



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:24 AM UTC

PDB ID : 3POR / pdb_00003por
Title : PORIN CONFORMATION IN THE ABSENCE OF CALCIUM; REFINED
STRUCTURE AT 2.5 ANGSTROMS RESOLUTION
Authors : Weiss, M.S.; Schulz, G.E.
Deposited on : 1992-11-09
Resolution : 2.50 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

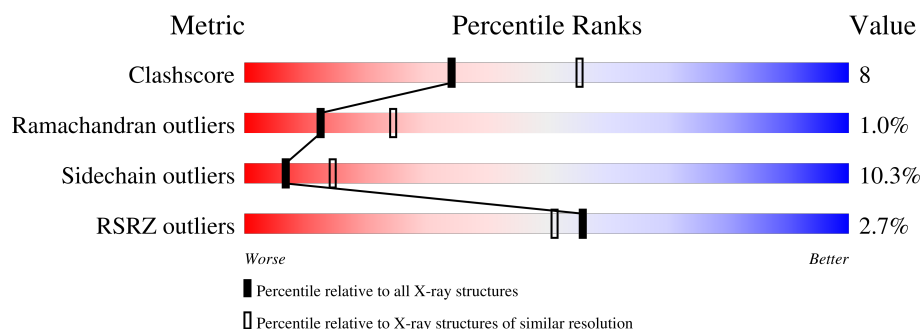
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	301	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TRS	A	700	-	X	-	-

2 Entry composition [i](#)

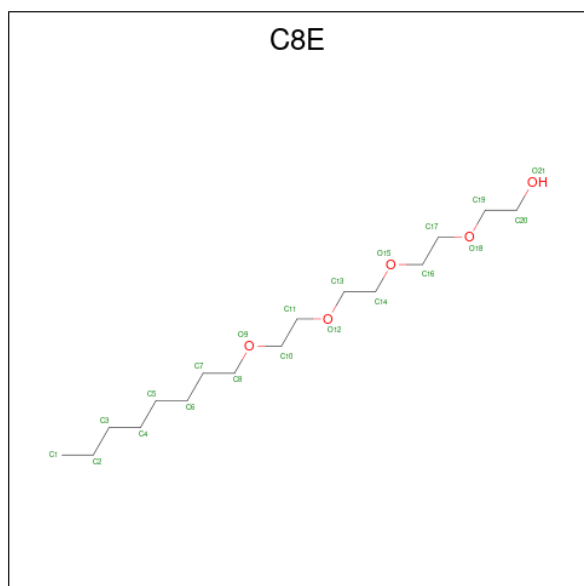
There are 4 unique types of molecules in this entry. The entry contains 2325 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PORIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2219	1389	348	473	9			

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: $C_{16}H_{34}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			21	16	5		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



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

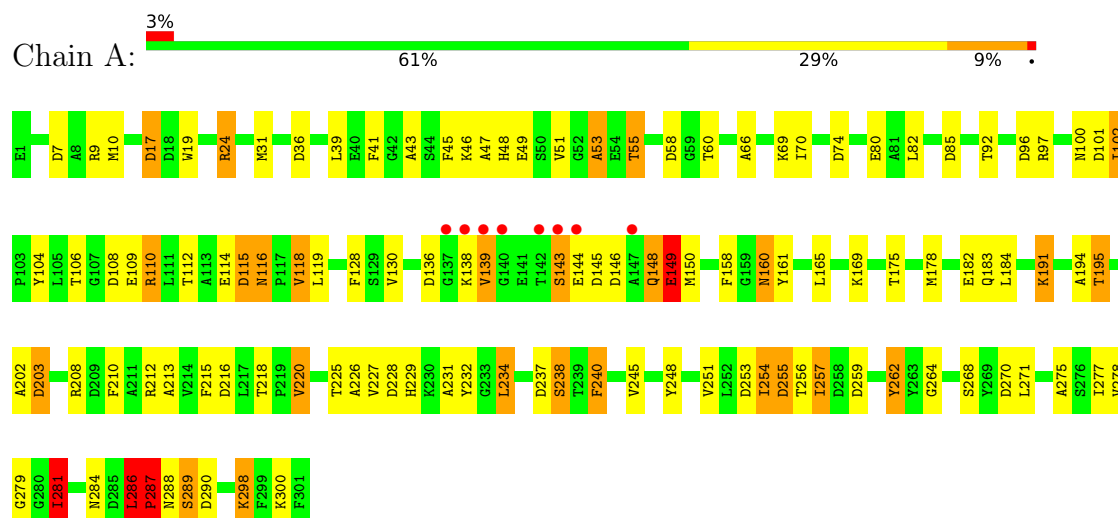
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	77	Total	O	0	0
			77	77		

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: PORIN



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	95.30Å 95.30Å 146.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.50 10.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.50) 93.7 (10.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.188 , (Not available) 0.178 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 105.4	EDS
L-test for twinning ¹	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.066 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2325	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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: C8E, TRS

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	1.48	18/2258 (0.8%)	2.12	89/3061 (2.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	ILE	CA-CB	-10.01	1.42	1.54
1	A	49	GLU	CA-CB	-7.66	1.41	1.53
1	A	48	HIS	CG-ND1	-6.98	1.30	1.38
1	A	229	HIS	CD2-NE2	-6.52	1.30	1.37
1	A	161	TYR	CA-C	-6.40	1.44	1.52
1	A	254	ILE	CA-CB	-6.30	1.46	1.54
1	A	48	HIS	CD2-NE2	-6.13	1.31	1.37
1	A	146	ASP	CA-CB	6.11	1.62	1.54
1	A	195	THR	CA-C	-5.80	1.45	1.52
1	A	148	GLN	N-CA	-5.73	1.39	1.46
1	A	195	THR	CA-CB	-5.62	1.40	1.53
1	A	213	ALA	CA-CB	-5.57	1.44	1.53
1	A	139	VAL	CA-CB	5.42	1.61	1.53
1	A	277	ILE	CA-CB	-5.34	1.48	1.54
1	A	256	THR	CA-CB	5.15	1.62	1.53
1	A	259	ASP	CA-CB	-5.13	1.43	1.53
1	A	39	LEU	CA-CB	-5.13	1.44	1.53
1	A	53	ALA	CA-CB	-5.03	1.45	1.53

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	ASP	CA-CB-CG	12.56	125.16	112.60
1	A	253	ASP	CA-CB-CG	10.39	122.99	112.60
1	A	183	GLN	OE1-CD-NE2	-9.24	113.36	122.60
1	A	289	SER	CA-C-O	9.17	133.62	120.51
1	A	96	ASP	N-CA-C	9.04	120.74	111.07
1	A	216	ASP	N-CA-CB	-8.53	99.07	112.46
1	A	136	ASP	CA-CB-CG	8.39	120.99	112.60
1	A	106	THR	N-CA-C	8.37	122.44	110.14
1	A	183	GLN	CG-CD-NE2	8.15	128.62	116.40
1	A	41	PHE	CA-CB-CG	7.89	121.69	113.80
1	A	36	ASP	CA-C-O	-7.63	112.39	120.63
1	A	203	ASP	CA-CB-CG	7.31	119.91	112.60
1	A	19	TRP	CG-CD2-CE3	7.29	141.19	133.90
1	A	289	SER	N-CA-C	7.18	126.10	110.80
1	A	281	ILE	CB-CG1-CD1	-7.15	98.78	113.80
1	A	45	PHE	CA-CB-CG	6.95	120.75	113.80
1	A	7	ASP	CA-CB-CG	6.91	119.51	112.60
1	A	298	LYS	N-CA-CB	-6.85	98.91	111.37
1	A	257	ILE	CA-C-O	-6.83	112.24	120.78
1	A	17	ASP	CA-CB-CG	6.82	119.42	112.60
1	A	149	GLU	O-C-N	-6.82	114.37	123.23
1	A	116	ASN	O-C-N	-6.68	115.90	121.38
1	A	55	THR	CA-CB-OG1	6.60	119.50	109.60
1	A	216	ASP	CA-CB-CG	6.51	119.11	112.60
1	A	110	ARG	CA-CB-CG	-6.45	101.20	114.10
1	A	148	GLN	N-CA-C	-6.37	98.35	108.73
1	A	148	GLN	OE1-CD-NE2	-6.35	116.25	122.60
1	A	70	ILE	CB-CG1-CD1	-6.34	100.48	113.80
1	A	288	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	A	60	THR	CA-C-O	-6.31	113.73	121.06
1	A	279	GLY	CA-C-O	-6.31	114.49	121.37
1	A	119	LEU	CA-C-O	-6.31	113.50	120.38
1	A	116	ASN	N-CA-C	6.29	117.31	109.57
1	A	268	SER	CA-CB-OG	6.22	123.54	111.10
1	A	229	HIS	CB-CG-CD2	-6.21	123.13	131.20
1	A	10	MET	CA-CB-CG	6.18	126.45	114.10
1	A	139	VAL	N-CA-CB	-6.08	106.20	112.28
1	A	257	ILE	O-C-N	-6.06	114.99	122.57
1	A	85	ASP	O-C-N	-6.05	114.54	122.59
1	A	232	TYR	O-C-N	-6.03	116.97	123.42
1	A	101	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	216	ASP	N-CA-C	5.99	119.95	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ASN	O-C-N	5.87	128.13	122.03
1	A	66	ALA	N-CA-C	-5.86	105.03	111.82
1	A	10	MET	CG-SD-CE	-5.83	88.07	100.90
1	A	160	ASN	CA-CB-CG	5.81	118.41	112.60
1	A	286	LEU	CA-C-N	5.76	127.05	119.84
1	A	286	LEU	C-N-CA	5.76	127.05	119.84
1	A	231	ALA	CA-C-O	-5.74	114.39	121.11
1	A	119	LEU	O-C-N	-5.74	116.52	123.29
1	A	245	VAL	O-C-N	-5.74	116.96	123.10
1	A	114	GLU	CB-CG-CD	5.72	122.33	112.60
1	A	279	GLY	O-C-N	-5.72	118.24	123.56
1	A	19	TRP	CB-CG-CD1	-5.71	118.33	126.90
1	A	24	ARG	CB-CG-CD	-5.69	98.20	111.30
1	A	149	GLU	CB-CG-CD	5.67	122.23	112.60
1	A	149	GLU	CA-C-O	-5.66	114.59	120.70
1	A	226	ALA	O-C-N	-5.65	116.77	123.22
1	A	240	PHE	CA-C-O	5.63	127.66	120.57
1	A	102	ILE	N-CA-C	-5.60	103.46	108.95
1	A	46	LYS	CA-C-O	-5.56	115.16	121.72
1	A	74	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	9	ARG	O-C-N	-5.56	116.92	123.25
1	A	270	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	212	ARG	N-CA-C	-5.53	105.33	111.36
1	A	45	PHE	CA-C-O	-5.52	115.32	121.23
1	A	130	VAL	CA-CB-CG1	-5.49	101.06	110.40
1	A	287	PRO	N-CA-C	5.46	123.71	112.47
1	A	115	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	145	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	96	ASP	O-C-N	5.42	127.65	122.07
1	A	268	SER	CB-CA-C	-5.40	98.09	109.38
1	A	46	LYS	CA-CB-CG	-5.39	103.32	114.10
1	A	97	ARG	N-CA-CB	-5.37	103.15	110.56
1	A	48	HIS	CB-CG-CD2	-5.36	124.23	131.20
1	A	275	ALA	O-C-N	-5.36	116.41	123.16
1	A	69	LYS	CA-CB-CG	5.33	124.77	114.10
1	A	47	ALA	N-CA-C	5.29	117.04	111.28
1	A	92	THR	N-CA-C	-5.29	106.68	113.02
1	A	92	THR	OG1-CB-CG2	-5.25	98.81	109.30
1	A	271	LEU	CA-C-O	5.18	125.91	119.12
1	A	51	VAL	O-C-N	-5.16	116.86	121.91
1	A	85	ASP	CA-CB-CG	-5.12	107.48	112.60
1	A	100	ASN	OD1-CG-ND2	-5.10	117.50	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	THR	CA-CB-CG2	-5.09	101.85	110.50
1	A	225	THR	CA-CB-OG1	5.04	117.16	109.60
1	A	82	LEU	N-CA-C	5.02	118.55	112.23
1	A	80	GLU	N-CA-C	-5.01	106.01	111.82
1	A	118	VAL	N-CA-CB	-5.00	106.37	112.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	286	LEU	Peptide

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	2219	0	2072	33	0
2	A	21	0	34	1	0
3	A	8	0	12	1	0
4	A	77	0	0	2	0
All	All	2325	0	2118	33	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 8.

All (33) 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:112:THR:HG21	1:A:149:GLU:HG3	1.67	0.77
1:A:138:LYS:HA	1:A:144:GLU:O	1.87	0.73
1:A:108:ASP:CG	1:A:109:GLU:H	2.04	0.65
1:A:215:PHE:HE2	1:A:254:ILE:HD12	1.64	0.62
1:A:191:LYS:HE3	4:A:933:HOH:O	2.01	0.61
1:A:116:ASN:HA	1:A:118:VAL:HG13	1.84	0.60
1:A:148:GLN:OE1	1:A:148:GLN:HA	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ALA:HA	1:A:58:ASP:O	2.01	0.59
1:A:112:THR:O	1:A:115:ASP:HB2	2.05	0.56
1:A:175:THR:HA	1:A:178:MET:O	2.06	0.56
1:A:210:PHE:HZ	2:A:545:C8E:H42	1.71	0.55
1:A:234:LEU:O	1:A:248:TYR:HA	2.06	0.55
1:A:108:ASP:CG	1:A:109:GLU:N	2.65	0.55
1:A:31:MET:HE3	1:A:43:ALA:HB3	1.91	0.53
1:A:278:VAL:HG21	1:A:298:LYS:HD3	1.92	0.52
1:A:194:ALA:O	1:A:238:SER:HA	2.13	0.49
1:A:264:GLY:HA2	1:A:281:ILE:O	2.13	0.48
1:A:227:VAL:HG21	1:A:257:ILE:HD12	1.95	0.47
1:A:138:LYS:HB3	1:A:143:SER:HA	1.96	0.47
1:A:208:ARG:HH11	1:A:208:ARG:HD3	1.61	0.46
1:A:24:ARG:HH22	3:A:700:TRS:H31	1.81	0.46
1:A:104:TYR:HB2	1:A:110:ARG:NE	2.31	0.45
1:A:262:TYR:HB3	1:A:284:ASN:HB3	1.99	0.45
1:A:208:ARG:NE	1:A:220:VAL:HG22	2.32	0.44
1:A:286:LEU:HA	1:A:287:PRO:HD2	1.79	0.44
1:A:228:ASP:O	1:A:255:ASP:HB3	2.18	0.44
1:A:184:LEU:O	1:A:202:ALA:HA	2.19	0.42
1:A:109:GLU:HG2	4:A:927:HOH:O	2.18	0.42
1:A:215:PHE:CE2	1:A:254:ILE:HD12	2.51	0.42
1:A:102:ILE:HB	1:A:104:TYR:CE2	2.56	0.41
1:A:138:LYS:HD3	1:A:144:GLU:O	2.21	0.41
1:A:139:VAL:HB	1:A:144:GLU:HB3	2.02	0.41
1:A:195:THR:HA	1:A:237:ASP:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	299/301 (99%)	284 (95%)	12 (4%)	3 (1%)	12	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	PRO
1	A	143	SER
1	A	289	SER

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	224/224 (100%)	201 (90%)	23 (10%)	7	14

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	55	THR
1	A	128	PHE
1	A	149	GLU
1	A	150	MET
1	A	158	PHE
1	A	160	ASN
1	A	165	LEU
1	A	169	LYS
1	A	182	GLU
1	A	191	LYS
1	A	203	ASP
1	A	218	THR
1	A	220	VAL
1	A	234	LEU
1	A	238	SER
1	A	240	PHE
1	A	251	VAL

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Mol	Chain	Res	Type
1	A	255	ASP
1	A	262	TYR
1	A	281	ILE
1	A	290	ASP
1	A	300	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TRS	A	700	-	7,7,7	1.22	0	9,9,9	1.85	3 (33%)
2	C8E	A	545	-	20,20,20	0.87	0	19,19,19	1.78	5 (26%)

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	TRS	A	700	-	-	7/9/9/9	-
2	C8E	A	545	-	-	6/18/18/18	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	545	C8E	O15-C16-C17	3.48	126.23	110.35
2	A	545	C8E	O18-C17-C16	3.45	126.06	110.35
3	A	700	TRS	O1-C1-C	3.03	119.32	110.88
2	A	545	C8E	O18-C19-C20	2.63	121.70	110.11
2	A	545	C8E	O9-C10-C11	2.63	122.32	110.35
2	A	545	C8E	O12-C11-C10	2.32	120.95	110.35
3	A	700	TRS	C1-C-N	2.29	114.02	108.17
3	A	700	TRS	C3-C-C2	2.11	116.27	110.66

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	700	TRS	C3-C-C2-O2
3	A	700	TRS	N-C-C2-O2
2	A	545	C8E	C4-C5-C6-C7
3	A	700	TRS	C2-C-C1-O1
3	A	700	TRS	N-C-C1-O1
3	A	700	TRS	C1-C-C2-O2
2	A	545	C8E	C14-C13-O12-C11
3	A	700	TRS	C3-C-C1-O1
2	A	545	C8E	C3-C4-C5-C6
2	A	545	C8E	C17-C16-O15-C14
2	A	545	C8E	C5-C6-C7-C8
3	A	700	TRS	C2-C-C3-O3
2	A	545	C8E	C10-C11-O12-C13

There are no ring outliers.

2 monomers are involved in 2 short contacts:

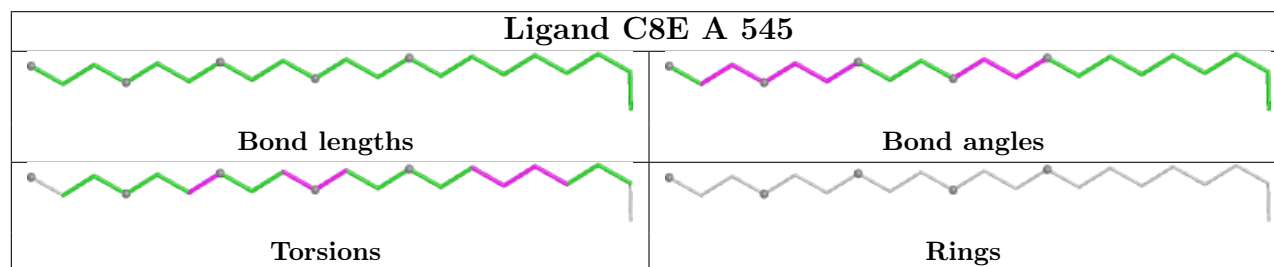
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	700	TRS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	545	C8E	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.



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	301/301 (100%)	-0.74	8 (2%) 56 51	12, 30, 64, 121	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	VAL	3.8
1	A	138	LYS	3.2
1	A	137	GLY	3.0
1	A	140	GLY	2.9
1	A	144	GLU	2.5
1	A	142	THR	2.3
1	A	147	ALA	2.3
1	A	143	SER	2.2

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](#)

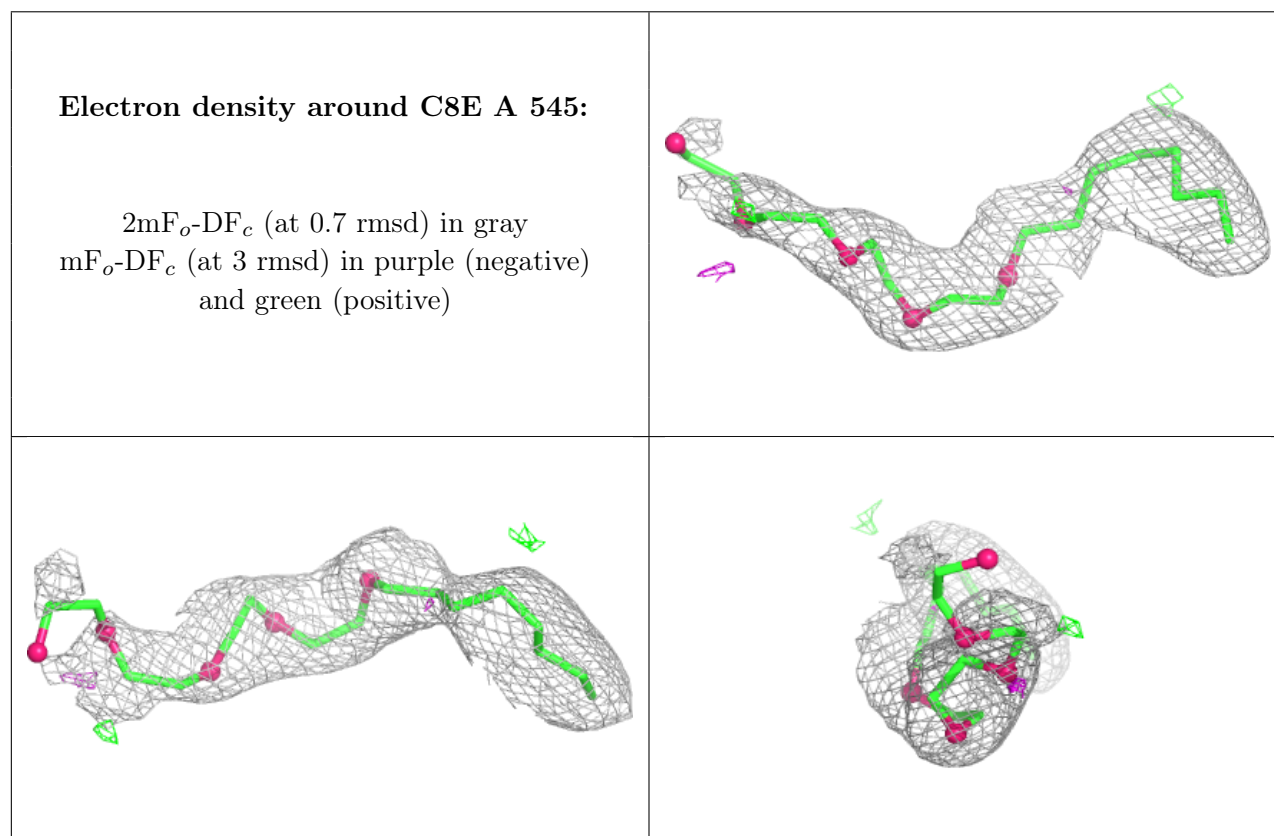
There are no oligosaccharides in this entry.

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	TRS	A	700	8/8	0.79	0.12	56,63,65,65	0
2	C8E	A	545	21/21	0.90	0.09	35,57,114,118	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.