



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:14 pm BST

PDB ID : 6KR4
Title : Crystal structure of the liprin-alpha3_SAM123/LAR_D1D2 complex
Authors : Xie, X.; Liang, M.; Luo, L.; Wei, Z.
Deposited on : 2019-08-20
Resolution : 2.85 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

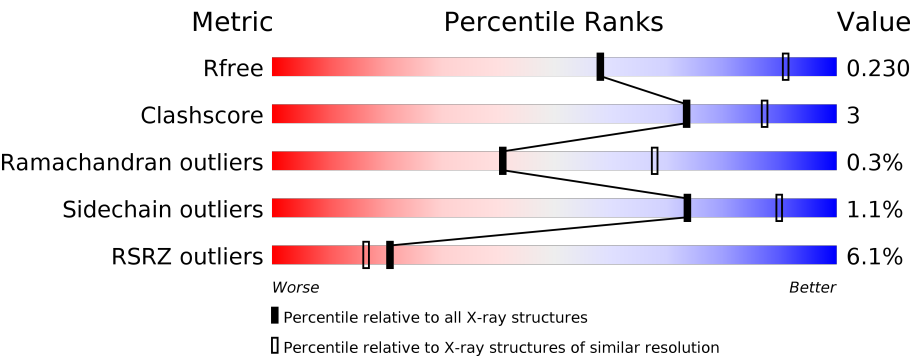
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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.



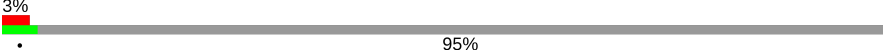

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 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	580	<div><div></div><div>93%7%</div></div>
1	B	580	<div><div>2%</div><div>89%9%</div></div>
1	C	580	<div><div>%</div><div>90%9%</div></div>
1	D	580	<div><div>7%</div><div>87%11%</div></div>
2	E	325	<div><div>5%</div><div>72%10%18%</div></div>
2	F	325	<div><div>16%</div><div>68%13%19%</div></div>

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Mol	Chain	Length	Quality of chain
2	G	325	 3% 95%
2	H	325	 15% 62% 8% 29%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24833 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 Receptor-type tyrosine-protein phosphatase F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	575	Total	C	N	O	S	0	6	0
			4669	2956	818	861	34			
1	B	571	Total	C	N	O	S	0	2	0
			4597	2910	799	855	33			
1	C	575	Total	C	N	O	S	0	4	0
			4638	2933	812	859	34			
1	D	568	Total	C	N	O	S	0	3	0
			4566	2896	791	846	33			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1328	HIS	-	expression tag	UNP P10586
A	1329	MET	-	expression tag	UNP P10586
A	1330	GLY	-	expression tag	UNP P10586
A	1331	SER	-	expression tag	UNP P10586
B	1328	HIS	-	expression tag	UNP P10586
B	1329	MET	-	expression tag	UNP P10586
B	1330	GLY	-	expression tag	UNP P10586
B	1331	SER	-	expression tag	UNP P10586
C	1328	HIS	-	expression tag	UNP P10586
C	1329	MET	-	expression tag	UNP P10586
C	1330	GLY	-	expression tag	UNP P10586
C	1331	SER	-	expression tag	UNP P10586
D	1328	HIS	-	expression tag	UNP P10586
D	1329	MET	-	expression tag	UNP P10586
D	1330	GLY	-	expression tag	UNP P10586
D	1331	SER	-	expression tag	UNP P10586

- Molecule 2 is a protein called Liprin-alpha-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	266	Total	C	N	O	S	0	0	0
			2111	1332	380	386	13			
2	F	264	Total	C	N	O	S	0	0	0
			2091	1315	372	391	13			
2	H	231	Total	C	N	O	S	0	0	0
			1789	1135	317	325	12			
2	G	15	Total	C	N	O	S	0	0	0
			108	71	18	18	1			

There are 16 discrepancies between the modelled and reference sequences:

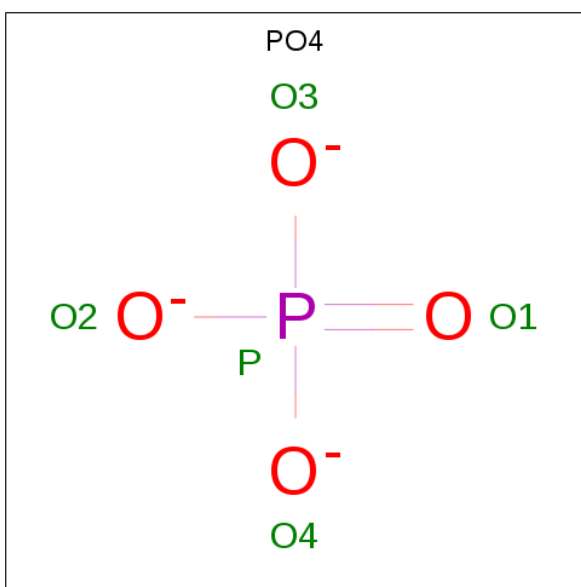
Chain	Residue	Modelled	Actual	Comment	Reference
E	802	GLY	-	expression tag	UNP P60469
E	803	PRO	-	expression tag	UNP P60469
E	804	GLY	-	expression tag	UNP P60469
E	805	SER	-	expression tag	UNP P60469
F	802	GLY	-	expression tag	UNP P60469
F	803	PRO	-	expression tag	UNP P60469
F	804	GLY	-	expression tag	UNP P60469
F	805	SER	-	expression tag	UNP P60469
H	802	GLY	-	expression tag	UNP P60469
H	803	PRO	-	expression tag	UNP P60469
H	804	GLY	-	expression tag	UNP P60469
H	805	SER	-	expression tag	UNP P60469
G	802	GLY	-	expression tag	UNP P60469
G	803	PRO	-	expression tag	UNP P60469
G	804	GLY	-	expression tag	UNP P60469
G	805	SER	-	expression tag	UNP P60469

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	B	1	Total	C	O	0	0
			13	8	5		
3	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



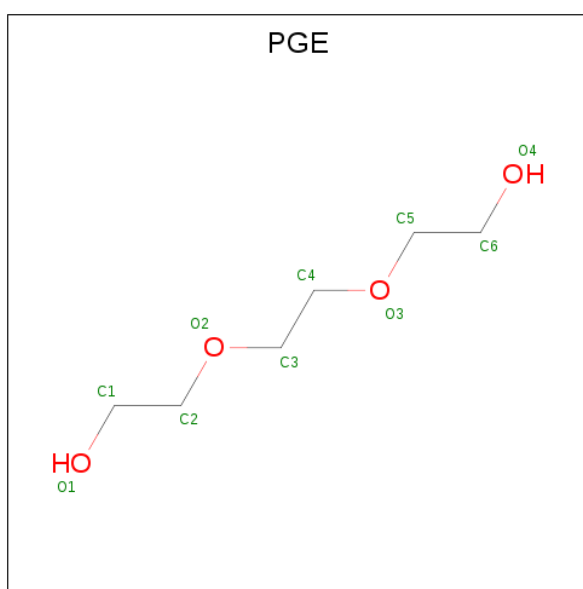
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

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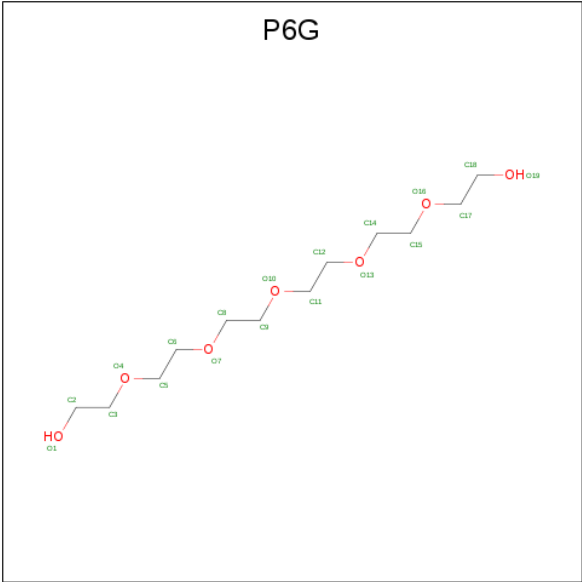
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



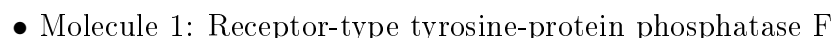
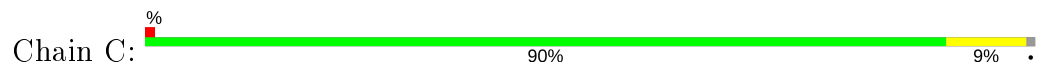
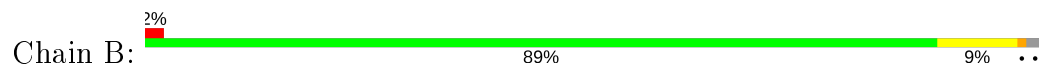
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			19	12	7		

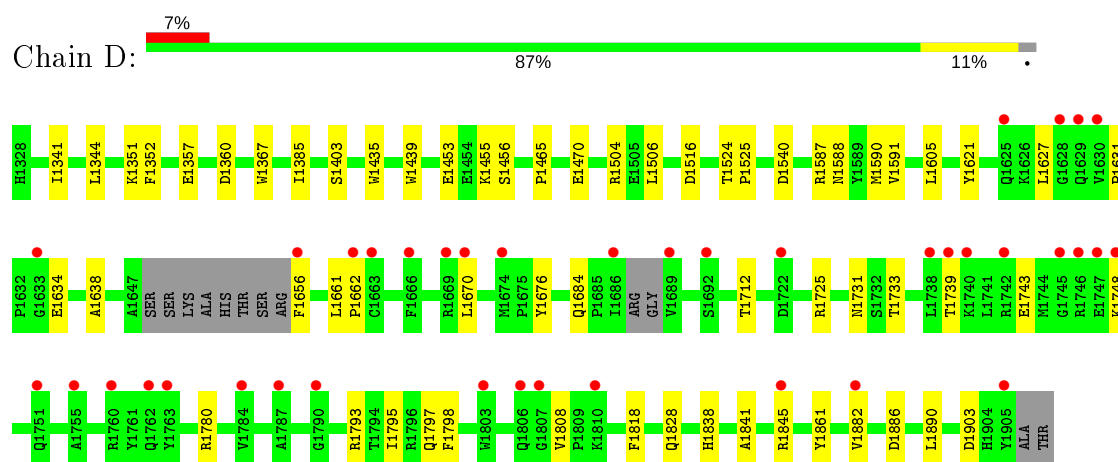
- Molecule 7 is water.

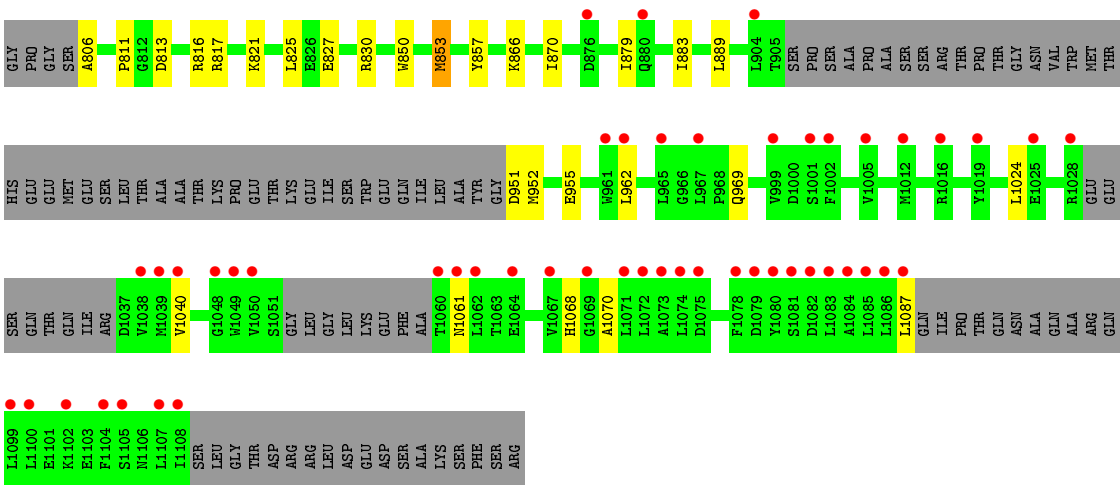
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	94	Total	O	0	0
			94	94		
7	B	4	Total	O	0	0
			4	4		
7	C	43	Total	O	0	0
			43	43		
7	D	16	Total	O	0	0
			16	16		
7	E	3	Total	O	0	0
			3	3		
7	F	1	Total	O	0	0
			1	1		

These plots are drawn for all protein, RNA and DNA 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.

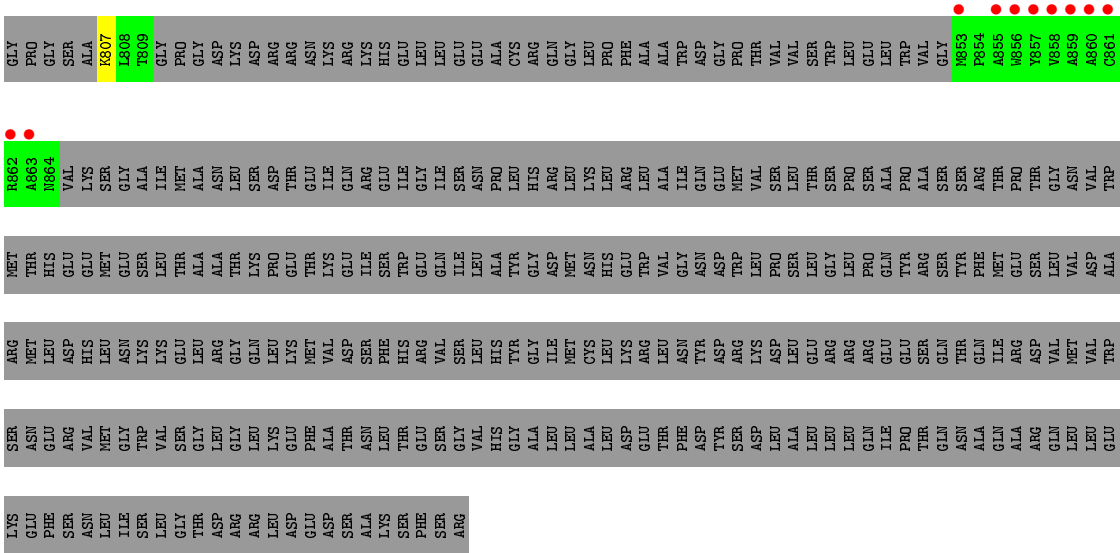
- Chain A:  93% 7%







● Molecule 2: Liprin-alpha-3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	250.38 Å 147.68 Å 143.97 Å 90.00° 103.85° 90.00°	Depositor
Resolution (Å)	42.17 – 2.85 45.30 – 2.84	Depositor EDS
% Data completeness (in resolution range)	98.7 (42.17-2.85) 91.1 (45.30-2.84)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.86 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.192 , 0.230 0.195 , 0.230	Depositor DCC
R_{free} test set	2000 reflections (1.69%)	wwPDB-VP
Wilson B-factor (Å ²)	60.1	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24833	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, PGE, PG4, P6G

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	0.51	0/4795	0.55	0/6494
1	B	0.34	0/4709	0.47	0/6383
1	C	0.43	0/4756	0.51	0/6444
1	D	0.36	0/4680	0.49	0/6345
2	E	0.34	0/2151	0.47	0/2908
2	F	0.28	0/2132	0.43	0/2886
2	G	0.20	0/110	0.34	0/150
2	H	0.27	0/1821	0.42	0/2463
All	All	0.39	0/25154	0.49	0/34073

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4669	0	4572	17	0
1	B	4597	0	4475	29	0
1	C	4638	0	4526	28	0
1	D	4566	0	4441	31	0
2	E	2111	0	2091	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2091	0	2038	23	0
2	G	108	0	99	1	0
2	H	1789	0	1747	17	0
3	A	13	0	18	1	0
3	B	13	0	18	1	0
3	C	13	0	18	2	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	1	0
5	C	10	0	14	0	0
5	D	10	0	14	1	0
6	D	19	0	26	0	0
7	A	94	0	0	0	0
7	B	4	0	0	0	0
7	C	43	0	0	1	0
7	D	16	0	0	0	0
7	E	3	0	0	0	0
7	F	1	0	0	0	0
All	All	24833	0	24097	162	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 3.

All (162) 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:1540:ASP:HB2	5:D:2002:PGE:H62	1.62	0.79
2:E:1027:ARG:HG2	2:E:1040:VAL:HG21	1.66	0.76
2:F:1028:ARG:HG3	2:F:1040:VAL:HG12	1.67	0.75
2:E:1028:ARG:HG3	2:E:1040:VAL:HG12	1.69	0.74
2:F:827:GLU:OE2	2:F:830:ARG:NH2	2.21	0.73
1:C:1826:LYS:HD2	1:C:1835:ILE:HD11	1.69	0.73
1:D:1439:TRP:O	1:D:1504:ARG:NH1	2.26	0.68
1:B:1754:PRO:HB2	1:B:1757:ARG:O	1.94	0.68
2:F:876:ASP:OD1	2:F:895:ARG:NH2	2.27	0.68
1:C:1367:TRP:HB3	1:C:1385:ILE:HD13	1.77	0.65
1:A:1344:LEU:HD23	1:A:1351:LYS:HB3	1.79	0.65
1:A:1857:GLU:HB2	3:A:2001:PG4:H51	1.78	0.65
1:A:1556:GLY:O	1:A:1560:VAL:HG12	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:864:ASN:ND2	2:F:882:GLU:O	2.28	0.64
1:A:1439:TRP:O	1:A:1504:ARG:NH1	2.31	0.64
1:A:1684:GLN:O	1:A:1725:ARG:NH2	2.31	0.63
2:E:992:LEU:HD22	2:E:998:MET:HE2	1.81	0.63
1:B:1439:TRP:O	1:B:1504:ARG:NH1	2.33	0.61
2:H:827:GLU:OE1	2:H:830:ARG:NH2	2.35	0.60
2:E:1038:VAL:HA	2:E:1041:TRP:CD1	2.37	0.59
2:F:1024:LEU:HD12	2:F:1040:VAL:HG13	1.84	0.59
1:C:1657:ILE:HG22	1:C:1659:ALA:H	1.68	0.58
1:C:1886:ASP:OD1	1:C:1886:ASP:N	2.36	0.58
1:B:1718:GLU:N	1:B:1718:GLU:OE1	2.36	0.58
2:H:811:PRO:HA	2:H:816:ARG:HG2	1.84	0.58
2:H:879:ILE:HG23	2:H:883:ILE:HD12	1.85	0.57
1:A:1718:GLU:N	1:A:1718:GLU:OE1	2.36	0.57
1:B:1826:LYS:HD2	1:B:1835:ILE:HD11	1.84	0.57
1:D:1627:LEU:HA	1:D:1638:ALA:HB3	1.85	0.56
2:E:827:GLU:OE1	2:E:830:ARG:NH2	2.40	0.55
1:C:1872:LYS:O	1:C:1876:THR:HG23	2.07	0.55
1:A:1886:ASP:OD1	1:A:1886:ASP:N	2.40	0.55
2:E:1024:LEU:HD12	2:E:1040:VAL:HG13	1.88	0.55
2:E:970:TYR:CE1	2:E:998:MET:HG2	2.42	0.55
2:H:1024:LEU:HD12	2:H:1040:VAL:HG13	1.87	0.55
1:C:1556:GLY:O	1:C:1560:VAL:HG12	2.07	0.54
1:D:1712:THR:HG23	1:D:1838:HIS:HB3	1.89	0.54
1:C:1435:TRP:HZ3	1:C:1506:LEU:HD22	1.73	0.54
2:H:1061:ASN:ND2	2:H:1087:LEU:O	2.31	0.54
2:F:1091:THR:HA	2:F:1097:ARG:HE	1.72	0.53
1:B:1556:GLY:O	1:B:1560:VAL:HG12	2.09	0.53
1:B:1403:SER:O	1:B:1436:ARG:NH2	2.42	0.53
1:B:1446:VAL:HG23	1:B:1506:LEU:HD11	1.90	0.53
1:B:1415:ARG:NH2	1:D:1360:ASP:OD2	2.42	0.53
1:D:1341:ILE:HD12	1:D:1605:LEU:HD22	1.92	0.52
2:E:998:MET:HE3	2:E:1004:ARG:HG2	1.91	0.52
1:A:1781:GLU:HG2	1:A:1796[B]:ARG:HG2	1.90	0.52
2:F:820:ARG:O	2:F:824:LEU:HD13	2.10	0.51
2:E:824:LEU:HD12	2:E:849:LEU:HD22	1.91	0.51
2:F:1068:HIS:CE1	2:F:1070:ALA:HB3	2.46	0.51
1:D:1587:ARG:O	1:D:1590:MET:HG2	2.11	0.51
2:H:866:LYS:H	2:H:870:ILE:HD12	1.76	0.51
1:C:1700:LEU:HD23	1:C:1874:LEU:HD22	1.92	0.51
1:D:1435:TRP:HZ3	1:D:1506:LEU:HD22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1075:ASP:O	2:F:1114:ARG:NH2	2.43	0.50
2:H:813:ASP:O	2:H:817:ARG:HG3	2.12	0.50
1:C:1857:GLU:HB2	3:C:2001:PG4:H51	1.92	0.50
1:C:1718:GLU:N	1:C:1718:GLU:OE1	2.44	0.50
1:D:1465:PRO:HB3	1:D:1470:GLU:HG3	1.94	0.49
1:C:1534:LYS:NZ	1:C:1566:GLU:OE2	2.30	0.49
1:B:1758:SER:OG	1:B:1767:ASP:OD1	2.24	0.49
1:C:1367:TRP:CB	1:C:1385:ILE:HD13	2.43	0.48
1:D:1903:ASP:OD2	2:H:816:ARG:NH2	2.45	0.48
2:H:1068:HIS:CE1	2:H:1070:ALA:HB3	2.48	0.48
1:A:1435:TRP:HZ3	1:A:1506:LEU:HD22	1.79	0.48
1:A:1400:VAL:O	1:A:1403:SER:OG	2.28	0.48
1:B:1700:LEU:HD23	1:B:1874:LEU:HD22	1.95	0.48
1:B:1624:ILE:HD12	1:B:1896:LEU:HD22	1.94	0.48
1:C:1627:LEU:HA	1:C:1638:ALA:HB3	1.96	0.48
1:D:1808:VAL:HB	1:D:1890:LEU:HD22	1.94	0.48
1:B:1886:ASP:OD1	1:B:1886:ASP:N	2.47	0.48
2:F:866:LYS:H	2:F:870:ILE:HD12	1.78	0.48
1:C:1733:THR:HA	1:C:1795:ILE:HG13	1.96	0.47
1:C:1863:GLY:HA3	2:G:807:LYS:HD3	1.96	0.47
1:C:1446:VAL:HG23	1:C:1506:LEU:HD11	1.96	0.47
2:E:951:ASP:OD1	2:E:952:MET:N	2.43	0.47
1:B:1684:GLN:O	1:B:1725:ARG:NH2	2.47	0.47
1:D:1798:PHE:HB3	1:D:1818:PHE:CE1	2.49	0.47
2:F:968:PRO:HD2	2:F:1064:GLU:HG2	1.97	0.46
1:D:1684:GLN:O	1:D:1725:ARG:NH2	2.48	0.46
1:D:1524:THR:HB	1:D:1525:PRO:HD3	1.97	0.46
1:A:1595:ASP:OD1	1:A:1596:GLN:N	2.49	0.46
1:C:1341:ILE:HD12	1:C:1605:LEU:HD22	1.97	0.46
1:A:1341:ILE:HD12	1:A:1605:LEU:HD22	1.98	0.46
2:E:1023:ASP:OD1	2:E:1026:ARG:NH1	2.49	0.46
2:E:1045:ARG:NH1	4:E:1201:PO4:O3	2.49	0.46
1:B:1567:ARG:HG2	1:B:1573:THR:O	2.16	0.45
1:C:1684:GLN:O	1:C:1725:ARG:NH2	2.45	0.45
2:F:1043:ASN:ND2	2:F:1067:VAL:O	2.37	0.45
1:B:1480:LEU:HD11	1:B:1494:ALA:HB2	1.98	0.45
1:D:1455:LYS:HG3	1:D:1516:ASP:OD2	2.16	0.45
2:E:876:ASP:OD1	2:E:891:ARG:NE	2.49	0.45
1:C:1438:VAL:HG13	1:C:1443:THR:HB	1.99	0.45
2:F:841:PRO:HA	2:F:844:VAL:HG22	1.99	0.45
2:E:952:MET:HB2	2:E:952:MET:HE2	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1524:THR:HB	1:A:1525:PRO:HD3	1.98	0.44
2:F:1051:SER:HB2	2:F:1056:LYS:HG2	1.99	0.44
2:F:1091:THR:HA	2:F:1097:ARG:NE	2.31	0.44
1:A:1367:TRP:HB3	1:A:1385:ILE:HD13	1.98	0.44
1:D:1344:LEU:HD23	1:D:1351:LYS:HB3	1.98	0.44
2:E:1041:TRP:HB2	2:E:1069:GLY:HA3	1.98	0.44
1:B:1739:THR:HG22	1:B:1845:ARG:NH1	2.32	0.44
1:D:1733:THR:HA	1:D:1795:ILE:HG13	1.98	0.44
1:D:1453:GLU:OE2	1:D:1456:SER:HA	2.18	0.44
1:D:1656:PHE:HE1	1:D:1676:TYR:CD1	2.35	0.44
2:H:951:ASP:OD1	2:H:952:MET:N	2.48	0.43
2:F:1038:VAL:HA	2:F:1041:TRP:CD1	2.53	0.43
2:H:889:LEU:HD23	2:H:889:LEU:HA	1.84	0.43
1:B:1355:GLU:OE2	1:B:1597:TYR:OH	2.26	0.43
1:B:1878:ARG:O	1:B:1881:MET:HG2	2.18	0.43
2:H:825:LEU:HA	2:H:825:LEU:HD23	1.76	0.43
1:D:1661:LEU:HA	1:D:1662:PRO:HD3	1.86	0.43
1:C:1823:HIS:HB3	3:C:2001:PG4:H72	2.00	0.43
1:B:1414:TYR:OH	1:B:1571:GLU:OE2	2.22	0.42
1:A:1872:LYS:O	1:A:1876:THR:HG23	2.20	0.42
1:B:1334:ILE:HA	1:B:1337:LEU:HB2	2.02	0.42
1:C:1786:ASP:HB3	1:C:1789:ASP:OD1	2.20	0.42
1:D:1731:ASN:HA	1:D:1793:ARG:NH1	2.35	0.42
2:F:1041:TRP:HB2	2:F:1069:GLY:HA3	2.01	0.42
2:H:853:MET:HG3	2:H:857:TYR:HD2	1.85	0.42
1:B:1621:TYR:O	1:B:1625:GLN:HG2	2.20	0.42
1:B:1819:ILE:HG22	3:B:2001:PG4:H61	2.01	0.42
1:D:1367:TRP:HB3	1:D:1385:ILE:HD13	2.02	0.42
1:D:1631:PRO:HB2	1:D:1634:GLU:HG3	2.00	0.42
2:E:998:MET:CE	2:E:1004:ARG:HG2	2.50	0.42
2:E:1053:LEU:HD22	2:E:1103:GLU:HG3	2.01	0.42
1:A:1344:LEU:HA	1:A:1351:LYS:HB3	2.02	0.42
1:B:1614:GLU:OE1	1:B:1858:ARG:NH2	2.47	0.42
1:C:1698:SER:HB2	1:C:1878:ARG:HD2	2.01	0.42
1:D:1886:ASP:OD1	1:D:1886:ASP:N	2.44	0.42
2:F:847:LEU:HA	2:F:847:LEU:HD23	1.85	0.41
1:A:1627:LEU:HA	1:A:1638:ALA:HB3	2.01	0.41
1:B:1570[A]:HIS:ND1	1:D:1357:GLU:O	2.53	0.41
1:B:1588:ASN:HD22	1:B:1588:ASN:C	2.21	0.41
2:F:1034:GLN:O	2:F:1045:ARG:NH2	2.53	0.41
1:C:1621:TYR:O	1:C:1625:GLN:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1006:SER:OG	2:F:1066:GLY:O	2.24	0.41
1:D:1861:TYR:HA	2:H:806:ALA:HA	2.02	0.41
1:C:1819:ILE:HG12	1:C:1849:PHE:CE1	2.55	0.41
2:E:992:LEU:HD23	2:E:996:LEU:HD12	2.01	0.41
2:H:962:LEU:HA	2:H:962:LEU:HD12	1.86	0.41
2:E:998:MET:HE1	2:E:1004:ARG:HA	2.02	0.41
2:H:821:LYS:HG3	2:H:850:TRP:HD1	1.86	0.41
1:B:1414:TYR:OH	1:B:1570[A]:HIS:HD2	2.04	0.41
1:C:1808:VAL:HB	1:C:1890:LEU:HD22	2.03	0.41
2:E:810:GLY:O	2:E:816:ARG:HG3	2.21	0.41
2:F:957:VAL:O	2:F:962:LEU:HB2	2.20	0.41
1:D:1828:GLN:NE2	2:H:955:GLU:OE2	2.54	0.41
1:B:1886:ASP:HA	1:B:1889:GLN:HB2	2.03	0.41
2:E:967:LEU:N	2:E:968:PRO:HD3	2.35	0.41
2:F:1083:LEU:HD23	2:F:1100:LEU:HD11	2.03	0.41
2:F:813:ASP:O	2:F:817:ARG:HG3	2.21	0.41
1:D:1743:GLU:HB2	1:D:1748:LYS:HG3	2.02	0.40
1:C:1856:LEU:HD22	1:C:1898:TYR:CD2	2.55	0.40
1:D:1780:ARG:HD2	1:D:1797:GLN:OE1	2.21	0.40
1:C:1334:ILE:HD12	7:C:2121:HOH:O	2.20	0.40
1:C:1859:MET:HE2	1:C:1865:VAL:HG22	2.03	0.40
1:D:1739:THR:HG22	1:D:1845:ARG:NH1	2.36	0.40
1:B:1420:TYR:OH	1:B:1562:ASP:OD2	2.29	0.40
1:B:1344:LEU:HB3	1:B:1352:PHE:CG	2.55	0.40
1:D:1670:LEU:HD12	1:D:1841:ALA:HB2	2.03	0.40
2:E:962:LEU:HA	2:E:962:LEU:HD12	1.94	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	577/580 (100%)	558 (97%)	17 (3%)	2 (0%)	41	68
1	B	569/580 (98%)	553 (97%)	14 (2%)	2 (0%)	34	62
1	C	575/580 (99%)	558 (97%)	15 (3%)	2 (0%)	41	68
1	D	565/580 (97%)	550 (97%)	13 (2%)	2 (0%)	34	62
2	E	262/325 (81%)	254 (97%)	8 (3%)	0	100	100
2	F	260/325 (80%)	250 (96%)	10 (4%)	0	100	100
2	G	11/325 (3%)	11 (100%)	0	0	100	100
2	H	221/325 (68%)	215 (97%)	6 (3%)	0	100	100
All	All	3040/3620 (84%)	2949 (97%)	83 (3%)	8 (0%)	41	68

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1882	VAL
1	C	1882	VAL
1	D	1882	VAL
1	A	1591	VAL
1	A	1882	VAL
1	B	1591	VAL
1	C	1591	VAL
1	D	1591	VAL

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	505/504 (100%)	498 (99%)	7 (1%)	67	86
1	B	495/504 (98%)	489 (99%)	6 (1%)	71	89
1	C	499/504 (99%)	493 (99%)	6 (1%)	71	89
1	D	489/504 (97%)	485 (99%)	4 (1%)	81	93
2	E	223/280 (80%)	220 (99%)	3 (1%)	69	88
2	F	222/280 (79%)	221 (100%)	1 (0%)	88	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	9/280 (3%)	9 (100%)	0	100	100
2	H	186/280 (66%)	184 (99%)	2 (1%)	73	90
All	All	2628/3136 (84%)	2599 (99%)	29 (1%)	73	90

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1348	ASP
1	A	1352	PHE
1	A	1415	ARG
1	A	1417	GLN
1	A	1588	ASN
1	A	1615	VAL
1	A	1860	ARG
1	B	1348	ASP
1	B	1352	PHE
1	B	1588	ASN
1	B	1615	VAL
1	B	1621	TYR
1	B	1744	MET
1	C	1348	ASP
1	C	1352	PHE
1	C	1531[A]	ARG
1	C	1531[B]	ARG
1	C	1532	ARG
1	C	1588	ASN
1	D	1352	PHE
1	D	1403	SER
1	D	1588	ASN
1	D	1621	TYR
2	E	807	LYS
2	E	969	GLN
2	E	1027	ARG
2	F	969	GLN
2	H	853	MET
2	H	969	GLN

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
4	PO4	B	2002	-	4,4,4	0.95	0	6,6,6	0.45	0
4	PO4	A	2002	-	4,4,4	0.94	0	6,6,6	0.48	0
4	PO4	D	2003	-	4,4,4	0.94	0	6,6,6	0.44	0
4	PO4	E	1201	-	4,4,4	0.97	0	6,6,6	0.39	0
3	PG4	A	2001	-	12,12,12	0.16	0	11,11,11	0.31	0
3	PG4	B	2001	-	12,12,12	0.15	0	11,11,11	0.24	0
5	PGE	C	2002	-	9,9,9	0.19	0	8,8,8	0.09	0
5	PGE	D	2002	-	9,9,9	0.17	0	8,8,8	0.22	0
3	PG4	C	2001	-	12,12,12	0.18	0	11,11,11	0.21	0
4	PO4	C	2003	-	4,4,4	0.94	0	6,6,6	0.48	0
6	P6G	D	2001	-	18,18,18	0.50	0	17,17,17	0.33	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	PG4	A	2001	-	-	2/10/10/10	-
3	PG4	B	2001	-	-	1/10/10/10	-
5	PGE	C	2002	-	-	0/7/7/7	-
5	PGE	D	2002	-	-	1/7/7/7	-
3	PG4	C	2001	-	-	0/10/10/10	-
6	P6G	D	2001	-	-	3/16/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	2001	P6G	O13-C14-C15-O16
3	B	2001	PG4	O4-C7-C8-O5
6	D	2001	P6G	O10-C11-C12-O13
6	D	2001	P6G	C15-C14-O13-C12
3	A	2001	PG4	C1-C2-O2-C3
3	A	2001	PG4	O2-C3-C4-O3
5	D	2002	PGE	O3-C5-C6-O4

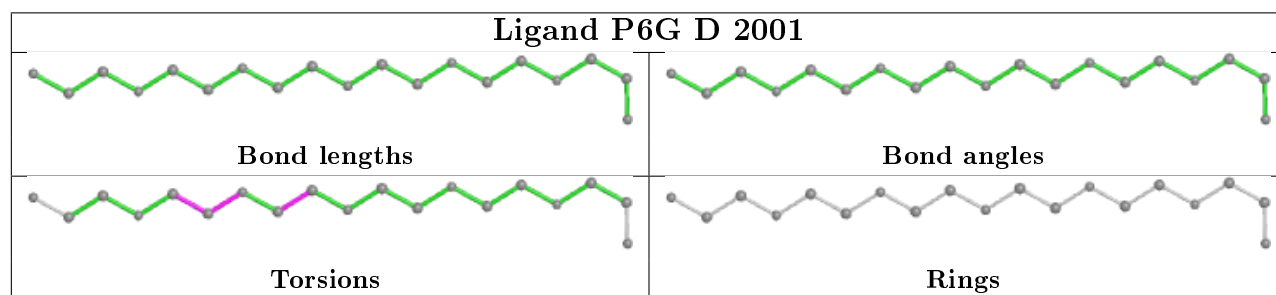
There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1201	PO4	1	0
3	A	2001	PG4	1	0
3	B	2001	PG4	1	0
5	D	2002	PGE	1	0
3	C	2001	PG4	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	575/580 (99%)	-0.36	2 (0%) 94 94	26, 42, 75, 159	0
1	B	571/580 (98%)	-0.15	12 (2%) 63 60	44, 77, 125, 155	0
1	C	575/580 (99%)	-0.32	3 (0%) 91 90	31, 58, 103, 196	0
1	D	568/580 (97%)	0.05	39 (6%) 16 12	32, 80, 169, 212	0
2	E	266/325 (81%)	0.06	17 (6%) 19 15	48, 85, 161, 236	0
2	F	264/325 (81%)	0.73	53 (20%) 1 0	61, 118, 198, 267	0
2	G	15/325 (4%)	3.26	10 (66%) 0 0	145, 168, 208, 212	0
2	H	231/325 (71%)	1.08	50 (21%) 0 0	85, 135, 224, 283	0
All	All	3065/3620 (84%)	0.02	186 (6%) 21 17	26, 72, 169, 283	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1100	LEU	11.6
2	H	1107	LEU	10.1
2	H	1072	LEU	9.3
2	F	825	LEU	9.0
2	H	1071	LEU	6.9
2	H	1073	ALA	6.8
2	H	1083	LEU	6.8
2	H	1086	LEU	6.1
2	H	1087	LEU	6.0
2	H	1049	TRP	5.9
2	G	861	CYS	5.8
2	H	1074	LEU	5.8
2	F	1089	ILE	5.7
2	H	961	TRP	5.7
2	G	858	VAL	5.4
1	D	1669	ARG	5.3

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Mol	Chain	Res	Type	RSRZ
2	H	1085	LEU	5.2
2	G	860	ALA	5.2
2	H	1081	SER	5.2
2	F	1055	LEU	5.1
2	H	1005	VAL	5.0
1	B	1635	SER	4.9
2	F	818	ASN	4.9
2	F	850	TRP	4.7
2	F	1053	LEU	4.6
2	E	833	LEU	4.6
2	G	862	ARG	4.5
2	G	863	ALA	4.5
2	H	1061	ASN	4.3
2	F	1034	GLN	4.3
2	G	853	MET	4.3
2	H	1040	VAL	4.3
2	H	1067	VAL	4.2
1	D	1745	GLY	4.2
1	D	1656	PHE	4.2
1	D	1674	MET	4.1
2	F	1054	GLY	4.1
2	F	1100	LEU	4.0
2	F	826	GLU	3.9
2	F	1092	GLN	3.8
2	F	1090	PRO	3.8
2	F	822	HIS	3.8
2	H	1012	MET	3.8
2	H	1075	ASP	3.8
2	E	834	PRO	3.8
2	E	829	CYS	3.7
2	E	835	PHE	3.7
2	F	811	PRO	3.6
1	D	1806	GLN	3.6
2	F	1111	GLY	3.6
2	F	1072	LEU	3.5
2	H	967	LEU	3.4
2	G	855	ALA	3.4
2	F	829	CYS	3.4
2	F	817	ARG	3.4
2	H	1099	LEU	3.4
1	B	1656	PHE	3.4
1	D	1760	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
2	H	999	VAL	3.3
2	G	856	TRP	3.3
2	H	1108	ILE	3.3
1	D	1787	ALA	3.3
2	E	811	PRO	3.3
2	H	1062	LEU	3.3
1	D	1810	LYS	3.3
2	E	830	ARG	3.2
2	F	1049	TRP	3.2
2	F	816	ARG	3.2
2	E	831	GLN	3.2
2	H	1016	ARG	3.1
1	D	1663	CYS	3.1
1	D	1692	SER	3.1
2	H	1084	ALA	3.1
1	B	1663	CYS	3.0
1	B	1665	LYS	3.0
2	G	857	TYR	3.0
1	D	1747	GLU	3.0
2	H	1060	THR	3.0
1	B	1399	GLY	3.0
2	H	1038	VAL	3.0
1	D	1630	VAL	3.0
2	F	1023	ASP	3.0
1	C	1904	HIS	3.0
1	D	1625	GLN	2.9
2	F	835	PHE	2.9
2	F	819	LYS	2.9
2	F	1051	SER	2.9
1	B	1666	PHE	2.9
2	F	809	THR	2.9
2	F	1088	GLN	2.8
2	E	826	GLU	2.8
2	H	1102	LYS	2.8
2	H	1001	SER	2.8
2	F	1039	MET	2.8
2	F	812	GLY	2.7
2	F	1087	LEU	2.7
1	D	1748	LYS	2.7
1	D	1763	TYR	2.7
2	H	1069	GLY	2.7
1	D	1905	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	1048	GLY	2.7
2	G	859	ALA	2.7
1	C	1687	ARG	2.7
2	F	1033	THR	2.7
1	D	1662	PRO	2.7
1	D	1803	TRP	2.6
2	H	1078	PHE	2.6
1	D	1755	ALA	2.6
2	E	1089	ILE	2.6
1	D	1807	GLY	2.6
1	D	1740	LYS	2.5
1	D	1790	GLY	2.5
2	H	1025	GLU	2.5
1	D	1666	PHE	2.5
2	F	849	LEU	2.5
2	E	850	TRP	2.5
2	F	813	ASP	2.5
2	H	1019	TYR	2.5
2	F	1107	LEU	2.5
1	D	1686	ILE	2.5
1	D	1742	ARG	2.4
2	H	1082	ASP	2.4
2	H	1002	PHE	2.4
1	C	1903	ASP	2.4
2	F	831	GLN	2.4
2	F	1037	ASP	2.4
2	F	815	ASP	2.4
2	H	876	ASP	2.4
2	F	1073	ALA	2.4
2	E	825	LEU	2.4
2	H	1064	GLU	2.4
2	F	1086	LEU	2.4
2	H	1028	ARG	2.3
1	A	1649	SER	2.3
2	F	824	LEU	2.3
2	F	1017	LEU	2.3
2	H	1104	PHE	2.3
1	B	1739	THR	2.3
2	F	1050	VAL	2.3
1	B	1664	ASN	2.3
2	F	868	GLY	2.3
2	F	820	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	838	TRP	2.3
1	B	1662	PRO	2.3
1	D	1633	GLY	2.3
2	F	1027	ARG	2.3
1	A	1636	VAL	2.2
2	H	1050	VAL	2.2
2	H	1105	SER	2.2
1	D	1722	ASP	2.2
2	F	1059	ALA	2.2
2	F	1099	LEU	2.2
2	H	904	LEU	2.2
2	H	962	LEU	2.2
2	F	823	GLU	2.2
2	F	838	TRP	2.2
1	D	1689	VAL	2.2
1	D	1882	VAL	2.2
1	D	1628	GLY	2.2
1	D	1746	ARG	2.2
1	B	1660	ASN	2.2
1	D	1784	VAL	2.2
1	D	1739	THR	2.2
2	F	1058	PHE	2.1
2	E	814	LYS	2.1
1	D	1738	LEU	2.1
1	D	1762	GLN	2.1
2	F	808	LEU	2.1
2	E	871	MET	2.1
2	F	814	LYS	2.1
2	H	1080	TYR	2.1
1	D	1751	GLN	2.1
1	B	1343	ARG	2.1
1	D	1845	ARG	2.1
1	B	1329	MET	2.1
2	E	1055	LEU	2.0
2	H	880	GLN	2.0
2	F	1071	LEU	2.0
2	E	837	ALA	2.0
2	H	965	LEU	2.0
2	H	1079	ASP	2.0
2	F	1052	GLY	2.0
2	E	828	ALA	2.0
2	H	1039	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	1629	GLN	2.0
1	D	1670	LEU	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](#)

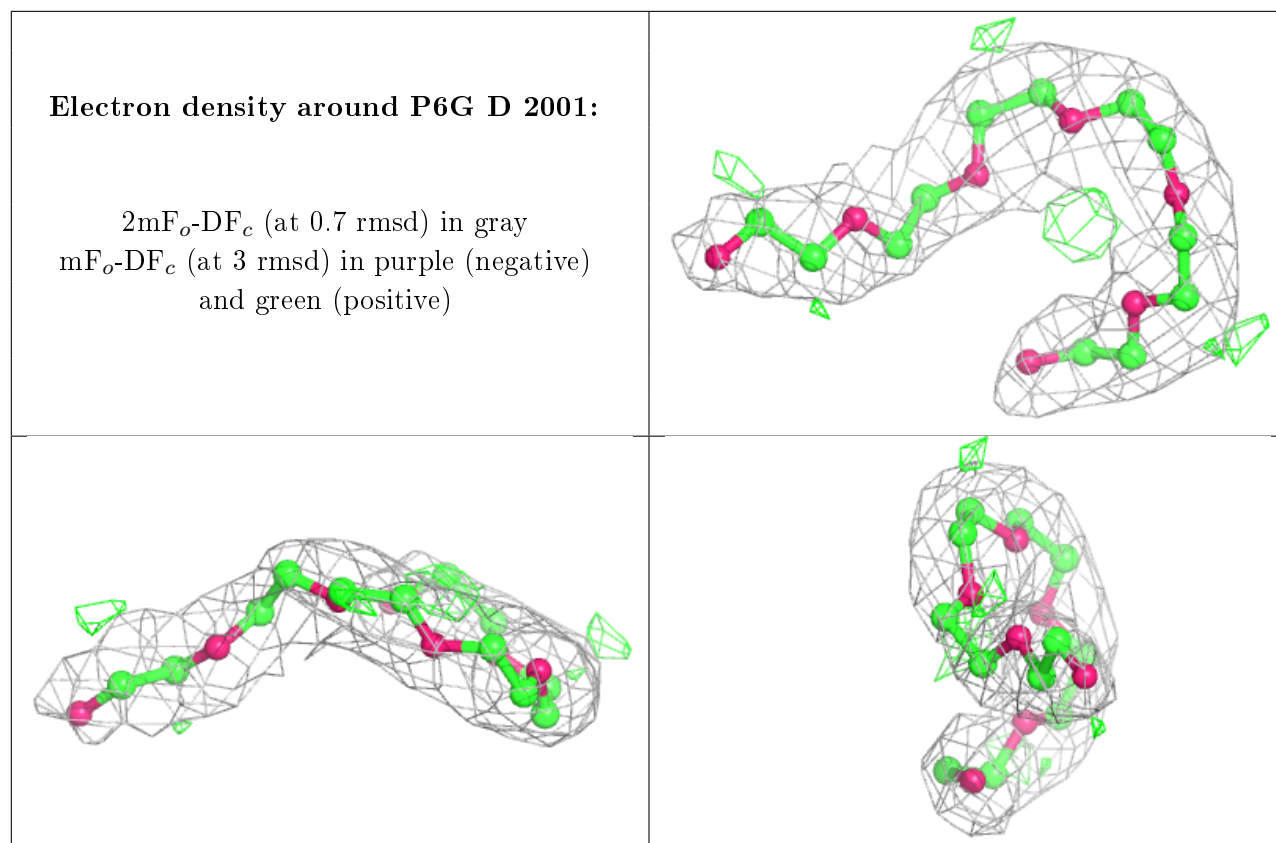
There are no carbohydrates in this entry.

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(\AA^2)	Q<0.9
4	PO4	A	2002	5/5	0.60	0.30	207,207,209,210	0
4	PO4	D	2003	5/5	0.73	0.17	172,172,174,175	0
4	PO4	C	2003	5/5	0.76	0.21	156,159,161,164	0
4	PO4	B	2002	5/5	0.83	0.28	195,195,196,196	0
5	PGE	C	2002	10/10	0.86	0.21	66,86,94,94	0
4	PO4	E	1201	5/5	0.87	0.11	157,157,158,159	0
5	PGE	D	2002	10/10	0.90	0.27	78,80,87,90	0
6	P6G	D	2001	19/19	0.90	0.17	51,69,87,87	0
3	PG4	B	2001	13/13	0.91	0.15	53,59,72,72	0
3	PG4	C	2001	13/13	0.93	0.19	60,67,73,77	0
3	PG4	A	2001	13/13	0.97	0.16	29,40,45,57	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.