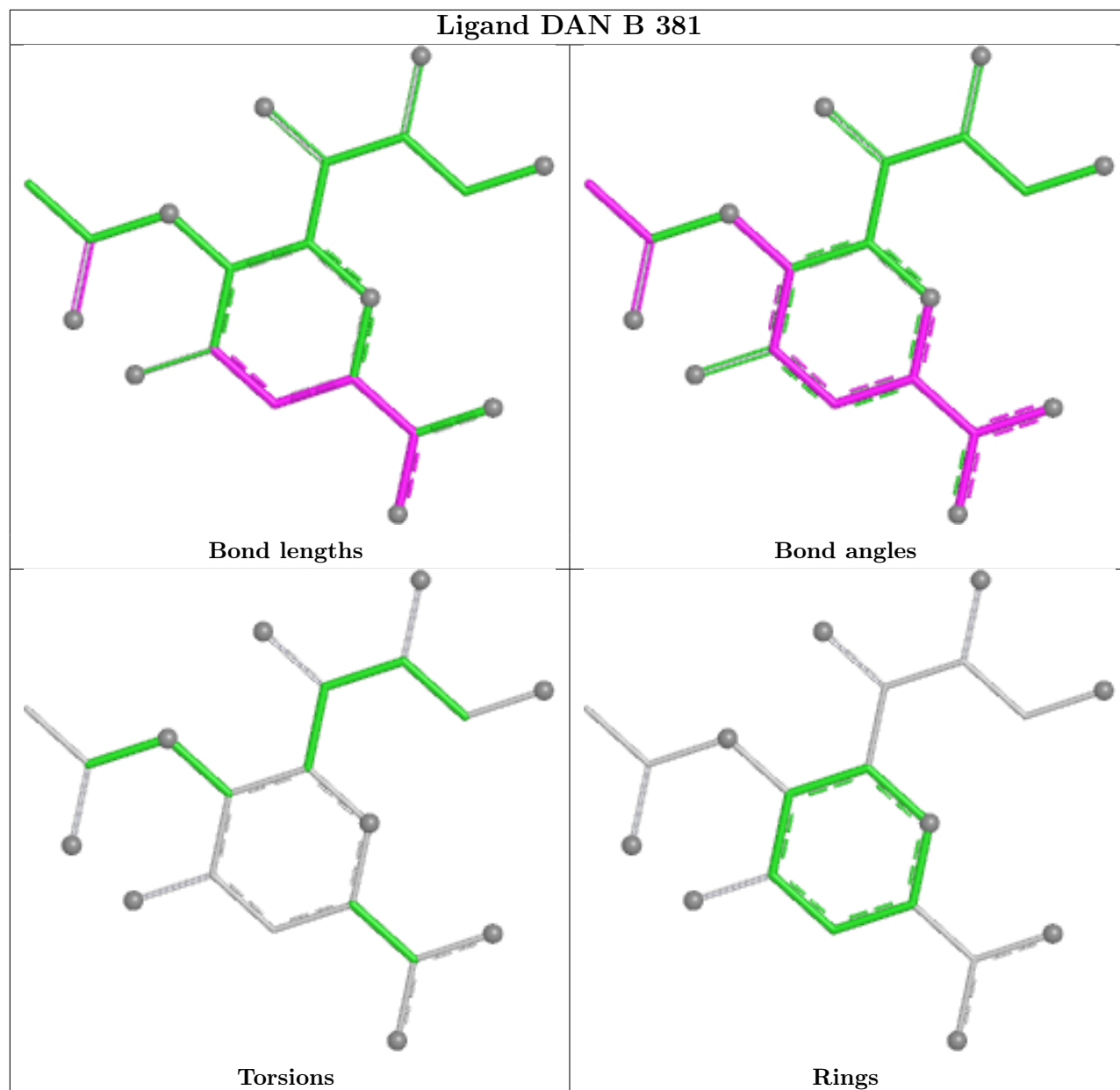
Mol	Chain	Res	Type	Atoms
3	B	383	EPE	N4-C7-C8-O8
3	A	382	EPE	N4-C7-C8-O8
3	B	383	EPE	C8-C7-N4-C3
3	B	383	EPE	C8-C7-N4-C5
3	B	382	EPE	N4-C7-C8-O8

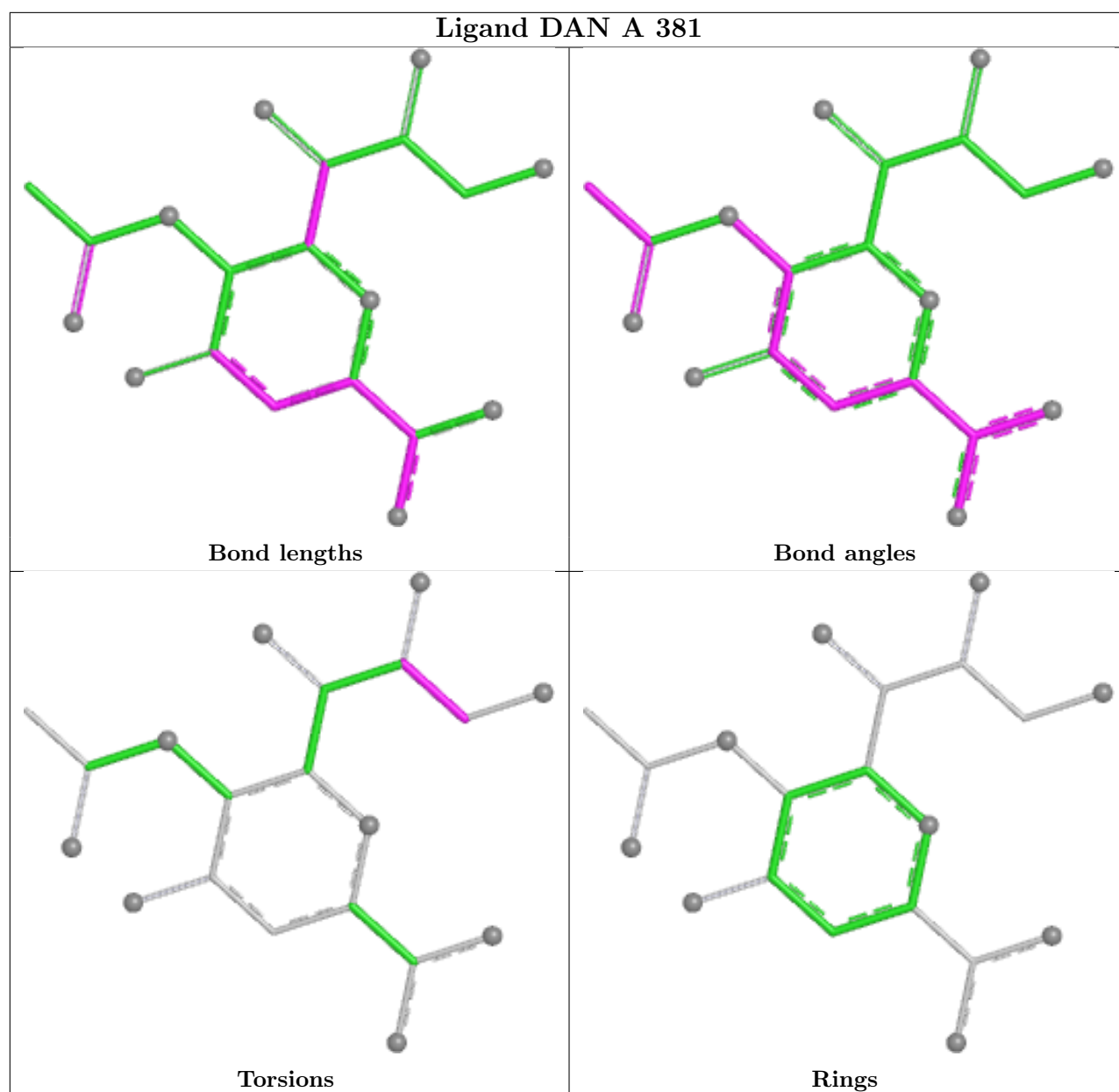
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	381	DAN	1	0
2	A	381	DAN	1	0
3	A	382	EPE	3	0
3	B	382	EPE	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	370/382 (96%)	-0.18	5 (1%) 73 65	10, 26, 44, 54	0
1	B	370/382 (96%)	-0.11	3 (0%) 82 76	12, 28, 44, 53	0
All	All	740/764 (96%)	-0.15	8 (1%) 78 71	10, 27, 44, 54	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	78	ARG	3.6
1	B	268	PRO	3.3
1	A	268	PRO	2.7
1	A	257	GLU	2.6
1	B	213	ALA	2.5
1	A	170	ARG	2.5
1	A	241	ARG	2.3
1	A	86	ASN	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.

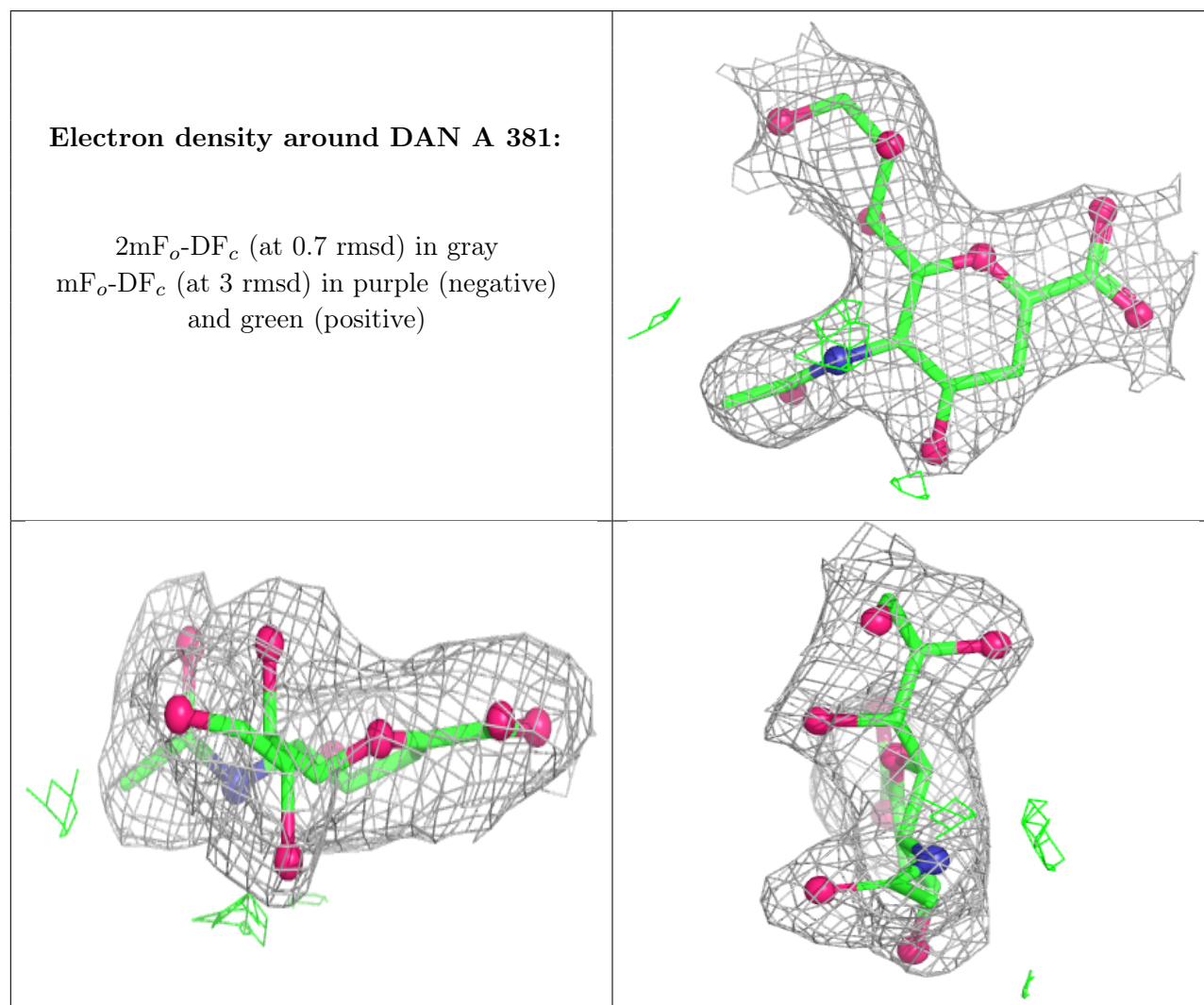
### 6.4 Ligands [i](#)

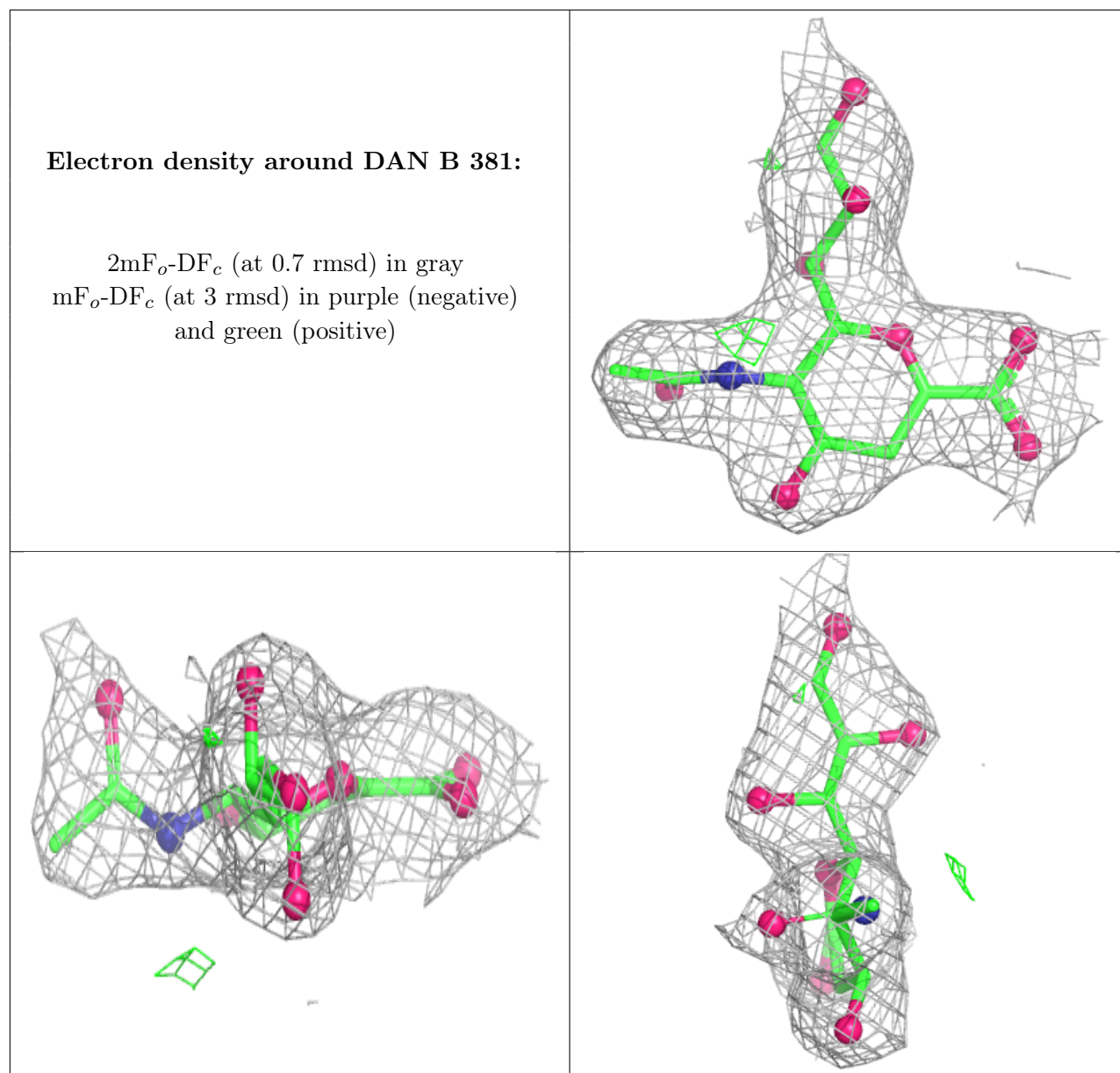
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	EPE	B	383	15/15	0.91	0.14	41,43,51,52	0
3	EPE	A	383	15/15	0.93	0.14	47,48,53,54	0
3	EPE	A	382	15/15	0.95	0.11	26,30,31,33	0
2	DAN	A	381	20/20	0.95	0.08	14,17,20,21	0
2	DAN	B	381	20/20	0.95	0.09	17,21,26,28	0
3	EPE	B	382	15/15	0.97	0.08	19,21,24,25	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.