



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2026 – 11:16 AM UTC

PDB ID : 3DWB / pdb_00003dwb
Title : structure of human ECE-1 complexed with phosphoramidon
Authors : Oefner, C.
Deposited on : 2008-07-22
Resolution : 2.38 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

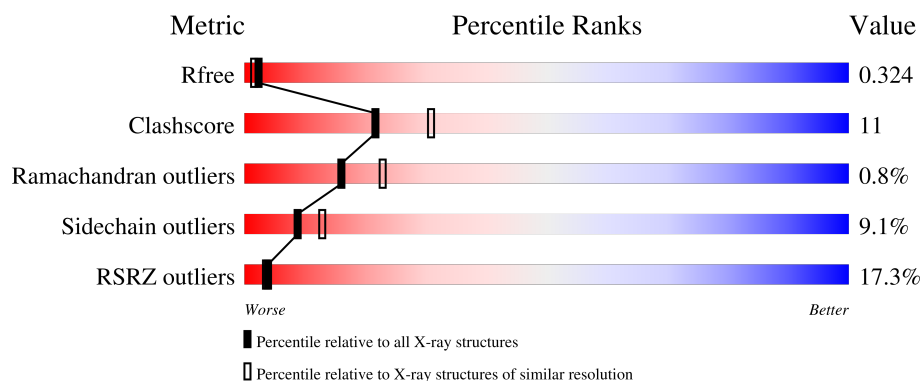
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	670	17% 71% 24% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5580 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 Endothelin-converting enzyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	660	5305	3371	896	1011	27	0	0	0

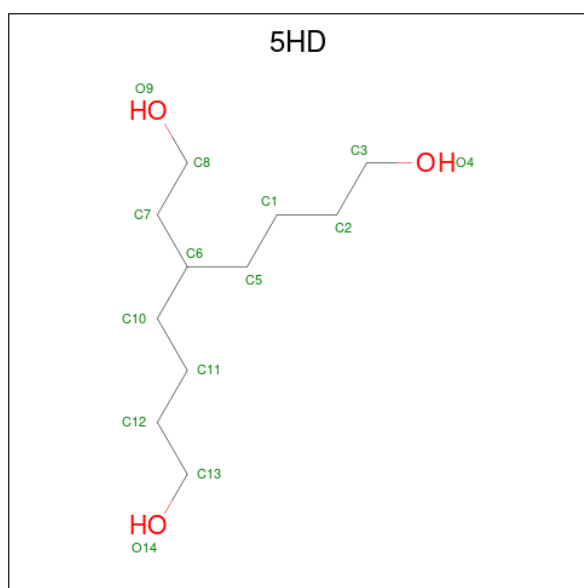
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	428	SER	CYS	engineered mutation	UNP P42892

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

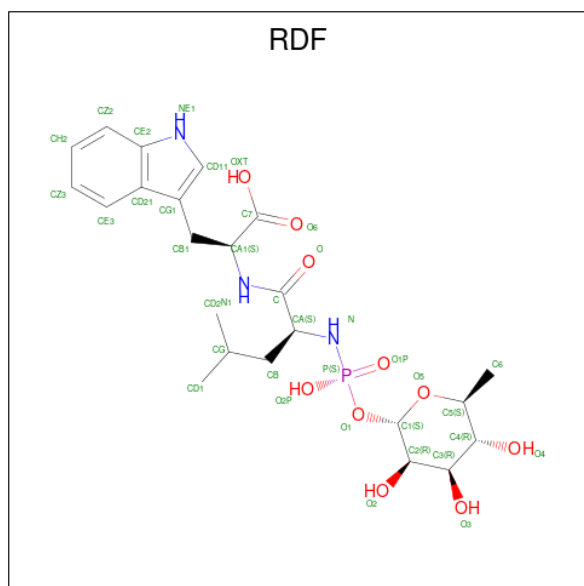
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 5-(2-hydroxyethyl)nonane-1,9-diol (CCD ID: 5HD) (formula: C₁₁H₂₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	11	3		

- Molecule 4 is N-ALPHA-L-RHAMNOPYRANOSYLOXY(HYDROXYPHOSPHINYL)-L-L EUCYL-L-TRYPTOPHAN (CCD ID: RDF) (formula: $C_{23}H_{34}N_3O_{10}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			37	23	3	10	1		

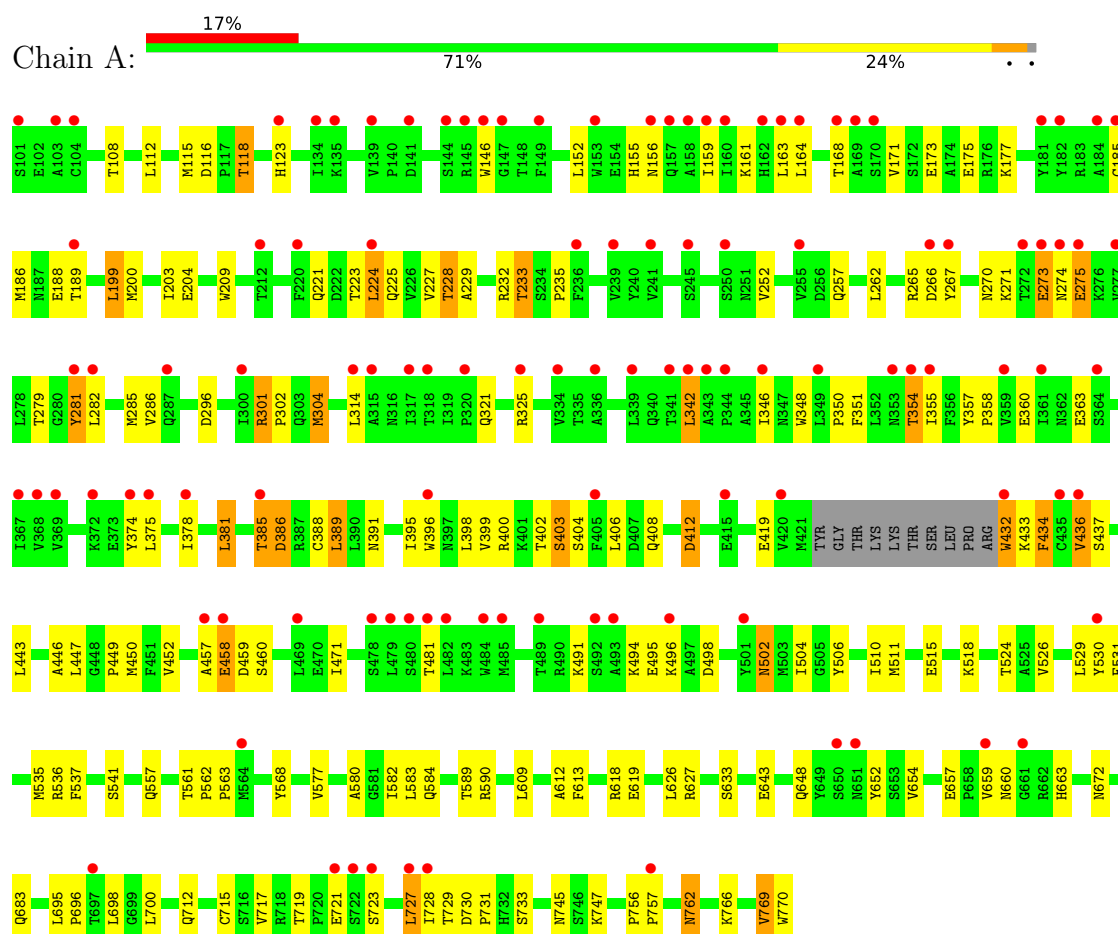
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	223	Total	O	0	0
			223	223		

3 Residue-property plots

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

- Molecule 1: Endothelin-converting enzyme 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	120.88Å 120.88Å 192.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.38 20.00 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.38) 98.8 (20.00-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.262 , 0.345 0.251 , 0.324	Depositor DCC
R_{free} test set	1705 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5580	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: RDF, 5HD, ZN

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	0.95	13/5445 (0.2%)	1.04	10/7393 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	GLU	CD-OE2	19.37	1.62	1.25
1	A	412	ASP	CG-OD1	13.28	1.50	1.25
1	A	281	TYR	C-O	7.88	1.34	1.24
1	A	459	ASP	CG-OD2	7.18	1.39	1.25
1	A	275	GLU	CD-OE2	7.05	1.38	1.25
1	A	408	GLN	C-O	7.00	1.33	1.24
1	A	279	THR	C-O	6.48	1.31	1.24
1	A	419	GLU	CD-OE1	6.01	1.36	1.25
1	A	188	GLU	CG-CD	5.66	1.66	1.52
1	A	279	THR	C-N	5.52	1.41	1.33
1	A	275	GLU	CD-OE1	5.38	1.35	1.25
1	A	458	GLU	CD-OE1	5.28	1.35	1.25
1	A	281	TYR	C-N	5.21	1.41	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	GLU	CG-CD-OE2	-10.38	94.53	118.40
1	A	756	PRO	CA-C-N	7.84	129.64	119.84
1	A	756	PRO	C-N-CA	7.84	129.64	119.84
1	A	562	PRO	N-CA-C	7.28	119.58	110.70
1	A	188	GLU	OE1-CD-OE2	6.77	139.14	122.90
1	A	769	VAL	CB-CA-C	5.96	121.06	111.29
1	A	279	THR	CA-C-O	5.39	126.48	120.82
1	A	348	TRP	N-CA-C	5.07	116.61	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	762	ASN	CA-C-N	5.00	125.53	120.38
1	A	762	ASN	C-N-CA	5.00	125.53	120.38

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	5305	0	5097	108	0
2	A	1	0	0	0	0
3	A	14	0	24	1	0
4	A	37	0	32	5	0
5	A	223	0	0	8	2
All	All	5580	0	5153	113	2

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 11.

All (113) 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)
4:A:817:RDF:HD1	4:A:817:RDF:CD11	0.97	1.10
4:A:817:RDF:HD1	4:A:817:RDF:CG1	2.10	0.82
1:A:648:GLN:HE22	1:A:745:ASN:HD21	1.28	0.81
1:A:363:GLU:HB2	5:A:987:HOH:O	1.80	0.81
1:A:580:ALA:HA	1:A:583:LEU:HD12	1.64	0.80
1:A:381:LEU:O	1:A:385:THR:HG23	1.82	0.79
4:A:817:RDF:CG1	4:A:817:RDF:CE3	2.52	0.77
1:A:175:GLU:HB3	1:A:450:MET:HE3	1.67	0.76
1:A:391:ASN:O	1:A:395:ILE:HD12	1.86	0.76
1:A:526:VAL:HG11	1:A:529:LEU:HD12	1.67	0.75
1:A:209:TRP:HB3	1:A:395:ILE:HD13	1.70	0.73
4:A:817:RDF:CE3	4:A:817:RDF:CE2	2.41	0.72
1:A:458:GLU:OE2	1:A:506:TYR:OH	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ILE:HD11	1:A:209:TRP:CD1	2.26	0.70
1:A:270:ASN:HB3	1:A:274:ASN:HD21	1.57	0.70
1:A:654:VAL:O	1:A:657:GLU:HG3	1.93	0.68
1:A:199:LEU:HB2	1:A:406:LEU:HD21	1.74	0.68
1:A:233:THR:HG22	1:A:235:PRO:HD3	1.73	0.68
1:A:524:THR:O	1:A:536:ARG:HD2	1.94	0.68
4:A:817:RDF:HD1	4:A:817:RDF:NE1	2.08	0.68
1:A:171:VAL:HG11	1:A:450:MET:HE2	1.75	0.68
1:A:123:HIS:ND1	5:A:874:HOH:O	2.26	0.67
1:A:164:LEU:HD21	1:A:447:LEU:HD21	1.79	0.65
1:A:285:MET:HB3	1:A:304:MET:HG3	1.76	0.65
1:A:672:ASN:HD21	1:A:745:ASN:HD22	1.46	0.64
1:A:285:MET:HB3	1:A:304:MET:CG	2.28	0.64
1:A:200:MET:O	1:A:203:ILE:HG22	1.98	0.62
1:A:654:VAL:O	1:A:657:GLU:CG	2.48	0.62
1:A:224:LEU:O	1:A:228:THR:HG23	1.99	0.62
1:A:199:LEU:HD12	1:A:406:LEU:HD11	1.82	0.62
1:A:510:ILE:HD11	1:A:511:MET:HE2	1.82	0.61
1:A:116:ASP:OD1	1:A:118:THR:HG22	2.01	0.61
1:A:224:LEU:O	1:A:228:THR:CG2	2.49	0.60
1:A:502:ASN:ND2	1:A:504:ILE:HD11	2.17	0.59
1:A:185:CYS:HB3	1:A:530:TYR:CD1	2.38	0.58
1:A:399:VAL:O	1:A:403:SER:OG	2.21	0.58
1:A:173:GLU:O	1:A:177:LYS:HG3	2.05	0.57
1:A:386:ASP:OD1	1:A:389:LEU:HB2	2.05	0.57
1:A:281:TYR:O	1:A:285:MET:HG3	2.05	0.56
1:A:156:ASN:HA	1:A:159:ILE:HD12	1.86	0.56
1:A:449:PRO:HD3	1:A:510:ILE:HD12	1.86	0.56
1:A:203:ILE:HG23	1:A:204:GLU:N	2.20	0.56
1:A:161:LYS:HG3	1:A:436:VAL:HG21	1.87	0.55
1:A:648:GLN:NE2	1:A:745:ASN:HD21	2.01	0.55
1:A:229:ALA:HB2	1:A:355:ILE:HG22	1.89	0.55
1:A:203:ILE:CD1	1:A:209:TRP:CD1	2.90	0.55
1:A:515:GLU:OE1	1:A:518:LYS:NZ	2.35	0.54
1:A:557:GLN:HE21	3:A:816:5HD:H11	1.74	0.52
1:A:185:CYS:HB3	1:A:530:TYR:CE1	2.45	0.52
1:A:582:ILE:C	1:A:584:GLN:H	2.18	0.52
1:A:762:ASN:OD1	1:A:766:LYS:NZ	2.42	0.52
1:A:396:TRP:O	1:A:399:VAL:HG22	2.09	0.52
1:A:350:PRO:O	1:A:354:THR:HG22	2.09	0.51
1:A:723:SER:O	1:A:727:LEU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:LEU:O	1:A:446:ALA:HB3	2.10	0.51
1:A:496:LYS:HE2	1:A:612:ALA:HB1	1.91	0.51
1:A:325:ARG:NH2	5:A:846:HOH:O	2.43	0.51
1:A:155:HIS:NE2	1:A:159:ILE:HD11	2.27	0.50
1:A:186:MET:SD	1:A:432:TRP:HE3	2.35	0.50
1:A:257:GLN:HB3	1:A:374:TYR:CZ	2.47	0.50
1:A:729:THR:O	5:A:929:HOH:O	2.19	0.50
1:A:203:ILE:CG2	1:A:204:GLU:N	2.75	0.49
1:A:282:LEU:O	1:A:286:VAL:HG23	2.12	0.49
1:A:683:GLN:HG3	5:A:993:HOH:O	2.13	0.49
1:A:163:LEU:HD22	1:A:450:MET:HB3	1.94	0.49
1:A:374:TYR:CZ	1:A:378:ILE:HD11	2.48	0.49
1:A:695:LEU:HB2	1:A:698:LEU:HD12	1.95	0.48
1:A:672:ASN:ND2	1:A:745:ASN:HD22	2.10	0.47
1:A:730:ASP:OD1	1:A:731:PRO:HD2	2.14	0.47
1:A:223:THR:O	1:A:227:VAL:HG22	2.13	0.47
1:A:342:LEU:HD11	1:A:375:LEU:HB2	1.96	0.47
1:A:267:TYR:O	1:A:271:LYS:HB2	2.14	0.47
1:A:357:TYR:CG	1:A:358:PRO:HA	2.49	0.47
1:A:618:ARG:HG3	1:A:619:GLU:N	2.29	0.47
1:A:164:LEU:HD21	1:A:447:LEU:CD2	2.44	0.47
1:A:203:ILE:HD11	1:A:209:TRP:CG	2.51	0.46
1:A:285:MET:HG2	1:A:396:TRP:CZ2	2.51	0.46
1:A:613:PHE:HB3	1:A:770:TRP:CZ2	2.51	0.46
1:A:561:THR:C	1:A:563:PRO:HD2	2.41	0.46
1:A:712:GLN:HA	1:A:715:CYS:SG	2.56	0.45
1:A:747:LYS:HD2	5:A:1021:HOH:O	2.14	0.45
1:A:698:LEU:HD22	1:A:700:LEU:HD12	1.98	0.45
1:A:342:LEU:C	1:A:342:LEU:HD13	2.42	0.45
1:A:346:ILE:H	1:A:346:ILE:HD12	1.82	0.45
1:A:262:LEU:HD21	1:A:281:TYR:CD2	2.52	0.44
1:A:350:PRO:O	1:A:354:THR:CG2	2.66	0.44
1:A:449:PRO:CD	1:A:510:ILE:HD12	2.48	0.44
1:A:395:ILE:O	1:A:399:VAL:HG13	2.18	0.44
1:A:537:PHE:CD1	1:A:537:PHE:C	2.96	0.44
1:A:568:TYR:CE1	1:A:577:VAL:HB	2.52	0.44
1:A:657:GLU:HB3	5:A:902:HOH:O	2.18	0.43
1:A:357:TYR:HA	5:A:1014:HOH:O	2.18	0.43
1:A:502:ASN:ND2	1:A:504:ILE:CD1	2.82	0.43
1:A:273:GLU:HG2	1:A:274:ASN:OD1	2.19	0.42
1:A:457:ALA:O	1:A:460:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:LYS:NZ	1:A:498:ASP:OD2	2.50	0.42
1:A:108:THR:HG23	1:A:698:LEU:HG	2.00	0.42
1:A:221:GLN:HG2	1:A:225:GLN:NE2	2.33	0.42
1:A:531:PHE:O	1:A:535:MET:HG2	2.19	0.42
1:A:225:GLN:HE21	1:A:351:PHE:HA	1.85	0.42
1:A:301:ARG:HB2	1:A:302:PRO:HD3	2.00	0.42
1:A:155:HIS:CE1	1:A:159:ILE:HD11	2.54	0.42
1:A:285:MET:HB3	1:A:304:MET:HG2	2.02	0.42
1:A:433:LYS:O	1:A:434:PHE:C	2.63	0.42
1:A:471:ILE:HG22	1:A:609:LEU:HD12	2.02	0.42
1:A:395:ILE:O	1:A:398:LEU:HB3	2.20	0.41
1:A:285:MET:HA	1:A:396:TRP:CH2	2.55	0.41
1:A:652:TYR:C	1:A:659:VAL:HG23	2.46	0.41
1:A:745:ASN:HA	1:A:766:LYS:HG2	2.01	0.41
1:A:660:ASN:HB3	1:A:663:HIS:HB3	2.02	0.41
1:A:402:THR:CG2	1:A:531:PHE:CE2	3.03	0.40
1:A:112:LEU:HD21	1:A:698:LEU:HD23	2.03	0.40
1:A:502:ASN:HD21	1:A:504:ILE:HD11	1.84	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:887:HOH:O	5:A:887:HOH:O[12_555]	1.84	0.36
5:A:821:HOH:O	5:A:987:HOH:O[7_655]	1.97	0.23

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	656/670 (98%)	621 (95%)	30 (5%)	5 (1%)	16 23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	PHE
1	A	696	PRO
1	A	727	LEU
1	A	275	GLU
1	A	757	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	581/590 (98%)	528 (91%)	53 (9%)	9 13

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	118	THR
1	A	146	TRP
1	A	152	LEU
1	A	168	THR
1	A	189	THR
1	A	199	LEU
1	A	224	LEU
1	A	228	THR
1	A	232	ARG
1	A	233	THR
1	A	252	VAL
1	A	265	ARG
1	A	266	ASP
1	A	273	GLU
1	A	296	ASP
1	A	301	ARG
1	A	304	MET
1	A	314	LEU
1	A	321	GLN

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Mol	Chain	Res	Type
1	A	342	LEU
1	A	354	THR
1	A	360	GLU
1	A	381	LEU
1	A	385	THR
1	A	386	ASP
1	A	388	CYS
1	A	389	LEU
1	A	400	ARG
1	A	403	SER
1	A	404	SER
1	A	412	ASP
1	A	432	TRP
1	A	436	VAL
1	A	437	SER
1	A	452	VAL
1	A	481	THR
1	A	491	LYS
1	A	495	GLU
1	A	502	ASN
1	A	541	SER
1	A	589	THR
1	A	590	ARG
1	A	626	LEU
1	A	627	ARG
1	A	633	SER
1	A	643	GLU
1	A	717	VAL
1	A	719	THR
1	A	721	GLU
1	A	728	ILE
1	A	733	SER
1	A	769	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	179	GLN
1	A	225	GLN
1	A	247	ASN
1	A	321	GLN

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Mol	Chain	Res	Type
1	A	332	HIS
1	A	347	ASN
1	A	392	ASN
1	A	411	GLN
1	A	442	ASN
1	A	502	ASN
1	A	548	GLN
1	A	632	ASN
1	A	641	GLN
1	A	648	GLN
1	A	655	ASN
1	A	672	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	5HD	A	816	-	13,13,13	0.35	0	13,13,13	0.51	0
4	RDF	A	817	2	38,39,39	1.27	3 (7%)	53,57,57	2.12	10 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	5HD	A	816	-	-	4/13/13/13	-
4	RDF	A	817	2	-	4/27/50/50	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	817	RDF	P-N	4.05	1.66	1.61
4	A	817	RDF	CD21-CG1	-3.09	1.38	1.44
4	A	817	RDF	CD21-CE2	-2.21	1.38	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	817	RDF	O1-P-O1P	-9.86	98.10	115.32
4	A	817	RDF	O2P-P-O1P	5.51	121.69	109.87
4	A	817	RDF	O5-C1-O1	-3.85	106.34	111.36
4	A	817	RDF	CZ2-CE2-CD21	-3.20	119.09	122.19
4	A	817	RDF	P-N-CA	-3.16	116.98	124.03
4	A	817	RDF	C3-C4-C5	-2.63	105.82	109.81
4	A	817	RDF	O5-C5-C6	2.47	112.22	106.74
4	A	817	RDF	CE3-CD21-CG1	-2.46	130.18	133.85
4	A	817	RDF	CA1-CB1-CG1	-2.26	109.16	113.44
4	A	817	RDF	C4-C3-C2	-2.01	107.30	110.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

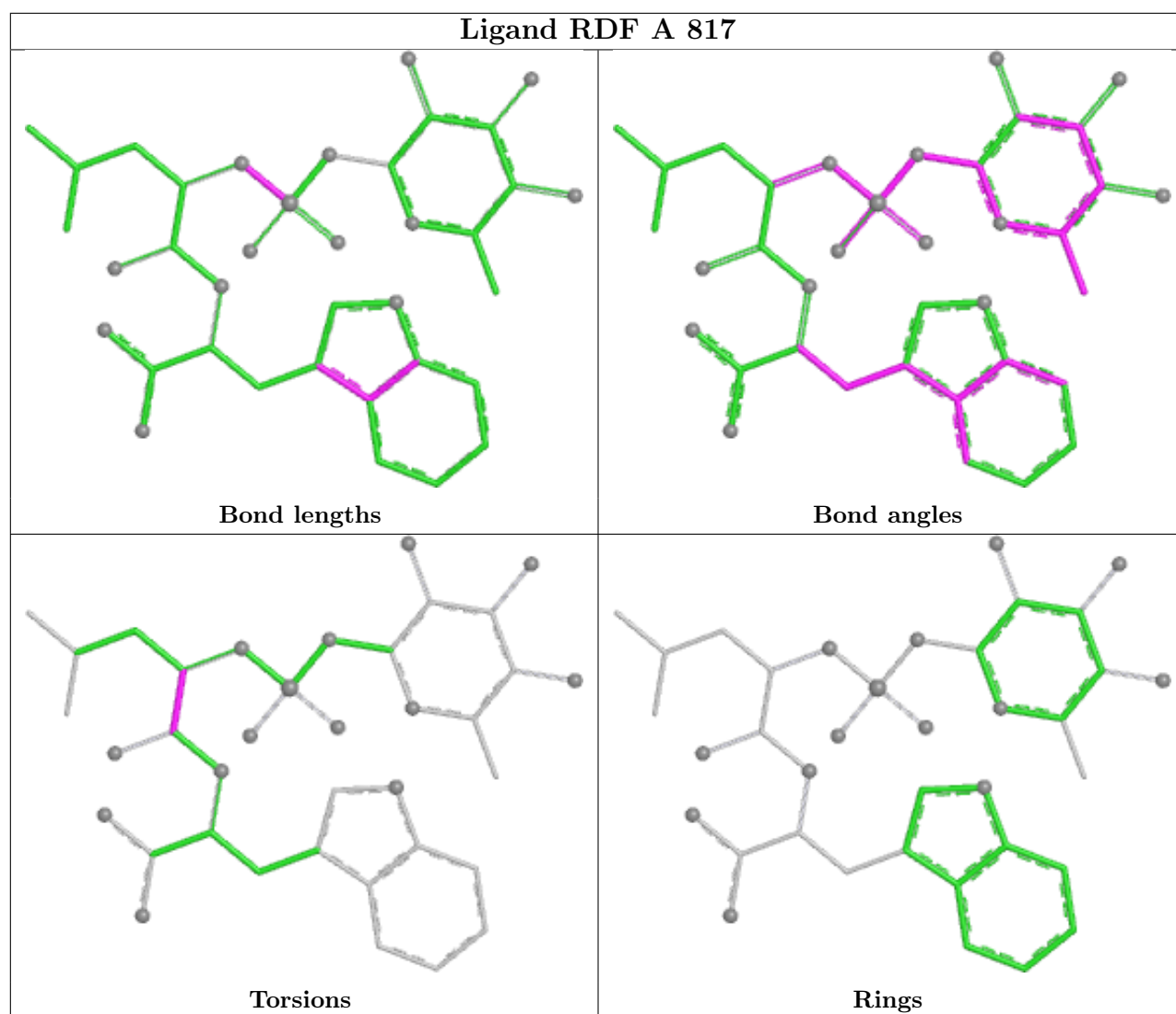
Mol	Chain	Res	Type	Atoms
3	A	816	5HD	C5-C6-C7-C8
4	A	817	RDF	N1-C-CA-N
4	A	817	RDF	O-C-CA-CB
3	A	816	5HD	C6-C10-C11-C12
4	A	817	RDF	N1-C-CA-CB
4	A	817	RDF	O-C-CA-N
3	A	816	5HD	C1-C2-C3-O4
3	A	816	5HD	C5-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	816	5HD	1	0
4	A	817	RDF	5	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	660/670 (98%)	1.08	114 (17%) 4 3	24, 47, 77, 86	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	275	GLU	5.3
1	A	159	ILE	4.5
1	A	169	ALA	4.2
1	A	277	VAL	4.1
1	A	432	TRP	4.0
1	A	160	ILE	4.0
1	A	182	TYR	3.7
1	A	697	THR	3.6
1	A	163	LEU	3.6
1	A	336	ALA	3.5
1	A	435	CYS	3.5
1	A	315	ALA	3.4
1	A	436	VAL	3.4
1	A	378	ILE	3.3
1	A	530	TYR	3.3
1	A	457	ALA	3.2
1	A	367	ILE	3.2
1	A	420	VAL	3.2
1	A	266	ASP	3.2
1	A	484	TRP	3.1
1	A	103	ALA	3.1
1	A	272	THR	3.0
1	A	274	ASN	3.0
1	A	479	LEU	3.0
1	A	659	VAL	3.0
1	A	650	SER	3.0
1	A	318	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	314	LEU	2.9
1	A	355	ILE	2.9
1	A	361	ILE	2.9
1	A	661	GLY	2.8
1	A	501	TYR	2.8
1	A	139	VAL	2.8
1	A	212	THR	2.8
1	A	481	THR	2.8
1	A	162	HIS	2.8
1	A	267	TYR	2.8
1	A	339	LEU	2.8
1	A	359	VAL	2.8
1	A	480	SER	2.8
1	A	493	ALA	2.8
1	A	369	VAL	2.8
1	A	164	LEU	2.7
1	A	415	GLU	2.7
1	A	273	GLU	2.7
1	A	651	ASN	2.6
1	A	341	THR	2.6
1	A	728	ILE	2.6
1	A	405	PHE	2.6
1	A	145	ARG	2.6
1	A	757	PRO	2.6
1	A	478	SER	2.6
1	A	364	SER	2.6
1	A	342	LEU	2.6
1	A	287	GLN	2.5
1	A	146	TRP	2.5
1	A	385	THR	2.5
1	A	250	SER	2.5
1	A	496	LYS	2.5
1	A	354	THR	2.5
1	A	317	ILE	2.5
1	A	282	LEU	2.5
1	A	156	ASN	2.5
1	A	123	HIS	2.5
1	A	158	ALA	2.5
1	A	168	THR	2.4
1	A	149	PHE	2.4
1	A	220	PHE	2.4
1	A	239	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	349	LEU	2.4
1	A	375	LEU	2.4
1	A	157	GLN	2.4
1	A	104	CYS	2.3
1	A	153	TRP	2.3
1	A	281	TYR	2.3
1	A	320	PRO	2.3
1	A	300	ILE	2.3
1	A	255	VAL	2.3
1	A	374	TYR	2.3
1	A	245	SER	2.3
1	A	343	ALA	2.3
1	A	189	THR	2.3
1	A	492	SER	2.3
1	A	144	SER	2.2
1	A	722	SER	2.2
1	A	134	ILE	2.2
1	A	334	VAL	2.2
1	A	485	MET	2.2
1	A	184	ALA	2.2
1	A	181	TYR	2.2
1	A	346	ILE	2.2
1	A	368	VAL	2.2
1	A	147	GLY	2.2
1	A	396	TRP	2.2
1	A	564	MET	2.2
1	A	721	GLU	2.1
1	A	185	CYS	2.1
1	A	723	SER	2.1
1	A	224	LEU	2.1
1	A	353	ASN	2.1
1	A	458	GLU	2.1
1	A	482	LEU	2.1
1	A	170	SER	2.1
1	A	489	THR	2.1
1	A	135	LYS	2.1
1	A	469	LEU	2.1
1	A	141	ASP	2.1
1	A	241	VAL	2.1
1	A	101	SER	2.0
1	A	344	PRO	2.0
1	A	236	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	727	LEU	2.0
1	A	325	ARG	2.0
1	A	372	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

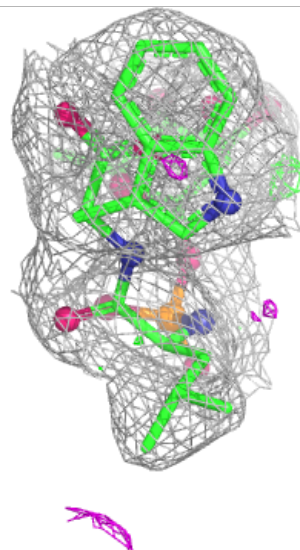
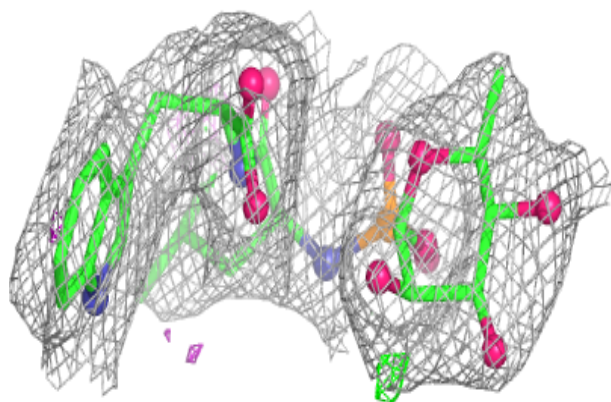
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	5HD	A	816	14/14	0.74	0.18	50,55,56,56	0
4	RDF	A	817	37/37	0.91	0.09	36,42,45,48	0
2	ZN	A	771	1/1	1.00	0.01	41,41,41,41	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 RDF A 817:

$2mF_o-DF_c$ (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.