



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:13 PM UTC

PDB ID : 1T0T / pdb_00001t0t
Title : Crystallographic structure of a putative chlorite dismutase
Authors : Gilski, M.; Borek, D.; Chen, Y.; Collart, F.; Joachimiak, A.; Otwinowski, Z.;
Midwest Center for Structural Genomics (MCSG)
Deposited on : 2004-04-12
Resolution : 1.75 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

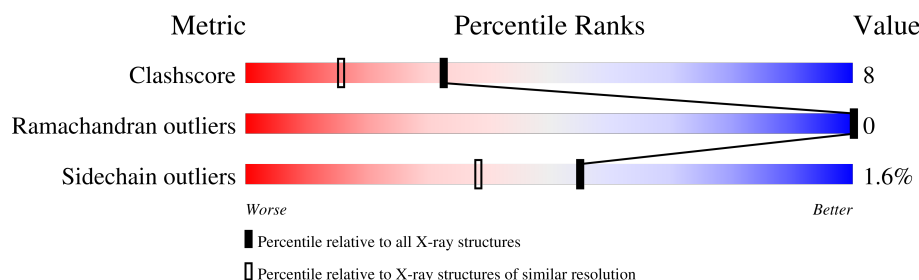
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	V	248	86% 11% .
1	W	248	81% 16% ..
1	X	248	84% 13% .
1	Y	248	88% 10% .
1	Z	248	88% 10% ..

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
3	P33	Y	4572	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11420 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.

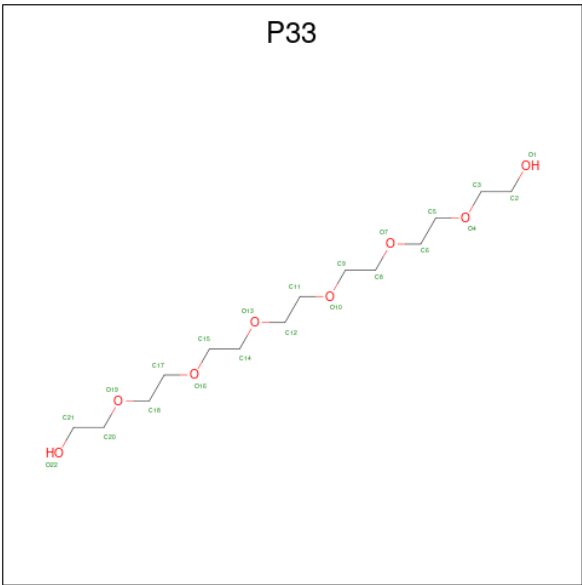
- Molecule 1 is a protein called APC35880.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	V	243	Total	C	N	O	S	0	0	0
			1996	1282	331	373	10			
1	W	243	Total	C	N	O	S	0	0	0
			1996	1282	331	373	10			
1	X	243	Total	C	N	O	S	0	0	0
			1996	1282	331	373	10			
1	Y	243	Total	C	N	O	S	0	0	0
			1996	1282	331	373	10			
1	Z	243	Total	C	N	O	S	0	0	0
			1996	1282	331	373	10			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	V	1	Total	Mg	0	0
			1	1		
2	W	1	Total	Mg	0	0
			1	1		
2	X	1	Total	Mg	0	0
			1	1		
2	Y	1	Total	Mg	0	0
			1	1		
2	Z	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 3,6,9,12,15,18-HEXAOSAICOSANE-1,20-DIOL (CCD ID: P33) (formula: C₁₄H₃₀O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	V	1	Total	C	O	0	0
			22	14	8		
3	W	1	Total	C	O	0	0
			22	14	8		
3	X	1	Total	C	O	0	0
			22	14	8		
3	Y	1	Total	C	O	0	0
			22	14	8		
3	Z	1	Total	C	O	0	0
			22	14	8		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	V	259	Total	O	0	0
			259	259		
4	W	255	Total	O	0	0
			255	255		
4	X	278	Total	O	0	0
			278	278		
4	Y	263	Total	O	0	0
			263	263		
4	Z	270	Total	O	0	0
			270	270		

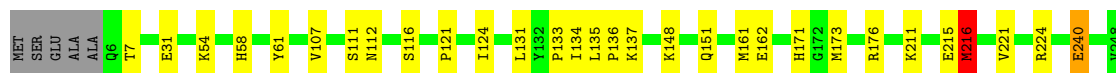
3 Residue-property plots

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

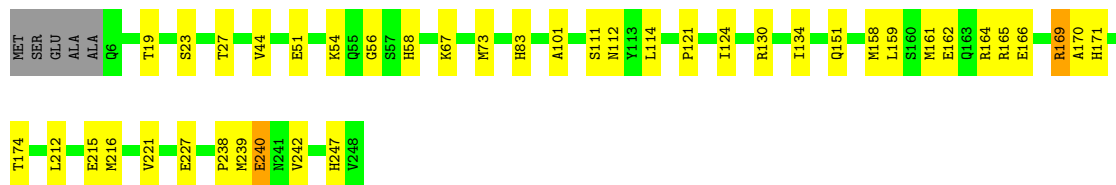
• Molecule 1: APC35880

Chain V: 



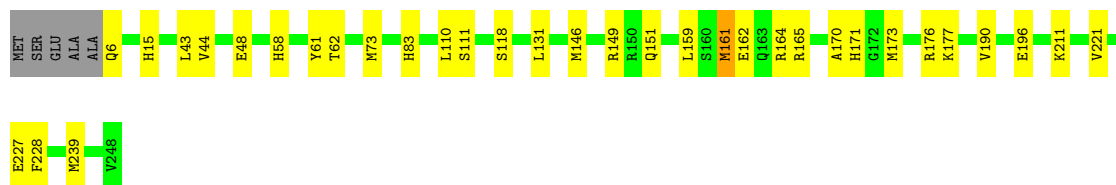
• Molecule 1: APC35880

Chain W: 



• Molecule 1: APC35880

Chain X: 



• Molecule 1: APC35880

Chain Y: 



• Molecule 1: APC35880

Chain Z: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	202.84Å 202.84Å 202.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.75	Depositor
% Data completeness (in resolution range)	99.8 (25.00-1.75)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0001	Depositor
R, R_{free}	0.156 , 0.194	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11420	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P33, MG

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	V	0.99	2/2048 (0.1%)	0.92	0/2774
1	W	1.00	0/2048	0.95	1/2774 (0.0%)
1	X	1.00	0/2048	0.94	0/2774
1	Y	0.95	0/2048	0.92	0/2774
1	Z	1.01	1/2048 (0.0%)	0.94	0/2774
All	All	0.99	3/10240 (0.0%)	0.93	1/13870 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	V	0	1
1	X	0	2
1	Z	0	2
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	216	MET	SD-CE	-6.63	1.62	1.79
1	Z	18	ARG	CG-CD	-6.54	1.32	1.52
1	V	215	GLU	C-O	-5.01	1.18	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	242	VAL	N-CA-C	6.39	117.14	110.62

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	V	61	TYR	Sidechain
1	X	61	TYR	Sidechain
1	X	62	THR	Mainchain
1	Z	18	ARG	Sidechain
1	Z	62	THR	Mainchain

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	V	1996	0	1931	23	0
1	W	1996	0	1931	46	0
1	X	1996	0	1931	26	0
1	Y	1996	0	1931	33	0
1	Z	1996	0	1931	21	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
2	Y	1	0	0	0	0
2	Z	1	0	0	0	0
3	V	22	0	30	3	0
3	W	22	0	30	8	0
3	X	22	0	30	1	0
3	Y	22	0	30	9	0
3	Z	22	0	30	5	0
4	V	259	0	0	17	0
4	W	255	0	0	18	0
4	X	278	0	0	16	0
4	Y	263	0	0	22	0
4	Z	270	0	0	13	0
All	All	11420	0	9805	157	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 8.

All (157) 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)
3:Z:5572:P33:C3	3:Z:5572:P33:O4	1.65	1.44
4:V:4140:HOH:O	1:W:83:HIS:HD2	1.32	1.11
1:Y:216:MET:HE1	3:Y:4572:P33:C11	1.80	1.11
1:W:212:LEU:HD11	1:W:216:MET:HE3	1.27	1.07
1:Y:216:MET:HE1	3:Y:4572:P33:H111	1.14	1.07
1:Z:146:MET:HB3	4:Z:5822:HOH:O	1.63	0.98
1:X:83:HIS:HD2	4:X:670:HOH:O	1.49	0.96
1:W:227:GLU:HG3	4:W:4202:HOH:O	1.68	0.93
1:Z:151:GLN:HG2	4:Z:5750:HOH:O	1.70	0.91
1:Y:216:MET:CE	3:Y:4572:P33:C11	2.50	0.90
1:X:151:GLN:HG2	4:X:677:HOH:O	1.78	0.84
1:Y:227:GLU:HG3	4:Y:974:HOH:O	1.77	0.83
1:Y:216:MET:CE	3:Y:4572:P33:H112	2.11	0.81
1:Z:146:MET:CB	4:Z:5822:HOH:O	2.27	0.78
1:V:31:GLU:CG	4:V:4183:HOH:O	2.31	0.77
3:Z:5572:P33:C3	3:Z:5572:P33:C5	2.62	0.77
1:Y:171:HIS:HD2	4:Y:772:HOH:O	1.67	0.77
1:Z:162:GLU:O	1:Z:166:GLU:HG2	1.83	0.76
1:X:146:MET:HE2	4:X:1285:HOH:O	1.84	0.76
1:W:171:HIS:HD2	4:W:4066:HOH:O	1.68	0.76
1:W:212:LEU:CD1	1:W:216:MET:HE3	2.12	0.75
1:Y:216:MET:CE	3:Y:4572:P33:H111	2.05	0.74
1:X:211:LYS:NZ	4:X:604:HOH:O	2.21	0.74
1:W:227:GLU:CD	4:W:4202:HOH:O	2.32	0.72
1:Z:148:LYS:NZ	1:Z:156:TRP:CZ2	2.56	0.72
1:Z:146:MET:HE3	1:Z:228:PHE:CE1	2.24	0.72
1:Y:171:HIS:CE1	3:Y:4572:P33:H121	2.27	0.70
1:Z:171:HIS:HD2	4:Z:5646:HOH:O	1.74	0.70
1:Y:171:HIS:HE1	4:Y:252:HOH:O	1.75	0.69
1:Y:148:LYS:NZ	4:Y:913:HOH:O	2.27	0.68
1:W:134:ILE:HD11	4:W:4092:HOH:O	1.92	0.68
1:X:161:MET:HE2	1:X:164:ARG:HH21	1.57	0.68
1:Y:6:GLN:N	4:Y:1355:HOH:O	2.25	0.68
1:V:31:GLU:HG2	4:V:4183:HOH:O	1.90	0.67
4:W:4034:HOH:O	1:Y:83:HIS:HE1	1.76	0.67
1:V:134:ILE:HD11	4:V:4182:HOH:O	1.94	0.66
1:Z:160:SER:OG	1:Z:163:GLN:HG3	1.96	0.66
3:X:3572:P33:H82	4:X:783:HOH:O	1.95	0.66
1:V:134:ILE:CD1	4:V:4182:HOH:O	2.43	0.65
1:Z:171:HIS:HE1	4:Z:5579:HOH:O	1.79	0.65
3:Y:4572:P33:H51	4:Y:282:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:134:ILE:CD1	4:W:4092:HOH:O	2.46	0.64
1:W:171:HIS:HE1	4:W:4005:HOH:O	1.81	0.64
1:W:112:ASN:O	1:W:130:ARG:NH2	2.26	0.64
1:W:216:MET:HE2	3:W:2572:P33:H112	1.80	0.64
1:V:211:LYS:NZ	4:V:4224:HOH:O	2.33	0.61
1:W:19:THR:HG22	4:W:4079:HOH:O	1.98	0.61
1:V:171:HIS:CD2	3:V:1572:P33:H121	2.36	0.61
1:V:173:MET:HE2	1:V:176:ARG:HD3	1.83	0.61
1:W:227:GLU:CG	4:W:4202:HOH:O	2.31	0.61
1:X:146:MET:HE3	1:X:228:PHE:CE1	2.36	0.60
1:W:216:MET:HE1	3:W:2572:P33:C11	2.32	0.59
1:Y:6:GLN:CA	4:Y:1355:HOH:O	2.50	0.59
1:V:107:VAL:CG1	1:Z:210:LYS:HE2	2.33	0.59
1:X:173:MET:HE3	4:X:691:HOH:O	2.03	0.59
4:V:4140:HOH:O	1:W:83:HIS:CD2	2.22	0.58
1:V:151:GLN:HG2	4:V:4143:HOH:O	2.04	0.58
1:W:216:MET:CE	3:W:2572:P33:H112	2.34	0.58
1:Y:34:GLU:HG3	4:Y:968:HOH:O	2.04	0.57
3:Z:5572:P33:H51	4:Z:5578:HOH:O	2.05	0.57
1:V:151:GLN:CG	4:V:4143:HOH:O	2.53	0.57
1:W:161:MET:SD	1:W:165:ARG:NH1	2.77	0.57
1:Y:227:GLU:CG	4:Y:974:HOH:O	2.44	0.56
1:Y:236:ARG:NH1	4:Y:1302:HOH:O	2.22	0.56
1:V:148:LYS:NZ	4:V:4066:HOH:O	2.38	0.56
1:Y:34:GLU:CG	4:Y:968:HOH:O	2.54	0.56
1:X:6:GLN:HB2	4:X:636:HOH:O	2.05	0.55
3:Y:4572:P33:H82	4:Y:282:HOH:O	2.05	0.55
1:Z:173:MET:HE3	4:Z:5709:HOH:O	2.06	0.55
1:W:19:THR:HG23	1:W:101:ALA:HB2	1.88	0.55
1:W:162:GLU:HB2	4:W:4246:HOH:O	2.06	0.55
1:W:44:VAL:HG11	1:W:239:MET:SD	2.47	0.55
1:W:54:LYS:HA	4:W:4092:HOH:O	2.06	0.54
1:W:239:MET:HG3	4:W:4135:HOH:O	2.08	0.54
1:W:216:MET:HE1	3:W:2572:P33:H92	1.89	0.53
1:Z:146:MET:HE2	4:Z:5775:HOH:O	2.08	0.53
1:X:110:LEU:HG	1:X:131:LEU:HD23	1.91	0.53
1:Z:15:HIS:HD2	4:Z:5593:HOH:O	1.92	0.53
1:Y:15:HIS:HD2	4:Y:758:HOH:O	1.91	0.53
1:V:240:GLU:H	1:V:240:GLU:CD	2.17	0.52
1:Z:58:HIS:HE1	4:Z:5610:HOH:O	1.91	0.52
1:X:15:HIS:HD2	4:X:497:HOH:O	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:216:MET:CE	3:W:2572:P33:C11	2.88	0.51
1:Y:208:GLN:NE2	4:Y:1001:HOH:O	2.42	0.50
1:X:58:HIS:HD2	4:X:500:HOH:O	1.96	0.49
1:Y:110:LEU:HD21	1:Y:130:ARG:HB2	1.93	0.49
1:Z:171:HIS:HB2	1:Z:221:VAL:HG11	1.93	0.49
1:X:173:MET:HE1	1:X:176:ARG:NE	2.28	0.49
1:X:162:GLU:HG3	1:X:165:ARG:NH2	2.26	0.49
1:Y:135:LEU:O	4:Y:811:HOH:O	2.20	0.48
3:V:1572:P33:H82	4:V:4240:HOH:O	2.12	0.48
1:X:149:ARG:NE	1:X:227:GLU:OE2	2.40	0.48
1:V:121:PRO:HA	1:V:124:ILE:HD12	1.96	0.48
1:W:166:GLU:OE2	1:W:169:ARG:NH2	2.47	0.48
1:V:216:MET:HG2	4:V:4031:HOH:O	2.13	0.48
1:Y:162:GLU:H	1:Y:162:GLU:CD	2.23	0.47
1:Y:169:ARG:O	1:Y:173:MET:HG2	2.15	0.47
1:W:216:MET:HE1	3:W:2572:P33:H111	1.96	0.47
1:X:58:HIS:HE1	4:X:536:HOH:O	1.98	0.47
1:Z:166:GLU:CD	1:Z:169:ARG:HH22	2.23	0.47
1:V:31:GLU:CB	4:V:4183:HOH:O	2.61	0.47
1:Y:58:HIS:HE1	4:Y:807:HOH:O	1.96	0.47
1:Y:7:THR:HG21	4:Y:969:HOH:O	2.15	0.47
1:W:171:HIS:HB2	1:W:221:VAL:HG11	1.97	0.46
1:Y:160:SER:OG	1:Y:163:GLN:HG3	2.16	0.46
1:V:173:MET:CE	1:V:176:ARG:HD3	2.45	0.46
1:V:224:ARG:HD2	1:W:158:MET:HE2	1.98	0.46
3:V:1572:P33:H51	4:V:4240:HOH:O	2.15	0.46
1:Y:171:HIS:ND1	3:Y:4572:P33:H121	2.31	0.46
1:V:116:SER:OG	4:V:4133:HOH:O	2.20	0.46
1:V:171:HIS:HB2	1:V:221:VAL:HG11	1.97	0.46
1:W:216:MET:CE	3:W:2572:P33:H92	2.47	0.45
1:X:44:VAL:HG11	1:X:239:MET:SD	2.55	0.45
1:X:83:HIS:CD2	4:X:670:HOH:O	2.38	0.45
1:X:171:HIS:HB2	1:X:221:VAL:HG11	1.98	0.45
1:Z:148:LYS:HE3	4:Z:5704:HOH:O	2.16	0.45
1:W:121:PRO:HA	1:W:124:ILE:HD12	1.99	0.45
1:V:58:HIS:HE1	4:V:4028:HOH:O	2.00	0.45
1:Z:227:GLU:HG3	4:Z:5782:HOH:O	2.17	0.45
1:Y:31:GLU:CD	4:Y:1013:HOH:O	2.60	0.44
1:W:170:ALA:HB2	4:W:4209:HOH:O	2.17	0.44
1:X:48:GLU:OE2	4:X:536:HOH:O	2.21	0.44
1:Z:110:LEU:HD21	1:Z:130:ARG:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:207:LEU:O	1:Z:211:LYS:HG3	2.17	0.44
3:Z:5572:P33:H82	4:Z:5578:HOH:O	2.17	0.44
1:W:247:HIS:HD2	4:W:4193:HOH:O	2.01	0.43
1:X:190:VAL:HG22	1:X:196:GLU:HG2	1.99	0.43
1:W:169:ARG:CD	4:W:4217:HOH:O	2.66	0.43
1:W:238:PRO:HB2	1:W:240:GLU:CD	2.43	0.43
1:Z:161:MET:HE2	1:Z:161:MET:HB2	1.59	0.43
1:W:171:HIS:CE1	3:W:2572:P33:H121	2.53	0.43
1:Y:93:LYS:NZ	4:Y:951:HOH:O	2.33	0.43
1:W:174:THR:HG23	1:W:215:GLU:HG2	2.00	0.43
1:X:170:ALA:HB2	4:X:754:HOH:O	2.18	0.43
3:Z:5572:P33:O4	3:Z:5572:P33:C2	2.59	0.43
1:W:114:LEU:C	1:W:114:LEU:HD23	2.44	0.42
1:X:151:GLN:CG	4:X:677:HOH:O	2.53	0.42
1:W:169:ARG:CG	4:W:4217:HOH:O	2.68	0.42
1:W:19:THR:HG21	4:W:4049:HOH:O	2.19	0.42
1:W:51:GLU:HA	1:W:56:GLY:O	2.20	0.42
1:X:43:LEU:HD11	4:X:611:HOH:O	2.19	0.42
1:W:23:SER:O	1:W:27:THR:HG23	2.20	0.41
1:X:159:LEU:O	1:X:164:ARG:NH1	2.53	0.41
1:V:131:LEU:C	1:V:133:PRO:HD3	2.46	0.41
1:Y:236:ARG:HD3	4:Y:1302:HOH:O	2.19	0.41
1:Y:135:LEU:HA	1:Y:136:PRO:HD3	1.85	0.41
1:Y:34:GLU:OE1	4:Y:887:HOH:O	2.22	0.41
1:W:58:HIS:HA	1:W:73:MET:O	2.21	0.41
1:V:135:LEU:HA	1:V:136:PRO:HD3	1.91	0.41
1:X:58:HIS:HA	1:X:73:MET:O	2.20	0.41
1:W:169:ARG:HD2	4:W:4217:HOH:O	2.19	0.41
1:W:67:LYS:HB2	1:W:67:LYS:HE2	1.96	0.40
1:W:151:GLN:NE2	4:Y:950:HOH:O	2.54	0.40
1:X:177:LYS:HE2	4:X:646:HOH:O	2.20	0.40
1:W:159:LEU:O	1:W:164:ARG:NH1	2.54	0.40
1:V:7:THR:HG21	4:V:4212:HOH:O	2.20	0.40
1:Y:221:VAL:O	1:Y:225:PHE:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	V	241/248 (97%)	236 (98%)	5 (2%)	0	100	100
1	W	241/248 (97%)	236 (98%)	5 (2%)	0	100	100
1	X	241/248 (97%)	235 (98%)	6 (2%)	0	100	100
1	Y	241/248 (97%)	236 (98%)	5 (2%)	0	100	100
1	Z	241/248 (97%)	236 (98%)	5 (2%)	0	100	100
All	All	1205/1240 (97%)	1179 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	V	215/218 (99%)	207 (96%)	8 (4%)	30	11
1	W	215/218 (99%)	212 (99%)	3 (1%)	59	44
1	X	215/218 (99%)	212 (99%)	3 (1%)	59	44
1	Y	215/218 (99%)	215 (100%)	0	100	100
1	Z	215/218 (99%)	212 (99%)	3 (1%)	59	44
All	All	1075/1090 (99%)	1058 (98%)	17 (2%)	55	38

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	54	LYS
1	V	111	SER
1	V	112	ASN
1	V	137	LYS
1	V	161	MET
1	V	162	GLU
1	V	216	MET
1	V	240	GLU
1	W	111	SER
1	W	169	ARG
1	W	240	GLU
1	X	111	SER
1	X	118	SER
1	X	161	MET
1	Z	118	SER
1	Z	161	MET
1	Z	244	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	V	58	HIS
1	V	83	HIS
1	V	184	GLN
1	W	30	ASN
1	W	83	HIS
1	W	153	ASN
1	W	171	HIS
1	W	208	GLN
1	W	241	ASN
1	X	15	HIS
1	X	30	ASN
1	X	58	HIS
1	X	83	HIS
1	X	112	ASN
1	X	208	GLN
1	X	247	HIS
1	Y	15	HIS
1	Y	30	ASN
1	Y	58	HIS
1	Y	83	HIS
1	Y	171	HIS
1	Z	15	HIS

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Mol	Chain	Res	Type
1	Z	58	HIS
1	Z	83	HIS
1	Z	151	GLN
1	Z	171	HIS
1	Z	184	GLN
1	Z	208	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

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	P33	Y	4572	-	21,21,21	1.14	3 (14%)	20,20,20	1.86	2 (10%)
3	P33	X	3572	-	21,21,21	1.14	3 (14%)	20,20,20	1.61	3 (15%)
3	P33	V	1572	-	21,21,21	1.25	3 (14%)	20,20,20	2.07	5 (25%)
3	P33	W	2572	-	21,21,21	1.12	2 (9%)	20,20,20	1.79	2 (10%)
3	P33	Z	5572	-	21,21,21	1.82	4 (19%)	20,20,20	2.29	3 (15%)

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	P33	Y	4572	-	-	6/19/19/19	-
3	P33	X	3572	-	-	4/19/19/19	-
3	P33	V	1572	-	-	4/19/19/19	-
3	P33	W	2572	-	-	5/19/19/19	-
3	P33	Z	5572	-	-	5/19/19/19	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Z	5572	P33	O4-C3	5.41	1.65	1.42
3	Z	5572	P33	C8-C9	3.71	1.67	1.49
3	V	1572	P33	O10-C9	3.18	1.55	1.42
3	X	3572	P33	O10-C9	2.99	1.55	1.42
3	W	2572	P33	O10-C9	2.97	1.54	1.42
3	Z	5572	P33	O4-C5	2.94	1.54	1.42
3	Z	5572	P33	O7-C6	2.89	1.54	1.42
3	V	1572	P33	C8-C9	2.83	1.63	1.49
3	Y	4572	P33	C8-C9	2.74	1.62	1.49
3	V	1572	P33	O7-C6	2.52	1.53	1.42
3	Y	4572	P33	O10-C9	2.47	1.52	1.42
3	X	3572	P33	C8-C9	2.34	1.60	1.49
3	W	2572	P33	C8-C9	2.23	1.60	1.49
3	Y	4572	P33	O7-C6	2.09	1.51	1.42
3	X	3572	P33	O4-C3	2.01	1.50	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	4572	P33	O7-C8-C9	7.12	142.79	110.35
3	Z	5572	P33	O7-C8-C9	6.96	142.08	110.35
3	V	1572	P33	O7-C8-C9	6.78	141.27	110.35
3	W	2572	P33	O7-C8-C9	6.08	138.05	110.35
3	Z	5572	P33	O4-C5-C6	5.44	135.16	110.35
3	X	3572	P33	O7-C8-C9	4.75	131.99	110.35
3	V	1572	P33	C9-O10-C11	3.89	130.29	113.26
3	X	3572	P33	C9-O10-C11	3.61	129.05	113.26
3	Z	5572	P33	C9-O10-C11	3.40	128.12	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	4572	P33	C9-O10-C11	3.11	126.89	113.26
3	W	2572	P33	C9-O10-C11	2.82	125.59	113.26
3	V	1572	P33	C15-O16-C17	-2.41	102.70	113.26
3	V	1572	P33	O13-C14-C15	-2.19	100.39	110.35
3	V	1572	P33	O10-C9-C8	-2.15	100.54	110.35
3	X	3572	P33	O10-C11-C12	-2.07	100.91	110.35

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	W	2572	P33	O7-C8-C9-O10
3	Z	5572	P33	O7-C8-C9-O10
3	X	3572	P33	O7-C8-C9-O10
3	Y	4572	P33	O7-C8-C9-O10
3	V	1572	P33	C5-C6-O7-C8
3	X	3572	P33	C5-C6-O7-C8
3	V	1572	P33	O7-C8-C9-O10
3	W	2572	P33	C5-C6-O7-C8
3	X	3572	P33	C8-C9-O10-C11
3	V	1572	P33	O19-C20-C21-O22
3	Y	4572	P33	C2-C3-O4-C5
3	Y	4572	P33	C5-C6-O7-C8
3	X	3572	P33	O19-C20-C21-O22
3	Z	5572	P33	C2-C3-O4-C5
3	Y	4572	P33	O10-C11-C12-O13
3	Z	5572	P33	O1-C2-C3-O4
3	Y	4572	P33	C8-C9-O10-C11
3	W	2572	P33	C11-C12-O13-C14
3	Y	4572	P33	C11-C12-O13-C14
3	W	2572	P33	C8-C9-O10-C11
3	V	1572	P33	O4-C5-C6-O7
3	W	2572	P33	O4-C5-C6-O7
3	Z	5572	P33	C8-C9-O10-C11
3	Z	5572	P33	O4-C5-C6-O7

There are no ring outliers.

5 monomers are involved in 26 short contacts:

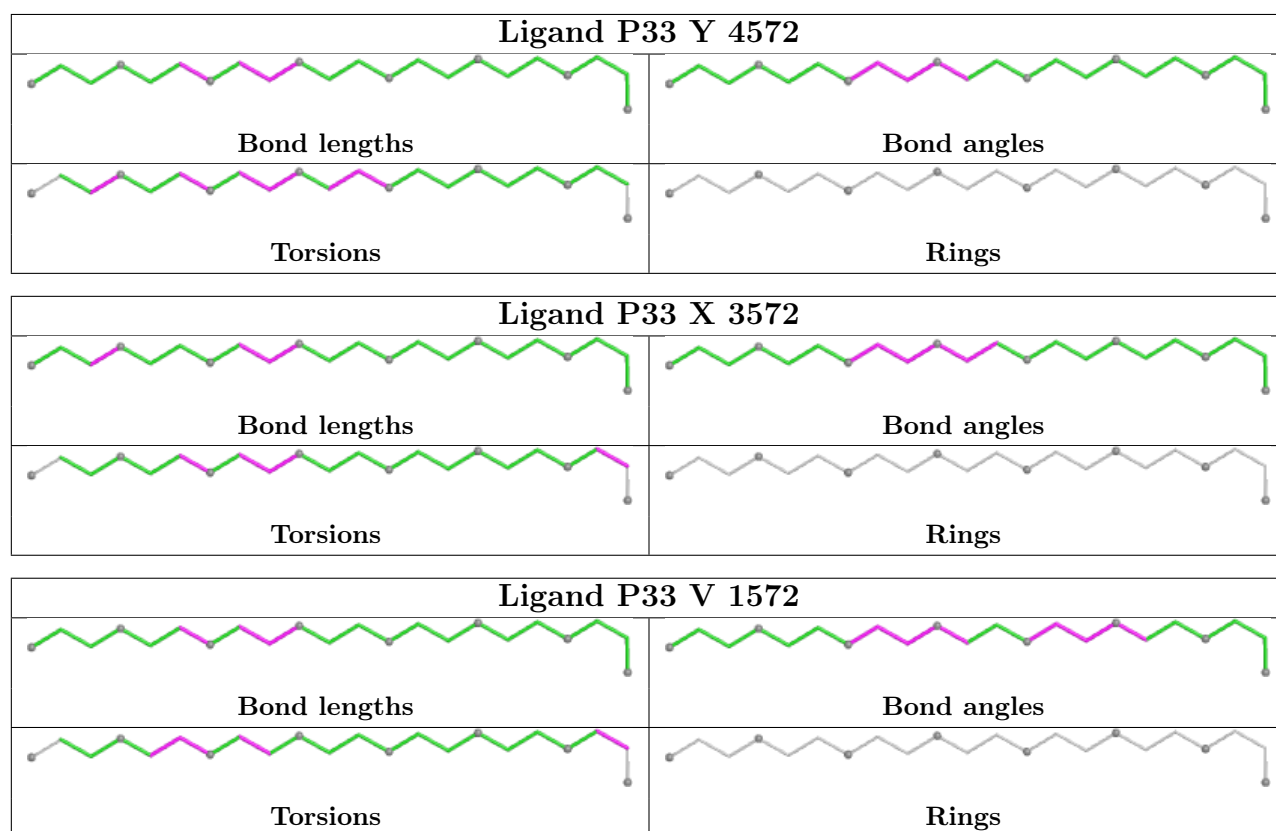
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Y	4572	P33	9	0

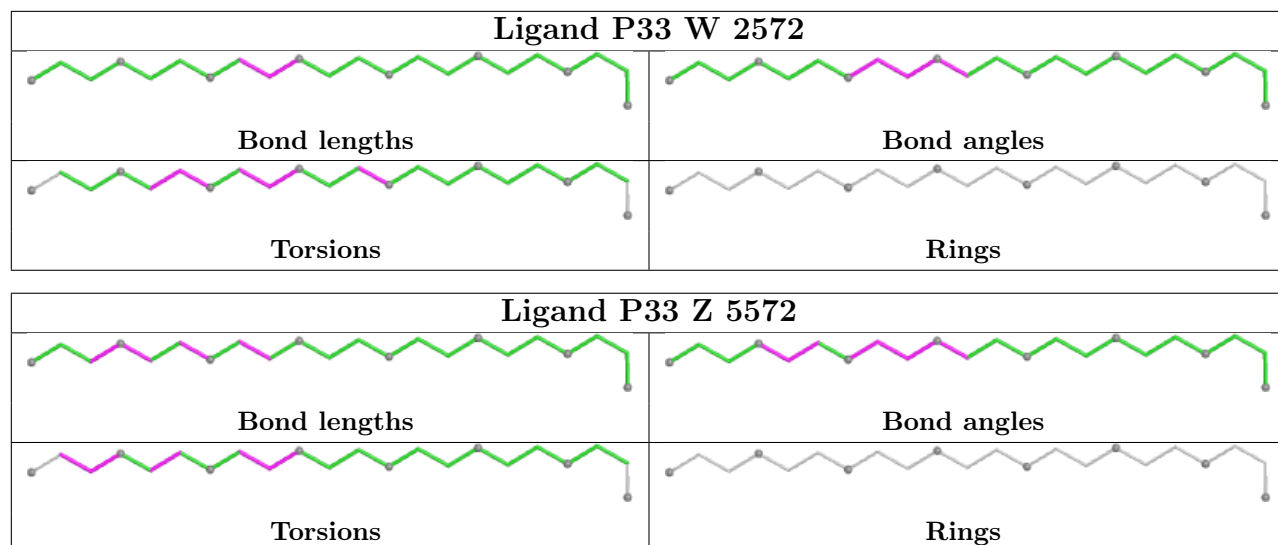
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	3572	P33	1	0
3	V	1572	P33	3	0
3	W	2572	P33	8	0
3	Z	5572	P33	5	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.