



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:32 AM UTC

PDB ID : 1SZR / pdb_00001sZR
Title : A Dimer interface mutant of ornithine decarboxylase reveals structure of gem diamine intermediate
Authors : Jackson, L.K.; Baldwin, J.; Goldsmith, E.J.; Phillips, M.A.
Deposited on : 2004-04-06
Resolution : 2.15 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

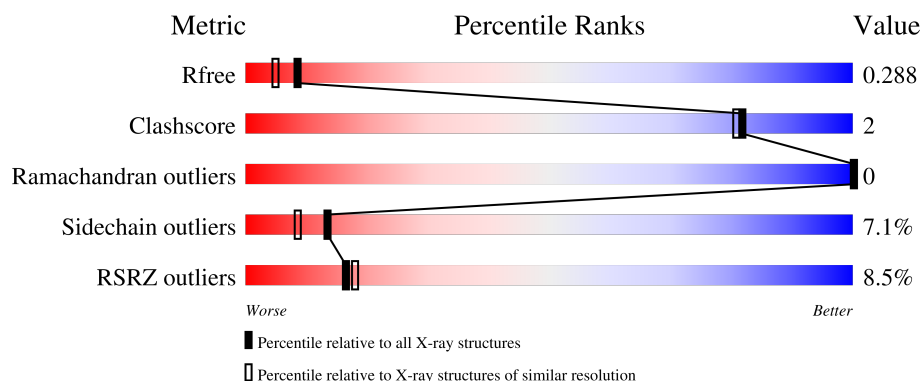
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	425	4% 76% 5% 19%
1	B	425	7% 72% 10% 17%
1	C	425	7% 72% 9% 18%
1	D	425	9% 77% 9% 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11393 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.

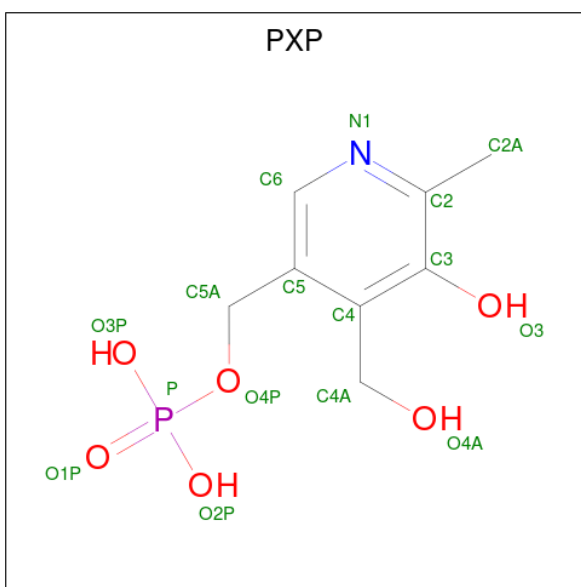
- Molecule 1 is a protein called Ornithine decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	347	Total	C	N	O	S	0	0	0
			2715	1747	450	503	15			
1	D	368	Total	C	N	O	S	0	0	0
			2879	1851	480	532	16			
1	A	345	Total	C	N	O	S	0	0	0
			2695	1732	447	501	15			
1	B	354	Total	C	N	O	S	0	0	0
			2768	1780	461	512	15			

There are 12 discrepancies between the modelled and reference sequences:

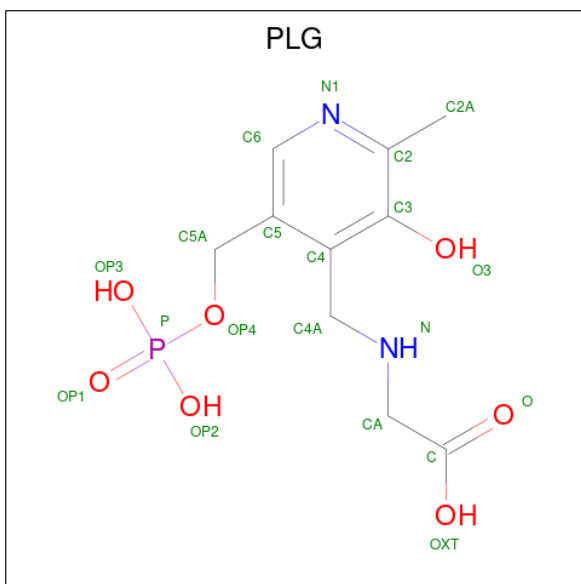
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P07805
A	2	ALA	-	cloning artifact	UNP P07805
A	294	ALA	LYS	engineered mutation	UNP P07805
B	1	GLY	-	cloning artifact	UNP P07805
B	2	ALA	-	cloning artifact	UNP P07805
B	294	ALA	LYS	engineered mutation	UNP P07805
C	1	GLY	-	cloning artifact	UNP P07805
C	2	ALA	-	cloning artifact	UNP P07805
C	294	ALA	LYS	engineered mutation	UNP P07805
D	1	GLY	-	cloning artifact	UNP P07805
D	2	ALA	-	cloning artifact	UNP P07805
D	294	ALA	LYS	engineered mutation	UNP P07805

- Molecule 2 is PYRIDOXINE-5'-PHOSPHATE (CCD ID: PXP) (formula: C₈H₁₂NO₆P).



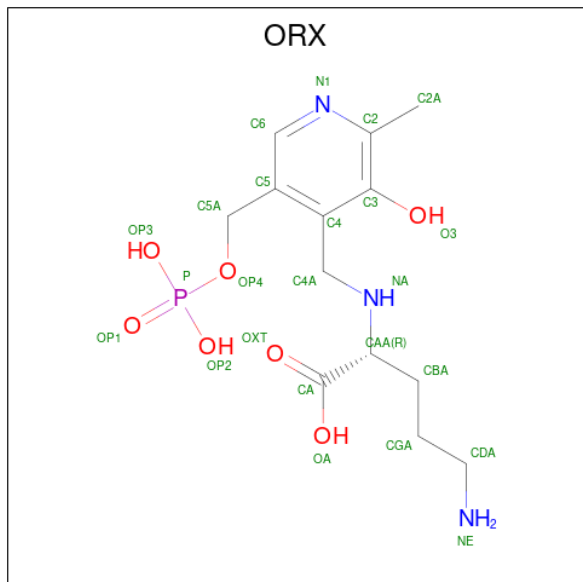
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 3 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL-METHANE] (CCD ID: PLG) (formula: $C_{10}H_{15}N_2O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

- Molecule 4 is N 2 -({3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL}METHYL)-D-ORNITHINE (CCD ID: ORX) (formula: $C_{13}H_{22}N_3O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			24	13	3	7	1		

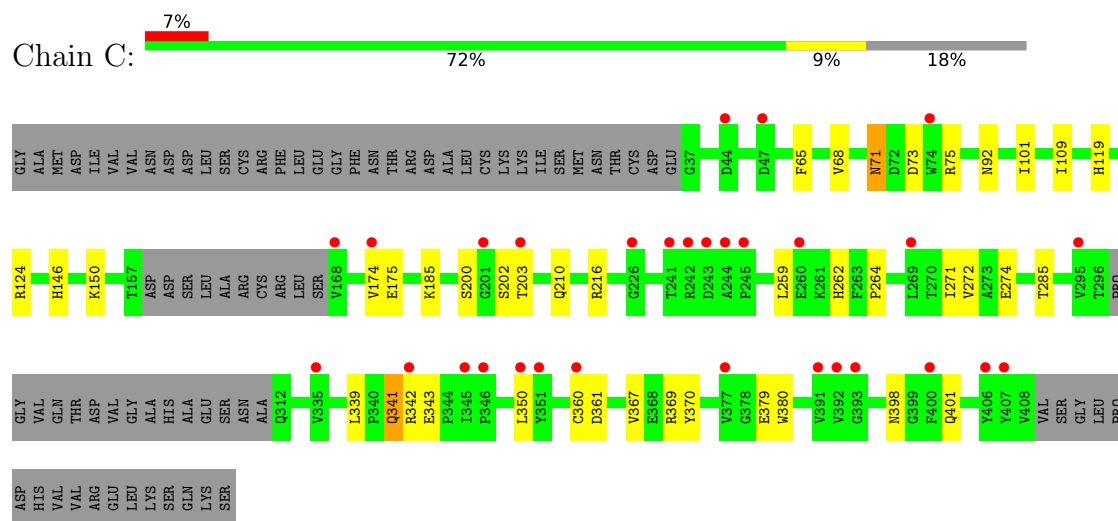
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	60	Total	O	0	0
			60	60		
5	D	57	Total	O	0	0
			57	57		
5	A	65	Total	O	0	0
			65	65		
5	B	78	Total	O	0	0
			78	78		

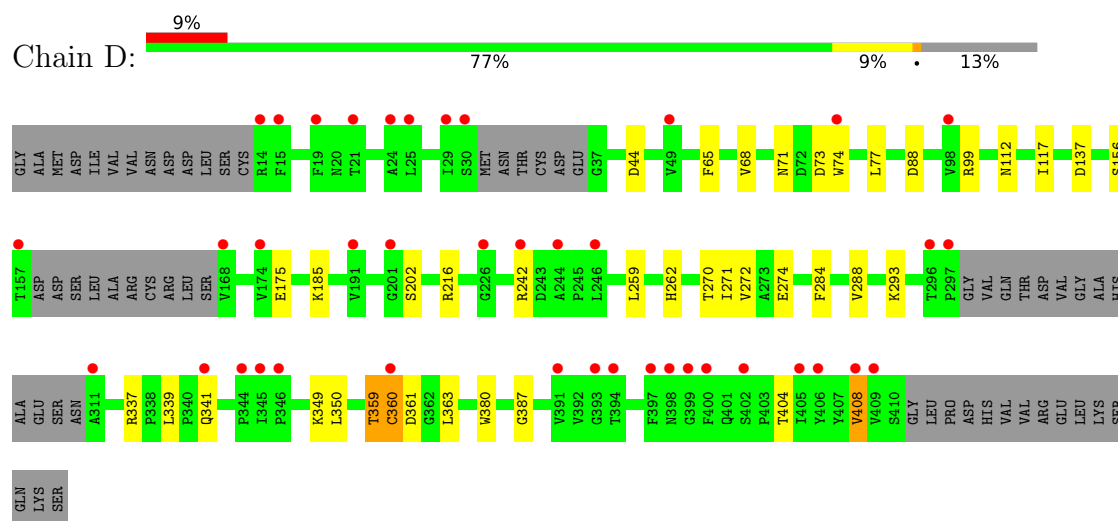
3 Residue-property plots [i](#)

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.

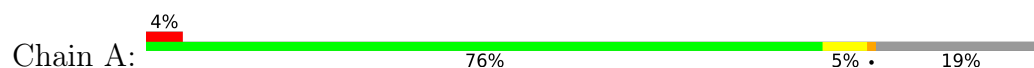
• Molecule 1: Ornithine decarboxylase

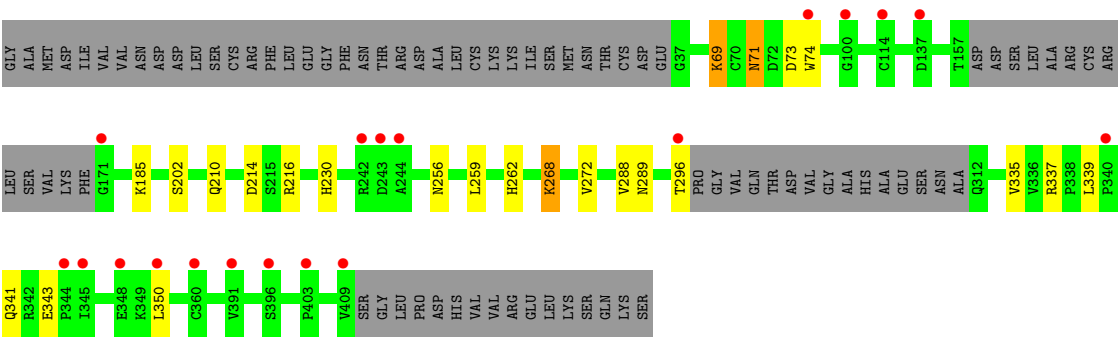


• Molecule 1: Ornithine decarboxylase

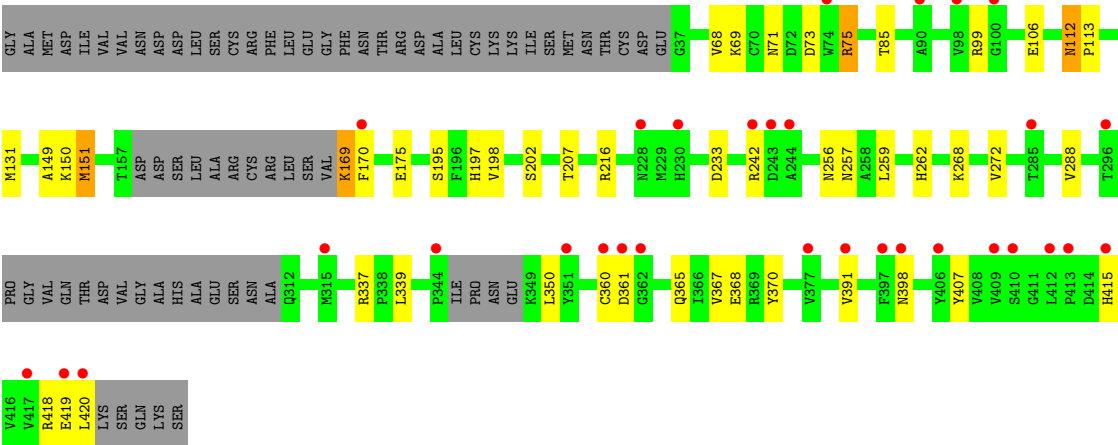


• Molecule 1: Ornithine decarboxylase





● Molecule 1: Ornithine decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.47Å 152.44Å 155.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.15 35.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	77.6 (35.00-2.15) 89.1 (35.00-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.13 (at 2.12Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.244 , 0.279 0.251 , 0.288	Depositor DCC
R_{free} test set	4213 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.722	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11393	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9527e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ORX, PXP, PLG

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	0.50	0/2762	0.79	0/3752
1	B	0.58	1/2836 (0.0%)	0.80	0/3849
1	C	0.49	0/2783	0.80	1/3779 (0.0%)
1	D	0.52	0/2949	0.80	1/4000 (0.0%)
All	All	0.52	1/11330 (0.0%)	0.80	2/15380 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	151	MET	SD-CE	-14.57	1.43	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	264	PRO	O-C-N	6.16	124.05	121.15
1	D	361	ASP	CA-CB-CG	5.08	117.68	112.60

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	2695	0	2643	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2768	0	2719	22	0
1	C	2715	0	2665	15	0
1	D	2879	0	2834	11	0
2	C	16	0	7	0	0
2	D	16	0	7	0	0
3	A	20	0	9	0	0
4	B	24	0	16	2	0
5	A	65	0	0	2	0
5	B	78	0	0	2	0
5	C	60	0	0	1	0
5	D	57	0	0	0	0
All	All	11393	0	10900	55	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 2.

All (55) 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:69:LYS:HE3	1:B:360:CYS:SG	2.32	0.70
1:C:216:ARG:HD3	1:C:262:HIS:O	1.96	0.65
1:D:216:ARG:HD3	1:D:262:HIS:O	1.96	0.64
1:C:342:ARG:HH22	1:C:379:GLU:CD	2.07	0.62
1:A:216:ARG:HD3	1:A:262:HIS:O	2.01	0.60
1:B:169:LYS:N	5:B:606:HOH:O	2.37	0.58
1:B:149:ALA:HB3	1:B:151:MET:HE3	1.85	0.57
1:C:360:CYS:SG	1:C:361:ASP:N	2.77	0.57
1:B:112:ASN:C	1:B:112:ASN:HD22	2.15	0.55
1:A:71:ASN:HD22	1:A:71:ASN:C	2.16	0.54
1:C:342:ARG:HG3	1:C:343:GLU:N	2.24	0.53
1:C:341:GLN:HG2	1:C:380:TRP:HB2	1.90	0.53
1:B:198:VAL:HG13	1:B:207:THR:HG21	1.93	0.49
1:C:367:VAL:HG11	1:C:370:TYR:HB2	1.95	0.48
1:D:68:VAL:HG23	1:D:77:LEU:HD21	1.97	0.47
1:B:169:LYS:HD2	1:B:170:PHE:CE1	2.50	0.47
1:B:71:ASN:HD22	1:B:71:ASN:C	2.23	0.47
1:A:71:ASN:HD22	1:A:73:ASP:H	1.62	0.47
1:B:256:ASN:ND2	5:B:572:HOH:O	2.48	0.46
1:C:71:ASN:C	1:C:71:ASN:HD22	2.24	0.46
1:D:359:THR:HG23	1:D:360:CYS:N	2.29	0.46
1:A:289:ASN:ND2	5:A:602:HOH:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:GLN:HG2	1:D:380:TRP:HB2	1.98	0.46
1:B:131:MET:HE3	1:B:151:MET:HE1	1.97	0.45
1:A:230:HIS:HB2	1:A:268:LYS:O	2.15	0.45
1:D:112:ASN:HD22	1:D:112:ASN:C	2.25	0.45
1:C:124:ARG:HG3	1:C:146:HIS:CD2	2.52	0.45
1:B:216:ARG:HD3	1:B:262:HIS:O	2.17	0.44
1:C:216:ARG:CD	1:C:262:HIS:O	2.65	0.44
1:B:365:GLN:HE21	1:B:368:GLU:HA	1.82	0.43
1:B:71:ASN:HD22	1:B:73:ASP:H	1.65	0.43
1:A:256:ASN:ND2	5:A:577:HOH:O	2.52	0.43
1:C:65:PHE:CD2	1:C:109:ILE:HD12	2.54	0.42
1:B:195:SER:HA	1:B:233:ASP:O	2.18	0.42
1:B:197:HIS:HE2	4:B:571:ORX:HNA	1.67	0.42
1:C:401:GLN:NE2	5:C:624:HOH:O	2.52	0.42
1:C:71:ASN:HD22	1:C:73:ASP:H	1.65	0.42
1:C:92:ASN:CG	1:C:119:HIS:CE1	2.98	0.42
1:B:149:ALA:CB	1:B:151:MET:HE3	2.48	0.41
1:C:101:ILE:HA	1:A:74:TRP:CH2	2.55	0.41
1:D:44:ASP:HA	1:D:408:VAL:HG13	2.03	0.41
1:B:75:ARG:HD3	1:B:407:TYR:CE1	2.56	0.41
1:B:112:ASN:C	1:B:112:ASN:ND2	2.78	0.41
1:D:71:ASN:C	1:D:71:ASN:HD22	2.28	0.41
1:D:284:PHE:HB2	1:D:387:GLY:CA	2.51	0.41
1:B:195:SER:CB	1:B:233:ASP:HB3	2.51	0.41
1:D:65:PHE:O	1:D:274:GLU:HA	2.21	0.41
1:D:73:ASP:O	1:D:77:LEU:HG	2.20	0.41
1:D:88:ASP:OD1	1:D:88:ASP:C	2.63	0.41
1:B:367:VAL:HG11	1:B:370:TYR:HB2	2.02	0.41
1:C:65:PHE:O	1:C:274:GLU:HA	2.19	0.41
1:B:69:LYS:NZ	4:B:571:ORX:HBA1	2.35	0.41
1:B:131:MET:CE	1:B:151:MET:HE1	2.51	0.41
1:A:210:GLN:NE2	1:A:214:ASP:OD2	2.51	0.40
1:B:112:ASN:HD22	1:B:113:PRO:N	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	339/425 (80%)	329 (97%)	10 (3%)	0	100	100
1	B	346/425 (81%)	338 (98%)	8 (2%)	0	100	100
1	C	341/425 (80%)	329 (96%)	12 (4%)	0	100	100
1	D	360/425 (85%)	347 (96%)	13 (4%)	0	100	100
All	All	1386/1700 (82%)	1343 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	292/361 (81%)	277 (95%)	15 (5%)	21	18
1	B	300/361 (83%)	274 (91%)	26 (9%)	9	5
1	C	294/361 (81%)	274 (93%)	20 (7%)	14	10
1	D	312/361 (86%)	288 (92%)	24 (8%)	12	7
All	All	1198/1444 (83%)	1113 (93%)	85 (7%)	13	8

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	68	VAL
1	C	71	ASN

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Mol	Chain	Res	Type
1	C	75	ARG
1	C	150	LYS
1	C	174	VAL
1	C	175	GLU
1	C	185	LYS
1	C	200	SER
1	C	202	SER
1	C	203	THR
1	C	210	GLN
1	C	259	LEU
1	C	271	ILE
1	C	272	VAL
1	C	285	THR
1	C	339	LEU
1	C	341	GLN
1	C	350	LEU
1	C	369	ARG
1	C	398	ASN
1	D	74	TRP
1	D	99	ARG
1	D	117	ILE
1	D	137	ASP
1	D	156	SER
1	D	175	GLU
1	D	185	LYS
1	D	202	SER
1	D	242	ARG
1	D	259	LEU
1	D	270	THR
1	D	271	ILE
1	D	272	VAL
1	D	288	VAL
1	D	293	LYS
1	D	337	ARG
1	D	339	LEU
1	D	349	LYS
1	D	350	LEU
1	D	359	THR
1	D	360	CYS
1	D	363	LEU
1	D	404	THR
1	D	408	VAL

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Mol	Chain	Res	Type
1	A	69	LYS
1	A	71	ASN
1	A	185	LYS
1	A	202	SER
1	A	259	LEU
1	A	268	LYS
1	A	272	VAL
1	A	288	VAL
1	A	296	THR
1	A	335	VAL
1	A	337	ARG
1	A	339	LEU
1	A	341	GLN
1	A	343	GLU
1	A	350	LEU
1	B	68	VAL
1	B	75	ARG
1	B	85	THR
1	B	99	ARG
1	B	106	GLU
1	B	112	ASN
1	B	150	LYS
1	B	169	LYS
1	B	175	GLU
1	B	202	SER
1	B	242	ARG
1	B	257	ASN
1	B	259	LEU
1	B	268	LYS
1	B	272	VAL
1	B	288	VAL
1	B	337	ARG
1	B	339	LEU
1	B	350	LEU
1	B	361	ASP
1	B	391	VAL
1	B	398	ASN
1	B	415	HIS
1	B	418	ARG
1	B	419	GLU
1	B	420	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30)

such sidechains are listed below:

Mol	Chain	Res	Type
1	C	71	ASN
1	C	112	ASN
1	C	119	HIS
1	C	256	ASN
1	C	289	ASN
1	C	312	GLN
1	C	341	GLN
1	D	71	ASN
1	D	112	ASN
1	D	116	GLN
1	D	146	HIS
1	D	230	HIS
1	D	256	ASN
1	D	289	ASN
1	D	347	ASN
1	A	71	ASN
1	A	112	ASN
1	A	116	GLN
1	A	119	HIS
1	A	256	ASN
1	A	289	ASN
1	A	347	ASN
1	A	398	ASN
1	B	71	ASN
1	B	112	ASN
1	B	116	GLN
1	B	146	HIS
1	B	183	GLN
1	B	256	ASN
1	B	398	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 ⓘ

4 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	PXP	D	575	1	16,16,16	1.30	2 (12%)	22,23,23	1.37	5 (22%)
4	ORX	B	571	1	24,24,24	0.97	2 (8%)	29,33,33	1.47	7 (24%)
2	PXP	C	575	1	16,16,16	1.16	1 (6%)	22,23,23	1.17	3 (13%)
3	PLG	A	572	1	20,20,20	1.14	2 (10%)	26,28,28	1.60	5 (19%)

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	PXP	D	575	1	-	0/8/8/8	0/1/1/1
4	ORX	B	571	1	-	7/19/19/19	0/1/1/1
2	PXP	C	575	1	-	0/8/8/8	0/1/1/1
3	PLG	A	572	1	-	4/12/12/12	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	575	PXP	P-O1P	3.01	1.59	1.50
2	D	575	PXP	C4A-C4	2.73	1.54	1.51
2	D	575	PXP	P-O1P	2.57	1.58	1.50
4	B	571	ORX	P-OP1	2.44	1.58	1.50
3	A	572	PLG	P-OP1	2.42	1.58	1.50
3	A	572	PLG	OXT-C	-2.15	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	571	ORX	OA-CA	-2.04	1.24	1.30

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	572	PLG	C4A-C4-C5	3.53	123.59	119.75
4	B	571	ORX	C4A-NA-CAA	3.28	119.99	113.84
4	B	571	ORX	C4A-C4-C5	3.26	123.29	119.75
2	D	575	PXP	C3-C4-C5	-3.11	115.91	118.73
3	A	572	PLG	C4-C4A-N	-2.99	105.98	111.50
3	A	572	PLG	OP3-P-OP4	2.76	113.86	106.67
4	B	571	ORX	OP3-P-OP4	2.48	113.14	106.67
4	B	571	ORX	C5A-C5-C6	-2.47	115.34	119.36
2	D	575	PXP	C6-C5-C4	2.39	119.87	118.06
3	A	572	PLG	C4A-N-CA	2.35	115.46	112.72
4	B	571	ORX	OA-CA-OXT	-2.31	118.85	124.08
2	D	575	PXP	C4A-C4-C5	2.20	123.27	119.91
4	B	571	ORX	C3-C4-C5	-2.20	116.73	118.73
2	C	575	PXP	C3-C4-C5	-2.18	116.75	118.73
4	B	571	ORX	OA-CA-CAA	2.11	120.67	113.51
2	D	575	PXP	O3P-P-O4P	2.05	112.00	106.67
3	A	572	PLG	C3-C4-C5	-2.02	116.89	118.73
2	C	575	PXP	O3P-P-O4P	2.01	111.90	106.67
2	C	575	PXP	C6-C5-C4	2.00	119.58	118.06
2	D	575	PXP	C5A-C5-C6	-2.00	116.10	119.36

There are no chirality outliers.

All (11) torsion outliers are listed below:

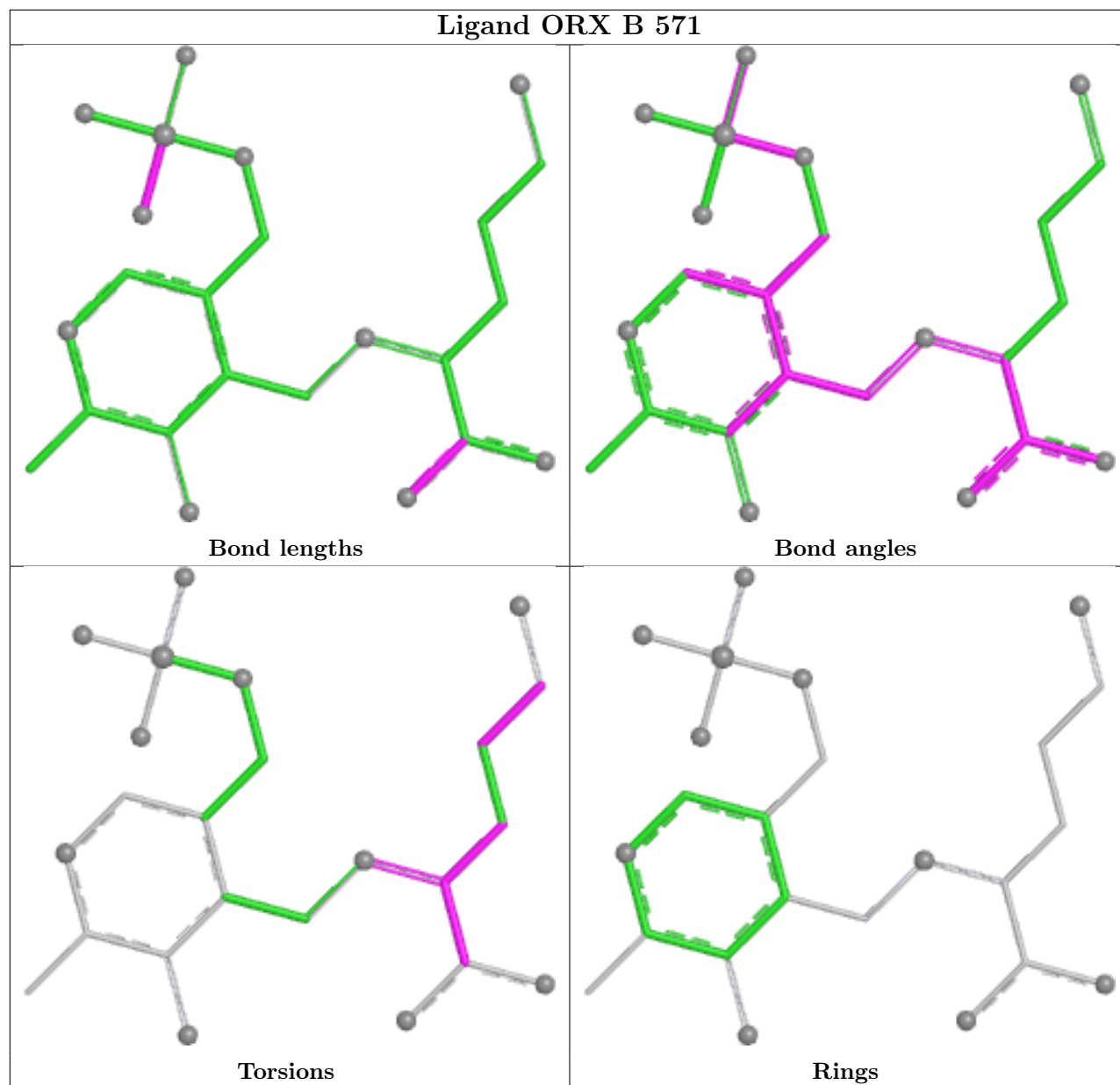
Mol	Chain	Res	Type	Atoms
4	B	571	ORX	CA-CAA-NA-C4A
4	B	571	ORX	CBA-CAA-NA-C4A
4	B	571	ORX	NA-CAA-CBA-CGA
3	A	572	PLG	O-C-CA-N
4	B	571	ORX	CA-CAA-CBA-CGA
3	A	572	PLG	OXT-C-CA-N
3	A	572	PLG	C4-C4A-N-CA
3	A	572	PLG	C-CA-N-C4A
4	B	571	ORX	OXT-CA-CAA-NA
4	B	571	ORX	OA-CA-CAA-NA
4	B	571	ORX	NE-CDA-CGA-CBA

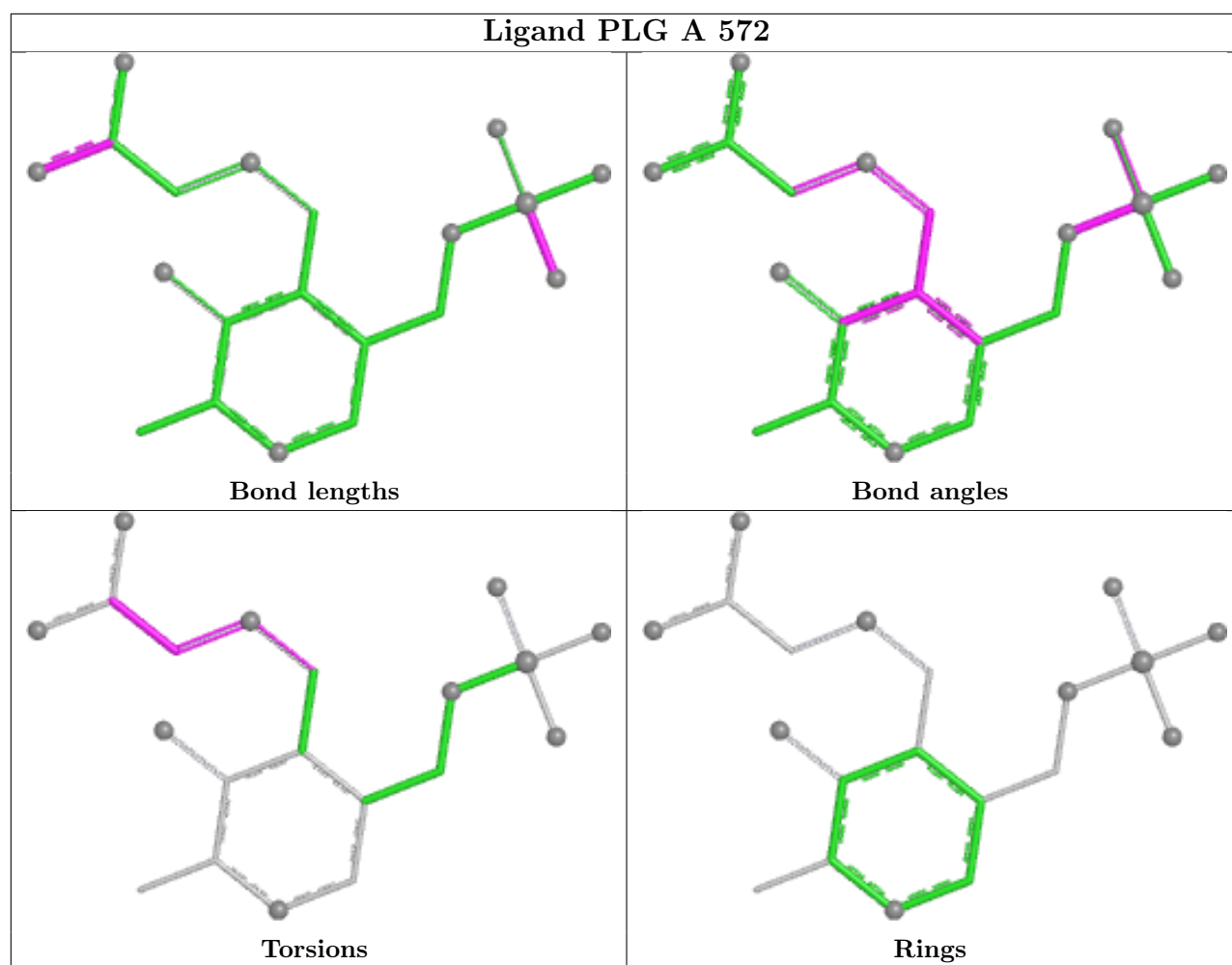
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	571	ORX	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	345/425 (81%)	0.70	19 (5%)	30 34	25, 37, 52, 68	0
1	B	354/425 (83%)	0.84	31 (8%)	15 17	25, 38, 55, 67	0
1	C	347/425 (81%)	0.84	30 (8%)	16 17	26, 38, 52, 68	0
1	D	368/425 (86%)	0.88	40 (10%)	10 12	26, 38, 67, 80	0
All	All	1414/1700 (83%)	0.82	120 (8%)	16 18	25, 38, 56, 80	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	415	HIS	6.9
1	D	74	TRP	6.3
1	B	420	LEU	6.0
1	A	243	ASP	5.5
1	C	360	CYS	5.1
1	B	412	LEU	4.6
1	B	413	PRO	4.5
1	B	74	TRP	4.5
1	D	311	ALA	4.4
1	B	360	CYS	4.3
1	C	243	ASP	4.1
1	C	345	ILE	4.1
1	A	74	TRP	3.9
1	C	74	TRP	3.8
1	D	399	GLY	3.8
1	C	168	VAL	3.7
1	D	21	THR	3.7
1	B	228	ASN	3.6
1	B	398	ASN	3.6
1	D	242	ARG	3.6
1	A	345	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	345	ILE	3.6
1	B	409	VAL	3.5
1	D	19	PHE	3.5
1	B	417	VAL	3.3
1	C	245	PRO	3.3
1	B	419	GLU	3.2
1	B	170	PHE	3.2
1	B	242	ARG	3.2
1	B	296	THR	3.2
1	C	335	VAL	3.1
1	A	391	VAL	3.1
1	B	243	ASP	3.1
1	C	342	ARG	3.0
1	D	244	ALA	3.0
1	D	405	ILE	3.0
1	C	400	PHE	3.0
1	D	408	VAL	3.0
1	D	174	VAL	2.9
1	C	226	GLY	2.9
1	C	377	VAL	2.9
1	C	260	GLU	2.9
1	D	297	PRO	2.8
1	D	398	ASN	2.8
1	C	407	TYR	2.8
1	D	246	LEU	2.8
1	D	360	CYS	2.8
1	D	346	PRO	2.8
1	B	351	TYR	2.8
1	A	242	ARG	2.7
1	D	341	GLN	2.7
1	B	230	HIS	2.7
1	D	29	ILE	2.7
1	B	285	THR	2.7
1	A	100	GLY	2.7
1	B	344	PRO	2.6
1	C	244	ALA	2.6
1	C	242	ARG	2.6
1	B	377	VAL	2.6
1	D	393	GLY	2.6
1	A	396	SER	2.6
1	A	171	GLY	2.6
1	C	174	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	351	TYR	2.5
1	B	361	ASP	2.5
1	D	157	THR	2.5
1	B	315	MET	2.5
1	D	296	THR	2.5
1	C	201	GLY	2.5
1	D	49	VAL	2.4
1	D	191	VAL	2.4
1	D	406	TYR	2.4
1	A	344	PRO	2.4
1	C	350	LEU	2.4
1	C	393	GLY	2.4
1	D	30	SER	2.4
1	B	406	TYR	2.4
1	C	47	ASP	2.4
1	D	344	PRO	2.4
1	A	350	LEU	2.3
1	B	410	SER	2.3
1	C	241	THR	2.3
1	C	406	TYR	2.3
1	A	114	CYS	2.3
1	B	90	ALA	2.3
1	B	362	GLY	2.3
1	D	402	SER	2.2
1	B	98	VAL	2.2
1	C	269	LEU	2.2
1	A	348	GLU	2.2
1	D	15	PHE	2.2
1	C	203	THR	2.2
1	A	409	VAL	2.2
1	A	137	ASP	2.2
1	C	44	ASP	2.2
1	C	391	VAL	2.2
1	A	360	CYS	2.2
1	A	340	PRO	2.1
1	D	400	PHE	2.1
1	B	397	PHE	2.1
1	C	392	VAL	2.1
1	A	244	ALA	2.1
1	D	14	ARG	2.1
1	A	296	THR	2.1
1	D	409	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	394	THR	2.1
1	A	403	PRO	2.1
1	B	100	GLY	2.1
1	D	397	PHE	2.1
1	D	25	LEU	2.1
1	C	346	PRO	2.1
1	D	201	GLY	2.1
1	D	98	VAL	2.1
1	D	168	VAL	2.1
1	B	391	VAL	2.1
1	D	24	ALA	2.1
1	B	244	ALA	2.1
1	C	295	VAL	2.0
1	D	391	VAL	2.0
1	D	226	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](#)

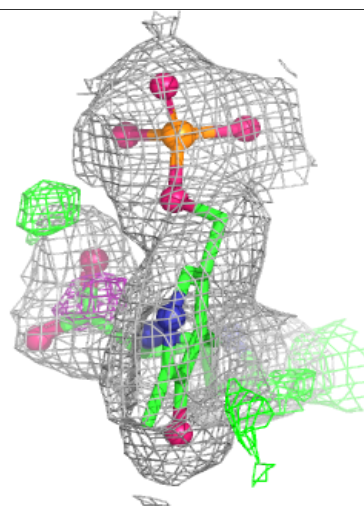
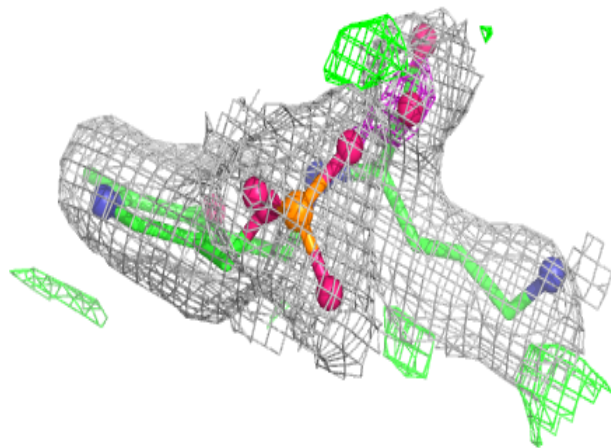
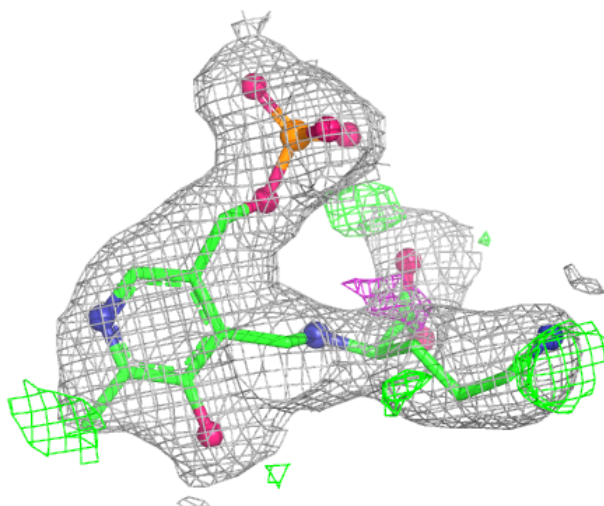
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

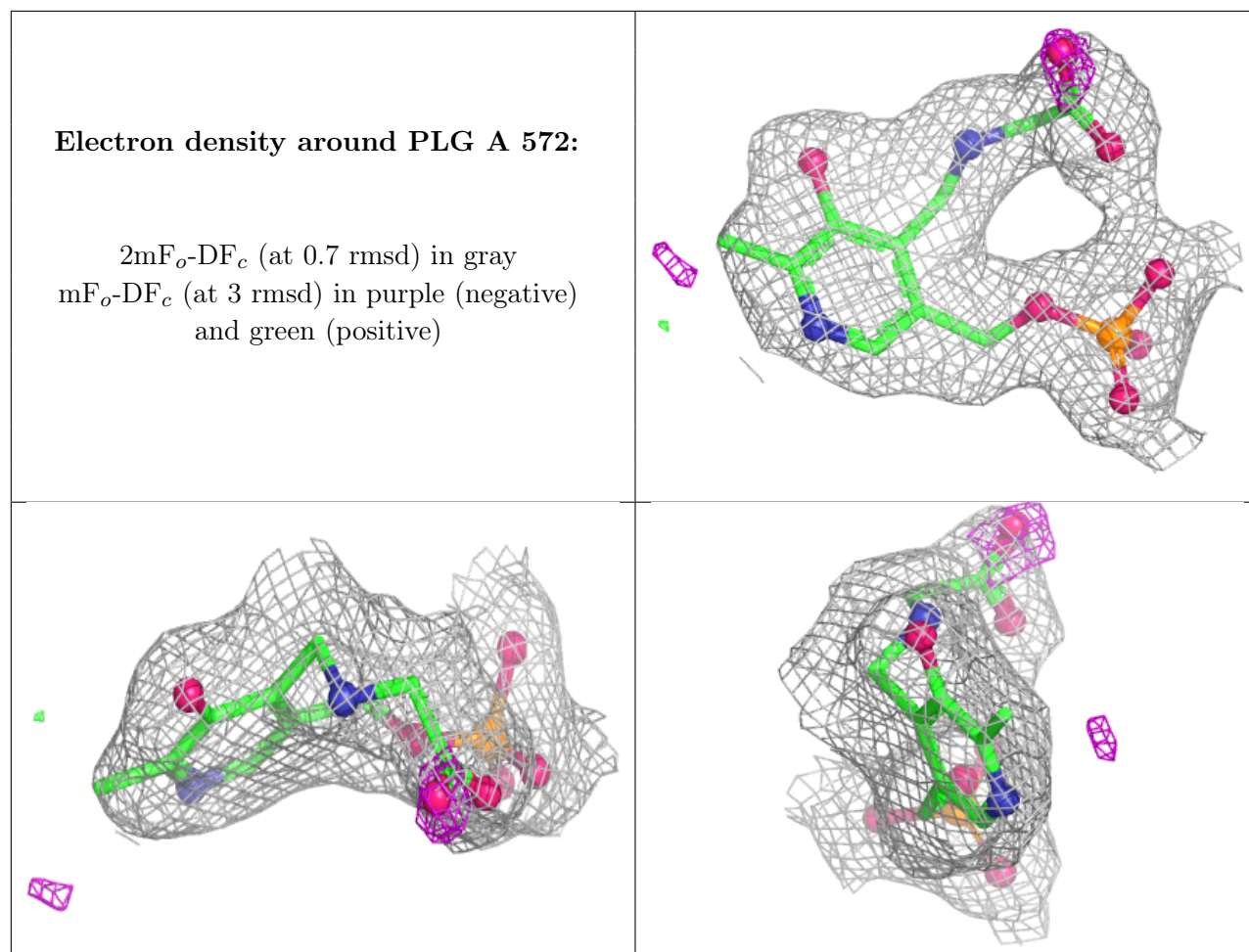
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ORX	B	571	24/24	0.93	0.11	22,34,43,44	0
3	PLG	A	572	20/20	0.95	0.08	22,30,37,38	0
2	PXP	D	575	16/16	0.97	0.07	24,32,37,38	0
2	PXP	C	575	16/16	0.98	0.05	27,33,37,38	0

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 ORX B 571:

$2mF_o-DF_c$ (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.