



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 10:11 AM EDT

PDB ID : 5E5U  
Title : Crystal structure of the complex between Carbonic anhydrase-like domain of PTPRG and Immunoglobulin domains 2-3 of CNTN6  
Authors : Nikolaienko, R.M.; Bouyain, S.  
Deposited on : 2015-10-09  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

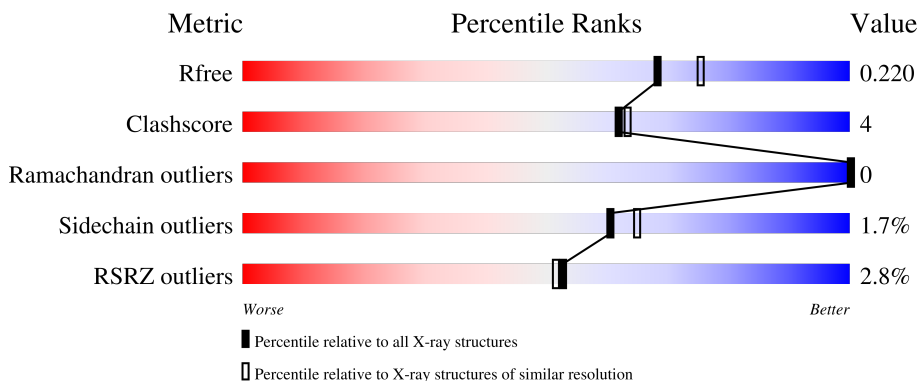
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	264	 7% 92% 8%
1	C	264	 2% 91% 8% .
2	B	199	 % 88% 11% .
2	D	199	 % 92% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FMT	A	404	-	X	-	-
4	FMT	B	402	-	X	-	-
5	MLI	A	405	-	-	X	-
7	MLT	D	401	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8039 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 gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2123	1353	364	401	5	0	0	0
1	C	264	2123	1353	364	401	5	0	0	0

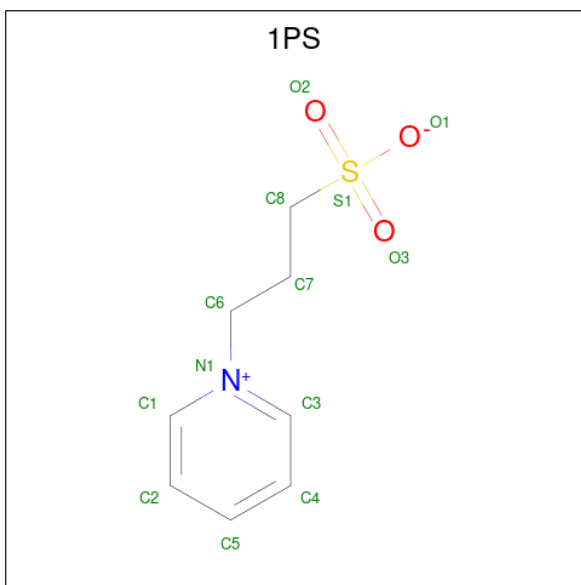
- Molecule 2 is a protein called Contactin-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	199	1573	1003	264	300	6	0	0	0
2	D	199	1573	1003	264	300	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

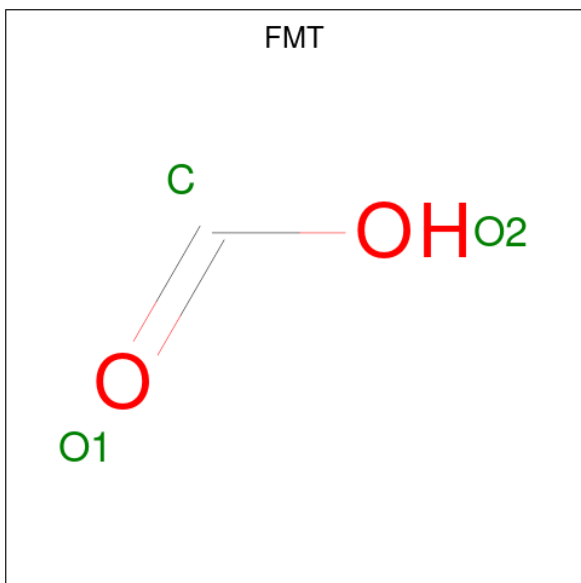
Chain	Residue	Modelled	Actual	Comment	Reference
B	118	SER	-	expression tag	UNP Q9JMB8
D	118	SER	-	expression tag	UNP Q9JMB8

- Molecule 3 is 3-PYRIDINIUM-1-YLPROPANE-1-SULFONATE (three-letter code: 1PS) (formula: C<sub>8</sub>H<sub>11</sub>NO<sub>3</sub>S).



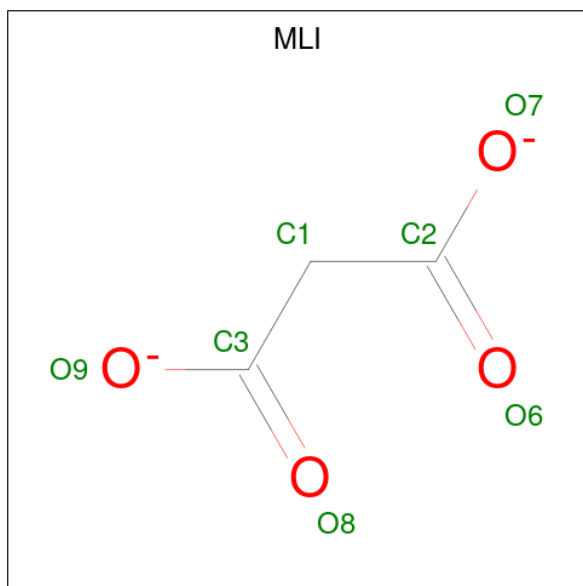
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	S			
3	A	1	Total	13	8	1	3	1	0	0
3	A	1	Total	13	8	1	3	1	0	0
3	C	1	Total	13	8	1	3	1	0	0
3	C	1	Total	13	8	1	3	1	0	0

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula:  $\text{CH}_2\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).



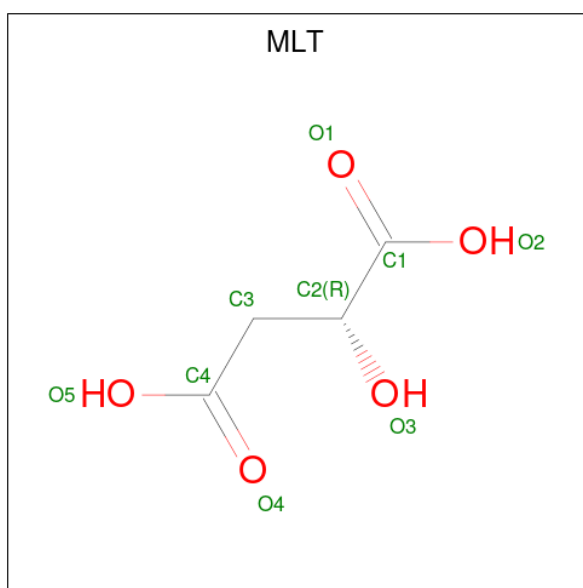
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 6 is ACETIC ACID (three-letter code: ACY) (formula:  $C_2H_4O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is D-MALATE (three-letter code: MLT) (formula:  $C_4H_6O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			9	4	5		
7	C	1	Total	C	O	0	0
			9	4	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			9	4	5		
7	D	1	Total	C	O	0	0
			9	4	5		

- Molecule 8 is water.

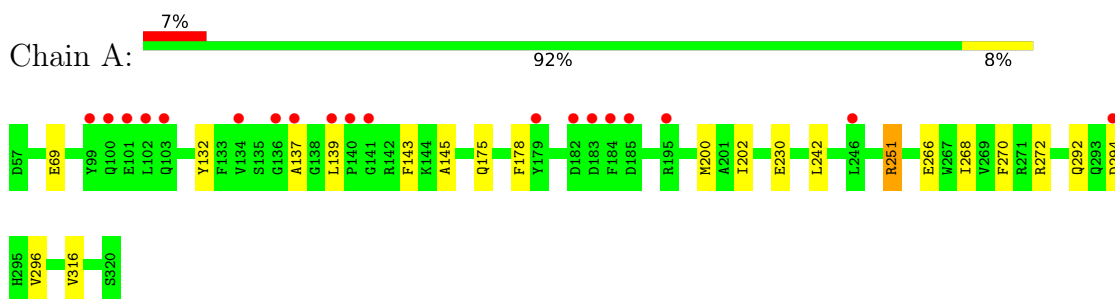
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	116	Total	O	0	0
			116	116		
8	B	126	Total	O	0	0
			126	126		
8	C	179	Total	O	0	0
			179	179		
8	D	114	Total	O	0	0
			114	114		



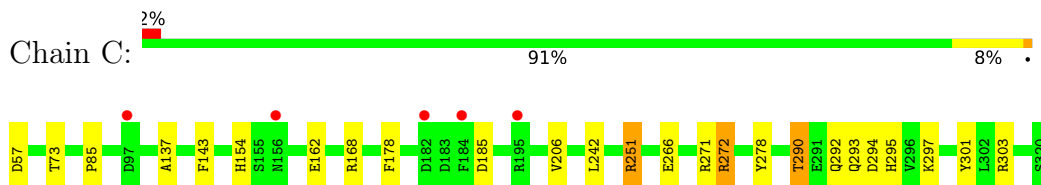
### 3 Residue-property plots [i](#)

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.

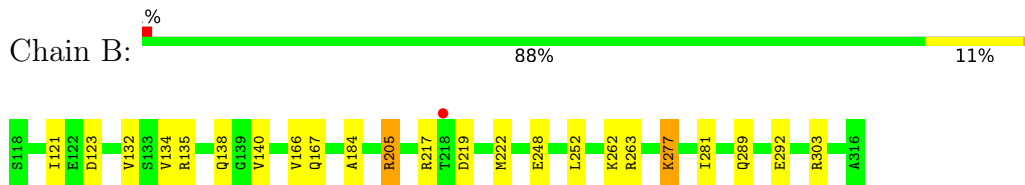
- Molecule 1: Receptor-type tyrosine-protein phosphatase gamma



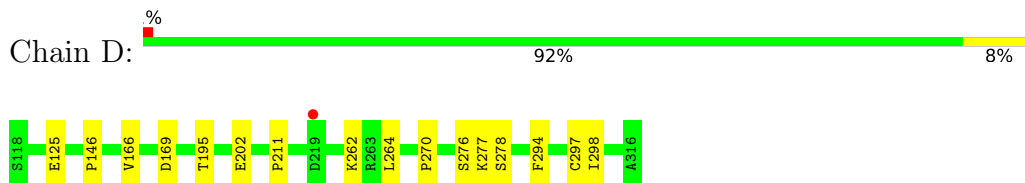
- Molecule 1: Receptor-type tyrosine-protein phosphatase gamma



- Molecule 2: Contactin-6



- Molecule 2: Contactin-6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.64Å 113.53Å 117.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.89 – 2.00 46.95 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (24.89-2.00) 93.2 (46.95-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.9	Depositor
R, $R_{free}$	0.168 , 0.217 0.171 , 0.220	Depositor DCC
$R_{free}$ test set	3524 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtrriage
Anisotropy	0.435	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.015 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8039	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MLI, ACY, FMT, 1PS, MLT

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	0.35	0/2188	0.50	0/2973
1	C	0.40	0/2188	0.53	0/2973
2	B	0.38	0/1613	0.52	0/2186
2	D	0.38	0/1613	0.51	0/2186
All	All	0.38	0/7602	0.51	0/10318

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	2123	0	1999	19	0
1	C	2123	0	1999	19	0
2	B	1573	0	1534	20	0
2	D	1573	0	1534	12	0
3	A	26	0	22	1	0
3	C	26	0	22	1	0
4	A	6	0	4	0	0
4	B	3	0	2	1	0
5	A	7	0	2	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	4	0	3	0	0
6	D	4	0	3	0	0
7	B	9	0	4	2	0
7	C	9	0	4	2	0
7	D	18	0	8	4	0
8	A	116	0	0	0	0
8	B	126	0	0	0	0
8	C	179	0	0	2	0
8	D	114	0	0	3	0
All	All	8039	0	7140	65	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (65) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLU:H	5:A:405:MLI:H12	1.44	0.83
1:C:290:THR:HG21	1:C:297:LYS:HE3	1.64	0.78
1:A:251:ARG:NH2	1:A:266:GLU:OE1	2.24	0.69
1:A:69:GLU:HB2	5:A:405:MLI:O7	1.93	0.68
2:B:166:VAL:O	4:B:402:FMT:H	1.97	0.65
2:D:169:ASP:O	8:D:501:HOH:O	2.15	0.65
1:C:292:GLN:O	3:C:402:1PS:H5	2.00	0.62
2:B:123:ASP:OD1	2:B:205:ARG:NH2	2.33	0.61
2:B:277:LYS:HD3	2:B:281:ILE:HD12	1.81	0.61
1:A:69:GLU:N	5:A:405:MLI:H12	2.16	0.60
2:B:121:ILE:O	2:B:205:ARG:NH1	2.35	0.60
1:A:200:MET:HE3	1:A:270:PHE:HE2	1.67	0.57
1:C:290:THR:CG2	1:C:297:LYS:HE3	2.34	0.56
1:A:143:PHE:HB3	1:A:178:PHE:HB3	1.88	0.56
1:C:143:PHE:HB3	1:C:178:PHE:HB3	1.88	0.55
1:A:251:ARG:HD2	1:A:268:ILE:HG12	1.89	0.55
2:B:138:GLN:HB2	2:B:222:MET:HE3	1.89	0.55
2:D:278:SER:HA	7:D:401:MLT:O3	2.07	0.54
2:D:166:VAL:O	8:D:501:HOH:O	2.18	0.54
2:B:205:ARG:HG2	2:B:205:ARG:HH11	1.73	0.54
1:C:57:ASP:N	1:C:57:ASP:OD1	2.40	0.54
2:B:248:GLU:HG2	2:B:281:ILE:HG12	1.91	0.53
2:B:303:ARG:NH1	7:B:403:MLT:H32	2.24	0.52
1:A:200:MET:HE1	1:A:242:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:HIS:HA	1:C:303:ARG:HD3	1.92	0.51
2:B:217:ARG:NH1	2:D:125:GLU:HG3	2.26	0.51
1:A:137:ALA:O	1:A:251:ARG:HD3	2.12	0.49
1:A:200:MET:CE	1:A:202:ILE:HD11	2.42	0.49
1:A:200:MET:HE2	1:A:202:ILE:HD11	1.95	0.49
1:C:57:ASP:HA	8:C:660:HOH:O	2.12	0.49
2:B:205:ARG:NH1	2:B:205:ARG:HG2	2.27	0.48
2:B:134:VAL:HG11	2:B:140:VAL:HG21	1.96	0.48
2:B:134:VAL:HG11	2:B:140:VAL:CG2	2.44	0.47
1:A:294:ASP:OD2	1:C:293:GLN:HB3	2.14	0.47
1:A:296:VAL:HG21	2:B:132:VAL:HG22	1.97	0.47
1:C:301:TYR:HD1	8:C:520:HOH:O	1.96	0.46
2:B:217:ARG:NH2	2:B:219:ASP:OD2	2.48	0.46
1:A:294:ASP:CG	1:C:294:ASP:H	2.19	0.46
1:C:85:PRO:HG3	1:C:162:GLU:HB3	1.97	0.46
1:C:294:ASP:HB3	1:C:295:HIS:ND1	2.30	0.46
2:B:262:LYS:HG2	2:B:263:ARG:O	2.16	0.45
2:D:270:PRO:HG3	8:D:566:HOH:O	2.16	0.45
2:B:303:ARG:HH12	7:B:403:MLT:H32	1.81	0.45
1:C:251:ARG:NH2	1:C:266:GLU:OE1	2.27	0.44
2:D:276:SER:HA	7:D:401:MLT:O1	2.16	0.44
5:A:405:MLI:C2	2:D:146:PRO:HD2	2.48	0.44
1:C:168:ARG:HE	7:C:403:MLT:C4	2.31	0.44
1:A:139:LEU:HD11	1:A:268:ILE:HD11	1.99	0.43
1:A:175:GLN:HA	1:A:200:MET:O	2.18	0.43
2:D:195:THR:HG22	2:D:211:PRO:HA	2.01	0.43
1:C:271:ARG:NE	7:C:403:MLT:O1	2.49	0.43
2:B:184:ALA:HA	2:B:252:LEU:HA	2.00	0.43
2:B:135:ARG:HD2	2:B:222:MET:HE2	2.01	0.42
2:D:264:LEU:HD12	2:D:294:PHE:HB3	2.01	0.42
1:A:294:ASP:H	1:C:294:ASP:CG	2.23	0.42
1:C:137:ALA:O	1:C:251:ARG:HD3	2.20	0.42
1:C:206:VAL:HG11	1:C:278:TYR:CE2	2.55	0.42
1:A:230:GLU:OE1	3:A:401:1PS:H1	2.19	0.42
2:D:278:SER:H	7:D:401:MLT:C1	2.33	0.41
2:D:277:LYS:N	7:D:401:MLT:O1	2.52	0.41
2:B:167:GLN:OE1	2:B:277:LYS:HE2	2.20	0.41
1:C:272:ARG:N	1:C:272:ARG:HD2	2.35	0.41
2:D:262:LYS:HG2	2:D:298:ILE:HD11	2.02	0.41
1:A:132:TYR:HB2	1:A:145:ALA:HB3	2.04	0.40
2:B:289:GLN:O	2:B:292:GLU:HG2	2.22	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	262/264 (99%)	250 (95%)	12 (5%)	0	100	100
1	C	262/264 (99%)	250 (95%)	12 (5%)	0	100	100
2	B	197/199 (99%)	197 (100%)	0	0	100	100
2	D	197/199 (99%)	196 (100%)	1 (0%)	0	100	100
All	All	918/926 (99%)	893 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	231/231 (100%)	227 (98%)	4 (2%)	60	65
1	C	231/231 (100%)	225 (97%)	6 (3%)	46	48
2	B	172/172 (100%)	170 (99%)	2 (1%)	71	76
2	D	172/172 (100%)	170 (99%)	2 (1%)	71	76
All	All	806/806 (100%)	792 (98%)	14 (2%)	60	65

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	ARG
1	A	272	ARG
1	A	292	GLN
1	A	316	VAL
2	B	205	ARG
2	B	277	LYS
1	C	73	THR
1	C	185	ASP
1	C	242	LEU
1	C	251	ARG
1	C	272	ARG
1	C	290	THR
2	D	202	GLU
2	D	297	CYS

Sometimes 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

14 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
3	1PS	A	402	-	13,13,13	2.86	6 (46%)	17,17,17	0.88	1 (5%)
3	1PS	A	401	-	13,13,13	2.83	6 (46%)	17,17,17	0.95	1 (5%)
6	ACY	B	401	-	3,3,3	0.67	0	3,3,3	0.98	0
7	MLT	C	403	-	8,8,8	1.28	0	10,10,10	1.92	2 (20%)
7	MLT	D	401	-	8,8,8	1.24	0	10,10,10	2.50	4 (40%)
4	FMT	A	404	-	2,2,2	2.63	2 (100%)	1,1,1	1.55	0
6	ACY	D	402	-	3,3,3	0.86	0	3,3,3	0.63	0
7	MLT	D	403	-	8,8,8	1.41	0	10,10,10	1.77	2 (20%)
7	MLT	B	403	-	8,8,8	1.41	1 (12%)	10,10,10	1.77	2 (20%)
5	MLI	A	405	-	6,6,6	1.22	0	7,7,7	1.65	1 (14%)
4	FMT	A	403	-	2,2,2	2.57	1 (50%)	1,1,1	1.60	0
4	FMT	B	402	-	2,2,2	2.82	2 (100%)	1,1,1	0.89	0
3	1PS	C	402	-	13,13,13	2.81	6 (46%)	17,17,17	1.04	2 (11%)
3	1PS	C	401	-	13,13,13	2.83	6 (46%)	17,17,17	1.02	1 (5%)

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	1PS	A	402	-	-	1/7/7/7	0/1/1/1
3	1PS	A	401	-	-	0/7/7/7	0/1/1/1
7	MLT	C	403	-	-	2/8/8/8	-
7	MLT	D	401	-	-	4/8/8/8	-
7	MLT	D	403	-	-	6/8/8/8	-
7	MLT	B	403	-	-	0/8/8/8	-
5	MLI	A	405	-	-	1/4/4/4	-
3	1PS	C	402	-	-	0/7/7/7	0/1/1/1
3	1PS	C	401	-	-	0/7/7/7	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	1PS	C1-C2	5.99	1.51	1.38
3	A	401	1PS	C1-C2	5.80	1.51	1.38
3	A	402	1PS	C1-C2	5.80	1.51	1.38
3	C	402	1PS	C1-C2	5.69	1.51	1.38
3	A	401	1PS	C5-C4	4.82	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	1PS	C5-C4	4.76	1.50	1.38
3	A	402	1PS	C5-C4	4.74	1.50	1.38
3	C	402	1PS	C5-C4	4.72	1.50	1.38
3	A	402	1PS	C3-C4	4.23	1.48	1.38
3	C	401	1PS	C3-C4	4.16	1.47	1.38
3	C	402	1PS	C3-C4	4.11	1.47	1.38
3	A	401	1PS	C3-C4	4.06	1.47	1.38
3	A	402	1PS	C1-N1	3.89	1.43	1.34
3	A	401	1PS	C1-N1	3.79	1.43	1.34
3	C	402	1PS	C1-N1	3.76	1.43	1.34
3	C	401	1PS	C1-N1	3.76	1.43	1.34
4	B	402	FMT	O1-C	3.28	1.39	1.22
4	A	403	FMT	O1-C	3.11	1.38	1.22
4	A	404	FMT	O1-C	3.09	1.38	1.22
3	A	402	1PS	C7-C8	-3.07	1.42	1.52
3	C	402	1PS	C7-C8	-3.03	1.42	1.52
3	A	401	1PS	C7-C8	-2.96	1.42	1.52
3	C	401	1PS	C7-C8	-2.82	1.43	1.52
3	A	402	1PS	C3-N1	2.49	1.40	1.34
3	A	401	1PS	C3-N1	2.43	1.40	1.34
3	C	402	1PS	C3-N1	2.38	1.40	1.34
4	B	402	FMT	O2-C	2.26	1.40	1.28
3	C	401	1PS	C3-N1	2.19	1.39	1.34
7	B	403	MLT	O3-C2	-2.09	1.38	1.42
4	A	404	FMT	O2-C	2.08	1.39	1.28

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	401	MLT	O2-C1-C2	5.13	123.98	112.72
7	C	403	MLT	O2-C1-C2	4.31	122.19	112.72
7	D	401	MLT	C2-C3-C4	3.63	121.11	112.13
7	B	403	MLT	O2-C1-C2	3.54	120.50	112.72
7	D	403	MLT	O2-C1-C2	3.37	120.12	112.72
7	D	401	MLT	O1-C1-C2	-3.16	116.36	122.54
3	C	401	1PS	O1-S1-C8	3.09	110.76	105.77
5	A	405	MLI	C3-C1-C2	3.00	123.37	112.87
3	A	401	1PS	O2-S1-C8	2.86	110.36	106.92
7	D	403	MLT	C2-C3-C4	2.74	118.91	112.13
7	C	403	MLT	O1-C1-C2	-2.26	118.12	122.54
3	A	402	1PS	O1-S1-C8	2.21	109.34	105.77
3	C	402	1PS	O3-S1-C8	2.11	109.46	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	1PS	O1-S1-C8	2.11	109.18	105.77
7	D	401	MLT	O5-C4-C3	2.10	120.79	114.07
7	B	403	MLT	C2-C3-C4	2.00	117.08	112.13

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	403	MLT	C1-C2-C3-C4
7	C	403	MLT	O3-C2-C3-C4
7	D	403	MLT	O1-C1-C2-O3
7	D	403	MLT	O1-C1-C2-C3
7	D	403	MLT	O2-C1-C2-O3
7	D	403	MLT	O2-C1-C2-C3
7	D	401	MLT	O1-C1-C2-O3
7	D	401	MLT	O2-C1-C2-O3
3	A	402	1PS	C6-C7-C8-S1
7	D	403	MLT	C2-C3-C4-O4
7	D	403	MLT	C2-C3-C4-O5
5	A	405	MLI	C2-C1-C3-O9
7	D	401	MLT	O1-C1-C2-C3
7	D	401	MLT	O2-C1-C2-C3

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	1PS	1	0
7	C	403	MLT	2	0
7	D	401	MLT	4	0
7	B	403	MLT	2	0
5	A	405	MLI	4	0
4	B	402	FMT	1	0
3	C	402	1PS	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	264/264 (100%)	0.14	19 (7%) 15 14	25, 39, 67, 90	0
1	C	264/264 (100%)	-0.22	5 (1%) 66 65	21, 32, 63, 89	0
2	B	199/199 (100%)	-0.30	1 (0%) 91 90	24, 37, 63, 94	0
2	D	199/199 (100%)	-0.27	1 (0%) 91 90	20, 38, 62, 93	0
All	All	926/926 (100%)	-0.15	26 (2%) 53 51	20, 37, 65, 94	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	PHE	5.1
1	A	195	ARG	3.9
1	C	184	PHE	3.9
1	A	102	LEU	3.5
1	A	137	ALA	3.4
1	A	141	GLY	3.1
1	A	182	ASP	3.1
1	C	156	ASN	3.0
1	A	136	GLY	2.9
1	A	139	LEU	2.8
1	A	183	ASP	2.7
1	A	185	ASP	2.6
1	A	294	ASP	2.6
1	C	97	ASP	2.6
1	C	195	ARG	2.5
1	A	100	GLN	2.5
1	C	182	ASP	2.4
1	A	134	VAL	2.4
2	B	218	THR	2.4
1	A	99	TYR	2.4
1	A	246	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	101	GLU	2.3
2	D	219	ASP	2.2
1	A	103	GLN	2.2
1	A	179	TYR	2.1
1	A	140	PRO	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	MLT	C	403	9/9	0.67	0.33	73,82,87,88	0
4	FMT	A	404	3/3	0.69	0.26	61,61,61,64	0
4	FMT	B	402	3/3	0.70	0.20	38,38,41,44	0
3	1PS	C	402	13/13	0.72	0.35	79,84,163,165	0
7	MLT	D	403	9/9	0.80	0.14	61,67,71,72	0
7	MLT	D	401	9/9	0.81	0.29	39,74,87,88	0
5	MLI	A	405	7/7	0.83	0.29	85,90,93,96	0
7	MLT	B	403	9/9	0.84	0.19	74,82,88,91	0
6	ACY	B	401	4/4	0.85	0.15	47,47,52,53	0
3	1PS	A	402	13/13	0.89	0.24	54,62,116,117	0
6	ACY	D	402	4/4	0.89	0.18	46,50,51,52	0
4	FMT	A	403	3/3	0.91	0.16	48,48,59,67	0
3	1PS	C	401	13/13	0.95	0.12	33,43,69,73	0
3	1PS	A	401	13/13	0.97	0.13	43,46,61,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.