Full wwPDB X-ray Structure Validation Report ⓘ

Jun 30, 2021 – 06:02 am BST

PDB ID	:	6ZZC
Title	:	MB_CRS6-1 bound to CrSAS-6_6HR
Authors	:	Hatzopoulos, G.N.; Kukenshoner, T.; Banterle, N.; Favez, T.; Fluckiger, I.; Hantschel, O.; Gonczy, P.
Deposited on	:	2020-08-04
Resolution	:	2.93 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:

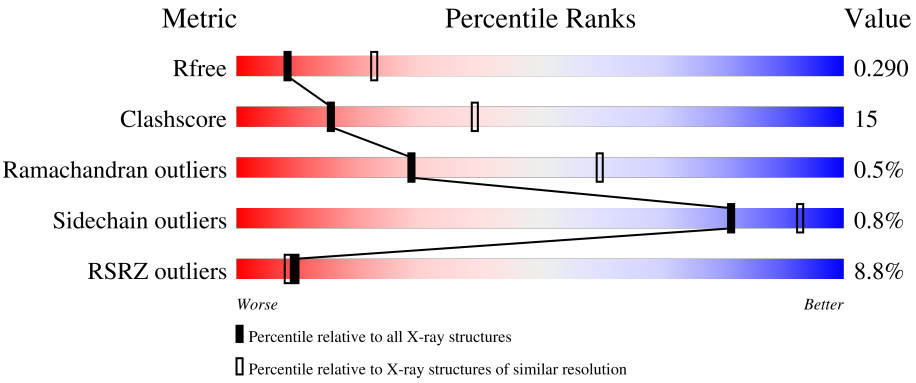
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.22
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

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 2.93 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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 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 <=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	227	5% 74% 19% 7%
1	B000	227	9% 90% 10%
1	C	227	4% 65% 19% . 15%
2	D	93	14% 58% 39% .
2	D0A0	93	16% 95% . .

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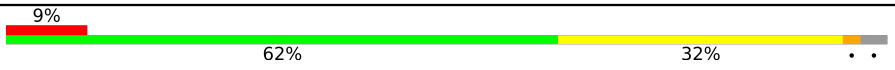
Mol	Chain	Length	Quality of chain
2	F	93	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7033 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 Centriole protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1687	1063	299	321	4			
1	B000	205	Total	C	N	O	S	0	0	0
			1650	1041	292	313	4			
1	C	193	Total	C	N	O	S	0	0	0
			1539	970	272	293	4			

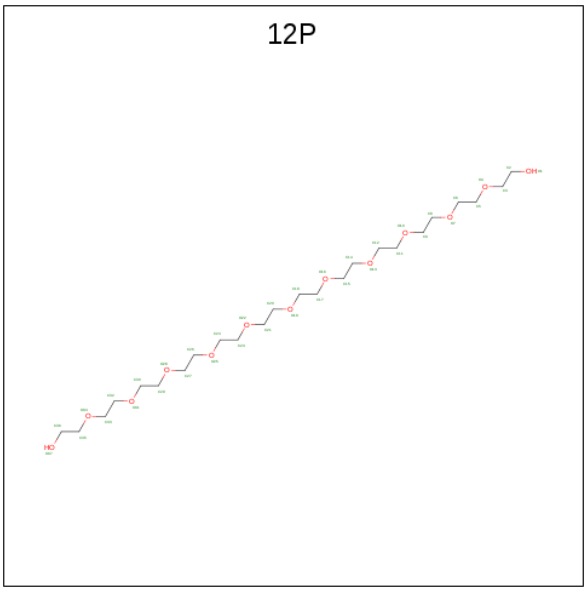
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A9CQL4
A	1	SER	-	expression tag	UNP A9CQL4
A	145	GLU	PHE	engineered mutation	UNP A9CQL4
B000	0	GLY	-	expression tag	UNP A9CQL4
B000	1	SER	-	expression tag	UNP A9CQL4
B000	145	GLU	PHE	engineered mutation	UNP A9CQL4
C	0	GLY	-	expression tag	UNP A9CQL4
C	1	SER	-	expression tag	UNP A9CQL4
C	145	GLU	PHE	engineered mutation	UNP A9CQL4

- Molecule 2 is a protein called MB_CrS6-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	90	Total	C	N	O	S	0	0	0
			687	446	104	136	1			
2	D0A0	90	Total	C	N	O	S	0	0	0
			687	446	104	136	1			
2	F	90	Total	C	N	O	S	0	0	0
			687	446	104	136	1			

- Molecule 3 is DODECAETHYLENE GLYCOL (three-letter code: 12P) (formula: $C_{24}H_{50}O_{13}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 37 24 13	0	0

- Molecule 4 is water.

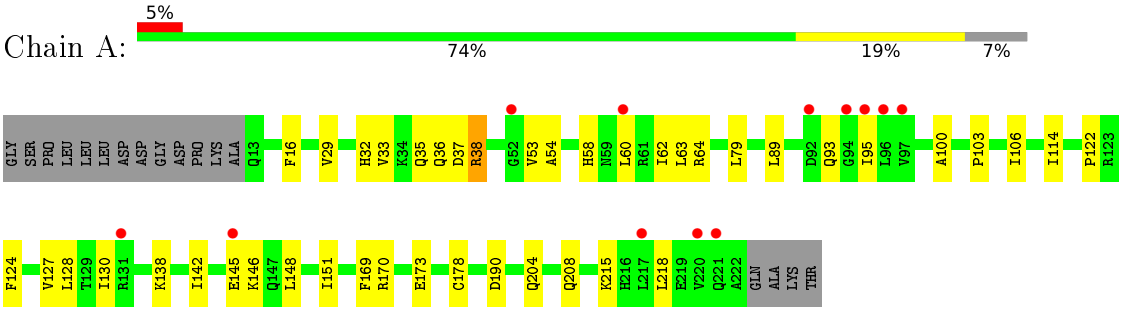
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B000	14	Total O 14 14	0	0
4	C	24	Total O 24 24	0	0
4	D	3	Total O 3 3	0	0
4	D0A0	2	Total O 2 2	0	0
4	F	7	Total O 7 7	0	0

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.

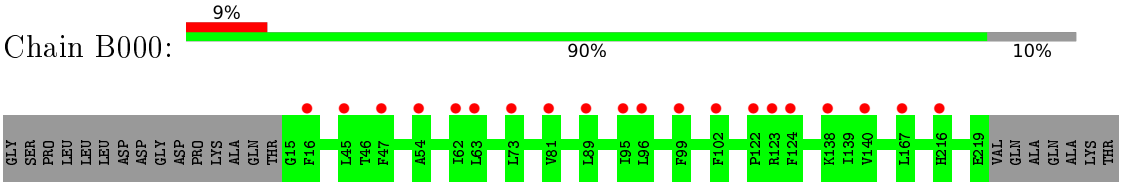
- Molecule 1: Centriole protein

Chain A:



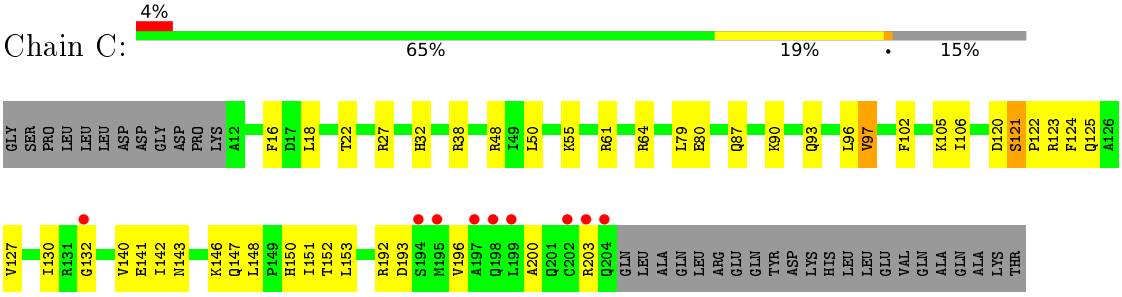
- Molecule 1: Centriole protein

Chain B000:



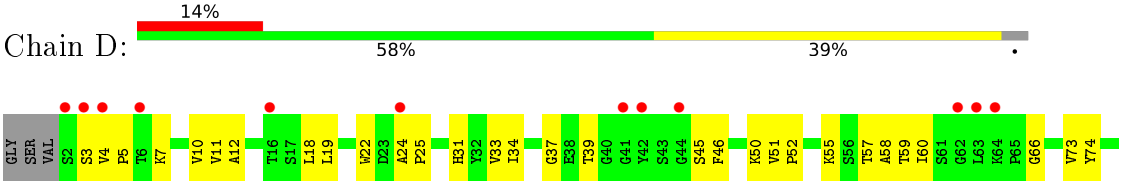
- Molecule 1: Centriole protein

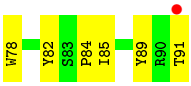
Chain C:



- Molecule 2: MB_CrS6-1

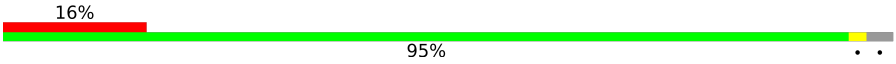
Chain D:

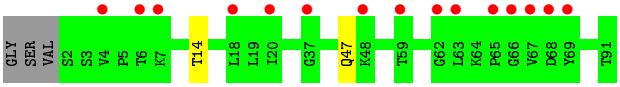




- Molecule 2: MB_CrS6-1

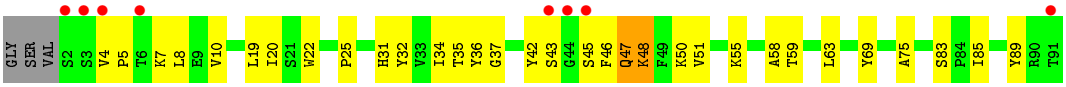
Chain D0A0:





- Molecule 2: MB_CrS6-1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	153.42Å 123.17Å 73.13Å 90.00° 107.90° 90.00°	Depositor
Resolution (Å)	47.07 – 2.93 47.07 – 2.93	Depositor EDS
% Data completeness (in resolution range)	97.4 (47.07-2.93) 97.3 (47.07-2.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.244 , 0.290 0.244 , 0.290	Depositor DCC
R_{free} test set	1348 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	97.6	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 83.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7033	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 12P

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	0.30	0/1716	0.52	0/2319
1	B000	0.30	0/1679	0.56	0/2268
1	C	0.29	0/1566	0.54	0/2117
2	D	0.36	0/707	0.60	0/969
2	D0A0	0.28	0/707	0.60	0/969
2	F	0.34	0/707	0.63	0/969
All	All	0.31	0/7082	0.56	0/9611

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

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	1687	0	1681	34	1
1	B000	1650	0	0	0	0
1	C	1539	0	1535	39	0
2	D	687	0	675	25	0
2	D0A0	687	0	0	0	0
2	F	687	0	675	34	1
3	C	37	0	50	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	9	0	0	0	0
4	B000	14	0	0	0	0
4	C	24	0	0	2	1
4	D	3	0	0	0	0
4	D0A0	2	0	0	0	0
4	F	7	0	0	0	0
All	All	7033	0	4616	120	2

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 15.

All (120) 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)
2:F:4:VAL:HG23	2:F:25:PRO:HB3	1.39	1.04
2:F:4:VAL:HG13	2:F:5:PRO:HD3	1.48	0.93
1:C:200:ALA:HA	1:C:203:ARG:HD3	1.54	0.89
2:F:4:VAL:HG11	2:F:75:ALA:HB2	1.56	0.85
2:D:5:PRO:HB3	2:D:24:ALA:HB2	1.63	0.80
1:A:148:LEU:HD23	1:C:148:LEU:HD23	1.63	0.80
1:C:93:GLN:NE2	1:C:152:THR:O	2.16	0.79
1:A:32:HIS:HB2	1:A:127:VAL:HG12	1.67	0.77
2:F:4:VAL:CG1	2:F:75:ALA:HB2	2.16	0.76
1:C:32:HIS:HB2	1:C:127:VAL:HG12	1.72	0.71
2:F:4:VAL:CG1	2:F:5:PRO:HD3	2.21	0.71
1:C:192:ARG:NH1	1:C:193:ASP:OD1	2.25	0.69
1:A:204:GLN:HE22	1:A:208:GLN:HE21	1.38	0.69
1:C:97:VAL:HG11	1:C:105:LYS:HG3	1.75	0.69
2:D:66:GLY:N	2:D:91:THR:O	2.26	0.69
2:D:37:GLY:HA3	2:D:46:PHE:CD1	2.29	0.68
2:F:19:LEU:HD13	2:F:59:THR:HG22	1.77	0.65
1:C:32:HIS:CD2	1:C:125:GLN:HE21	2.16	0.64
1:C:146:LYS:HB3	1:C:148:LEU:HD13	1.80	0.63
1:A:170:ARG:HD2	1:A:173:GLU:OE1	1.99	0.63
2:D:4:VAL:HG21	2:D:82:TYR:CD2	2.33	0.62
1:A:29:VAL:HG12	1:A:114:ILE:HD11	1.82	0.61
1:C:22:THR:OG1	2:F:48:LYS:NZ	2.30	0.61
2:D:34:ILE:HG12	2:D:73:VAL:HG22	1.83	0.60
1:C:200:ALA:HA	1:C:203:ARG:CD	2.29	0.59
2:D:7:LYS:O	2:D:22:TRP:HA	2.02	0.59
2:F:5:PRO:HG2	2:F:85:ILE:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:VAL:HG23	1:A:138:LYS:HG3	1.86	0.58
2:D:19:LEU:HD13	2:D:59:THR:HG22	1.85	0.57
2:F:5:PRO:CB	2:F:22:TRP:HB2	2.35	0.57
2:F:31:HIS:CD2	2:F:50:LYS:HE3	2.39	0.57
1:C:142:ILE:HA	1:C:146:LYS:O	2.04	0.57
1:C:120:ASP:O	1:C:143:ASN:ND2	2.38	0.56
1:A:95:ILE:HG13	1:C:147:GLN:H	1.70	0.56
2:F:5:PRO:HB3	2:F:22:TRP:HB2	1.88	0.56
2:D:39:THR:O	2:D:46:PHE:HZ	1.89	0.56
1:A:145:GLU:HG2	1:C:96:LEU:HB3	1.87	0.56
1:C:122:PRO:HB2	1:C:124:PHE:CE1	2.41	0.56
2:F:4:VAL:HG13	2:F:5:PRO:CD	2.31	0.54
1:A:64:ARG:HA	1:A:79:LEU:O	2.07	0.54
2:D:12:ALA:HB3	2:D:19:LEU:HB3	1.89	0.54
2:D:31:HIS:CD2	2:D:50:LYS:HE2	2.41	0.54
1:A:204:GLN:NE2	1:A:208:GLN:HE21	2.04	0.54
2:D:74:TYR:CD2	2:D:84:PRO:HB3	2.43	0.53
1:C:48:ARG:HG2	1:C:50:LEU:HD11	1.90	0.53
2:D:18:LEU:HD11	2:D:60:ILE:HD12	1.90	0.53
1:A:54:ALA:HB2	1:A:60:LEU:HD12	1.91	0.53
1:C:130:ILE:HG22	1:C:132:GLY:H	1.73	0.52
1:A:178:CYS:HB3	2:D:78:TRP:CH2	2.44	0.52
2:F:31:HIS:CG	2:F:50:LYS:HE3	2.45	0.52
1:A:89:LEU:O	1:A:93:GLN:HB2	2.10	0.52
1:C:200:ALA:CA	1:C:203:ARG:HD3	2.36	0.51
2:D:24:ALA:N	2:D:25:PRO:HD3	2.26	0.51
1:C:64:ARG:NH1	1:C:80:GLU:OE1	2.44	0.51
1:A:169:PHE:CZ	1:A:173:GLU:OE2	2.64	0.49
2:F:7:LYS:O	2:F:22:TRP:HA	2.12	0.49
2:F:32:TYR:HB2	2:F:51:VAL:CG2	2.43	0.49
1:C:61:ARG:HB3	2:F:42:TYR:CZ	2.48	0.49
2:D:33:VAL:HG12	2:D:74:TYR:HB2	1.95	0.49
1:A:95:ILE:HG13	1:C:146:LYS:HA	1.94	0.48
1:C:61:ARG:HD3	2:F:42:TYR:CD1	2.48	0.48
2:F:32:TYR:HB2	2:F:51:VAL:HG23	1.96	0.47
1:A:53:VAL:HG11	1:A:58:HIS:HA	1.96	0.47
1:A:63:LEU:HD12	1:A:103:PRO:HG3	1.97	0.47
1:C:141:GLU:HB3	1:C:148:LEU:HB2	1.96	0.47
1:A:127:VAL:CG2	1:A:138:LYS:HG3	2.44	0.47
2:F:20:ILE:HD11	2:F:34:ILE:HD13	1.97	0.46
2:F:43:SER:HB3	2:F:46:PHE:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HD21	1:C:150:HIS:CE1	2.51	0.46
2:F:42:TYR:O	2:F:46:PHE:HD1	1.98	0.46
1:C:192:ARG:HD2	1:C:192:ARG:C	2.36	0.46
1:C:192:ARG:O	1:C:196:VAL:HG23	2.16	0.46
2:D:37:GLY:HA3	2:D:46:PHE:CG	2.51	0.46
2:D:11:VAL:HG12	2:D:19:LEU:O	2.16	0.46
1:A:122:PRO:HB2	1:A:124:PHE:CE1	2.51	0.46
1:A:33:VAL:HA	1:A:128:LEU:O	2.16	0.46
1:C:22:THR:HG1	2:F:46:PHE:HB2	1.81	0.46
1:C:97:VAL:CG1	1:C:105:LYS:HG3	2.46	0.45
2:F:36:TYR:O	2:F:47:GLN:HB3	2.17	0.45
1:C:102:PHE:HE1	1:C:151:ILE:HD12	1.82	0.45
2:F:10:VAL:HG11	2:F:89:TYR:CE1	2.52	0.45
2:D:19:LEU:HD12	2:D:58:ALA:O	2.16	0.45
1:A:215:LYS:HE3	1:A:215:LYS:HB3	1.88	0.45
2:D:19:LEU:HD11	2:D:57:THR:OG1	2.17	0.45
2:F:4:VAL:HG11	2:F:32:TYR:HE1	1.82	0.45
2:D:3:SER:HB2	2:D:85:ILE:HB	1.99	0.44
2:F:8:LEU:HD22	2:F:85:ILE:HG23	1.99	0.44
1:C:87:GLN:OE1	4:C:401:HOH:O	2.21	0.44
1:C:102:PHE:CZ	1:C:106:ILE:HD11	2.53	0.44
1:A:151:ILE:HD13	1:A:151:ILE:HA	1.87	0.44
1:C:79:LEU:HD11	1:C:153:LEU:HD22	1.99	0.44
2:F:63:LEU:HB3	2:F:69:TYR:CE2	2.53	0.44
1:A:100:ALA:O	1:A:103:PRO:HD2	2.18	0.44
2:F:42:TYR:CG	2:F:43:SER:N	2.86	0.44
1:A:37:ASP:OD1	1:A:38:ARG:N	2.51	0.43
1:A:16:PHE:HD1	1:A:62:ILE:HD12	1.84	0.43
2:F:19:LEU:HD12	2:F:58:ALA:O	2.19	0.43
1:A:142:ILE:HA	1:A:146:LYS:O	2.19	0.42
2:D:10:VAL:HG11	2:D:89:TYR:CD1	2.53	0.42
1:A:35:GLN:NE2	1:A:130:ILE:HG12	2.34	0.42
1:C:55:LYS:HD2	1:C:55:LYS:HA	1.74	0.42
1:A:103:PRO:O	1:A:106:ILE:HG22	2.20	0.42
1:C:140:VAL:HA	1:C:148:LEU:O	2.18	0.42
2:D:52:PRO:HD2	2:D:55:LYS:HE2	2.01	0.41
2:F:35:THR:HG23	2:F:47:GLN:H	1.84	0.41
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.82	0.41
2:F:4:VAL:HG21	2:F:32:TYR:HE1	1.85	0.41
1:C:90:LYS:NZ	4:C:401:HOH:O	2.53	0.41
2:F:43:SER:HB3	2:F:46:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:PHE:HD1	1:C:18:LEU:HD12	1.86	0.41
1:A:36:GLN:O	1:A:38:ARG:HD3	2.21	0.41
1:A:178:CYS:HB3	2:D:78:TRP:CZ3	2.56	0.41
2:D:66:GLY:H	2:D:91:THR:C	2.22	0.41
2:F:37:GLY:HA3	2:F:45:SER:HB2	2.03	0.41
1:A:63:LEU:CD1	1:A:103:PRO:HG3	2.50	0.41
1:C:27:ARG:NH2	2:F:83:SER:OG	2.54	0.40
1:C:122:PRO:HB2	1:C:124:PHE:HE1	1.85	0.40
2:D:51:VAL:HG13	2:D:55:LYS:HD2	2.02	0.40
1:A:145:GLU:HG2	1:A:145:GLU:O	2.22	0.40
1:C:123:ARG:HB3	1:C:143:ASN:HB2	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASP:OD2	2:F:55:LYS:NZ[3_546]	2.14	0.06
4:C:407:HOH:O	4:C:417:HOH:O[2_555]	2.19	0.01

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	208/227 (92%)	199 (96%)	9 (4%)	0	100	100
1	B000	203/227 (89%)	197 (97%)	6 (3%)	0	100	100
1	C	191/227 (84%)	181 (95%)	9 (5%)	1 (0%)	29	60
2	D	88/93 (95%)	80 (91%)	7 (8%)	1 (1%)	14	40
2	D0A0	88/93 (95%)	81 (92%)	6 (7%)	1 (1%)	14	40
2	F	88/93 (95%)	82 (93%)	5 (6%)	1 (1%)	14	40
All	All	866/960 (90%)	820 (95%)	42 (5%)	4 (0%)	29	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	47	GLN
2	D0A0	47	GLN
2	D	45	SER
1	C	121	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	190/203 (94%)	189 (100%)	1 (0%)	88 96
1	B000	186/203 (92%)	186 (100%)	0	100 100
1	C	174/203 (86%)	171 (98%)	3 (2%)	60 83
2	D	77/79 (98%)	77 (100%)	0	100 100
2	D0A0	77/79 (98%)	76 (99%)	1 (1%)	69 88
2	F	77/79 (98%)	76 (99%)	1 (1%)	69 88
All	All	781/846 (92%)	775 (99%)	6 (1%)	81 93

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	C	38	ARG
1	C	97	VAL
1	C	121	SER
2	D0A0	14	THR
2	F	48	LYS

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	204	GLN
1	A	208	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	12P	C	301	-	36,36,36	0.55	0	35,35,35	0.25	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	12P	C	301	-	-	23/34/34/34	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

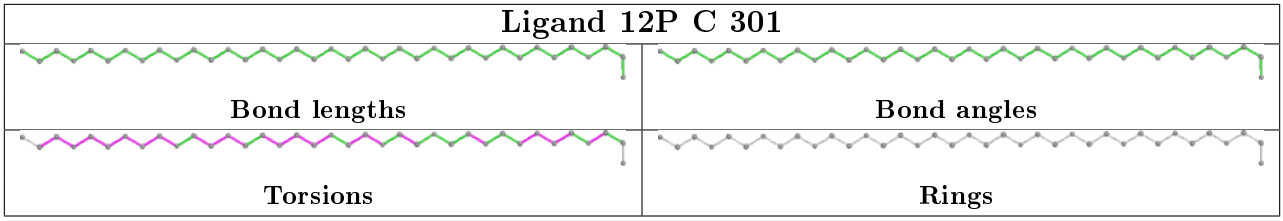
All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	301	12P	O16-C17-C18-O19
3	C	301	12P	O19-C20-C21-O22
3	C	301	12P	C17-C18-O19-C20
3	C	301	12P	O10-C11-C12-O13
3	C	301	12P	O1-C2-C3-O4
3	C	301	12P	O7-C8-C9-O10
3	C	301	12P	O31-C32-C33-O34
3	C	301	12P	C15-C14-O13-C12
3	C	301	12P	C6-C5-O4-C3
3	C	301	12P	C36-C35-O34-C33
3	C	301	12P	C11-C12-O13-C14
3	C	301	12P	C26-C27-O28-C29
3	C	301	12P	C9-C8-O7-C6
3	C	301	12P	C18-C17-O16-C15
3	C	301	12P	C2-C3-O4-C5
3	C	301	12P	C20-C21-O22-C23
3	C	301	12P	O22-C23-C24-O25
3	C	301	12P	C29-C30-O31-C32
3	C	301	12P	O4-C5-C6-O7
3	C	301	12P	C14-C15-O16-C17
3	C	301	12P	C33-C32-O31-C30
3	C	301	12P	C8-C9-O10-C11
3	C	301	12P	C5-C6-O7-C8

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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

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, 95^{th} 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	210/227 (92%)	0.38	12 (5%) 23 22	70, 113, 193, 248	0
1	B000	205/227 (90%)	0.61	20 (9%) 7 6	78, 134, 202, 224	0
1	C	193/227 (85%)	0.43	9 (4%) 31 31	57, 103, 206, 276	0
2	D	90/93 (96%)	0.94	13 (14%) 2 2	88, 126, 221, 280	0
2	D0A0	90/93 (96%)	1.10	15 (16%) 1 1	88, 141, 193, 256	0
2	F	90/93 (96%)	0.66	8 (8%) 9 8	52, 85, 139, 256	0
All	All	878/960 (91%)	0.61	77 (8%) 10 8	52, 119, 201, 280	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D0A0	66	GLY	12.6
2	F	44	GLY	8.7
2	D0A0	65	PRO	7.3
1	B000	95	ILE	6.2
2	F	4	VAL	6.1
2	F	2	SER	6.0
2	D	41	GLY	5.9
1	C	195	MET	5.7
2	D0A0	67	VAL	5.2
1	C	132	GLY	5.0
1	B000	123	ARG	4.9
2	D0A0	63	LEU	4.9
1	C	194	SER	4.7
2	D0A0	59	THR	4.4
1	B000	124	PHE	4.3
1	C	202	CYS	4.3
1	A	92	ASP	4.3
2	D	44	GLY	4.2
1	C	197	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
2	D	2	SER	4.0
2	D	42	TYR	3.9
2	D0A0	18	LEU	3.8
2	D0A0	62	GLY	3.7
1	B000	62	ILE	3.7
1	A	52	GLY	3.5
2	D0A0	20	ILE	3.5
2	D0A0	6	THR	3.4
1	A	145	GLU	3.4
1	C	198	GLN	3.3
2	D	3	SER	3.3
1	B000	81	VAL	3.2
1	A	131	ARG	3.1
2	F	45	SER	3.0
2	D	16	THR	2.9
1	C	199	LEU	2.9
2	D	24	ALA	2.9
2	D0A0	7	LYS	2.8
1	A	220	VAL	2.8
2	D	63	LEU	2.8
1	B000	102	PHE	2.7
1	A	97	VAL	2.7
2	D	91	THR	2.7
1	B000	16	PHE	2.7
1	B000	96	LEU	2.7
2	F	91	THR	2.6
2	D0A0	37	GLY	2.6
1	B000	140	VAL	2.6
1	A	60	LEU	2.6
2	F	3	SER	2.6
1	B000	122	PRO	2.6
2	D	64	LYS	2.5
2	D0A0	48	LYS	2.5
1	A	94	GLY	2.5
2	D	62	GLY	2.5
2	D0A0	69	TYR	2.4
1	B000	54	ALA	2.4
2	F	6	THR	2.4
2	D	6	THR	2.4
2	F	43	SER	2.4
1	B000	216	HIS	2.3
1	B000	99	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	221	GLN	2.3
1	C	204	GLN	2.3
2	D0A0	4	VAL	2.3
1	C	203	ARG	2.3
1	B000	63	LEU	2.3
1	B000	73	LEU	2.2
1	B000	89	LEU	2.2
1	B000	45	LEU	2.2
1	B000	167	LEU	2.1
1	A	95	ILE	2.1
1	B000	138	LYS	2.1
1	A	96	LEU	2.1
2	D0A0	68	ASP	2.1
1	B000	47	PHE	2.1
1	A	217	LEU	2.1
2	D	4	VAL	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 monosaccharides 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, 95^{th} 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
3	12P	C	301	37/37	0.54	0.21	127,141,162,176	0

6.5 Other polymers (i)

There are no such residues in this entry.