



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:40 PM UTC

PDB ID : 7RE8 / pdb_00007re8
Title : Class I MHC (HLA-A*02) presenting alpha fetoprotein peptide (AFP)
Authors : Dasgupta, M.; Baker, B.M.
Deposited on : 2021-07-12
Resolution : 2.82 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

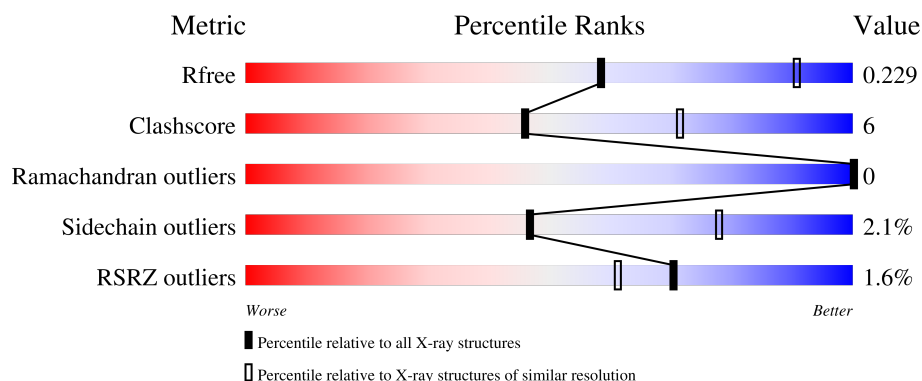
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	276	86% 13% .
1	D	276	85% 14%
2	B	100	80% 20%
2	E	100	84% 16%
3	C	9	67% 33%

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Mol	Chain	Length	Quality of chain
3	F	9	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (22%), green (56%), yellow (33%), and orange (11%). The percentages are labeled above or below the segments.

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6558 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 MHC class I antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2247	1403	409	426	9			
1	D	275	Total	C	N	O	S	0	0	0
			2247	1403	409	426	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A5B8RNS7
D	1	MET	-	initiating methionine	UNP A0A5B8RNS7

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	E	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

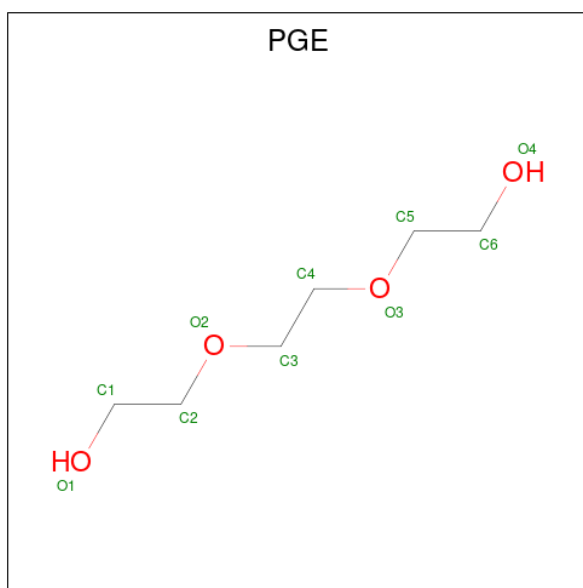
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P61769
E	1	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called PHE-MET-ASN-LYS-PHE-ILE-TYR-GLU-ILE.

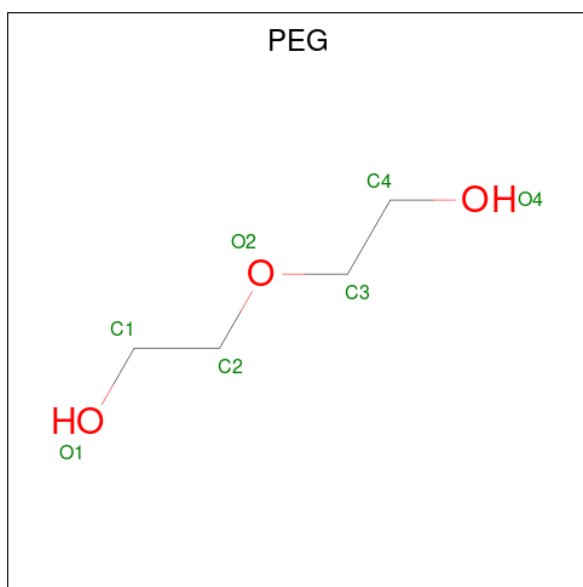
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			85	59	11	14	1			
3	F	9	Total	C	N	O	S	0	0	0
			85	59	11	14	1			

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



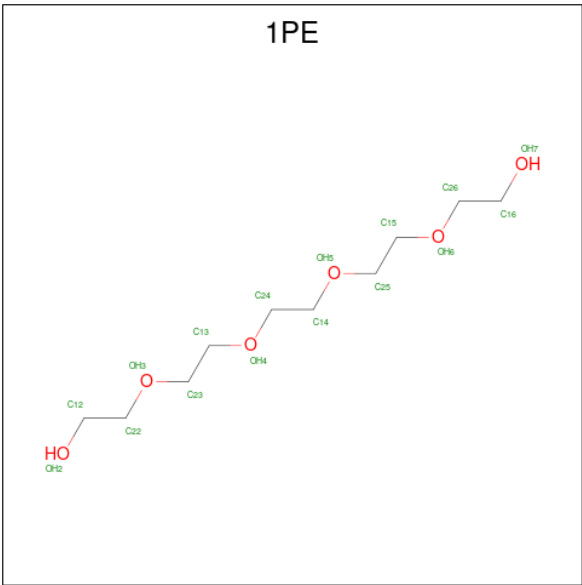
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		
4	E	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	10	6		
6	D	1	Total	C	O	0	0
			16	10	6		

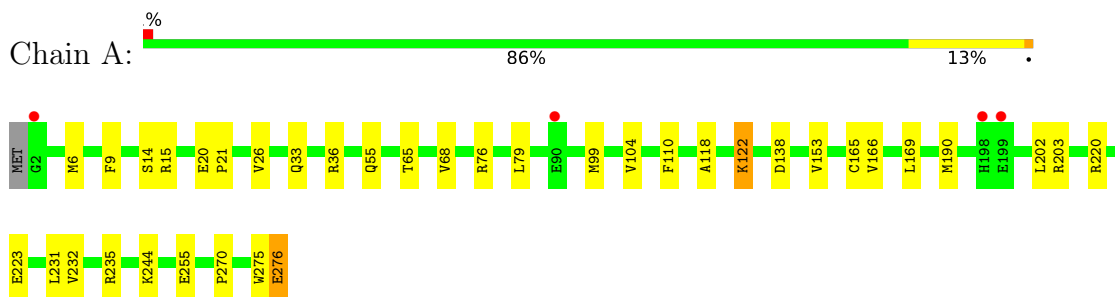
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	19	Total	O	0	0
			19	19		
7	B	11	Total	O	0	0
			11	11		
7	D	20	Total	O	0	0
			20	20		
7	E	8	Total	O	0	0
			8	8		

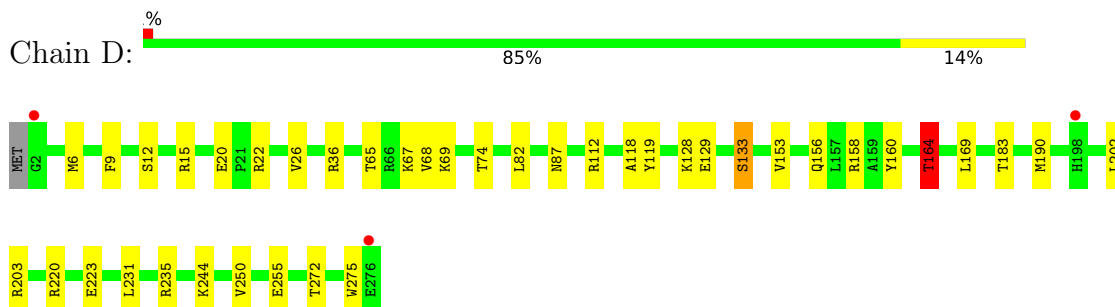
3 Residue-property plots [i](#)

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.

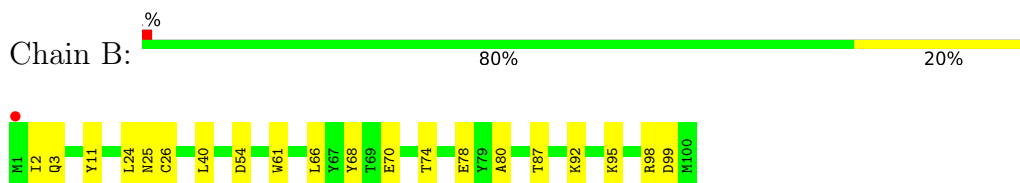
- Molecule 1: MHC class I antigen, A-2 alpha chain



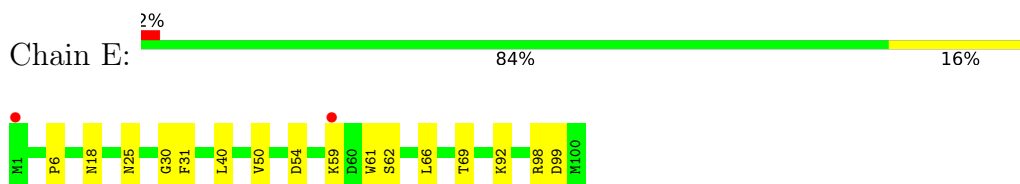
- Molecule 1: MHC class I antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin



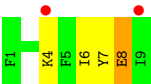
- Molecule 2: Beta-2-microglobulin



- Molecule 3: PHE-MET-ASN-LYS-PHE-ILE-TYR-GLU-ILE



● Molecule 3: PHE-MET-ASN-LYS-PHE-ILE-TYR-GLU-ILE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.21Å 87.31Å 78.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.47 – 2.82 58.47 – 2.82	Depositor EDS
% Data completeness (in resolution range)	97.2 (58.47-2.82) 97.0 (58.47-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.185 , 0.239 0.187 , 0.229	Depositor DCC
R_{free} test set	2049 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.135 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6558	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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: PEG, PGE, 1PE

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	0.48	2/2312 (0.1%)	0.69	1/3137 (0.0%)
1	D	0.54	2/2312 (0.1%)	0.76	1/3137 (0.0%)
2	B	0.32	0/860	0.50	0/1162
2	E	0.37	0/860	0.49	0/1162
3	C	0.72	0/87	0.75	0/113
3	F	0.73	0/87	0.51	0/113
All	All	0.48	4/6518 (0.1%)	0.67	2/8824 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	255	GLU	C-N	-7.20	1.23	1.33
1	A	255	GLU	C-N	-6.42	1.25	1.33
1	A	138	ASP	C-N	-5.46	1.25	1.33
1	D	272	THR	C-N	5.17	1.40	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	GLU	CB-CA-C	8.16	125.61	110.10
1	D	164	THR	CB-CA-C	5.07	119.21	110.79

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	2247	0	2093	26	0
1	D	2247	0	2093	27	0
2	B	837	0	803	14	0
2	E	837	0	803	12	0
3	C	85	0	85	1	0
3	F	85	0	85	5	0
4	A	10	0	14	0	0
4	B	10	0	14	1	0
4	C	10	0	14	2	0
4	D	20	0	28	5	0
4	E	10	0	14	0	0
5	A	28	0	40	2	0
5	B	7	0	10	1	0
5	D	21	0	30	0	0
5	E	14	0	20	3	0
6	A	16	0	22	0	0
6	D	16	0	22	2	0
7	A	19	0	0	0	0
7	B	11	0	0	0	0
7	D	20	0	0	0	0
7	E	8	0	0	0	0
All	All	6558	0	6190	73	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 6.

All (73) 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:D:160:TYR:HA	1:D:164:THR:CG2	2.07	0.84
1:D:153:VAL:HG13	4:D:304:PGE:H32	1.66	0.77
1:D:160:TYR:HA	1:D:164:THR:HG23	1.69	0.73
2:E:59:LYS:HA	5:E:202:PEG:H21	1.77	0.67
1:A:99:MET:HE2	4:B:202:PGE:H2	1.78	0.65
1:D:22:ARG:HH22	6:D:306:1PE:H252	1.60	0.65
2:B:74:THR:O	2:B:98:ARG:NH2	2.32	0.63
3:F:7:TYR:H	4:D:304:PGE:H3	1.64	0.61
2:B:26:CYS:HB2	2:B:40:LEU:HD21	1.84	0.57
2:B:25:ASN:HB3	2:B:66:LEU:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:MET:HB2	1:D:169:LEU:HD13	1.86	0.57
2:B:80:ALA:HB2	2:B:95:LYS:HD2	1.87	0.57
1:A:6:MET:HB2	1:A:169:LEU:HD13	1.88	0.56
3:F:4:LYS:HG2	1:D:67:LYS:HD3	1.86	0.56
2:E:6:PRO:HB3	2:E:31:PHE:HB3	1.92	0.52
2:E:92:LYS:HD2	5:E:201:PEG:H41	1.91	0.52
1:A:270:PRO:HG2	1:D:158:ARG:HH12	1.75	0.50
1:D:128:LYS:HD2	1:D:133:SER:HB2	1.93	0.50
1:D:160:TYR:CD1	1:D:164:THR:HG23	2.46	0.50
1:A:33:GLN:NE2	2:B:54:ASP:OD2	2.34	0.49
3:C:7:TYR:HB2	4:C:101:PGE:H32	1.93	0.49
2:E:30:GLY:HA2	2:E:62:SER:HB3	1.94	0.49
2:E:18:ASN:OD1	2:E:98:ARG:NH2	2.45	0.49
1:A:235:ARG:HD2	2:B:11:TYR:CE1	2.48	0.49
1:D:220:ARG:NH2	1:D:223:GLU:OE2	2.37	0.49
1:A:232:VAL:O	1:A:244:LYS:NZ	2.40	0.48
2:E:40:LEU:HD13	2:E:50:VAL:HG11	1.96	0.48
2:E:92:LYS:HD3	5:E:201:PEG:H12	1.96	0.48
1:D:190:MET:SD	1:D:275:TRP:HB2	2.55	0.47
2:B:78:GLU:HB3	2:B:95:LYS:NZ	2.30	0.47
1:D:202:LEU:HD12	1:D:250:VAL:HG21	1.96	0.47
1:D:231:LEU:HD11	1:D:244:LYS:HE3	1.97	0.46
1:D:82:LEU:HD13	1:D:119:TYR:CD1	2.51	0.46
1:D:36:ARG:HG3	2:E:54:ASP:CG	2.41	0.46
1:D:160:TYR:CA	1:D:164:THR:HG23	2.40	0.45
1:A:235:ARG:HD2	2:B:11:TYR:CZ	2.51	0.45
1:A:55:GLN:HB2	5:A:305:PEG:C2	2.47	0.45
1:A:231:LEU:HD11	1:A:244:LYS:HE3	1.98	0.45
2:B:3:GLN:HB3	2:B:87:THR:HG22	1.99	0.45
2:E:25:ASN:HB3	2:E:66:LEU:HD11	1.99	0.45
1:A:203:ARG:NH1	2:B:99:ASP:OD2	2.50	0.44
1:D:65:THR:HA	1:D:68:VAL:HG12	2.00	0.44
1:D:9:PHE:HB2	1:D:26:VAL:HG22	1.98	0.44
1:A:14:SER:HB3	1:A:79:LEU:HD13	2.00	0.44
1:A:202:LEU:HD12	1:A:202:LEU:HA	1.91	0.44
1:A:153:VAL:HG22	4:C:101:PGE:H12	2.00	0.44
1:D:15:ARG:NH1	1:D:20:GLU:O	2.51	0.44
1:D:22:ARG:NH1	6:D:306:1PE:H231	2.33	0.44
1:A:21:PRO:HG2	1:A:76:ARG:HG3	2.00	0.43
1:A:104:VAL:HG11	1:A:166:VAL:HG13	1.99	0.43
1:A:270:PRO:HG2	1:D:158:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLN:HB2	5:A:305:PEG:O2	2.18	0.43
3:F:6:ILE:HG12	1:D:74:THR:HG21	2.01	0.43
1:D:112:ARG:HG3	1:D:129:GLU:OE1	2.18	0.43
1:A:15:ARG:NH1	1:A:20:GLU:O	2.52	0.43
1:A:220:ARG:O	1:A:223:GLU:HG2	2.18	0.43
1:D:203:ARG:NH1	2:E:99:ASP:OD2	2.51	0.42
4:D:304:PGE:H62	4:D:304:PGE:H4	1.54	0.42
1:A:65:THR:HA	1:A:68:VAL:HG12	2.01	0.42
1:A:190:MET:SD	1:A:275:TRP:HB2	2.60	0.42
1:D:160:TYR:HA	1:D:164:THR:HG22	1.96	0.42
1:A:118:ALA:HB2	2:B:61:TRP:CE2	2.55	0.42
1:D:118:ALA:HB2	2:E:61:TRP:CE2	2.54	0.42
2:B:92:LYS:HZ3	5:B:201:PEG:H32	1.84	0.42
3:F:7:TYR:N	4:D:304:PGE:H3	2.32	0.41
1:D:156:GLN:OE1	4:D:304:PGE:H42	2.21	0.41
2:E:40:LEU:HD22	2:E:69:THR:HG22	2.02	0.41
1:A:9:PHE:HB2	1:A:26:VAL:HG22	2.02	0.41
3:F:8:GLU:H	3:F:8:GLU:HG3	1.66	0.41
1:A:6:MET:HE2	1:A:165:CYS:SG	2.60	0.41
1:A:122:LYS:HG3	2:B:2:ILE:HG13	2.03	0.41
2:B:24:LEU:O	2:B:68:TYR:HA	2.21	0.40
1:A:110:PHE:HB2	1:A:166:VAL:HG21	2.03	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	273/276 (99%)	266 (97%)	7 (3%)	0	100	100
1	D	273/276 (99%)	267 (98%)	6 (2%)	0	100	100
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	756/770 (98%)	737 (98%)	19 (2%)	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	231/232 (100%)	228 (99%)	3 (1%)	61	85
1	D	231/232 (100%)	224 (97%)	7 (3%)	36	69
2	B	95/95 (100%)	94 (99%)	1 (1%)	65	86
2	E	95/95 (100%)	95 (100%)	0	100	100
3	C	9/9 (100%)	7 (78%)	2 (22%)	1	3
3	F	9/9 (100%)	8 (89%)	1 (11%)	6	19
All	All	670/672 (100%)	656 (98%)	14 (2%)	47	78

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	122	LYS
1	A	276	GLU
2	B	70	GLU
3	C	8	GLU
3	C	9	ILE
3	F	8	GLU
1	D	12	SER
1	D	69	LYS
1	D	87	ASN

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Mol	Chain	Res	Type
1	D	133	SER
1	D	164	THR
1	D	183	THR
1	D	235	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
3	C	3	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](#)

18 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	$\# Z > 2$
5	PEG	A	302	-	6,6,6	0.50	0	5,5,5	0.24	0
5	PEG	A	306	-	6,6,6	0.49	0	5,5,5	0.25	0
4	PGE	B	202	-	9,9,9	0.52	0	8,8,8	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PGE	E	203	-	9,9,9	0.53	0	8,8,8	0.23	0
5	PEG	B	201	-	6,6,6	0.50	0	5,5,5	0.22	0
6	1PE	D	306	-	15,15,15	0.55	0	14,14,14	0.22	0
4	PGE	C	101	-	9,9,9	0.19	0	8,8,8	0.18	0
5	PEG	D	302	-	6,6,6	0.50	0	5,5,5	0.26	0
5	PEG	E	202	-	6,6,6	0.50	0	5,5,5	0.29	0
5	PEG	A	304	-	6,6,6	0.51	0	5,5,5	0.19	0
5	PEG	A	305	-	6,6,6	0.11	0	5,5,5	0.07	0
5	PEG	E	201	-	6,6,6	0.49	0	5,5,5	0.24	0
5	PEG	D	305	-	6,6,6	0.12	0	5,5,5	0.08	0
6	1PE	A	303	-	15,15,15	0.54	0	14,14,14	0.21	0
4	PGE	A	301	-	9,9,9	0.53	0	8,8,8	0.23	0
5	PEG	D	303	-	6,6,6	0.18	0	5,5,5	0.18	0
4	PGE	D	304	-	9,9,9	0.14	0	8,8,8	0.11	0
4	PGE	D	301	-	9,9,9	0.53	0	8,8,8	0.20	0

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
5	PEG	A	302	-	-	0/4/4/4	-
5	PEG	A	306	-	-	1/4/4/4	-
4	PGE	B	202	-	-	2/7/7/7	-
4	PGE	E	203	-	-	4/7/7/7	-
5	PEG	B	201	-	-	1/4/4/4	-
6	1PE	D	306	-	-	9/13/13/13	-
4	PGE	C	101	-	-	4/7/7/7	-
5	PEG	D	302	-	-	1/4/4/4	-
5	PEG	E	202	-	-	3/4/4/4	-
5	PEG	A	304	-	-	3/4/4/4	-
5	PEG	A	305	-	-	2/4/4/4	-
5	PEG	E	201	-	-	2/4/4/4	-
5	PEG	D	305	-	-	2/4/4/4	-
6	1PE	A	303	-	-	6/13/13/13	-
4	PGE	A	301	-	-	1/7/7/7	-
5	PEG	D	303	-	-	2/4/4/4	-
4	PGE	D	304	-	-	5/7/7/7	-
4	PGE	D	301	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	304	PGE	C1-C2-O2-C3
5	D	303	PEG	C4-C3-O2-C2
4	D	304	PGE	C6-C5-O3-C4
4	B	202	PGE	O2-C3-C4-O3
4	C	101	PGE	O2-C3-C4-O3
6	D	306	1PE	OH6-C15-C25-OH5
4	E	203	PGE	O3-C5-C6-O4
6	D	306	1PE	OH7-C16-C26-OH6
6	D	306	1PE	OH5-C14-C24-OH4
4	A	301	PGE	O2-C3-C4-O3
4	D	301	PGE	O2-C3-C4-O3
5	E	202	PEG	O2-C3-C4-O4
4	C	101	PGE	C1-C2-O2-C3
4	D	304	PGE	O2-C3-C4-O3
4	E	203	PGE	O1-C1-C2-O2
6	A	303	1PE	OH7-C16-C26-OH6
6	D	306	1PE	OH2-C12-C22-OH3
4	D	304	PGE	O1-C1-C2-O2
5	A	304	PEG	O1-C1-C2-O2
5	D	305	PEG	O2-C3-C4-O4
5	A	304	PEG	O2-C3-C4-O4
5	E	202	PEG	O1-C1-C2-O2
4	E	203	PGE	C4-C3-O2-C2
4	C	101	PGE	C3-C4-O3-C5
5	D	302	PEG	C1-C2-O2-C3
5	D	305	PEG	C1-C2-O2-C3
6	A	303	1PE	OH5-C14-C24-OH4
4	D	301	PGE	C1-C2-O2-C3
4	E	203	PGE	C3-C4-O3-C5
6	A	303	1PE	C23-C13-OH4-C24
5	E	201	PEG	C4-C3-O2-C2
6	A	303	1PE	OH6-C15-C25-OH5
6	D	306	1PE	C25-C15-OH6-C26
6	D	306	1PE	C23-C13-OH4-C24
5	E	202	PEG	C4-C3-O2-C2
6	D	306	1PE	C12-C22-OH3-C23
4	B	202	PGE	C4-C3-O2-C2

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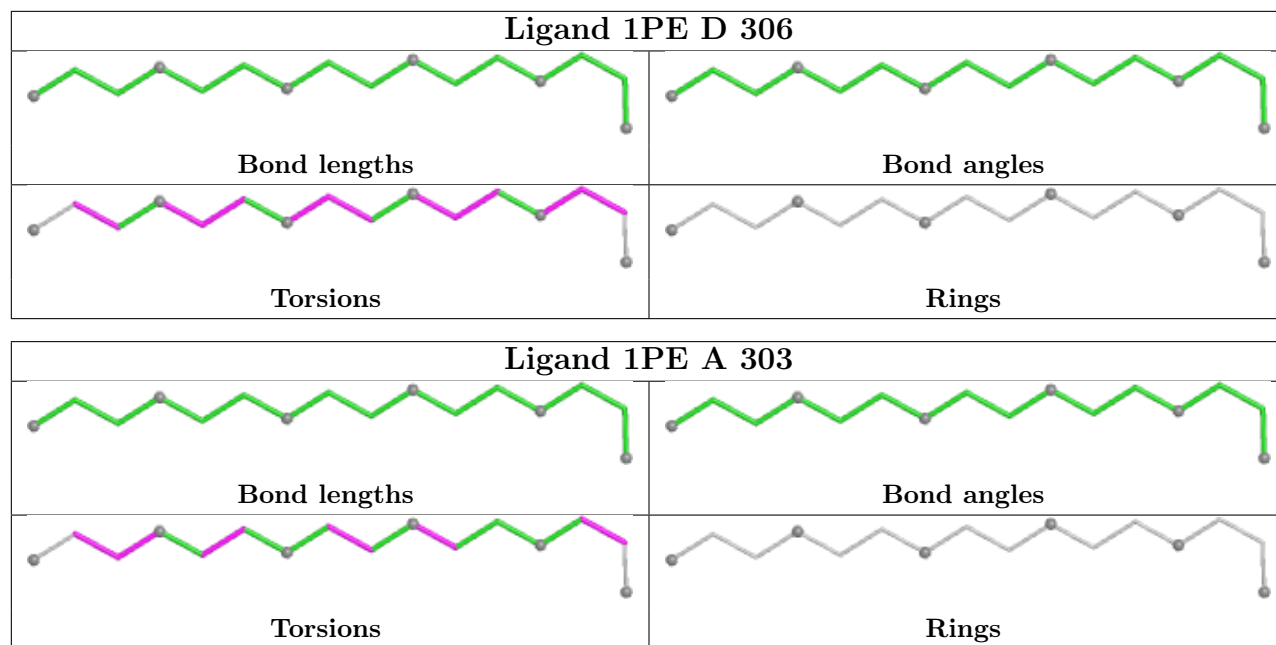
Mol	Chain	Res	Type	Atoms
4	C	101	PGE	C6-C5-O3-C4
5	A	306	PEG	C1-C2-O2-C3
5	B	201	PEG	O2-C3-C4-O4
4	D	304	PGE	C3-C4-O3-C5
6	D	306	1PE	C24-C14-OH5-C25
5	E	201	PEG	O2-C3-C4-O4
5	D	303	PEG	O1-C1-C2-O2
5	A	305	PEG	C4-C3-O2-C2
6	A	303	1PE	C16-C26-OH6-C15
6	D	306	1PE	OH4-C13-C23-OH3
5	A	304	PEG	C4-C3-O2-C2
6	A	303	1PE	OH2-C12-C22-OH3
5	A	305	PEG	C1-C2-O2-C3

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	202	PGE	1	0
5	B	201	PEG	1	0
6	D	306	1PE	2	0
4	C	101	PGE	2	0
5	E	202	PEG	1	0
5	A	305	PEG	2	0
5	E	201	PEG	2	0
4	D	304	PGE	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 [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	275/276 (99%)	0.07	4 (1%) 72 63	9, 26, 54, 92	0
1	D	275/276 (99%)	0.09	3 (1%) 78 70	12, 25, 54, 79	0
2	B	100/100 (100%)	0.16	1 (1%) 79 72	13, 29, 61, 73	0
2	E	100/100 (100%)	0.09	2 (2%) 65 55	9, 27, 52, 64	0
3	C	9/9 (100%)	0.72	0 100 100	24, 33, 42, 49	0
3	F	9/9 (100%)	1.02	2 (22%) 2 1	27, 37, 45, 52	0
All	All	768/770 (99%)	0.11	12 (1%) 70 61	9, 27, 54, 92	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	GLY	3.6
1	D	276	GLU	3.5
2	B	1	MET	3.1
2	E	1	MET	3.0
1	A	199	GLU	2.6
1	A	198	HIS	2.2
1	A	90	GLU	2.2
3	F	4	LYS	2.1
3	F	9	ILE	2.1
1	D	198	HIS	2.1
2	E	59	LYS	2.1
1	D	2	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

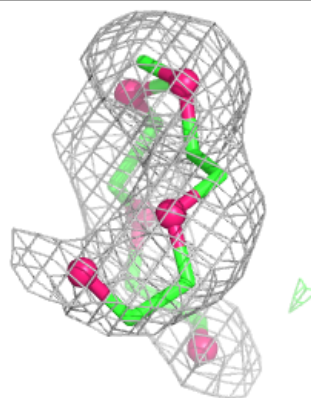
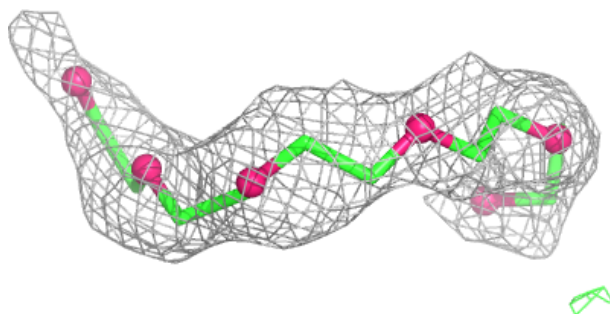
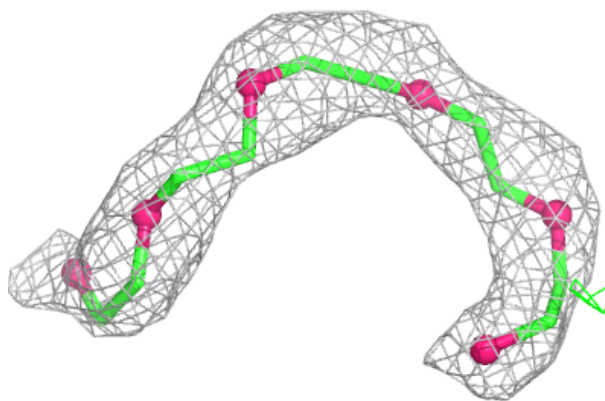
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PEG	A	305	7/7	0.78	0.22	20,20,20,20	0
5	PEG	B	201	7/7	0.78	0.16	32,39,44,46	0
5	PEG	A	304	7/7	0.80	0.18	37,43,46,48	0
5	PEG	D	302	7/7	0.81	0.16	51,52,56,57	0
5	PEG	D	305	7/7	0.81	0.18	20,20,20,20	0
4	PGE	D	304	10/10	0.82	0.19	43,55,57,58	0
4	PGE	B	202	10/10	0.82	0.17	41,50,53,54	0
5	PEG	D	303	7/7	0.83	0.15	37,39,52,52	0
5	PEG	E	201	7/7	0.84	0.14	28,33,48,48	0
4	PGE	E	203	10/10	0.86	0.14	45,51,54,55	0
4	PGE	C	101	10/10	0.87	0.18	36,42,54,54	0
5	PEG	A	306	7/7	0.88	0.11	14,23,38,41	0
6	1PE	D	306	16/16	0.88	0.13	31,41,45,45	0
5	PEG	E	202	7/7	0.89	0.15	31,35,38,40	0
6	1PE	A	303	16/16	0.90	0.12	40,43,50,52	0
4	PGE	A	301	10/10	0.91	0.12	28,35,40,40	0
5	PEG	A	302	7/7	0.92	0.09	31,31,33,36	0
4	PGE	D	301	10/10	0.92	0.11	28,33,42,45	0

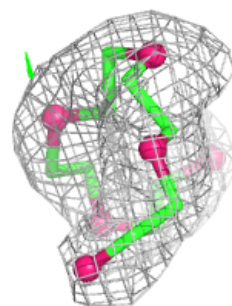
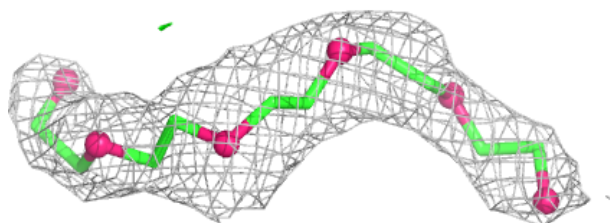
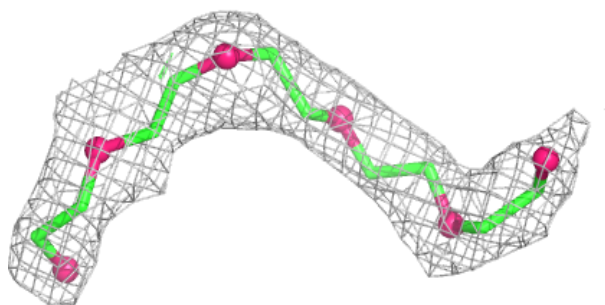
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1PE D 306:

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

**Electron density around 1PE A 303:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.