

Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2024 – 03:27 PM EDT

PTP) in

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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) 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	:	2.36.1
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)	:	2.36.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 3.10 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	А	215	69%		25%		• •	
1	В	215	75%		17%	•	·	
1	С	215	54%	34%		7%	•	
1	D	215	69%		23%	•	•	
1	Е	215	69%		24%	•	•	



Mol	Chain	Length	Quality	of chain		
1	F	215	53%	34%	8%	5%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10099 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace	
1	Δ	207	Total	С	Ν	0	S	0	0	0	
1	Л	201	1659	1060	295	296	8	0	0	0	
1	В	206	Total	С	Ν	0	S	0	0	0	
	D	200	1644	1048	293	295	8	0	0		
1	C	206	, Total	С	Ν	0	S	0	0	0	
		200	1637	1045	293	291	8	0	0	0	
1	П	206	Total	С	Ν	0	S	0	0	0	
	D	200	1651	1051	297	295	8	0	0		
1	F	207	Total	С	Ν	0	S	0	0	0	
		207	1653	1055	296	294	8	0	0	0	
1	Б	205	Total	С	Ν	0	S	0	0	0	
	Г	200	1621	1037	288	288	8	0	U		

• Molecule 1 is a protein called Glycolipid transfer protein domain-containing protein 1.

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	0	SER	-	expression tag	UNP Q5TA50
В	0	SER	-	expression tag	UNP Q5TA50
С	0	SER	-	expression tag	UNP Q5TA50
D	0	SER	-	expression tag	UNP Q5TA50
Е	0	SER	-	expression tag	UNP Q5TA50
F	0	SER	-	expression tag	UNP Q5TA50

• Molecule 2 is (2S,3R,4Z)-3-hydroxy-2-[(9E)-octadec-9-enoylamino]octadec-4-en-1-yl dihydrogen phosphate (three-letter code: 1Q0) (formula: $C_{36}H_{70}NO_6P$).





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
9	Λ	1	Total	С	Ν	0	Р	0	0
2	Л	T	44	36	1	6	1	0	0
2	В	1	Total	С	Ν	Ο	Р	0	0
	D	T	27	19	1	6	1	0	0
2	С	1	Total	С	Ν	Ο	Р	0	0
2	U	T	44	36	1	6	1	0	0
2	Л	1	Total	С	Ν	Ο	Р	0	0
2	D	T	44	36	1	6	1	0	0
2	F	1	Total	С	Ν	Ο	Р	0	0
2	Ľ	I	44	36	1	6	1	0	0
2	F	1	Total	Ċ	N	Ō	Р	0	0
	Ľ	L	16	8	1	6	1	0	

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	4	Total O 4 4	0	0
3	В	3	Total O 3 3	0	0
3	С	3	Total O 3 3	0	0
3	D	2	Total O 2 2	0	0
3	Е	3	Total O 3 3	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: Glycolipid transfer protein domain-containing protein 1



Chain D:

69%

•

23%



• Molecule 1: Glycolipid transfer protein domain-containing protein 1

Chain E:		69%		24%	•	·
SER MET ASP ASP SER GLU GLY GLY	L10 K11 V12 V12 V13 S16 F17 F17 F17 F17 F17 F17	E23 L29 L39 S51 F52 T53 T53	U55 V57 V58 S59 S59 K60 L61 R62 I63 I63 P71 P71	S78 L87 E95 R96	H100 P101 E102	R106 H116 W117 L118

• Molecule 1: Glycolipid transfer protein domain-containing protein 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	236.98Å 128.76Å 66.66Å	Depositor
a, b, c, α , β , γ	90.00° 93.53° 90.00°	Depositor
Bosolution(A)	30.05 - 3.10	Depositor
Resolution (A)	30.05 - 3.10	EDS
% Data completeness	98.5 (30.05-3.10)	Depositor
(in resolution range)	94.4 (30.05-3.10)	EDS
R_{merge}	0.11	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.96 (at 3.11 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
B B.	0.225 , 0.263	Depositor
Λ, Λ_{free}	0.225 , 0.263	DCC
R_{free} test set	1786 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	65.9	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.27, 38.1	EDS
L-test for $twinning^2$	$ < L >=0.46, < L^2>=0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10099	wwPDB-VP
Average B, all atoms $(Å^2)$	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.79% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: $1\mathrm{Q}0$

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).

Mal	Chain	Bond	lengths	Bond angles		
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.30	0/1697	0.46	0/2301	
1	В	0.30	0/1681	0.54	2/2281~(0.1%)	
1	С	0.29	0/1674	0.51	1/2272~(0.0%)	
1	D	0.28	0/1688	0.47	1/2288~(0.0%)	
1	Е	0.27	0/1691	0.44	0/2295	
1	F	0.27	0/1658	0.51	0/2252	
All	All	0.29	0/10089	0.49	4/13689~(0.0%)	

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	66	ARG	NE-CZ-NH2	9.70	125.15	120.30
1	В	66	ARG	NE-CZ-NH1	-8.51	116.05	120.30
1	С	165	LEU	CB-CA-C	6.71	122.96	110.20
1	D	131	ASP	CB-CA-C	-6.16	98.07	110.40

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	А	1659	0	1670	31	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	1644	0	1650	25	0
1	С	1637	0	1644	52	0
1	D	1651	0	1663	39	0
1	Ε	1653	0	1655	35	0
1	F	1621	0	1622	54	0
2	А	44	0	68	9	0
2	В	27	0	28	5	0
2	С	44	0	68	1	0
2	D	44	0	68	9	0
2	Е	44	0	68	11	0
2	F	16	0	8	3	0
3	А	4	0	0	0	0
3	В	3	0	0	0	0
3	С	3	0	0	0	0
3	D	2	0	0	0	0
3	Е	3	0	0	1	0
All	All	10099	0	10212	245	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 12.

All (245) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:E:301:1Q0:CAO	2:E:301:1Q0:H68	2.09	0.83	
1:D:53:ILE:HD12	2:D:301:1Q0:H38	1.65	0.77	
1:A:53:ILE:HD12	2:A:301:1Q0:H40	1.66	0.77	
1:E:117:TRP:CH2	2:E:301:1Q0:H8	2.23	0.73	
1:F:191:LEU:HG	1:F:195:GLN:HE22	1.53	0.73	
1:C:25:GLU:OE1	1:C:196:ARG:NH2	2.23	0.70	
1:B:58:VAL:HA	1:B:61:LEU:HD12	1.72	0.70	
1:D:74:GLU:O	1:D:77:ARG:NH1	2.26	0.69	
1:B:195:GLN:O	1:B:199:ASN:ND2	2.25	0.69	
2:E:301:1Q0:H68	2:E:301:1Q0:H44	1.74	0.69	
1:F:113:ARG:NH2	1:F:211:LEU:O	2.28	0.67	
1:B:119:GLN:HG3	1:B:195:GLN:HG2	1.76	0.66	
1:A:114:ALA:HB1	2:A:301:1Q0:H42	1.77	0.66	
1:D:128:SER:HB3	1:D:168:ARG:HE	1.60	0.65	
2:E:301:1Q0:H68	2:E:301:1Q0:H45	1.79	0.65	
1:C:143:ASN:HA	1:C:147:ALA:HB3	1.78	0.65	
2:A:301:1Q0:H55	2:A:301:1Q0:CAI	2.28	0.64	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:F:79:LEU:HA	1:F:82:MET:HB3	1.80	0.64	
1:C:195:GLN:O	1:C:199:ASN:ND2	2.31	0.63	
1:C:98:SER:OG	1:C:99:HIS:N	2.30	0.63	
1:C:30:ASP:OD1	1:C:30:ASP:N	2.30	0.63	
1:B:13:VAL:HG21	1:B:38:GLY:HA3	1.79	0.63	
1:C:126:ARG:NH1	1:C:187:LEU:O	2.33	0.62	
1:F:135:SER:HB2	1:F:162:PHE:HD1	1.63	0.62	
1:F:37:LYS:NZ	1:F:65:GLU:OE2	2.29	0.62	
1:F:49:ILE:HG13	1:F:50:PHE:N	2.14	0.62	
1:D:48:THR:OG1	1:D:49:ILE:N	2.30	0.62	
1:C:139:ALA:O	1:C:143:ASN:ND2	2.32	0.61	
1:D:122:LEU:HD21	2:D:301:1Q0:H63	1.83	0.61	
1:B:85:HIS:O	1:B:89:ASN:ND2	2.33	0.61	
1:A:26:GLU:OE1	1:A:77:ARG:NH2	2.34	0.60	
1:C:9:ASN:OD1	1:C:41:ARG:NH2	2.32	0.60	
1:A:149:TYR:OH	1:B:182:GLN:NE2	2.25	0.60	
2:F:301:1Q0:OAC	2:F:301:1Q0:H29	2.02	0.59	
1:C:22:ASP:OD1	1:C:26:GLU:N	2.35	0.58	
1:B:98:SER:OG	1:B:99:HIS:N	2.37	0.58	
1:C:147:ALA:O	1:C:155:ARG:NE	2.21	0.58	
1:B:116:HIS:HB2	1:B:198:TYR:CE1	2.39	0.57	
1:E:150:HIS:HE1	2:E:301:1Q0:H16	1.69	0.57	
1:B:70:GLY:O	1:B:73:SER:OG	2.23	0.57	
1:F:33:ILE:HD13	1:F:65:GLU:HG3	1.87	0.56	
1:F:51:SER:O	1:F:54:SER:OG	2.23	0.56	
1:F:93:ASP:HB3	1:F:96:ARG:O	2.04	0.56	
1:E:116:HIS:HB2	1:E:198:TYR:CE1	2.40	0.56	
1:C:40:VAL:HG13	1:C:54:SER:HB3	1.88	0.56	
1:B:39:LEU:HD23	2:B:301:1Q0:H50	1.88	0.55	
1:B:36:TRP:HB3	1:B:61:LEU:HD21	1.88	0.55	
1:B:125:LEU:HA	1:B:137:LEU:HD13	1.88	0.55	
2:B:301:1Q0:OBN	2:B:301:1Q0:OAE	2.22	0.55	
1:C:13:VAL:O	1:C:16:SER:OG	2.25	0.55	
1:D:30:ASP:OD1	1:D:68:ARG:NE	2.40	0.55	
1:A:169:GLU:O	1:A:172:LEU:N	2.38	0.55	
1:D:146:LEU:HG	1:D:150:HIS:HE1	1.71	0.55	
1:D:146:LEU:O	1:D:150:HIS:ND1	2.37	0.55	
1:F:72:GLN:HE21	1:F:85:HIS:CE1	2.25	0.54	
2:A:301:1Q0:H55	2:A:301:1Q0:H46	1.89	0.54	
1:D:97:ARG:HH21	1:D:106:ARG:HH12	1.53	0.54	
2:A:301:1Q0:H46	2:A:301:1Q0:CAX	2.38	0.54	



	lo do pagom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:116:HIS:HB2	1:B:198:TYR:CZ	2.43	0.54	
1:F:21:LEU:HB2	1:F:197:VAL:HG12	1.90	0.54	
1:D:106:ARG:NH2	2:D:301:1Q0:OAF	2.40	0.54	
1:A:114:ALA:HB2	2:A:301:1Q0:H70	1.90	0.54	
1:C:126:ARG:HG3	1:C:187:LEU:HB2	1.90	0.53	
1:A:146:LEU:HB3	1:A:150:HIS:CE1	2.44	0.53	
1:E:14:LEU:HG	1:E:190:ALA:HB2	1.89	0.53	
1:E:126:ARG:HG3	1:E:127:THR:H	1.73	0.53	
1:A:68:ARG:NH1	1:A:73:SER:O	2.42	0.53	
1:A:187:LEU:O	1:A:191:LEU:HB2	2.09	0.53	
1:F:25:GLU:OE2	1:F:196:ARG:NH2	2.42	0.53	
2:A:301:1Q0:CAI	2:A:301:1Q0:CAX	2.87	0.52	
1:F:68:ARG:NH1	1:F:73:SER:O	2.42	0.52	
1:B:56:ASP:OD2	2:B:301:1Q0:H24	2.09	0.52	
1:C:9:ASN:N	1:C:175:MET:O	2.42	0.52	
1:E:194:ILE:O	1:E:197:VAL:N	2.42	0.52	
1:E:150:HIS:NE2	2:E:301:1Q0:OAC	2.24	0.51	
1:C:14:LEU:HB3	1:C:190:ALA:HB1	1.92	0.51	
1:E:195:GLN:O	1:E:199:ASN:ND2	2.43	0.51	
1:B:56:ASP:OD2	2:B:301:1Q0:NBM	2.44	0.51	
1:C:19:GLN:OE1	1:C:19:GLN:N	2.43	0.51	
1:C:64:MET:CE	1:C:104:GLY:HA2	2.40	0.51	
1:E:129:PRO:HB3	3:E:402:HOH:O	2.10	0.51	
1:A:128:SER:OG	1:A:168:ARG:NE	2.42	0.51	
1:B:181:GLU:OE2	1:E:96:ARG:NH1	2.43	0.51	
1:A:159:THR:HA	1:A:162:PHE:CD2	2.45	0.51	
1:D:9:ASN:OD1	1:D:11:LYS:N	2.45	0.50	
1:E:39:LEU:HB3	2:E:301:1Q0:H53	1.93	0.50	
1:C:10:LEU:HD23	1:C:175:MET:SD	2.52	0.50	
1:C:28:LEU:HB2	1:C:31:PRO:HG2	1.94	0.50	
1:C:172:LEU:HA	1:C:175:MET:HE3	1.94	0.50	
1:E:8:PHE:O	1:E:10:LEU:N	2.45	0.50	
1:F:13:VAL:HG21	1:F:38:GLY:HA3	1.94	0.49	
1:E:126:ARG:HH21	1:E:188:GLY:HA3	1.77	0.49	
1:A:139:ALA:O	1:A:143:ASN:ND2	2.42	0.49	
1:E:117:TRP:HH2	2:E:301:1Q0:H4	1.78	0.49	
1:E:150:HIS:CE1	2:E:301:1Q0:H16	2.47	0.49	
1:C:205:TYR:HB3	1:C:211:LEU:HD23	1.95	0.49	
1:F:210:LEU:HD23	1:F:213:LEU:HD11	1.94	0.49	
1:D:150:HIS:HB3	1:D:154:VAL:CG2	2.42	0.49	
1:B:13:VAL:CG2	1:B:38:GLY:HA3	2.43	0.49	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:30:ASP:HB2	1:D:31:PRO:HD3	1.95	0.49	
1:A:53:ILE:CD1	2:A:301:1Q0:H40	2.40	0.49	
1:D:131:ASP:OD1	1:D:131:ASP:N	2.46	0.49	
1:B:43:LEU:HD22	1:B:50:PHE:HB3	1.95	0.48	
1:F:112:HIS:CE1	1:F:201:SER:HB2	2.48	0.48	
1:F:126:ARG:HD2	1:F:187:LEU:HD23	1.94	0.48	
1:D:101:PRO:O	1:D:106:ARG:NH1	2.46	0.48	
1:D:72:GLN:HG2	1:D:85:HIS:CE1	2.49	0.47	
1:D:117:TRP:CH2	2:D:301:1Q0:H66	2.49	0.47	
1:F:175:MET:H	1:F:175:MET:HG2	1.54	0.47	
1:C:50:PHE:O	1:C:53:ILE:HG12	2.14	0.47	
1:F:177:VAL:O	1:F:179:PRO:HD2	2.13	0.47	
1:A:36:TRP:HB3	1:A:61:LEU:HD11	1.96	0.47	
1:D:129:PRO:HG2	1:D:132:ALA:HB2	1.97	0.47	
1:F:116:HIS:O	1:F:119:GLN:HG2	2.14	0.47	
1:D:50:PHE:O	1:D:53:ILE:HG12	2.14	0.47	
1:A:131:ASP:N	1:A:131:ASP:OD1	2.47	0.47	
1:A:172:LEU:HD23	1:A:180:PRO:HB3	1.95	0.47	
1:A:191:LEU:O	1:A:194:ILE:HG22	2.14	0.47	
1:F:135:SER:HB2	1:F:162:PHE:CD1	2.48	0.47	
1:A:166:PRO:HD2	1:A:171:PHE:CZ	2.50	0.47	
1:C:64:MET:HE1	1:C:67:LEU:HD12	1.97	0.47	
1:E:12:VAL:O	1:E:16:SER:OG	2.32	0.47	
1:C:41:ARG:HA	1:C:44:ASN:HB2	1.97	0.47	
2:D:301:1Q0:H44	2:D:301:1Q0:H51	1.71	0.47	
1:F:28:LEU:HB3	1:F:31:PRO:HD2	1.96	0.47	
1:C:134:THR:HA	1:C:137:LEU:HD23	1.96	0.47	
1:B:167:THR:OG1	1:B:170:VAL:HG23	2.15	0.46	
1:E:126:ARG:NH2	1:E:188:GLY:HA3	2.30	0.46	
1:F:134:THR:O	1:F:138:CYS:HB2	2.15	0.46	
1:C:62:ARG:O	1:C:66:ARG:HG2	2.15	0.46	
1:D:153:VAL:HG21	2:F:301:1Q0:H26	1.97	0.46	
1:F:87:LEU:HD12	1:F:92:VAL:HG21	1.98	0.46	
1:F:205:TYR:CD1	1:F:210:LEU:HD22	2.51	0.46	
1:A:74:GLU:HG3	1:D:74:GLU:HB2	1.97	0.46	
1:C:138:CYS:O	1:C:142:TYR:N	2.46	0.46	
1:E:125:LEU:HA	1:E:137:LEU:HD13	1.97	0.46	
1:A:43:LEU:HG	2:A:301:1Q0:H54	1.98	0.46	
1:D:60:LYS:CE	2:D:301:1Q0:H30	2.46	0.46	
1:E:123:GLU:O	1:E:126:ARG:HG3	2.16	0.46	
1:C:116:HIS:HB2	1:C:198:TYR:CE1	2.51	0.46	



	lo uo pagem	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:42:PHE:HZ	1:D:175:MET:HA	1.81	0.46	
1:D:116:HIS:HB2	1:D:198:TYR:CE1	2.51	0.46	
1:C:179:PRO:C	1:C:181:GLU:H	2.20	0.45	
1:D:112:HIS:CE1	1:D:201:SER:HB2	2.52	0.45	
1:F:137:LEU:O	1:F:141:SER:OG	2.33	0.45	
1:F:187:LEU:HG	1:F:191:LEU:HB2	1.97	0.45	
1:F:103:SER:O	1:F:106:ARG:HG3	2.15	0.45	
1:F:50:PHE:CE1	1:F:161:ALA:HB1	2.51	0.45	
1:C:115:LEU:HD12	1:C:115:LEU:HA	1.83	0.45	
1:B:43:LEU:HD23	1:B:43:LEU:HA	1.85	0.45	
1:F:72:GLN:HE21	1:F:85:HIS:HE1	1.65	0.45	
1:D:159:THR:O	1:D:162:PHE:HB2	2.17	0.45	
1:B:53:ILE:HB	2:B:301:1Q0:CAU	2.46	0.44	
1:C:64:MET:HE3	1:C:104:GLY:HA2	1.99	0.44	
1:E:63:ILE:HD13	1:E:102:GLU:HB3	1.98	0.44	
1:F:22:ASP:HB3	1:F:26:GLU:HG3	1.99	0.44	
2:F:301:100:CAJ	2:F:301:100:NBM	2.78	0.44	
1:C:78:SER:OG	1:C:79:LEU:N	2.49	0.44	
1:F:36:TRP:HA	1:F:39:LEU:HD22	1.99	0.44	
2:D:301:1Q0:H36	2:D:301:1Q0:H20	2.00	0.44	
1:E:12:VAL:HA	1:E:15:VAL:HG13	1.98	0.44	
1:E:52:PHE:CE1	1:E:53:ILE:HG22	2.52	0.44	
1:F:106:ARG:NH2	1:F:214:PRO:OXT	2.36	0.44	
1:A:124:GLY:O	1:A:128:SER:HB3	2.18	0.44	
1:A:9:ASN:HB2	1:A:175:MET:O	2.18	0.44	
1:C:24:LYS:HE2	1:C:24:LYS:HB3	1.63	0.44	
1:D:146:LEU:HD12	1:D:146:LEU:HA	1.83	0.44	
1:F:93:ASP:CG	1:F:100:HIS:H	2.21	0.44	
1:D:106:ARG:HE	1:D:106:ARG:HB2	1.60	0.44	
1:E:146:LEU:HG	1:E:150:HIS:CE1	2.52	0.44	
1:F:49:ILE:O	1:F:52:PHE:N	2.50	0.44	
1:F:169:GLU:OE1	1:F:169:GLU:N	2.48	0.44	
1:A:76:TYR:OH	1:A:86:GLU:OE2	2.28	0.43	
1:E:179:PRO:HB2	1:E:182:GLN:OE1	2.18	0.43	
1:C:112:HIS:CE1	1:C:201:SER:HB2	2.54	0.43	
1:D:28:LEU:O	1:D:31:PRO:HD2	2.18	0.43	
1:B:10:LEU:O	1:B:13:VAL:N	2.48	0.43	
1:A:105:CYS:O	1:A:205:TYR:OH	2.27	0.43	
1:E:60:LYS:NZ	2:E:301:1Q0:OAF	2.52	0.43	
1:C:80:GLN:HG3	1:C:204:LEU:HD22	1.99	0.43	
1:F:27:VAL:HG13	1:F:79:LEU:HG	2.00	0.43	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:78:SER:OG	1:C:80:GLN:OE1	2.30	0.43	
1:D:114:ALA:HB1	2:D:301:1Q0:H40	2.00	0.43	
1:F:82:MET:O	1:F:85:HIS:N	2.51	0.43	
1:C:43:LEU:HG	2:C:301:1Q0:H54	2.01	0.43	
1:C:96:ARG:O	1:C:98:SER:N	2.52	0.43	
1:D:117:TRP:CH2	2:D:301:1Q0:CAW	3.02	0.43	
1:E:56:ASP:O	1:E:60:LYS:HG2	2.18	0.43	
1:F:72:GLN:H	1:F:72:GLN:HG2	1.68	0.43	
1:A:93:ASP:HB3	1:A:96:ARG:O	2.19	0.42	
1:C:191:LEU:O	1:C:195:GLN:HB2	2.19	0.42	
1:A:167:THR:OG1	1:A:170:VAL:HG23	2.19	0.42	
1:C:83:VAL:O	1:C:87:LEU:HB2	2.19	0.42	
1:C:24:LYS:H	1:C:24:LYS:HG2	1.48	0.42	
1:C:124:GLY:O	1:C:128:SER:HB3	2.20	0.42	
1:D:60:LYS:HE3	1:D:110:ARG:HG2	2.02	0.42	
1:C:62:ARG:HH11	1:C:62:ARG:HG3	1.85	0.42	
1:F:109:LEU:HD22	1:F:213:LEU:HD13	2.02	0.42	
1:F:179:PRO:HA	1:F:180:PRO:HD2	1.87	0.42	
1:F:195:GLN:HA	1:F:198:TYR:HB3	2.02	0.42	
1:C:36:TRP:CZ2	1:C:115:LEU:HD13	2.55	0.42	
1:E:8:PHE:O	1:E:10:LEU:HD22	2.19	0.42	
1:F:124:GLY:O	1:F:128:SER:HB3	2.19	0.42	
1:D:143:ASN:HA	1:D:147:ALA:HB3	2.02	0.42	
1:D:166:PRO:HD2	1:D:171:PHE:HE1	1.85	0.42	
1:B:17:PHE:CD2	1:B:194:ILE:HG12	2.54	0.42	
1:C:119:GLN:O	1:C:123:GLU:HB3	2.20	0.42	
1:F:90:ARG:HD3	1:F:90:ARG:HA	1.72	0.42	
1:C:90:ARG:HD3	1:E:208:HIS:O	2.20	0.41	
1:C:116:HIS:O	1:C:120:LEU:HB2	2.19	0.41	
2:E:301:1Q0:H42	2:E:301:1Q0:H50	2.02	0.41	
1:A:13:VAL:O	1:A:16:SER:OG	2.25	0.41	
1:A:98:SER:OG	1:A:99:HIS:N	2.53	0.41	
1:C:64:MET:HE1	1:C:104:GLY:HA2	2.02	0.41	
1:D:182:GLN:HA	1:D:185:GLN:HB2	2.01	0.41	
1:E:17:PHE:HD1	1:E:17:PHE:HA	1.73	0.41	
1:D:128:SER:O	1:D:168:ARG:NH2	2.53	0.41	
1:D:191:LEU:N	1:D:192:PRO:HD2	2.35	0.41	
1:E:59:SER:O	1:E:62:ARG:HB2	2.21	0.41	
1:F:79:LEU:O	1:F:83:VAL:HG23	2.21	0.41	
1:F:187:LEU:HD21	1:F:191:LEU:HD22	2.01	0.41	
1:F:135:SER:OG	1:F:136:ALA:N	2.53	0.41	



A + 1	A + 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:76:TYR:CE1	1:A:82:MET:HG3	2.54	0.41	
1:C:106:ARG:HG3	1:C:107:THR:N	2.34	0.41	
1:E:190:ALA:O	1:E:194:ILE:HG13	2.20	0.41	
1:A:30:ASP:HB2	1:A:31:PRO:HD3	2.01	0.41	
1:C:142:TYR:O	1:C:145:SER:N	2.39	0.41	
1:E:58:VAL:O	1:E:62:ARG:HG2	2.21	0.41	
1:E:71:PRO:HB2	1:E:72:GLN:OE1	2.20	0.41	
1:E:177:VAL:HG11	1:E:186:MET:SD	2.60	0.41	
1:F:31:PRO:HA	1:F:34:ALA:HB3	2.02	0.41	
1:F:117:TRP:NE1	1:F:141:SER:HB2	2.35	0.41	
1:F:108:VAL:HA	1:F:111:LEU:HD12	2.02	0.41	
1:B:53:ILE:HG13	1:B:54:SER:N	2.35	0.41	
1:D:22:ASP:OD1	1:D:26:GLU:N	2.45	0.41	
1:E:87:LEU:HD23	1:E:87:LEU:HA	1.82	0.41	
1:F:204:LEU:O	1:F:208:HIS:ND1	2.53	0.41	
1:F:11:LYS:O	1:F:15:VAL:HG13	2.21	0.40	
1:F:164:THR:O	1:F:164:THR:OG1	2.30	0.40	
1:F:175:MET:O	1:F:176:ASN:HB2	2.19	0.40	
1:C:76:TYR:CE1	1:C:82:MET:HG3	2.57	0.40	
1:A:177:VAL:HG21	1:A:183:ALA:HA	2.04	0.40	
1:B:138:CYS:HB3	1:B:162:PHE:CE2	2.56	0.40	
1:D:11:LYS:O	1:D:15:VAL:HG23	2.21	0.40	
1:C:49:ILE:H	1:C:49:ILE:HG12	1.58	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	Perce	ntiles
1	А	205/215~(95%)	195 (95%)	9 (4%)	1 (0%)	29	64
1	В	204/215~(95%)	188 (92%)	15 (7%)	1 (0%)	29	64



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	С	204/215~(95%)	174 (85%)	23 (11%)	7 (3%)	3	21
1	D	204/215~(95%)	190 (93%)	13~(6%)	1 (0%)	29	64
1	Ε	205/215~(95%)	188 (92%)	14 (7%)	3~(2%)	10	39
1	F	203/215~(94%)	180 (89%)	22 (11%)	1 (0%)	29	64
All	All	1225/1290~(95%)	1115 (91%)	96~(8%)	14 (1%)	14	46

All (14) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	Е	9	ASN
1	В	66	ARG
1	С	143	ASN
1	Е	166	PRO
1	С	97	ARG
1	С	186	MET
1	D	98	SER
1	С	17	PHE
1	С	166	PRO
1	С	188	GLY
1	F	98	SER
1	А	170	VAL
1	С	180	PRO
1	Е	194	ILE

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	Perc	centiles
1	А	182/190~(96%)	168 (92%)	14 (8%)	13	41
1	В	180/190~(95%)	164 (91%)	16 (9%)	9	34
1	\mathbf{C}	178/190~(94%)	153~(86%)	25 (14%)	3	15
1	D	181/190~(95%)	166 (92%)	15 (8%)	11	38
1	Е	180/190~(95%)	161 (89%)	19 (11%)	6	26



α \cdots 1	C		
Continued	trom	previous	<i>paae</i>
• • • • • • • • • • • •	J	<i>r</i> · · · · · · · · · · · · · · · · · · ·	r ~g ····

Mol	Chain	hain Analysed Rotameric Outliers		Percentiles	
1	F	175/190~(92%)	146 (83%)	29~(17%)	2 9
All	All	1076/1140~(94%)	958~(89%)	118 (11%)	6 25

All (118) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	29	LEU
1	А	43	LEU
1	А	72	GLN
1	А	73	SER
1	А	95	GLU
1	А	103	SER
1	А	106	ARG
1	А	146	LEU
1	А	152	TRP
1	А	164	THR
1	А	172	LEU
1	А	173	GLU
1	А	185	GLN
1	А	186	MET
1	В	10	LEU
1	В	13	VAL
1	В	14	LEU
1	В	23	GLU
1	В	43	LEU
1	В	53	ILE
1	В	62	ARG
1	В	68	ARG
1	В	97	ARG
1	В	106	ARG
1	В	115	LEU
1	В	120	LEU
1	В	134	THR
1	В	164	THR
1	В	181	GLU
1	В	182	GLN
1	С	14	LEU
1	С	23	GLU
1	С	24	LYS
1	С	26	GLU
1	С	30	ASP
1	С	43	LEU



Mol	Chain	Res	Type
1	С	49	ILE
1	С	72	GLN
1	С	78	SER
1	С	106	ARG
1	С	115	LEU
1	С	120	LEU
1	С	134	THR
1	С	137	LEU
1	С	138	CYS
1	С	146	LEU
1	С	153	VAL
1	С	164	THR
1	С	167	THR
1	С	171	PHE
1	С	182	GLN
1	С	191	LEU
1	С	195	GLN
1	С	197	VAL
1	С	200	VAL
1	D	45	SER
1	D	48	THR
1	D	73	SER
1	D	95	GLU
1	D	97	ARG
1	D	103	SER
1	D	106	ARG
1	D	128	SER
1	D	131	ASP
1	D	146	LEU
1	D	159	THR
1	D	170	VAL
1	D	171	PHE
1	D	189	GLU
1	D	203	LYS
1	Е	10	LEU
1	Е	15	VAL
1	Е	16	SER
1	Е	17	PHE
1	Е	21	LEU
1	Е	23	GLU
1	Е	29	LEU
1	Е	51	SER



Mol	Chain	Res	Type
1	Е	53	ILE
1	Е	78	SER
1	Е	95	GLU
1	Е	100	HIS
1	Е	106	ARG
1	Е	119	GLN
1	Е	128	SER
1	Е	156	ARG
1	Е	164	THR
1	Е	186	MET
1	Е	191	LEU
1	F	12	VAL
1	F	13	VAL
1	F	15	VAL
1	F	23	GLU
1	F	27	VAL
1	F	39	LEU
1	F	46	LEU
1	F	49	ILE
1	F	53	ILE
1	F	72	GLN
1	F	74	GLU
1	F	89	ASN
1	F	90	ARG
1	F	95	GLU
1	F	97	ARG
1	F	98	SER
1	F	103	SER
1	F	106	ARG
1	F	110	ARG
1	F	138	CYS
1	F	141	SER
1	F	153	VAL
1	F	154	VAL
1	F	175	MET
1	F	184	VAL
1	F	187	LEU
1	F	196	ARG
1	F	201	SER
1	F	205	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:



Mol	Chain	Res	Type
1	С	112	HIS
1	С	185	GLN
1	D	89	ASN
1	Е	89	ASN
1	F	85	HIS
1	F	116	HIS
1	F	195	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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).

Mal	Turne	Chain	Dec	Tinle	Bo	ond leng	$_{\rm ths}$	B	ond ang	gles		
IVIOI	туре	Chain	nes	nes	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1Q0	С	301	-	42,43,43	0.80	2 (4%)	46,48,48	0.81	3 (6%)		
2	1Q0	Е	301	-	42,43,43	0.81	2 (4%)	46,48,48	0.81	3 (6%)		
2	1Q0	F	301	-	14,15,43	1.10	2 (14%)	18,20,48	1.15	3 (16%)		
2	1Q0	А	301	-	42,43,43	0.81	2 (4%)	46,48,48	0.81	3 (6%)		
2	1Q0	В	301	-	$25,\!26,\!43$	1.05	2 (8%)	27,31,48	1.01	3 (11%)		
2	1Q0	D	301	-	42,43,43	0.97	3 (7%)	46,48,48	1.02	4 (8%)		



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	1Q0	С	301	-	-	23/46/46/46	-
2	1Q0	Е	301	-	-	23/46/46/46	-
2	1Q0	F	301	-	-	10/17/17/46	-
2	1Q0	А	301	-	-	18/46/46/46	-
2	1Q0	В	301	-	-	13/29/29/46	-
2	1Q0	D	301	-	-	22/46/46/46	_

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	301	1Q0	CBO-NBM	3.92	1.42	1.34
2	Е	301	1Q0	CBO-NBM	3.92	1.42	1.34
2	А	301	1Q0	CBO-NBM	3.91	1.42	1.34
2	С	301	1Q0	CBO-NBM	3.89	1.42	1.34
2	D	301	1Q0	CBQ-NBM	-3.38	1.40	1.46
2	D	301	1Q0	CBO-NBM	3.10	1.40	1.34
2	F	301	1Q0	CBO-NBM	2.31	1.42	1.34
2	Е	301	1Q0	CBQ-NBM	-2.26	1.42	1.46
2	А	301	1Q0	CBQ-NBM	-2.26	1.42	1.46
2	В	301	1Q0	CBQ-NBM	-2.24	1.42	1.46
2	С	301	1Q0	CBQ-NBM	-2.19	1.42	1.46
2	F	301	1Q0	CBQ-NBM	-2.17	1.42	1.46
2	D	301	1Q0	OAE-CBP	-2.03	1.39	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	D	301	1Q0	CBP-CBQ-NBM	-3.09	104.41	110.01
2	А	301	1Q0	CBK-CBO-NBM	2.42	120.02	115.83
2	С	301	1Q0	CBK-CBO-NBM	2.40	119.99	115.83
2	Е	301	1Q0	CBK-CBO-NBM	2.40	119.99	115.83
2	В	301	1Q0	CBK-CBO-NBM	2.39	119.98	115.83
2	F	301	1Q0	CBP-CAK-CAJ	-2.38	119.99	124.86
2	F	301	1Q0	CBK-CBO-NBM	2.30	119.99	116.10
2	D	301	1Q0	CBP-CAK-CAJ	-2.22	119.83	124.79
2	В	301	1Q0	CBP-CAK-CAJ	-2.17	119.94	124.79
2	А	301	1Q0	CBP-CAK-CAJ	-2.15	119.99	124.79



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	301	1Q0	CBP-CAK-CAJ	-2.15	119.99	124.79
2	Е	301	1Q0	CBP-CAK-CAJ	-2.13	120.04	124.79
2	D	301	1Q0	CBK-CBO-NBM	2.11	119.49	115.83
2	С	301	1Q0	CBQ-NBM-CBO	-2.07	119.99	123.48
2	Ε	301	1Q0	CBQ-NBM-CBO	-2.07	119.99	123.48
2	В	301	1Q0	CBQ-NBM-CBO	-2.07	119.99	123.48
2	D	301	1Q0	OAE-CBP-CAK	-2.07	105.31	110.85
2	А	301	1Q0	CBQ-NBM-CBO	-2.05	120.02	123.48
2	F	301	1Q0	CBQ-NBM-CBO	-2.05	119.99	122.90

There are no chirality outliers.

All (109) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	301	1Q0	CAK-CBP-CBQ-CBL
2	В	301	1Q0	OAE-CBP-CBQ-CBL
2	В	301	1Q0	OBN-CBL-CBQ-CBP
2	В	301	1Q0	OBN-CBL-CBQ-NBM
2	В	301	1Q0	CBL-OBN-PBR-OAG
2	С	301	1Q0	OBN-CBL-CBQ-NBM
2	С	301	1Q0	CBL-OBN-PBR-OAD
2	D	301	1Q0	OBN-CBL-CBQ-CBP
2	D	301	1Q0	OBN-CBL-CBQ-NBM
2	Е	301	1Q0	CBL-OBN-PBR-OAF
2	Е	301	1Q0	CBL-OBN-PBR-OAD
2	F	301	1Q0	CAP-CAJ-CAK-CBP
2	F	301	1Q0	CAJ-CAK-CBP-CBQ
2	F	301	1Q0	CBP-CBQ-NBM-CBO
2	F	301	1Q0	CBL-CBQ-NBM-CBO
2	F	301	1Q0	CBL-OBN-PBR-OAF
2	F	301	1Q0	CBL-OBN-PBR-OAD
2	Е	301	1Q0	CBJ-CBK-CBO-NBM
2	Е	301	1Q0	CBJ-CBK-CBO-OAC
2	D	301	1Q0	CBB-CBE-CBG-CBH
2	А	301	1Q0	CAM-CAR-CAW-CBB
2	F	301	1Q0	CAJ-CAK-CBP-OAE
2	С	301	1Q0	CAQ-CAV-CBA-CAX
2	А	301	1Q0	CAZ-CBC-CBF-CBH
2	D	301	1Q0	CAR-CAW-CBB-CBE
2	D	301	1Q0	CAQ-CAV-CBA-CAX
2	А	301	1Q0	CAP-CAU-CAZ-CBC
2	D	301	1Q0	CAP-CAU-CAZ-CBC



Mol	Chain	Res	Type	Atoms
2	С	301	1Q0	CAT-CAY-CBD-CBI
2	А	301	1Q0	CAL-CAQ-CAV-CBA
2	С	301	1Q0	CBE-CBG-CBH-CBF
2	С	301	1Q0	CBB-CBE-CBG-CBH
2	С	301	1Q0	CAU-CAZ-CBC-CBF
2	С	301	1Q0	CAL-CAQ-CAV-CBA
2	В	301	1Q0	CAT-CAY-CBD-CBI
2	А	301	1Q0	CBB-CBE-CBG-CBH
2	Е	301	1Q0	CAN-CAS-CAX-CBA
2	D	301	1Q0	CBC-CBF-CBH-CBG
2	D	301	1Q0	CAZ-CBC-CBF-CBH
2	D	301	1Q0	CAW-CBB-CBE-CBG
2	D	301	1Q0	CAY-CBD-CBI-CBJ
2	А	301	1Q0	CAU-CAZ-CBC-CBF
2	В	301	1Q0	CAI-CAH-CAN-CAS
2	А	301	1Q0	CBD-CBI-CBJ-CBK
2	Е	301	1Q0	CBB-CBE-CBG-CBH
2	А	301	1Q0	CAI-CAO-CAT-CAY
2	С	301	1Q0	CAI-CAO-CAT-CAY
2	С	301	1Q0	CAH-CAN-CAS-CAX
2	D	301	1Q0	CBE-CBG-CBH-CBF
2	А	301	1Q0	CAK-CAJ-CAP-CAU
2	В	301	1Q0	CAH-CAI-CAO-CAT
2	D	301	1Q0	CAK-CAJ-CAP-CAU
2	Е	301	1Q0	CAH-CAN-CAS-CAX
2	С	301	1Q0	CAN-CAS-CAX-CBA
2	D	301	1Q0	CAT-CAY-CBD-CBI
2	Е	301	1Q0	CAT-CAY-CBD-CBI
2	Е	301	1Q0	CAB-CAM-CAR-CAW
2	А	301	1Q0	CAB-CAM-CAR-CAW
2	С	301	1Q0	CBI-CBJ-CBK-CBO
2	Е	301	1Q0	CBL-OBN-PBR-OAG
2	D	301	1Q0	CAN-CAS-CAX-CBA
2	А	301	1Q0	CAY-CBD-CBI-CBJ
2	D	301	1Q0	CAB-CAM-CAR-CAW
2	Е	301	1Q0	CAK-CAJ-CAP-CAU
2	Е	301	1Q0	CAO-CAT-CAY-CBD
2	С	301	1Q0	CAO-CAT-CAY-CBD
2	Е	301	1Q0	CAA-CAL-CAQ-CAV
2	Е	301	1Q0	CAZ-CBC-CBF-CBH
2	F	301	1Q0	OBN-CBL-CBQ-CBP
2	Е	301	1Q0	CAM-CAR-CAW-CBB

Continued from previous page...



Mol	Chain	Res	Type	Atoms
2	С	301	1Q0	CAB-CAM-CAR-CAW
2	С	301	1Q0	CAY-CBD-CBI-CBJ
2	В	301	1Q0	CAO-CAT-CAY-CBD
2	С	301	1Q0	CBL-OBN-PBR-OAF
2	С	301	1Q0	CAK-CAJ-CAP-CAU
2	А	301	1Q0	OAE-CBP-CBQ-NBM
2	В	301	1Q0	OAE-CBP-CBQ-NBM
2	Е	301	1Q0	OAE-CBP-CBQ-NBM
2	F	301	1Q0	OAE-CBP-CBQ-NBM
2	D	301	1Q0	CAU-CAZ-CBC-CBF
2	Е	301	1Q0	CAS-CAX-CBA-CAV
2	Е	301	1Q0	OBN-CBL-CBQ-NBM
2	D	301	1Q0	CAO-CAT-CAY-CBD
2	В	301	1Q0	CAJ-CAK-CBP-OAE
2	С	301	1Q0	CBL-OBN-PBR-OAG
2	D	301	1Q0	CAS-CAX-CBA-CAV
2	Е	301	1Q0	CAH-CAI-CAO-CAT
2	А	301	1Q0	CAH-CAI-CAO-CAT
2	А	301	1Q0	CBC-CBF-CBH-CBG
2	А	301	1Q0	CAI-CAH-CAN-CAS
2	Е	301	1Q0	CAJ-CAP-CAU-CAZ
2	С	301	1Q0	CAA-CAL-CAQ-CAV
2	С	301	1Q0	CAZ-CBC-CBF-CBH
2	D	301	1Q0	CBI-CBJ-CBK-CBO
2	Е	301	1Q0	CBD-CBI-CBJ-CBK
2	А	301	1Q0	CBJ-CBK-CBO-OAC
2	В	301	1Q0	CBL-OBN-PBR-OAD
2	D	301	1Q0	CBL-OBN-PBR-OAF
2	D	301	1Q0	CBL-OBN-PBR-OAD
2	С	301	1Q0	CBJ-CBK-CBO-OAC
2	В	301	1Q0	CAJ-CAK-CBP-CBQ
2	D	301	1Q0	CBD-CBI-CBJ-CBK
2	F	301	1Q0	CBL-OBN-PBR-OAG
2	С	301	1Q0	OAE-CBP-CBQ-NBM
2	А	301	1Q0	CBJ-CBK-CBO-NBM
2	С	301	1Q0	CBJ-CBK-CBO-NBM
2	Е	301	1Q0	CAI-CAH-CAN-CAS
2	Е	301	1Q0	CAJ-CAK-CBP-OAE
2	А	301	1Q0	CBE-CBG-CBH-CBF

There are no ring outliers.

6 monomers are involved in 38 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	301	1Q0	1	0
2	Е	301	1Q0	11	0
2	F	301	1Q0	3	0
2	А	301	1Q0	9	0
2	В	301	1Q0	5	0
2	D	301	1Q0	9	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 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 sufficient must be highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.















5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	А	207/215~(96%)	-0.49	0 100 100	37, 63, 107, 132	0
1	В	206/215~(95%)	-0.35	1 (0%) 91 81	44, 79, 118, 142	0
1	С	206/215~(95%)	-0.28	0 100 100	49, 95, 140, 191	0
1	D	206/215~(95%)	-0.31	1 (0%) 91 81	47, 86, 130, 207	0
1	Е	207/215~(96%)	-0.42	0 100 100	44, 84, 129, 174	0
1	F	205/215~(95%)	0.32	14 (6%) 17 7	89, 149, 195, 226	0
All	All	1237/1290~(95%)	-0.26	16 (1%) 77 59	37, 89, 165, 226	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	185	GLN	3.5
1	F	71	PRO	3.1
1	F	26	GLU	2.8
1	F	91	LEU	2.6
1	F	132	ALA	2.4
1	В	62	ARG	2.4
1	F	170	VAL	2.1
1	F	95	GLU	2.1
1	F	209	SER	2.1
1	F	102	GLU	2.1
1	F	97	ARG	2.1
1	D	214	PRO	2.1
1	F	129	PRO	2.0
1	F	182	GLN	2.0
1	F	75	HIS	2.0
1	F	177	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	${f B} ext{-factors}({ m \AA}^2)$	Q < 0.9
2	1Q0	С	301	44/44	0.91	0.25	71,77,85,88	0
2	1Q0	D	301	44/44	0.92	0.23	82,85,88,89	0
2	1Q0	F	301	16/44	0.92	0.21	94,96,98,100	16
2	1Q0	Е	301	44/44	0.93	0.23	69,72,79,81	0
2	1Q0	А	301	44/44	0.93	0.25	$66,\!66,\!68,\!69$	0
2	1Q0	В	301	27/44	0.94	0.23	49,57,61,62	27

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.

