



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2016 – 12:14 AM EDT

PDB ID : 4WMO
Title : Selenomethionine derivative of *Xenopus laevis* embryonic epidermal lectin carbohydrate-binding domain
Authors : Wangkanont, K.; Kiessling, L.L.; Forest, K.T.
Deposited on : 2014-10-09
Resolution : 2.30 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

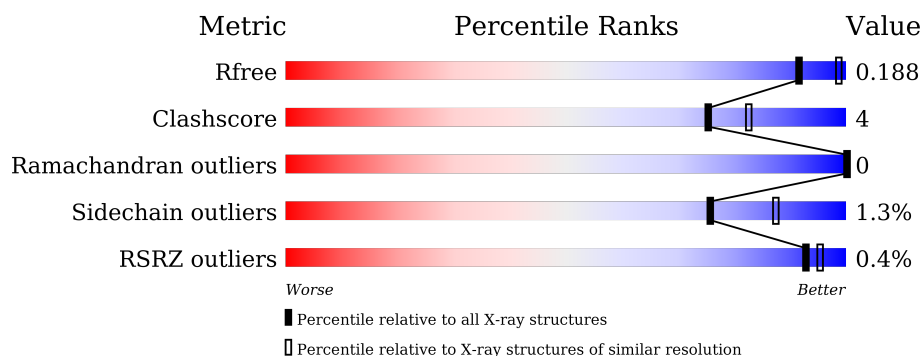
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	289	<div> <div>87%</div> <div>9%</div> <div>.</div> </div>
1	B	289	<div> <div>88%</div> <div>7%</div> <div>..</div> </div>
1	C	289	<div> <div>87%</div> <div>8%</div> <div>.</div> </div>
1	D	289	<div> <div>%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>
1	E	289	<div> <div>%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>
1	F	289	<div> <div>87%</div> <div>9%</div> <div>.</div> </div>

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	1PE	A	404	-	-	-	X
3	1PE	A	405	-	-	-	X
3	1PE	A	406	-	-	-	X
3	1PE	B	404	-	-	-	X
3	1PE	B	405	-	-	-	X
3	1PE	C	404	-	-	-	X
3	1PE	C	405	-	-	-	X
3	1PE	C	406	-	-	-	X
3	1PE	D	404	-	-	-	X
3	1PE	D	405	-	-	-	X
3	1PE	E	404	-	-	-	X
3	1PE	E	405	-	-	-	X
3	1PE	F	404	-	-	-	X
3	1PE	F	405	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14639 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.

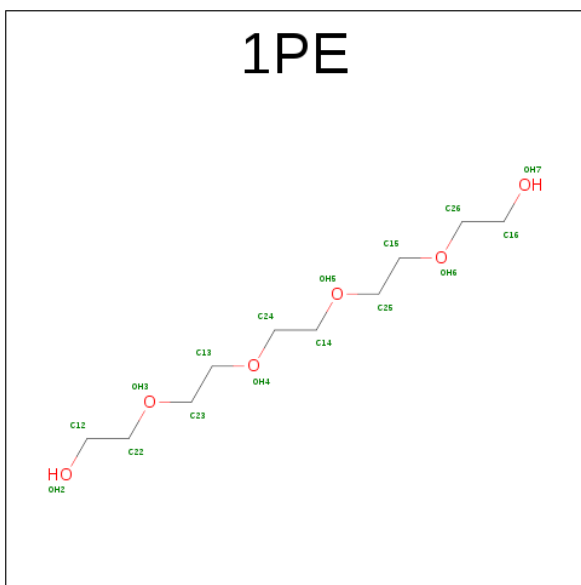
- Molecule 1 is a protein called XEEL protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	F	277	Total	C	N	O	S	Se	0	2	0
			2153	1350	367	421	8	7			
1	C	277	Total	C	N	O	S	Se	0	2	0
			2153	1350	367	421	8	7			
1	B	277	Total	C	N	O	S	Se	0	2	0
			2158	1353	370	420	8	7			
1	D	277	Total	C	N	O	S	Se	0	1	0
			2147	1347	366	419	8	7			
1	E	277	Total	C	N	O	S	Se	0	1	0
			2147	1347	366	419	8	7			
1	A	277	Total	C	N	O	S	Se	0	3	0
			2169	1359	374	421	8	7			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	3	Total	Ca	0	0
			3	3		
2	E	3	Total	Ca	0	0
			3	3		
2	B	3	Total	Ca	0	0
			3	3		
2	C	3	Total	Ca	0	0
			3	3		
2	A	3	Total	Ca	0	0
			3	3		
2	F	3	Total	Ca	0	0
			3	3		

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).

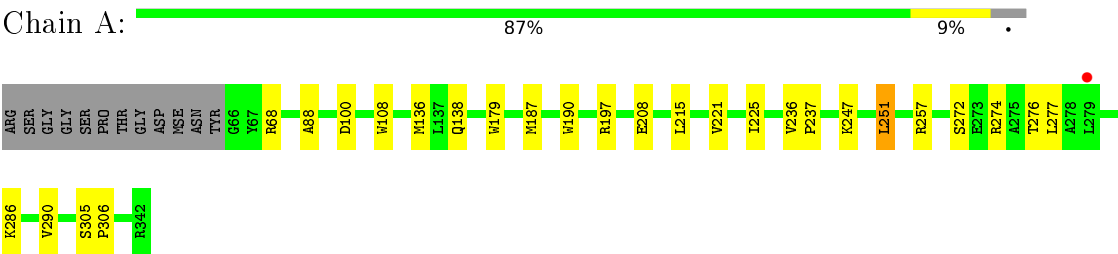


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total 16	C 10	O 6	0	0
3	F	1	Total 16	C 10	O 6	0	0
3	C	1	Total 16	C 10	O 6	0	0
3	C	1	Total 16	C 10	O 6	0	0
3	C	1	Total 16	C 10	O 6	0	0
3	B	1	Total 16	C 10	O 6	0	0
3	B	1	Total 16	C 10	O 6	0	0
3	D	1	Total 16	C 10	O 6	0	0
3	D	1	Total 16	C 10	O 6	0	0
3	E	1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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	236	Total 236	O 236	0	0
4	C	228	Total 228	O 228	0	0
4	B	236	Total 236	O 236	0	0
4	D	262	Total 262	O 262	0	0
4	E	241	Total 241	O 241	0	0
4	A	267	Total 267	O 267	0	0

● Molecule 1: XEEL protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	123.65Å 111.07Å 123.61Å 90.00° 119.72° 90.00°	Depositor
Resolution (Å)	30.09 – 2.30 30.09 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.09-2.30) 99.8 (30.09-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.160 , 0.188 0.157 , 0.188	Depositor DCC
R_{free} test set	12637 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 32.2	EDS
Estimated twinning fraction	0.000 for l,k,-h-l 0.000 for -h-l,k,h 0.000 for -h-l,-k,l 0.015 for h,-k,-h-l 0.000 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	3 of 128967 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14639	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.74 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.4617e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, 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	0.46	0/2219	0.61	2/2998 (0.1%)
1	B	0.46	0/2208	0.63	4/2984 (0.1%)
1	C	0.45	0/2203	0.61	2/2978 (0.1%)
1	D	0.47	0/2197	0.62	1/2970 (0.0%)
1	E	0.45	0/2197	0.62	4/2970 (0.1%)
1	F	0.44	0/2203	0.60	3/2978 (0.1%)
All	All	0.45	0/13227	0.61	16/17878 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136[A]	MSE	CG-SE-CE	6.37	112.90	98.90
1	B	136[B]	MSE	CG-SE-CE	6.37	112.90	98.90
1	B	189	MSE	CG-SE-CE	6.23	112.61	98.90
1	F	189	MSE	CG-SE-CE	6.05	112.22	98.90
1	E	101	MSE	CG-SE-CE	6.03	112.17	98.90
1	F	136[A]	MSE	CG-SE-CE	5.66	111.35	98.90
1	F	136[B]	MSE	CG-SE-CE	5.66	111.35	98.90
1	A	136[A]	MSE	CG-SE-CE	5.60	111.22	98.90
1	A	136[B]	MSE	CG-SE-CE	5.60	111.22	98.90
1	E	136[A]	MSE	CG-SE-CE	5.48	110.96	98.90
1	E	136[B]	MSE	CG-SE-CE	5.48	110.96	98.90
1	B	338	MSE	CA-CB-CG	-5.47	104.00	113.30
1	E	189	MSE	CG-SE-CE	5.46	110.91	98.90
1	C	189	MSE	CG-SE-CE	5.17	110.27	98.90
1	D	338	MSE	CG-SE-CE	5.09	110.09	98.90
1	C	338	MSE	CA-CB-CG	-5.03	104.75	113.30

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	2169	0	2031	18	0
1	B	2158	0	2019	14	0
1	C	2153	0	2011	17	0
1	D	2147	0	2007	12	0
1	E	2147	0	2007	20	0
1	F	2153	0	2011	19	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
3	A	48	0	66	5	0
3	B	32	0	44	7	0
3	C	48	0	66	5	0
3	D	32	0	44	1	0
3	E	32	0	44	10	0
3	F	32	0	44	7	0
4	A	267	0	0	3	0
4	B	236	0	0	0	0
4	C	228	0	0	3	0
4	D	262	0	0	1	0
4	E	241	0	0	3	0
4	F	236	0	0	2	0
All	All	14639	0	12394	99	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 4.

All (99) 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:E:286:LYS:HZ3	3:E:405:1PE:H261	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:CYS:HB3	3:B:405:IPE:H162	1.73	0.71
1:A:225:ILE:HD12	3:A:404:IPE:H131	1.74	0.69
1:D:100:ASP:HB3	1:D:108:TRP:HB2	1.76	0.68
1:B:222:LYS:HZ2	3:B:404:IPE:H151	1.59	0.67
1:D:222:LYS:HE2	3:D:404:IPE:H132	1.76	0.67
1:F:192:ASN:OD1	4:F:627:HOH:O	2.12	0.67
1:C:222:LYS:HZ3	3:C:404:IPE:H142	1.60	0.66
1:E:261:THR:HB	3:E:405:IPE:H242	1.77	0.66
1:D:66:GLY:N	4:D:687:HOH:O	2.29	0.65
1:F:222:LYS:HZ2	3:F:404:IPE:H242	1.62	0.65
1:F:286:LYS:NZ	3:F:405:IPE:H231	2.10	0.65
1:A:100:ASP:HB3	1:A:108:TRP:HB2	1.80	0.64
1:F:192:ASN:ND2	4:F:725:HOH:O	2.25	0.64
1:C:103:THR:OG1	1:C:191:ARG:NH1	2.33	0.61
1:A:286:LYS:HD3	3:A:405:IPE:H251	1.83	0.60
1:C:286:LYS:HE2	3:C:405:IPE:H122	1.83	0.59
1:C:100:ASP:HB3	1:C:108:TRP:HB2	1.85	0.59
1:F:100:ASP:HB3	1:F:108:TRP:HB2	1.84	0.59
1:E:225:ILE:HD11	3:E:404:IPE:H251	1.84	0.58
1:E:286:LYS:NZ	3:E:405:IPE:H261	2.20	0.57
1:F:286:LYS:NZ	3:F:405:IPE:H152	2.20	0.57
1:B:141:GLU:OE2	3:B:404:IPE:H252	2.05	0.57
1:B:222:LYS:NZ	3:B:404:IPE:H151	2.20	0.56
1:A:187:MSE:HA	1:A:190:TRP:CE2	2.41	0.55
1:F:225:ILE:CD1	3:F:404:IPE:H151	2.38	0.54
1:F:286:LYS:HE2	3:F:405:IPE:H222	1.88	0.54
1:D:187:MSE:HA	1:D:190:TRP:CE2	2.44	0.53
1:E:190:TRP:CH2	1:E:338:MSE:HE1	2.43	0.53
1:F:103:THR:OG1	1:F:191:ARG:NH1	2.41	0.53
1:F:286:LYS:HZ2	3:F:405:IPE:H231	1.71	0.53
1:F:318:ASP:OD1	1:C:79:ARG:NH1	2.41	0.52
1:E:191:ARG:NH1	4:E:683:HOH:O	2.29	0.52
1:E:286:LYS:HZ3	3:E:405:IPE:H251	1.74	0.52
1:F:222:LYS:NZ	3:F:404:IPE:H242	2.24	0.52
1:C:227:LYS:HD2	3:C:406:IPE:H221	1.91	0.52
1:C:261:THR:HB	3:C:405:IPE:H242	1.92	0.52
1:A:286:LYS:HZ3	3:A:405:IPE:H261	1.76	0.51
1:B:222:LYS:HZ3	3:B:404:IPE:H121	1.76	0.50
1:E:222:LYS:HZ3	3:E:404:IPE:H152	1.75	0.50
1:E:225:ILE:CD1	3:E:404:IPE:H251	2.41	0.50
1:D:177:ALA:HB3	1:D:340:PHE:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:LYS:HD3	3:E:405:1PE:H251	1.94	0.49
1:D:246:GLU:CD	1:D:246:GLU:H	2.15	0.48
1:B:292:HIS:O	1:B:315:LEU:HD22	2.13	0.48
1:C:218:LYS:HD2	1:C:219:TYR:CE2	2.48	0.48
1:F:118:ASN:HD21	1:E:136[B]:MSE:SE	2.47	0.48
1:A:274:ARG:NH1	4:A:502:HOH:O	2.46	0.47
1:E:225:ILE:HG22	4:E:586:HOH:O	2.14	0.47
1:C:192:ASN:ND2	4:C:666:HOH:O	2.48	0.47
1:A:68:ARG:HG2	1:A:88:ALA:O	2.15	0.46
1:C:187:MSE:HA	1:C:190:TRP:CE2	2.50	0.46
1:C:305:SER:HA	1:C:306:PRO:HA	1.75	0.46
1:F:98:PHE:HB2	1:F:187:MSE:HE2	1.97	0.46
1:F:266:GLN:OE1	1:F:285:VAL:HG22	2.16	0.46
1:C:98:PHE:HB2	1:C:187:MSE:HE2	1.99	0.45
1:B:220:PRO:HB2	1:B:225:ILE:HD12	1.98	0.45
1:B:113:SER:HB3	1:B:163:TYR:HB3	1.99	0.45
1:A:277:LEU:HD23	1:A:290:VAL:HG23	1.99	0.44
1:A:286:LYS:NZ	3:A:405:1PE:H261	2.31	0.44
1:D:103:THR:OG1	1:D:191:ARG:NH2	2.49	0.44
1:E:100:ASP:HB3	1:E:108:TRP:HB2	1.99	0.44
1:F:68:ARG:HG2	1:F:88:ALA:O	2.18	0.44
1:F:305:SER:HA	1:F:306:PRO:HA	1.76	0.44
1:E:305:SER:HA	1:E:306:PRO:HA	1.85	0.44
1:A:179:TRP:CG	1:A:197:ARG:HG2	2.53	0.44
1:C:191:ARG:NE	4:C:689:HOH:O	2.38	0.44
1:B:187:MSE:HA	1:B:190:TRP:CE2	2.52	0.44
1:C:190:TRP:CZ3	1:C:338:MSE:HE1	2.53	0.44
1:E:227:LYS:HE2	1:E:274:ARG:NH2	2.33	0.44
1:E:191:ARG:HD3	4:E:683:HOH:O	2.19	0.43
1:F:221:VAL:HA	1:F:276:THR:HG21	2.00	0.43
1:A:208:GLU:HG3	1:A:215:LEU:HD12	2.00	0.43
1:E:187:MSE:HA	1:E:190:TRP:CE2	2.54	0.43
1:C:141:GLU:HB2	4:C:554:HOH:O	2.19	0.42
1:A:225:ILE:HG22	4:A:548:HOH:O	2.18	0.42
1:A:247:LYS:HG2	1:A:251:LEU:HD22	2.01	0.42
1:A:221:VAL:HA	1:A:276:THR:HG21	2.01	0.42
1:E:84:ILE:HD11	1:E:187:MSE:HE1	2.01	0.42
1:F:190:TRP:CH2	1:F:338:MSE:HE1	2.54	0.42
1:A:286:LYS:CE	3:A:405:1PE:H261	2.49	0.42
1:B:305:SER:HA	1:B:306:PRO:HA	1.86	0.42
1:B:186:PRO:HD2	1:B:189:MSE:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:TYR:CE2	1:B:224:ASP:HB2	2.54	0.42
1:C:176:LEU:HD12	1:C:340:PHE:O	2.20	0.42
1:D:98:PHE:HB2	1:D:187:MSE:HE2	2.01	0.42
1:E:178:LEU:HA	1:E:338:MSE:O	2.20	0.42
1:E:222:LYS:HZ3	3:E:404:1PE:C15	2.34	0.41
1:B:222:LYS:NZ	3:B:404:1PE:H121	2.35	0.41
1:A:257[B]:ARG:NH2	4:A:691:HOH:O	2.22	0.41
1:C:258:SER:O	3:C:405:1PE:H231	2.20	0.41
3:E:405:1PE:H241	3:E:405:1PE:H251	1.88	0.41
1:D:251:LEU:HB3	1:D:332:ILE:HD12	2.01	0.41
1:A:305:SER:HA	1:A:306:PRO:HA	1.83	0.41
1:B:222:LYS:HE3	3:B:404:1PE:H262	2.03	0.41
1:D:187:MSE:HA	1:D:190:TRP:CD2	2.56	0.40
1:A:236:VAL:HA	1:A:237:PRO:HD3	1.99	0.40
1:D:305:SER:HA	1:D:306:PRO:HA	1.85	0.40
1:D:236:VAL:HA	1:D:237:PRO:HD3	1.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	278/289 (96%)	269 (97%)	9 (3%)	0	100	100
1	B	277/289 (96%)	268 (97%)	9 (3%)	0	100	100
1	C	277/289 (96%)	265 (96%)	12 (4%)	0	100	100
1	D	276/289 (96%)	263 (95%)	13 (5%)	0	100	100
1	E	276/289 (96%)	266 (96%)	10 (4%)	0	100	100
1	F	277/289 (96%)	266 (96%)	11 (4%)	0	100	100
All	All	1661/1734 (96%)	1597 (96%)	64 (4%)	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	226/225 (100%)	223 (99%)	3 (1%)	76	87
1	B	225/225 (100%)	221 (98%)	4 (2%)	66	82
1	C	225/225 (100%)	223 (99%)	2 (1%)	84	93
1	D	224/225 (100%)	222 (99%)	2 (1%)	84	93
1	E	224/225 (100%)	222 (99%)	2 (1%)	84	93
1	F	225/225 (100%)	221 (98%)	4 (2%)	66	82
All	All	1349/1350 (100%)	1332 (99%)	17 (1%)	76	87

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	191	ARG
1	F	251	LEU
1	F	260	PHE
1	F	272	SER
1	C	251	LEU
1	C	272	SER
1	B	251	LEU
1	B	261	THR
1	B	272	SER
1	B	315	LEU
1	D	251	LEU
1	D	272	SER
1	E	251	LEU
1	E	272	SER
1	A	138	GLN
1	A	251	LEU
1	A	272	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 18 are monoatomic - leaving 14 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	1PE	A	404	-	15,15,15	0.60	0	14,14,14	0.99	0
3	1PE	A	405	-	15,15,15	0.62	0	14,14,14	0.91	0
3	1PE	A	406	-	15,15,15	0.58	0	14,14,14	0.91	0
3	1PE	B	404	-	15,15,15	0.65	0	14,14,14	0.85	0
3	1PE	B	405	-	15,15,15	0.61	0	14,14,14	1.05	2 (14%)
3	1PE	C	404	-	15,15,15	0.62	0	14,14,14	0.97	0
3	1PE	C	405	-	15,15,15	0.63	0	14,14,14	1.00	1 (7%)
3	1PE	C	406	-	15,15,15	0.60	0	14,14,14	0.96	0
3	1PE	D	404	-	15,15,15	0.62	0	14,14,14	1.00	1 (7%)
3	1PE	D	405	-	15,15,15	0.65	0	14,14,14	0.96	0
3	1PE	E	404	-	15,15,15	0.62	0	14,14,14	1.03	2 (14%)
3	1PE	E	405	-	15,15,15	0.63	0	14,14,14	0.86	0
3	1PE	F	404	-	15,15,15	0.60	0	14,14,14	0.91	0
3	1PE	F	405	-	15,15,15	0.69	0	14,14,14	0.87	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
3	1PE	A	404	-	-	0/13/13/13	0/0/0/0
3	1PE	A	405	-	-	0/13/13/13	0/0/0/0
3	1PE	A	406	-	-	0/13/13/13	0/0/0/0
3	1PE	B	404	-	-	0/13/13/13	0/0/0/0
3	1PE	B	405	-	-	0/13/13/13	0/0/0/0
3	1PE	C	404	-	-	0/13/13/13	0/0/0/0
3	1PE	C	405	-	-	0/13/13/13	0/0/0/0
3	1PE	C	406	-	-	0/13/13/13	0/0/0/0
3	1PE	D	404	-	-	0/13/13/13	0/0/0/0
3	1PE	D	405	-	-	0/13/13/13	0/0/0/0
3	1PE	E	404	-	-	0/13/13/13	0/0/0/0
3	1PE	E	405	-	-	0/13/13/13	0/0/0/0
3	1PE	F	404	-	-	0/13/13/13	0/0/0/0
3	1PE	F	405	-	-	0/13/13/13	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	404	1PE	C26-OH6-C15	2.01	121.87	113.31
3	B	405	1PE	C25-OH5-C14	2.04	122.03	113.31
3	C	405	1PE	C24-OH4-C13	2.10	122.29	113.31
3	E	404	1PE	C25-OH5-C14	2.12	122.37	113.31
3	B	405	1PE	C23-OH3-C22	2.22	122.78	113.31
3	D	404	1PE	C25-OH5-C14	2.22	122.79	113.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	1PE	1	0
3	A	405	1PE	4	0
3	B	404	1PE	6	0
3	B	405	1PE	1	0
3	C	404	1PE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	405	1PE	3	0
3	C	406	1PE	1	0
3	D	404	1PE	1	0
3	E	404	1PE	4	0
3	E	405	1PE	6	0
3	F	404	1PE	3	0
3	F	405	1PE	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	271/289 (93%)	-0.70	1 (0%) 93 95	5, 10, 21, 28	0
1	B	271/289 (93%)	-0.67	0 100 100	4, 11, 23, 38	0
1	C	271/289 (93%)	-0.66	0 100 100	6, 13, 23, 38	0
1	D	271/289 (93%)	-0.70	2 (0%) 89 92	4, 10, 20, 33	0
1	E	271/289 (93%)	-0.61	2 (0%) 89 92	5, 12, 24, 36	0
1	F	271/289 (93%)	-0.63	1 (0%) 93 95	6, 14, 26, 36	0
All	All	1626/1734 (93%)	-0.66	6 (0%) 93 95	4, 12, 24, 38	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	66	GLY	2.5
1	D	114	VAL	2.3
1	D	279	LEU	2.2
1	E	279	LEU	2.2
1	A	279	LEU	2.2
1	E	337	VAL	2.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	1PE	C	404	16/16	0.81	0.28	9.09	33,44,56,62	0
3	1PE	A	404	16/16	0.86	0.27	8.18	28,44,51,54	0
3	1PE	D	405	16/16	0.91	0.32	8.06	31,43,50,54	0
3	1PE	A	406	16/16	0.89	0.27	6.69	31,43,54,57	0
3	1PE	B	405	16/16	0.88	0.29	5.93	37,47,53,57	0
3	1PE	B	404	16/16	0.92	0.24	5.57	35,41,51,54	0
3	1PE	D	404	16/16	0.86	0.25	5.38	31,40,45,50	0
3	1PE	A	405	16/16	0.86	0.24	5.35	30,41,49,51	0
3	1PE	F	404	16/16	0.89	0.20	5.26	33,41,54,62	0
3	1PE	F	405	16/16	0.91	0.28	5.17	30,35,51,52	0
3	1PE	E	405	16/16	0.89	0.30	5.07	33,43,53,56	0
3	1PE	C	406	16/16	0.86	0.21	4.72	36,45,54,64	0
3	1PE	C	405	16/16	0.92	0.24	4.35	26,34,49,52	0
3	1PE	E	404	16/16	0.84	0.19	3.46	34,46,53,57	0
2	CA	C	403	1/1	1.00	0.06	-1.09	5,5,5,5	0
2	CA	F	402	1/1	1.00	0.05	-1.37	6,6,6,6	0
2	CA	D	402	1/1	0.99	0.06	-1.41	4,4,4,4	0
2	CA	A	402	1/1	0.99	0.06	-1.63	5,5,5,5	0
2	CA	B	403	1/1	1.00	0.05	-1.87	4,4,4,4	0
2	CA	E	402	1/1	0.99	0.05	-1.98	3,3,3,3	0
2	CA	A	403	1/1	1.00	0.04	-2.11	3,3,3,3	0
2	CA	B	402	1/1	0.99	0.04	-2.17	6,6,6,6	0
2	CA	F	403	1/1	1.00	0.04	-2.18	8,8,8,8	0
2	CA	E	403	1/1	1.00	0.03	-2.76	5,5,5,5	0
2	CA	D	401	1/1	0.99	0.04	-2.86	11,11,11,11	0
2	CA	C	401	1/1	0.99	0.03	-2.94	13,13,13,13	0
2	CA	C	402	1/1	1.00	0.03	-3.28	8,8,8,8	0
2	CA	D	403	1/1	1.00	0.03	-3.42	6,6,6,6	0
2	CA	E	401	1/1	0.99	0.04	-3.55	11,11,11,11	0
2	CA	A	401	1/1	0.99	0.04	-4.07	12,12,12,12	0
2	CA	B	401	1/1	0.99	0.04	-6.23	13,13,13,13	0
2	CA	F	401	1/1	0.98	0.02	-7.40	12,12,12,12	0

6.5 Other polymers

There are no such residues in this entry.