



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:42 PM GMT

PDB ID : 1LN3  
Title : Structure of Human Phosphatidylcholine Transfer Protein in Complex with  
Palmitoyl-Linoleoyl Phosphatidylcholine (Seleno-Met Protein)  
Authors : Roderick, S.L.; Chan, W.W.; Agate, D.S.; Olsen, L.R.; Vetting, M.W.; Ra-  
jashankar, K.R.; Cohen, D.E.  
Deposited on : 2002-05-02  
Resolution : 2.90 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

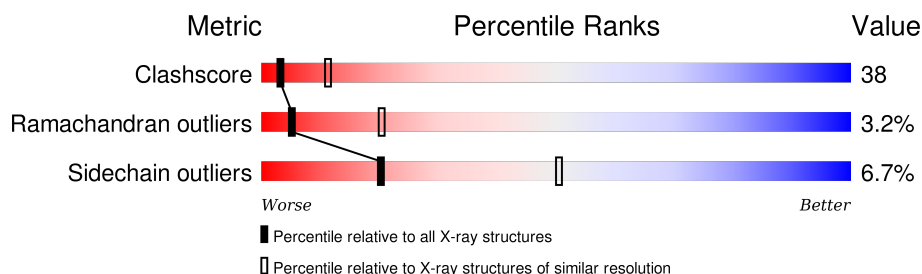
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	
1	B	214	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3513 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.

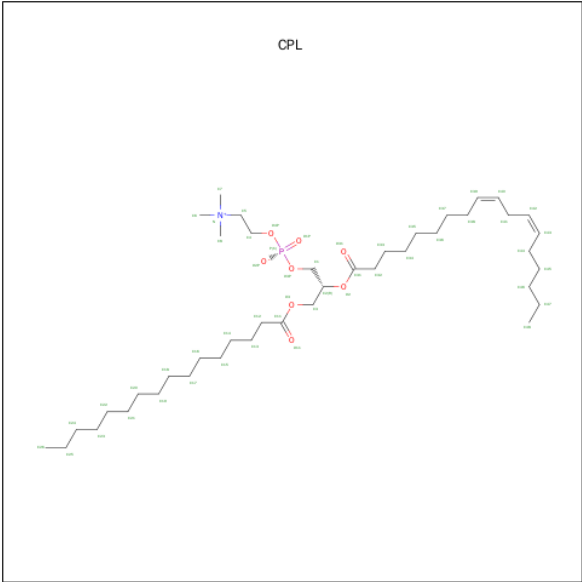
- Molecule 1 is a protein called Phosphatidylcholine transfer protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	Se	0	0	0
			1670	1070	278	312	4	6			
1	B	203	Total	C	N	O	S	Se	0	0	0
			1670	1070	278	312	4	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9UKL6
A	73	MSE	MET	MODIFIED RESIDUE	UNP Q9UKL6
A	109	MSE	MET	MODIFIED RESIDUE	UNP Q9UKL6
A	125	MSE	MET	MODIFIED RESIDUE	UNP Q9UKL6
A	140	MSE	MET	MODIFIED RESIDUE	UNP Q9UKL6
A	173	MSE	MET	MODIFIED RESIDUE	UNP Q9UKL6
A	203	MSE	MET	MODIFIED RESIDUE	UNP Q9UKL6
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9UKL6
B	73	MSE	MET	MODIFIED RESIDUE	UNP Q9UKL6
B	109	MSE	MET	MODIFIED RESIDUE	UNP Q9UKL6
B	125	MSE	MET	MODIFIED RESIDUE	UNP Q9UKL6
B	140	MSE	MET	MODIFIED RESIDUE	UNP Q9UKL6
B	173	MSE	MET	MODIFIED RESIDUE	UNP Q9UKL6
B	203	MSE	MET	MODIFIED RESIDUE	UNP Q9UKL6

- Molecule 2 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: CPL) (formula: C<sub>42</sub>H<sub>80</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 3 is water.

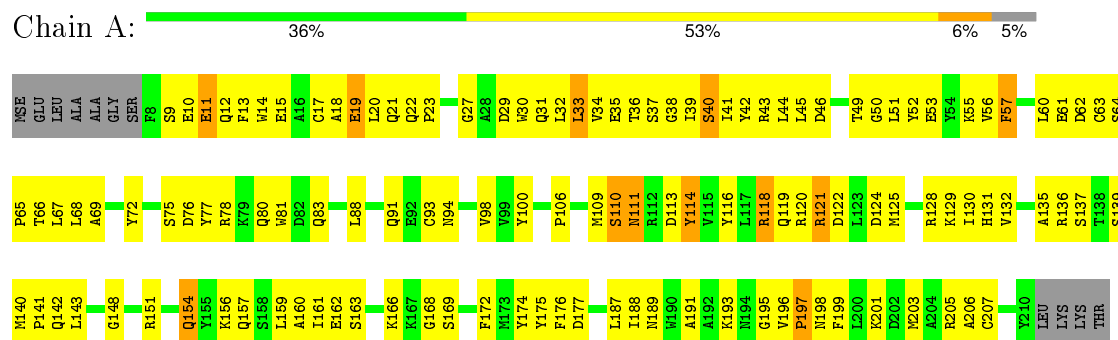
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		
3	B	34	Total	O	0	0
			34	34		

### 3 Residue-property plots

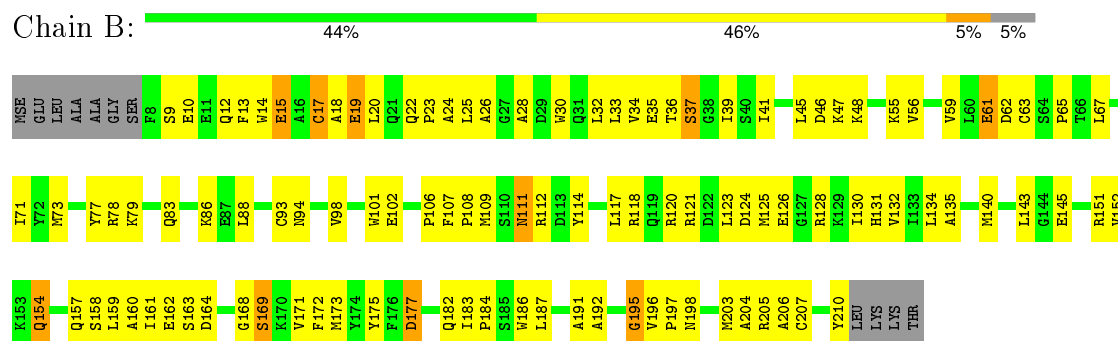
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: Phosphatidylcholine transfer protein



#### • Molecule 1: Phosphatidylcholine transfer protein



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.60 Å   134.60 Å   82.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	27.53 – 2.90	Depositor
% Data completeness (in resolution range)	93.5 (27.53-2.90)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.223 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3513	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CPL

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	0.66	1/1706 (0.1%)	0.82	0/2296
1	B	0.65	1/1706 (0.1%)	0.80	0/2296
All	All	0.65	2/3412 (0.1%)	0.81	0/4592

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	GLU	CD-OE2	7.02	1.33	1.25
1	B	19	GLU	CD-OE2	6.91	1.33	1.25

There are no bond angle outliers.

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	1670	0	1620	142	0
1	B	1670	0	1620	113	0
2	A	52	0	80	13	0
2	B	52	0	80	6	0
3	A	35	0	0	5	0
3	B	34	0	0	1	0
All	All	3513	0	3400	256	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 38.

All (256) 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:109:MSE:HE1	1:A:187:LEU:HD22	1.26	1.17
1:A:65:PRO:HG3	1:A:169:SER:HB3	1.43	1.01
1:B:65:PRO:HG3	1:B:169:SER:HB3	1.51	0.92
1:B:106:PRO:HD2	1:B:109:MSE:HE3	1.55	0.89
1:A:19:GLU:HA	1:A:22:GLN:O	1.73	0.88
1:A:109:MSE:HE1	1:A:187:LEU:CD2	2.04	0.86
1:B:98:VAL:HG11	1:B:140:MSE:HE2	1.56	0.86
1:A:9:SER:HB2	3:A:2023:HOH:O	1.80	0.82
1:A:61:GLU:HA	1:A:168:GLY:HA3	1.62	0.81
1:A:122:ASP:HB3	1:A:129:LYS:HE3	1.61	0.81
1:A:64:SER:HB2	1:A:67:LEU:HG	1.62	0.81
1:A:106:PRO:HD2	1:A:109:MSE:HE3	1.61	0.80
1:B:109:MSE:HE1	1:B:187:LEU:HD22	1.65	0.78
1:B:73:MSE:HE2	1:B:120:ARG:HB3	1.65	0.78
1:B:9:SER:OG	1:B:12:GLN:HG3	1.83	0.78
1:B:22:GLN:HE21	1:B:23:PRO:HD2	1.48	0.77
1:A:159:LEU:HD21	2:A:300:CPL:H482	1.65	0.76
1:A:14:TRP:HZ3	1:A:125:MSE:HB2	1.51	0.76
1:B:24:ALA:O	1:B:25:LEU:HD23	1.86	0.76
1:A:63:CYS:HG	1:A:207:CYS:HG	1.33	0.75
1:A:39:ILE:CD1	1:A:60:LEU:HD21	2.17	0.75
1:A:17:CYS:O	1:A:20:LEU:HB3	1.87	0.74
1:B:111:ASN:O	1:B:112:ARG:HD2	1.88	0.72
1:A:32:LEU:HG	1:A:33:LEU:H	1.55	0.71
1:B:117:LEU:O	1:B:135:ALA:HA	1.90	0.70
1:A:151:ARG:HH11	1:A:151:ARG:HG2	1.55	0.70
1:B:203:MSE:O	1:B:206:ALA:N	2.24	0.70
1:B:114:TYR:CZ	1:B:152:VAL:HG21	2.27	0.70
1:B:134:LEU:CD2	1:B:158:SER:HB2	2.21	0.69
1:A:35:GLU:HA	1:A:39:ILE:O	1.93	0.68
1:B:61:GLU:HA	1:B:168:GLY:HA3	1.76	0.68
1:A:198:ASN:HB2	3:A:2036:HOH:O	1.93	0.67
1:B:32:LEU:HG	1:B:33:LEU:N	2.08	0.67
1:B:56:VAL:HG11	2:B:301:CPL:H43	1.77	0.67
1:A:203:MSE:O	1:A:206:ALA:HB3	1.96	0.66
1:B:35:GLU:HA	1:B:39:ILE:O	1.97	0.65
1:A:110:SER:HB3	1:A:148:GLY:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:HD11	2:A:300:CPL:H482	1.79	0.65
1:A:43:ARG:HD2	1:A:52:TYR:CD2	2.31	0.65
1:B:196:VAL:HB	1:B:197:PRO:HD3	1.79	0.65
1:A:122:ASP:HB3	1:A:129:LYS:CE	2.27	0.64
1:A:159:LEU:HD23	1:A:160:ALA:N	2.13	0.64
1:B:79:LYS:HD3	1:B:88:LEU:O	1.99	0.63
1:B:114:TYR:CE2	1:B:152:VAL:HG11	2.34	0.63
1:B:79:LYS:HG2	1:B:88:LEU:HB3	1.80	0.63
1:B:71:ILE:HD11	1:B:210:TYR:CD2	2.34	0.62
1:B:106:PRO:HD2	1:B:109:MSE:CE	2.29	0.62
1:B:34:VAL:CG2	1:B:192:ALA:HB1	2.30	0.61
1:B:13:PHE:CE2	1:B:121:ARG:HB2	2.35	0.61
1:B:28:ALA:HB3	1:B:30:TRP:CD1	2.35	0.61
1:A:118:ARG:HH11	1:A:118:ARG:HB3	1.64	0.61
1:B:34:VAL:HG22	1:B:192:ALA:HB1	1.82	0.60
1:A:43:ARG:HH12	1:A:188:ILE:HD13	1.66	0.60
1:A:131:HIS:HB2	1:A:161:ILE:HB	1.83	0.60
1:A:39:ILE:HD11	1:A:60:LEU:HD21	1.84	0.60
1:B:93:CYS:O	1:B:94:ASN:HB2	2.03	0.59
1:B:73:MSE:HE2	1:B:120:ARG:CB	2.32	0.59
1:A:36:THR:HG21	1:A:197:PRO:HA	1.84	0.59
1:B:77:TYR:CE2	1:B:210:TYR:CD1	2.90	0.59
1:A:32:LEU:HG	1:A:33:LEU:N	2.16	0.59
1:A:39:ILE:HD12	1:A:60:LEU:HD21	1.85	0.59
1:A:45:LEU:HD11	1:A:50:GLY:HA2	1.85	0.59
1:B:107:PHE:CD1	1:B:108:PRO:HA	2.38	0.58
1:A:33:LEU:HD21	2:A:300:CPL:H252	1.84	0.58
1:B:46:ASP:O	1:B:48:LYS:N	2.36	0.58
1:A:116:TYR:HB2	1:A:136:ARG:O	2.03	0.58
1:B:157:GLN:NE2	1:B:175:TYR:HD1	2.02	0.57
1:A:98:VAL:HG11	1:A:140:MSE:HE2	1.87	0.57
2:B:301:CPL:H342	2:B:301:CPL:H222	1.87	0.57
1:B:77:TYR:CE2	1:B:210:TYR:HD1	2.23	0.57
1:A:130:ILE:O	1:A:132:VAL:HG23	2.04	0.57
1:B:154:GLN:N	1:B:154:GLN:NE2	2.53	0.56
1:B:67:LEU:HD23	1:B:71:ILE:HD13	1.87	0.56
1:B:20:LEU:HD21	1:B:162:GLU:HG3	1.86	0.56
1:B:203:MSE:O	1:B:206:ALA:HB3	2.05	0.56
1:A:91:GLN:NE2	1:A:140:MSE:HE1	2.22	0.55
1:A:151:ARG:HG2	1:A:151:ARG:NH1	2.19	0.55
1:B:63:CYS:HG	1:B:207:CYS:HG	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:HD12	1:A:51:LEU:O	2.07	0.55
1:B:17:CYS:SG	1:B:123:LEU:HD12	2.47	0.55
1:B:65:PRO:HG3	1:B:162:GLU:O	2.07	0.54
1:A:34:VAL:O	1:A:40:SER:HA	2.07	0.54
1:A:29:ASP:O	1:A:29:ASP:OD1	2.25	0.54
1:A:196:VAL:HG21	2:A:300:CPL:H263	1.89	0.54
1:A:23:PRO:HB3	1:A:57:PHE:CE2	2.43	0.54
1:A:19:GLU:HB2	1:A:172:PHE:CZ	2.43	0.54
1:B:32:LEU:HG	1:B:33:LEU:H	1.72	0.54
1:B:106:PRO:O	1:B:109:MSE:HB2	2.08	0.54
1:A:125:MSE:O	1:A:128:ARG:HB2	2.08	0.54
1:B:10:GLU:HG3	1:B:121:ARG:HH12	1.73	0.54
1:B:182:GLN:C	1:B:183:ILE:HD12	2.29	0.53
1:A:45:LEU:HD13	1:A:52:TYR:CE1	2.43	0.53
1:A:17:CYS:SG	1:A:132:VAL:HG21	2.48	0.53
1:A:13:PHE:CE2	1:A:121:ARG:HG3	2.44	0.53
1:A:9:SER:O	1:A:13:PHE:HD1	1.92	0.53
1:A:39:ILE:HD11	1:A:60:LEU:CD2	2.38	0.53
1:A:118:ARG:HH11	1:A:118:ARG:CG	2.22	0.53
1:A:14:TRP:CZ3	1:A:125:MSE:HB2	2.39	0.52
1:A:30:TRP:CD1	1:A:44:LEU:HD13	2.44	0.52
1:A:106:PRO:HD2	1:A:109:MSE:CE	2.37	0.52
1:B:159:LEU:HD13	1:B:173:MSE:HE3	1.91	0.52
1:A:36:THR:O	1:A:39:ILE:N	2.43	0.52
1:A:198:ASN:HD22	1:A:198:ASN:N	2.06	0.52
1:B:14:TRP:HA	1:B:17:CYS:HB2	1.91	0.52
1:B:41:ILE:HD12	2:B:301:CPL:H263	1.92	0.51
1:B:106:PRO:CD	1:B:109:MSE:HE3	2.35	0.51
1:A:22:GLN:NE2	1:A:23:PRO:N	2.59	0.51
1:B:154:GLN:N	1:B:154:GLN:HE21	2.09	0.51
1:A:93:CYS:O	1:A:94:ASN:HB2	2.10	0.51
1:B:126:GLU:OE2	1:B:128:ARG:NH2	2.43	0.51
1:B:61:GLU:O	1:B:62:ASP:HB2	2.10	0.51
1:B:17:CYS:O	1:B:20:LEU:HB3	2.11	0.51
1:A:159:LEU:HD21	2:A:300:CPL:C48	2.36	0.51
1:A:30:TRP:CZ3	1:A:55:LYS:HB2	2.46	0.51
1:B:19:GLU:HB2	1:B:172:PHE:CE2	2.46	0.51
1:B:14:TRP:CE3	1:B:125:MSE:HE3	2.46	0.50
1:B:88:LEU:HD13	1:B:101:TRP:CE3	2.46	0.50
1:A:33:LEU:CD2	2:A:300:CPL:H252	2.42	0.50
1:B:198:ASN:HD22	1:B:198:ASN:N	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HD21	1:A:35:GLU:HG3	1.92	0.50
1:A:65:PRO:CG	1:A:169:SER:HB3	2.29	0.50
1:B:161:ILE:CD1	1:B:171:VAL:HG12	2.42	0.50
1:B:19:GLU:HA	1:B:22:GLN:O	2.11	0.50
1:A:29:ASP:OD1	1:A:29:ASP:C	2.50	0.50
1:A:109:MSE:CE	1:A:187:LEU:HD22	2.19	0.49
1:B:34:VAL:HG12	1:B:35:GLU:N	2.28	0.49
1:A:77:TYR:O	1:A:80:GLN:HB3	2.11	0.49
1:A:41:ILE:HG13	1:A:56:VAL:HG22	1.93	0.49
1:B:36:THR:HG22	1:B:37:SER:N	2.28	0.49
1:B:65:PRO:HG2	1:B:163:SER:HA	1.95	0.49
1:A:78:ARG:HB2	3:A:2020:HOH:O	2.11	0.49
1:A:20:LEU:HA	1:A:172:PHE:HB2	1.95	0.49
1:A:43:ARG:HA	1:A:53:GLU:O	2.13	0.49
1:A:191:ALA:HB1	2:A:300:CPL:H242	1.95	0.48
1:B:125:MSE:O	1:B:128:ARG:CB	2.61	0.48
1:A:34:VAL:HG12	1:A:35:GLU:N	2.28	0.48
1:A:161:ILE:HG22	1:A:162:GLU:N	2.28	0.48
1:B:26:ALA:N	3:B:2061:HOH:O	2.29	0.48
1:A:64:SER:HB2	1:A:67:LEU:CG	2.39	0.48
1:B:114:TYR:CE1	1:B:152:VAL:HG21	2.48	0.48
1:B:56:VAL:HG11	2:B:301:CPL:C43	2.43	0.48
1:A:31:GLN:O	1:A:42:TYR:HA	2.14	0.48
1:B:65:PRO:HA	1:B:161:ILE:HG21	1.95	0.48
1:A:30:TRP:CZ2	1:A:55:LYS:HD2	2.49	0.48
1:A:46:ASP:OD2	1:A:49:THR:HG23	2.14	0.48
1:A:36:THR:O	1:A:38:GLY:N	2.47	0.47
1:B:79:LYS:CG	1:B:88:LEU:HB3	2.44	0.47
1:A:125:MSE:SE	1:A:128:ARG:HH21	2.47	0.47
1:A:65:PRO:HG2	1:A:163:SER:HA	1.96	0.47
1:B:134:LEU:HD23	1:B:158:SER:HB2	1.93	0.47
1:B:162:GLU:O	1:B:169:SER:HB3	2.15	0.47
1:B:126:GLU:C	1:B:128:ARG:H	2.17	0.47
1:A:39:ILE:CD1	1:A:60:LEU:CD2	2.91	0.47
1:A:157:GLN:NE2	1:A:175:TYR:HD1	2.13	0.47
1:B:71:ILE:CD1	1:B:71:ILE:N	2.77	0.47
1:A:22:GLN:NE2	1:A:23:PRO:O	2.48	0.46
1:B:56:VAL:O	1:B:172:PHE:HA	2.15	0.46
1:A:12:GLN:HA	1:A:15:GLU:OE1	2.16	0.46
1:A:196:VAL:O	1:A:197:PRO:C	2.54	0.46
1:A:118:ARG:HH11	1:A:118:ARG:CB	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ASP:OD2	1:A:177:ASP:C	2.54	0.46
1:B:161:ILE:HD13	1:B:171:VAL:HG12	1.96	0.46
1:A:64:SER:HB3	1:A:66:THR:HG22	1.97	0.46
1:B:65:PRO:CG	1:B:163:SER:HA	2.46	0.46
1:A:13:PHE:CD2	1:A:121:ARG:HB2	2.51	0.46
1:A:64:SER:CB	1:A:67:LEU:HG	2.42	0.46
1:A:88:LEU:HD12	1:A:100:TYR:O	2.15	0.46
1:B:184:PRO:CB	1:B:186:TRP:CD1	2.99	0.46
1:A:159:LEU:CD2	2:A:300:CPL:H482	2.42	0.46
1:A:110:SER:C	1:A:111:ASN:O	2.54	0.46
1:B:67:LEU:HD23	1:B:71:ILE:CD1	2.46	0.46
1:A:175:TYR:CD2	1:A:176:PHE:N	2.84	0.46
1:B:20:LEU:HD22	1:B:160:ALA:HB1	1.99	0.45
1:A:64:SER:O	1:A:67:LEU:N	2.50	0.45
1:B:78:ARG:CZ	1:B:101:TRP:HH2	2.29	0.45
1:A:154:GLN:NE2	3:A:2001:HOH:O	2.48	0.45
1:A:75:SER:O	1:A:76:ASP:C	2.55	0.45
1:B:59:VAL:HG13	1:B:169:SER:O	2.17	0.45
1:B:160:ALA:O	1:B:171:VAL:HA	2.17	0.45
1:A:66:THR:HG23	1:A:67:LEU:N	2.31	0.45
1:A:61:GLU:HA	1:A:168:GLY:CA	2.41	0.45
1:B:15:GLU:O	1:B:18:ALA:HB3	2.17	0.45
1:A:113:ASP:OD2	1:A:151:ARG:HA	2.17	0.45
1:A:198:ASN:O	1:A:201:LYS:HB3	2.17	0.45
1:A:45:LEU:HB2	1:A:52:TYR:CZ	2.52	0.45
1:B:71:ILE:HD12	1:B:71:ILE:N	2.31	0.45
1:B:86:LYS:HB3	1:B:102:GLU:HB3	1.98	0.45
1:A:57:PHE:N	1:A:57:PHE:CD1	2.84	0.44
1:B:67:LEU:O	1:B:71:ILE:HD13	2.16	0.44
1:B:107:PHE:CG	1:B:108:PRO:HA	2.52	0.44
1:A:196:VAL:HB	1:A:197:PRO:HD3	2.00	0.44
1:B:203:MSE:O	1:B:204:ALA:C	2.55	0.44
1:A:114:TYR:CD1	1:A:114:TYR:N	2.86	0.44
1:A:33:LEU:C	1:A:34:VAL:HG23	2.38	0.44
1:A:177:ASP:OD2	1:A:177:ASP:O	2.35	0.44
1:B:131:HIS:HB2	1:B:161:ILE:HB	2.00	0.44
1:B:41:ILE:HD11	2:B:301:CPL:H42	1.98	0.44
1:B:59:VAL:HG11	1:B:164:ASP:HB2	1.98	0.44
1:B:71:ILE:HD11	1:B:210:TYR:CE2	2.52	0.44
1:A:12:GLN:O	1:A:13:PHE:C	2.54	0.44
1:A:68:LEU:HD21	2:A:300:CPL:H483	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:THR:O	1:B:37:SER:C	2.54	0.44
1:A:198:ASN:N	1:A:198:ASN:ND2	2.66	0.44
1:A:45:LEU:HG	1:A:45:LEU:O	2.13	0.44
1:B:86:LYS:HG2	1:B:102:GLU:OE2	2.18	0.44
1:B:145:GLU:HG2	1:B:151:ARG:CB	2.47	0.44
1:A:11:GLU:HG3	3:A:2023:HOH:O	2.17	0.43
1:A:36:THR:C	1:A:38:GLY:N	2.71	0.43
1:A:49:THR:HB	1:A:51:LEU:HG	2.00	0.43
1:A:10:GLU:CD	1:A:121:ARG:HH22	2.20	0.43
1:A:140:MSE:HA	1:A:141:PRO:HD3	1.89	0.43
1:A:34:VAL:HG21	2:A:300:CPL:H261	2.00	0.43
1:A:78:ARG:HA	1:A:81:TRP:NE1	2.33	0.43
1:A:13:PHE:HZ	1:A:119:GLN:NE2	2.16	0.43
1:A:69:ALA:HB1	1:A:120:ARG:NH1	2.34	0.43
1:B:184:PRO:HB2	1:B:186:TRP:CD1	2.54	0.43
1:A:139:SER:O	1:A:140:MSE:HG2	2.19	0.43
1:A:30:TRP:CH2	1:A:55:LYS:HD2	2.53	0.43
1:B:34:VAL:CG1	1:B:35:GLU:N	2.82	0.42
1:B:175:TYR:HE2	1:B:177:ASP:OD2	2.02	0.42
1:B:36:THR:CG2	1:B:37:SER:N	2.82	0.42
1:A:157:GLN:HA	1:A:174:TYR:O	2.19	0.42
1:A:65:PRO:CG	1:A:163:SER:HA	2.49	0.42
1:B:114:TYR:CG	2:B:301:CPL:HC71	2.54	0.42
1:A:199:PHE:CZ	2:A:300:CPL:HC32	2.55	0.42
1:B:65:PRO:HB3	1:B:161:ILE:HG22	2.01	0.42
1:B:184:PRO:HB3	1:B:186:TRP:CD1	2.55	0.42
1:A:36:THR:C	1:A:38:GLY:H	2.23	0.42
1:B:24:ALA:O	1:B:55:LYS:NZ	2.50	0.41
1:A:159:LEU:HD11	2:A:300:CPL:H461	2.02	0.41
1:A:45:LEU:HB2	1:A:52:TYR:CE2	2.55	0.41
1:A:33:LEU:O	1:A:34:VAL:CG2	2.68	0.41
1:A:38:GLY:O	1:A:39:ILE:HG13	2.21	0.41
1:A:135:ALA:O	1:A:156:LYS:HA	2.21	0.41
1:B:22:GLN:HA	1:B:23:PRO:HD3	1.93	0.41
1:A:72:TYR:CE1	1:A:159:LEU:HD12	2.55	0.41
1:B:45:LEU:HD12	1:B:46:ASP:H	1.84	0.41
1:B:191:ALA:HA	1:B:195:GLY:HA3	2.03	0.41
1:B:158:SER:O	1:B:173:MSE:HA	2.19	0.41
1:B:196:VAL:CB	1:B:197:PRO:HD3	2.49	0.41
1:B:184:PRO:O	1:B:187:LEU:N	2.49	0.41
1:A:189:ASN:O	1:A:193:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLU:N	1:A:61:GLU:OE1	2.42	0.41
1:A:21:GLN:HE22	1:A:128:ARG:HH12	1.69	0.40
1:B:36:THR:O	1:B:39:ILE:N	2.54	0.40
1:A:131:HIS:CD2	1:A:131:HIS:H	2.39	0.40
1:B:157:GLN:HE21	1:B:175:TYR:HD1	1.64	0.40
1:A:33:LEU:HB3	1:A:41:ILE:O	2.20	0.40
1:A:21:GLN:NE2	1:A:128:ARG:HH22	2.19	0.40
1:A:61:GLU:O	1:A:62:ASP:CB	2.68	0.40
1:B:36:THR:O	1:B:39:ILE:HB	2.22	0.40
1:B:39:ILE:HA	1:B:39:ILE:HD13	1.83	0.40
1:B:130:ILE:HG22	1:B:132:VAL:HG23	2.03	0.40
1:A:159:LEU:HD11	2:A:300:CPL:C48	2.51	0.40
1:A:35:GLU:HG2	1:A:40:SER:HB3	2.04	0.40
1:A:63:CYS:O	1:A:64:SER:C	2.58	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	201/214 (94%)	172 (86%)	20 (10%)	9 (4%)	3	12
1	B	201/214 (94%)	183 (91%)	14 (7%)	4 (2%)	9	33
All	All	402/428 (94%)	355 (88%)	34 (8%)	13 (3%)	5	20

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	SER
1	B	47	LYS
1	A	27	GLY
1	A	83	GLN

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Mol	Chain	Res	Type
1	B	111	ASN
1	A	11	GLU
1	A	33	LEU
1	A	18	ALA
1	A	111	ASN
1	A	166	LYS
1	B	37	SER
1	A	195	GLY
1	B	195	GLY

### 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	178/179 (99%)	165 (93%)	13 (7%)	17	45
1	B	178/179 (99%)	167 (94%)	11 (6%)	23	55
All	All	356/358 (99%)	332 (93%)	24 (7%)	20	50

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	A	57	PHE
1	A	110	SER
1	A	114	TYR
1	A	118	ARG
1	A	121	ARG
1	A	124	ASP
1	A	137	SER
1	A	142	GLN
1	A	143	LEU
1	A	154	GLN
1	A	197	PRO
1	A	205	ARG
1	B	15	GLU

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Mol	Chain	Res	Type
1	B	17	CYS
1	B	61	GLU
1	B	83	GLN
1	B	118	ARG
1	B	124	ASP
1	B	143	LEU
1	B	154	GLN
1	B	169	SER
1	B	177	ASP
1	B	205	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	22	GLN
1	A	80	GLN
1	A	91	GLN
1	A	94	ASN
1	A	154	GLN
1	A	157	GLN
1	A	194	ASN
1	A	198	ASN
1	B	21	GLN
1	B	22	GLN
1	B	80	GLN
1	B	83	GLN
1	B	94	ASN
1	B	154	GLN
1	B	198	ASN

### 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

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	$\# Z  > 2$
2	CPL	A	300	-	51,51,51	1.41	3 (5%)	55,59,59	1.03	5 (9%)
2	CPL	B	301	-	51,51,51	1.43	3 (5%)	55,59,59	1.14	5 (9%)

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
2	CPL	A	300	-	-	0/55/55/55	0/0/0/0
2	CPL	B	301	-	-	0/55/55/55	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	CPL	C1-C2	2.64	1.58	1.50
2	B	301	CPL	C1-C2	3.02	1.59	1.50
2	A	300	CPL	O2-C31	5.23	1.50	1.34
2	B	301	CPL	O2-C31	5.43	1.50	1.34
2	B	301	CPL	O3-C11	5.84	1.50	1.33
2	A	300	CPL	O3-C11	5.99	1.51	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	CPL	P-O4P-C4	-3.29	102.69	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	CPL	P-O4P-C4	-2.87	105.11	121.50
2	B	301	CPL	O3-C3-C2	-2.36	102.34	108.69
2	A	300	CPL	O3-C3-C2	-2.32	102.43	108.69
2	A	300	CPL	O3-C11-C12	2.02	118.05	111.90
2	B	301	CPL	O3-C11-C12	2.38	119.15	111.90
2	A	300	CPL	O2-C31-C32	2.94	117.91	111.53
2	A	300	CPL	C2-O2-C31	3.31	125.83	117.89
2	B	301	CPL	C2-O2-C31	3.73	126.84	117.89
2	B	301	CPL	O2-C31-C32	3.85	119.90	111.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	CPL	13	0
2	B	301	CPL	6	0

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.