



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:57 AM UTC

PDB ID : 1ZDT / pdb_00001zdt
Title : The Crystal Structure of Human Steroidogenic Factor-1
Authors : Wang, W.; Zhang, C.; Marimuthu, A.; Krupka, H.I.; Tabrizizad, M.; Shelloe, R.; Mehra, U.; Eng, K.; Nguyen, H.; Settachatgul, C.; Powell, B.; Milburn, M.V.; West, B.L.
Deposited on : 2005-04-14
Resolution : 2.10 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

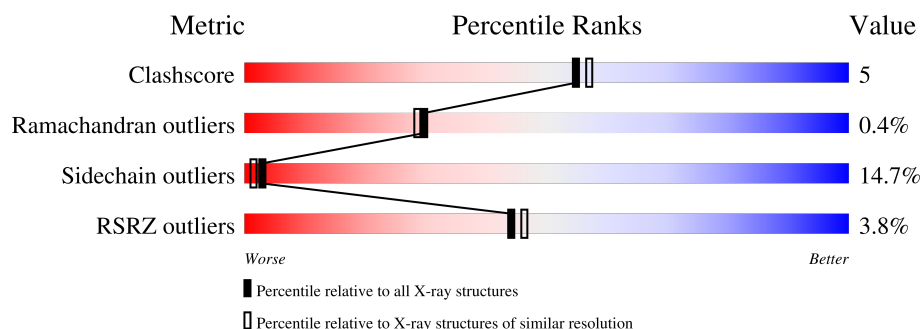
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	241	4% 76% 16% 5%
1	B	241	2% 76% 19% 5%
2	P	12	17% 58% 8% 17% 17%
2	Q	12	17% 42% 33% 17% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4320 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 Steroidogenic factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1873	1202	320	339	12			
1	B	239	Total	C	N	O	S	0	0	0
			1922	1231	330	349	12			

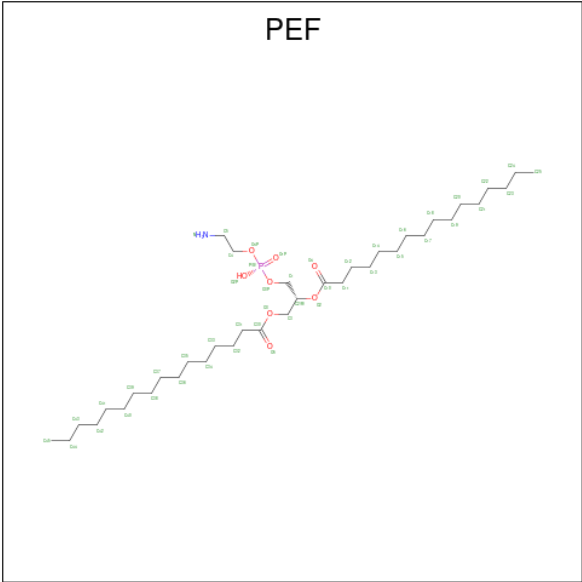
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	247	SER	CYS	engineered mutation	UNP Q13285
A	412	SER	CYS	engineered mutation	UNP Q13285
B	247	SER	CYS	engineered mutation	UNP Q13285
B	412	SER	CYS	engineered mutation	UNP Q13285

- Molecule 2 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	12	Total	C	N	O	0	0	0
			102	65	17	20			
2	Q	11	Total	C	N	O	0	0	0
			94	61	16	17			

- Molecule 3 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: C₃₇H₇₄NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
3	B	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

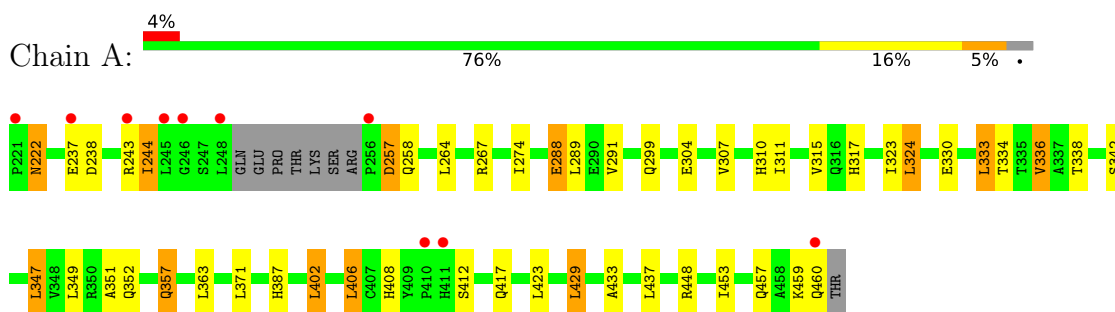
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	116	Total	O	0	0
			116	116		
4	B	114	Total	O	0	0
			114	114		
4	P	3	Total	O	0	0
			3	3		
4	Q	2	Total	O	0	0
			2	2		

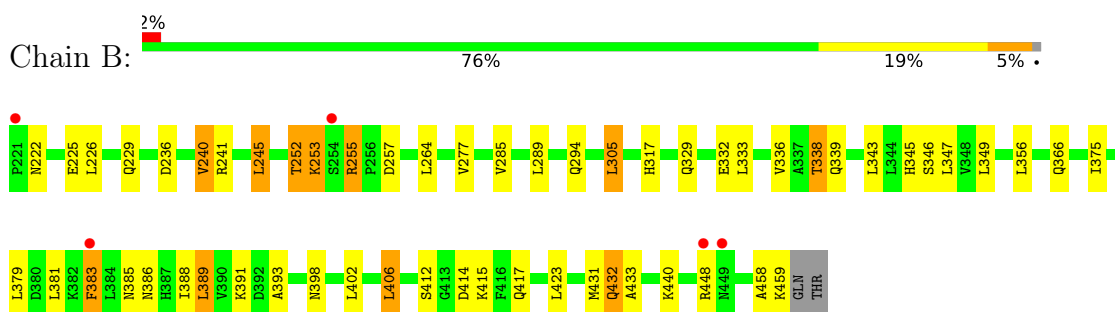
3 Residue-property plots [i](#)

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.

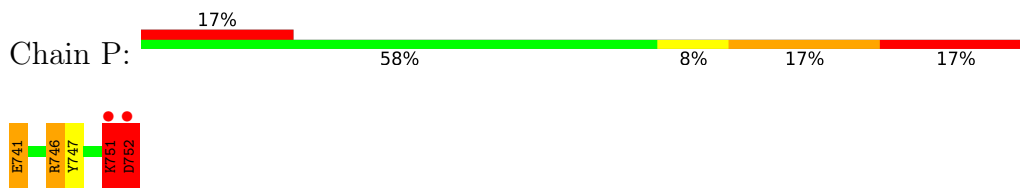
- Molecule 1: Steroidogenic factor 1



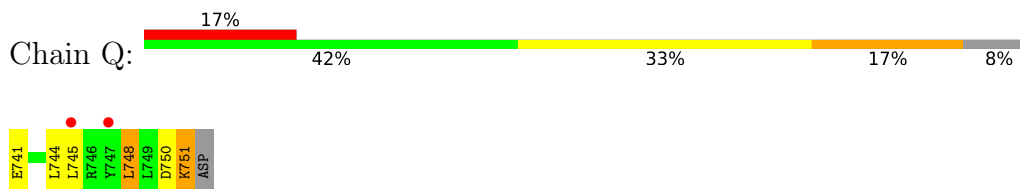
- Molecule 1: Steroidogenic factor 1



- Molecule 2: Nuclear receptor coactivator 2



- Molecule 2: Nuclear receptor coactivator 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	73.60Å 73.60Å 195.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.10) 98.4 (50.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.25	Depositor
R, R_{free}	0.216 , 0.265 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4320	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: PEF

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	1.02	8/1904 (0.4%)	1.07	6/2575 (0.2%)
1	B	1.01	10/1955 (0.5%)	1.06	4/2646 (0.2%)
2	P	1.84	4/102 (3.9%)	1.43	3/136 (2.2%)
2	Q	0.73	0/94	0.86	0/125
All	All	1.04	22/4055 (0.5%)	1.07	13/5482 (0.2%)

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	2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	751	LYS	CA-C	10.81	1.67	1.52
2	P	751	LYS	C-N	8.19	1.44	1.33
1	B	431	MET	SD-CE	8.00	1.99	1.79
2	P	751	LYS	N-CA	6.42	1.54	1.46
1	A	357	GLN	CD-OE1	6.04	1.35	1.23
1	B	329	GLN	CD-OE1	5.90	1.34	1.23
1	A	299	GLN	CD-OE1	5.71	1.34	1.23
1	A	336	VAL	CA-CB	5.64	1.62	1.54
1	B	366	GLN	CD-NE2	-5.56	1.21	1.33
2	P	752	ASP	N-CA	5.50	1.56	1.46
1	B	432	GLN	CD-OE1	5.49	1.33	1.23
1	B	385	ASN	CG-OD1	5.45	1.33	1.23
1	A	222	ASN	CG-OD1	5.43	1.33	1.23
1	B	345	HIS	ND1-CE1	5.32	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	398	ASN	CG-OD1	5.28	1.33	1.23
1	B	317	HIS	ND1-CE1	5.26	1.37	1.32
1	A	352	GLN	CD-NE2	-5.25	1.22	1.33
1	A	408	HIS	ND1-CE1	5.18	1.37	1.32
1	B	294	GLN	CD-OE1	5.16	1.33	1.23
1	B	317	HIS	CD2-NE2	-5.06	1.32	1.37
1	A	387	HIS	CD2-NE2	-5.03	1.32	1.37
1	A	317	HIS	CD2-NE2	-5.01	1.32	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	HIS	CB-CG-CD2	-6.93	122.18	131.20
1	B	317	HIS	CB-CG-CD2	-6.89	122.24	131.20
1	A	317	HIS	CB-CG-CD2	-6.85	122.30	131.20
1	A	387	HIS	CB-CG-CD2	-6.80	122.36	131.20
1	B	345	HIS	CB-CG-CD2	-6.66	122.54	131.20
1	A	317	HIS	CB-CG-ND1	5.90	131.55	122.70
1	B	317	HIS	CB-CG-ND1	5.86	131.49	122.70
2	P	751	LYS	CA-C-N	5.83	132.19	121.70
2	P	751	LYS	C-N-CA	5.83	132.19	121.70
1	A	408	HIS	CB-CG-ND1	5.81	131.41	122.70
1	B	345	HIS	CB-CG-ND1	5.81	131.41	122.70
2	P	751	LYS	N-CA-C	5.73	123.00	110.80
1	A	387	HIS	CB-CG-ND1	5.69	131.23	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	ILE	Peptide
1	A	257	ASP	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	1873	0	1918	15	1
1	B	1922	0	1969	20	0
2	P	102	0	103	3	0
2	Q	94	0	99	2	0
3	A	47	0	73	2	0
3	B	47	0	73	1	0
4	A	116	0	0	3	0
4	B	114	0	0	2	1
4	P	3	0	0	0	0
4	Q	2	0	0	0	0
All	All	4320	0	4235	40	1

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 5.

All (40) 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:453:ILE:O	1:A:457:GLN:HG2	1.88	0.73
1:B:236:ASP:O	1:B:240:VAL:HG12	1.97	0.64
1:A:304:GLU:HG2	4:A:1034:HOH:O	2.00	0.61
2:Q:750:ASP:O	2:Q:751:LYS:C	2.42	0.61
1:B:285:VAL:HG11	1:B:393:ALA:HB2	1.84	0.59
1:A:334:THR:O	1:A:338:THR:HG23	2.03	0.59
1:A:238:ASP:HA	4:A:1025:HOH:O	2.03	0.58
1:A:347:LEU:HD11	1:A:433:ALA:HA	1.85	0.58
1:A:288:GLU:HG3	4:A:1035:HOH:O	2.04	0.56
1:B:338:THR:HG23	1:B:339:GLN:OE1	2.05	0.56
1:A:324:LEU:HD23	1:A:330:GLU:HG2	1.87	0.56
1:B:402:LEU:O	1:B:406:LEU:HD22	2.06	0.54
1:B:277:VAL:HG11	2:Q:748:LEU:HB3	1.89	0.54
1:A:402:LEU:O	1:A:406:LEU:HB2	2.07	0.53
1:B:225:GLU:O	1:B:229:GLN:HG3	2.10	0.52
1:B:347:LEU:HD13	1:B:432:GLN:HB3	1.90	0.52
1:B:379:LEU:HD11	1:B:383:PHE:CE1	2.46	0.51
2:P:741:GLU:OE2	2:P:746:ARG:NH1	2.45	0.50
1:A:347:LEU:HD13	3:A:1001:PEF:H212	1.94	0.49
1:A:323:ILE:O	1:A:330:GLU:HA	2.12	0.49
1:B:347:LEU:HD21	1:B:433:ALA:HA	1.95	0.49
1:B:305:LEU:HD13	1:B:375:ILE:CG2	2.43	0.49
1:B:255:ARG:HD2	4:B:1060:HOH:O	2.13	0.48
1:A:351:ALA:HA	1:A:429:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:THR:CG2	1:B:339:GLN:OE1	2.64	0.45
1:B:386:ASN:OD1	1:B:388:ILE:HG22	2.17	0.44
2:P:747:TYR:OH	2:P:752:ASP:HB3	2.18	0.44
1:B:381:LEU:HD21	1:B:391:LYS:HB2	2.00	0.43
1:B:458:ALA:O	1:B:459:LYS:CB	2.66	0.43
1:B:241:ARG:HG2	1:B:245:LEU:HD22	2.00	0.43
1:A:310:HIS:CD2	3:A:1001:PEF:H241	2.53	0.43
1:A:237:GLU:O	1:A:238:ASP:HB2	2.18	0.43
1:B:305:LEU:HD13	1:B:375:ILE:HG21	2.00	0.42
1:B:252:THR:HG22	1:B:253:LYS:N	2.35	0.42
1:B:289:LEU:HD12	1:B:389:LEU:HD23	2.00	0.42
1:A:307:VAL:O	1:A:311:ILE:HG12	2.19	0.41
2:P:751:LYS:O	2:P:752:ASP:HB2	2.20	0.41
1:B:383:PHE:CD2	1:B:383:PHE:N	2.88	0.41
3:B:1002:PEF:H52	4:B:1115:HOH:O	2.21	0.40
1:A:333:LEU:HD13	1:A:333:LEU:HA	1.89	0.40

All (1) 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)
1:A:417:GLN:OE1	4:B:1003:HOH:O[5_555]	2.07	0.13

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	229/241 (95%)	220 (96%)	8 (4%)	1 (0%)	30	28
1	B	237/241 (98%)	233 (98%)	4 (2%)	0	100	100
2	P	10/12 (83%)	9 (90%)	0	1 (10%)	0	0
2	Q	9/12 (75%)	8 (89%)	1 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	485/506 (96%)	470 (97%)	13 (3%)	2 (0%)	30	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	459	LYS
2	P	751	LYS

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	208/216 (96%)	179 (86%)	29 (14%)	3	2
1	B	214/216 (99%)	186 (87%)	28 (13%)	4	2
2	P	11/11 (100%)	8 (73%)	3 (27%)	0	0
2	Q	10/11 (91%)	5 (50%)	5 (50%)	0	0
All	All	443/454 (98%)	378 (85%)	65 (15%)	3	1

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
1	A	243	ARG
1	A	244	ILE
1	A	257	ASP
1	A	258	GLN
1	A	264	LEU
1	A	267	ARG
1	A	274	ILE
1	A	288	GLU
1	A	289	LEU
1	A	291	VAL
1	A	315	VAL
1	A	324	LEU

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Mol	Chain	Res	Type
1	A	333	LEU
1	A	336	VAL
1	A	342	SER
1	A	347	LEU
1	A	349	LEU
1	A	357	GLN
1	A	363	LEU
1	A	371	LEU
1	A	402	LEU
1	A	406	LEU
1	A	412	SER
1	A	423	LEU
1	A	429	LEU
1	A	437	LEU
1	A	448	ARG
1	A	460	GLN
1	B	222	ASN
1	B	226	LEU
1	B	240	VAL
1	B	245	LEU
1	B	252	THR
1	B	253	LYS
1	B	255	ARG
1	B	257	ASP
1	B	264	LEU
1	B	305	LEU
1	B	332	GLU
1	B	333	LEU
1	B	336	VAL
1	B	338	THR
1	B	343	LEU
1	B	346	SER
1	B	349	LEU
1	B	356	LEU
1	B	383	PHE
1	B	389	LEU
1	B	406	LEU
1	B	412	SER
1	B	414	ASP
1	B	415	LYS
1	B	417	GLN
1	B	423	LEU

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Mol	Chain	Res	Type
1	B	440	LYS
1	B	448	ARG
2	P	741	GLU
2	P	746	ARG
2	P	752	ASP
2	Q	741	GLU
2	Q	744	LEU
2	Q	745	LEU
2	Q	748	LEU
2	Q	751	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	271	GLN

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	PEF	B	1002	-	46,46,46	1.06	4 (8%)	49,51,51	1.00	4 (8%)
3	PEF	A	1001	-	46,46,46	1.09	4 (8%)	49,51,51	1.00	3 (6%)

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	PEF	B	1002	-	-	13/50/50/50	-
3	PEF	A	1001	-	-	12/50/50/50	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	PEF	O3-C30	3.76	1.44	1.33
3	B	1002	PEF	O3-C30	3.55	1.43	1.33
3	A	1001	PEF	O2-C10	3.54	1.44	1.34
3	B	1002	PEF	O2-C10	3.35	1.43	1.34
3	B	1002	PEF	C44-C43	-2.83	1.34	1.51
3	A	1001	PEF	C44-C43	-2.80	1.34	1.51
3	B	1002	PEF	C5-N	-2.57	1.26	1.46
3	A	1001	PEF	C5-N	-2.43	1.27	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	PEF	O3-C30-O5	-2.98	116.17	123.63
3	B	1002	PEF	O2-C10-C11	2.93	117.81	111.48
3	B	1002	PEF	O3-C30-C31	2.45	119.30	111.83
3	B	1002	PEF	O2-C10-O4	-2.29	118.34	123.70
3	A	1001	PEF	O2P-P-O1P	2.16	122.52	112.44
3	B	1002	PEF	O3-C30-O5	-2.15	118.24	123.63
3	A	1001	PEF	O3-C30-C31	2.08	118.19	111.83

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1002	PEF	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
3	A	1001	PEF	C17-C18-C19-C20
3	B	1002	PEF	C17-C18-C19-C20
3	B	1002	PEF	C40-C41-C42-C43
3	B	1002	PEF	C16-C17-C18-C19
3	A	1001	PEF	C14-C15-C16-C17
3	A	1001	PEF	C16-C17-C18-C19
3	B	1002	PEF	C13-C14-C15-C16
3	A	1001	PEF	C19-C20-C21-C22
3	B	1002	PEF	C14-C15-C16-C17
3	A	1001	PEF	C39-C40-C41-C42
3	B	1002	PEF	C19-C20-C21-C22
3	B	1002	PEF	C21-C22-C23-C24
3	B	1002	PEF	C38-C39-C40-C41
3	B	1002	PEF	C15-C16-C17-C18
3	B	1002	PEF	C41-C42-C43-C44
3	B	1002	PEF	C36-C37-C38-C39
3	A	1001	PEF	C13-C14-C15-C16
3	A	1001	PEF	C32-C33-C34-C35
3	B	1002	PEF	C35-C36-C37-C38
3	A	1001	PEF	C31-C30-O3-C3
3	A	1001	PEF	C37-C38-C39-C40
3	A	1001	PEF	O3-C30-C31-C32
3	A	1001	PEF	O5-C30-O3-C3
3	A	1001	PEF	O5-C30-C31-C32

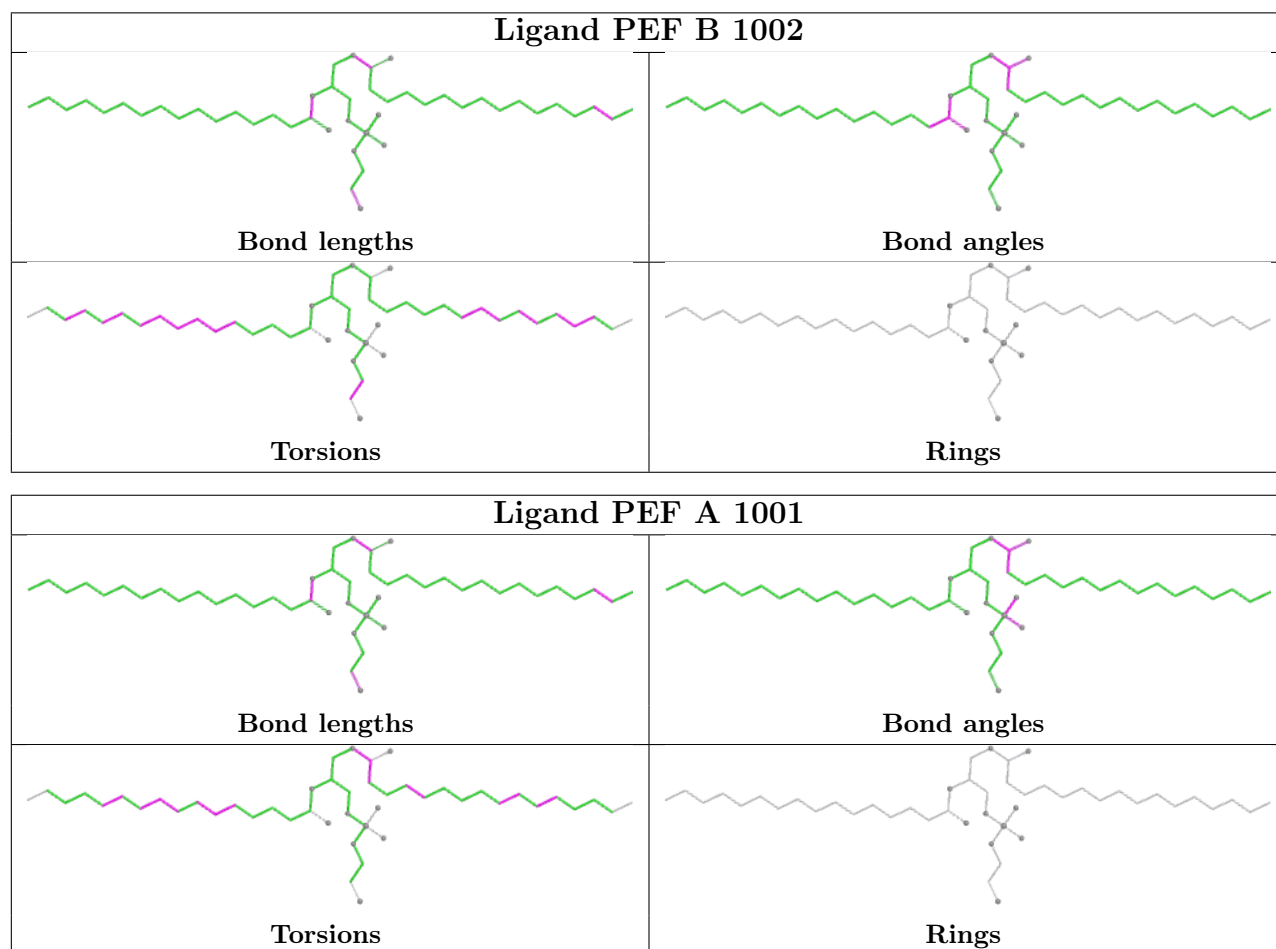
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	PEF	1	0
3	A	1001	PEF	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	233/241 (96%)	0.05	10 (4%) 40 41	16, 22, 32, 42	0
1	B	239/241 (99%)	0.11	5 (2%) 63 66	11, 23, 31, 36	0
2	P	12/12 (100%)	0.51	2 (16%) 4 4	16, 23, 27, 36	0
2	Q	11/12 (91%)	1.22	2 (18%) 3 3	20, 22, 26, 26	0
All	All	495/506 (97%)	0.11	19 (3%) 44 46	11, 23, 32, 42	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	752	ASP	4.5
1	A	256	PRO	3.9
1	B	254	SER	3.7
1	A	221	PRO	3.3
1	B	221	PRO	3.0
1	A	410	PRO	2.9
1	A	245	LEU	2.8
2	Q	747	TYR	2.7
1	A	237	GLU	2.7
1	A	246	GLY	2.5
1	A	243	ARG	2.4
2	Q	745	LEU	2.4
1	A	411	HIS	2.3
1	A	248	LEU	2.2
1	A	460	GLN	2.2
1	B	383	PHE	2.1
1	B	449	ASN	2.1
1	B	448	ARG	2.1
2	P	751	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](#)

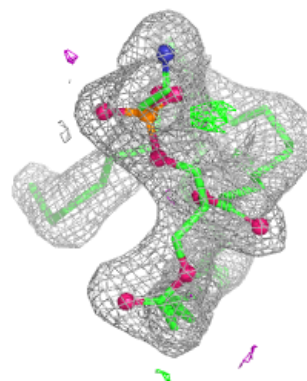
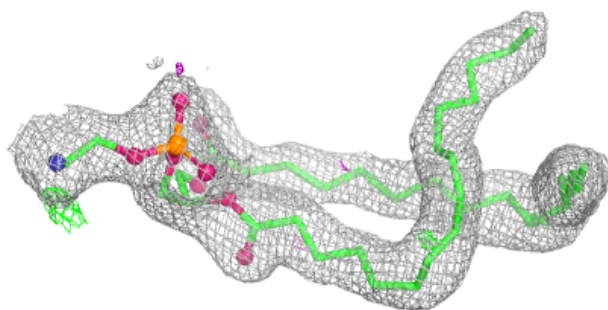
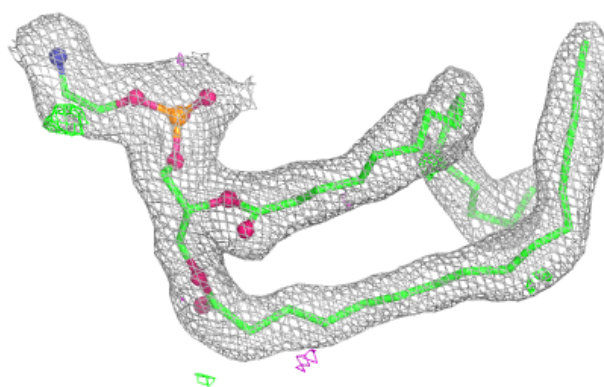
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PEF	A	1001	47/47	0.94	0.08	19,24,27,28	0
3	PEF	B	1002	47/47	0.94	0.08	19,24,27,29	0

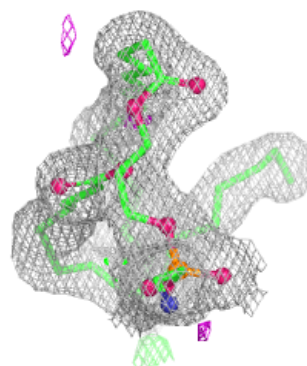
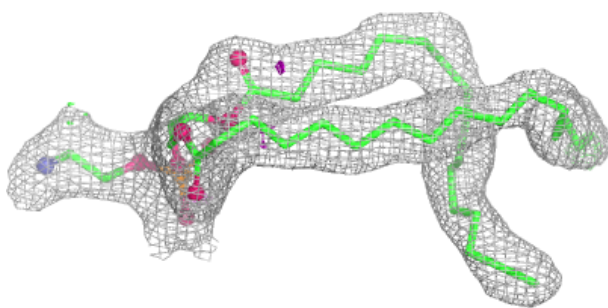
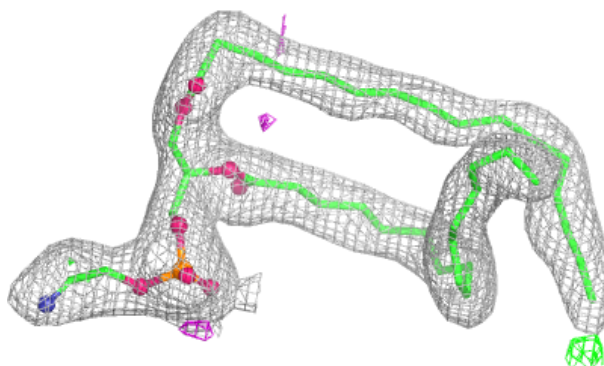
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PEF A 1001:

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

**Electron density around PEF B 1002:**

$2mF_o-DF_c$ (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.