



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:30 PM UTC

PDB ID : 2O95 / pdb_00002o95
Title : Crystal Structure of the Metal-Free Dimeric Human Mov34 MPN domain (residues 1-186)
Authors : Sanches, M.; Alves, B.S.C.; Zanchin, N.I.T.; Guimaraes, B.G.
Deposited on : 2006-12-13
Resolution : 1.95 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

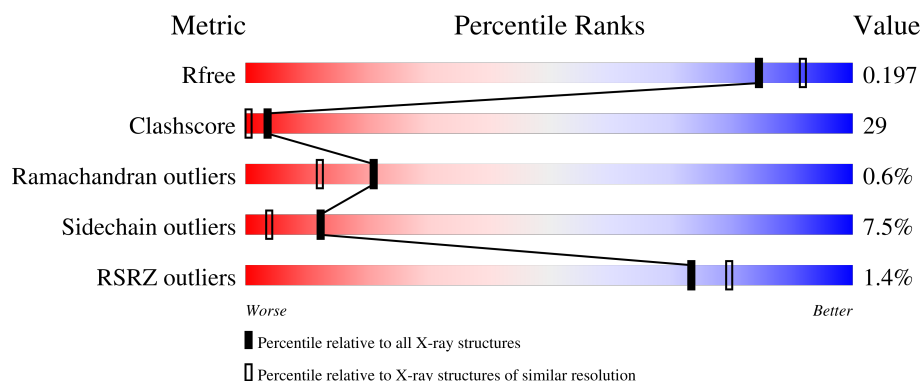
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 $\leq 5\%$. 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	187	2% 56% 33% 5%
1	B	187	% 58% 32% 6%

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	12P	A	2001	-	-	X	-
6	ETE	B	2002	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3358 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 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	35	6	0
			1472	940	248	277	7			
1	B	176	Total	C	N	O	S	25	4	0
			1437	919	242	270	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	cloning artifact	UNP P51665
B	0	GLY	-	cloning artifact	UNP P51665

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



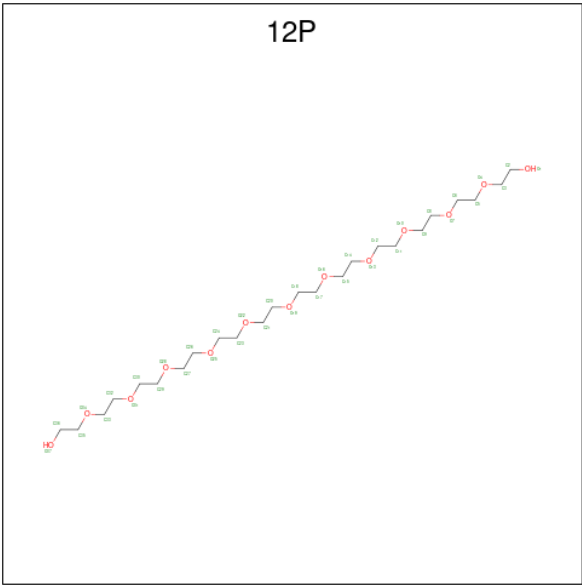
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	1
			10	8	2		

- Molecule 3 is DODECAETHYLENE GLYCOL (CCD ID: 12P) (formula: C₂₄H₅₀O₁₃).



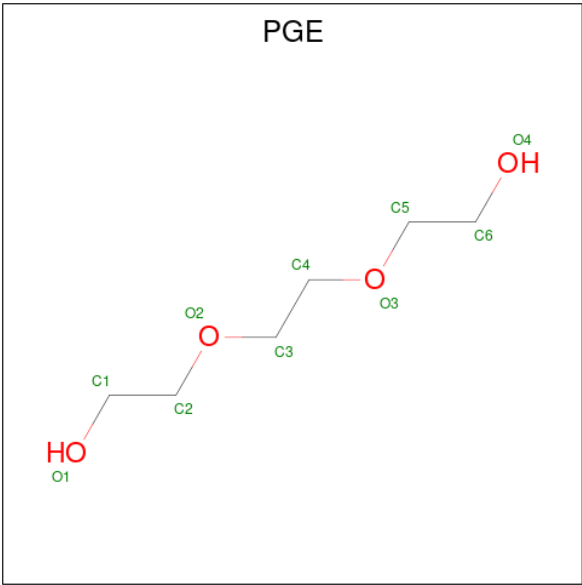
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			36	24	12		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			16	10	6		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



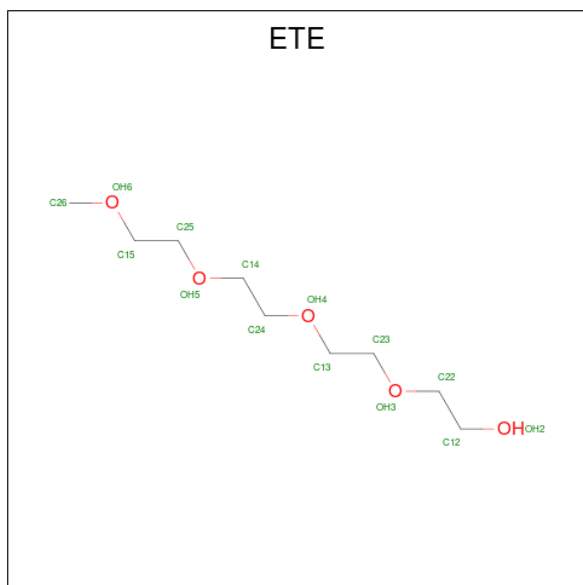
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	1
			13	8	5		

Continued on next page...

Continued from previous page...

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

- Molecule 6 is 2-{2-[2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: ETE) (formula: C₉H₂₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			14	9	5		

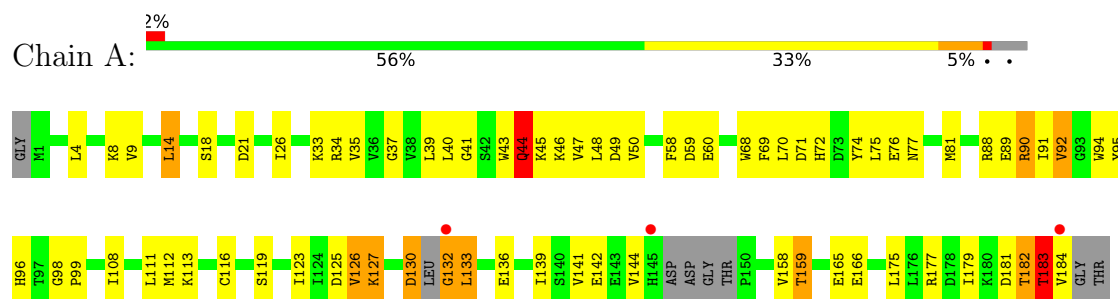
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	153	Total	O	0	0
			153	153		
7	B	167	Total	O	0	0
			167	167		

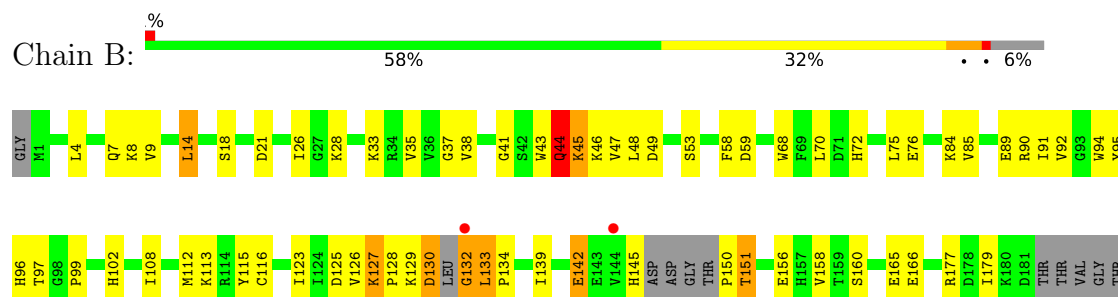
3 Residue-property plots

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 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: 26S proteasome non-ATPase regulatory subunit 7



- Molecule 1: 26S proteasome non-ATPase regulatory subunit 7



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	114.10Å 95.29Å 58.99Å 90.00° 121.13° 90.00°	Depositor
Resolution (Å)	30.21 – 1.95 30.21 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.21-1.95) 99.7 (30.21-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.240 (Not available) , 0.197	Depositor DCC
R_{free} test set	1973 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for k+l,h+l,-l 0.011 for -k+l,-h-l,-l 0.487 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3358	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, 12P, ETE, PG4, SO4

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	1.19	7/1505 (0.5%)	1.18	11/2038 (0.5%)
1	B	1.17	5/1470 (0.3%)	1.16	10/1990 (0.5%)
All	All	1.18	12/2975 (0.4%)	1.17	21/4028 (0.5%)

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	A	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	THR	C-O	-10.25	1.11	1.23
1	A	144	VAL	C-O	6.06	1.32	1.24
1	B	28	LYS	CD-CE	-5.96	1.34	1.52
1	B	72	HIS	C-O	-5.80	1.16	1.24
1	A	158	VAL	C-N	5.68	1.40	1.33
1	A	144	VAL	C-N	5.61	1.41	1.33
1	A	46	LYS	CG-CD	-5.58	1.35	1.52
1	B	132	GLY	N-CA	5.42	1.54	1.45
1	B	177	ARG	CB-CG	-5.22	1.36	1.52
1	A	132	GLY	N-CA	5.20	1.53	1.45
1	A	90	ARG	C-O	-5.18	1.17	1.23
1	B	90	ARG	C-O	-5.13	1.17	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	LYS	CA-C-N	7.72	128.12	119.32
1	B	127	LYS	C-N-CA	7.72	128.12	119.32
1	B	179	ILE	N-CA-C	6.86	118.43	109.58
1	A	89	GLU	N-CA-C	-6.73	99.08	109.24
1	A	127	LYS	CA-C-N	6.68	126.93	119.32
1	A	127	LYS	C-N-CA	6.68	126.93	119.32
1	A	126	VAL	CG1-CB-CG2	-6.66	96.15	110.80
1	B	44	GLN	CA-C-N	-6.51	114.31	123.03
1	B	44	GLN	C-N-CA	-6.51	114.31	123.03
1	A	179	ILE	N-CA-C	6.43	117.88	109.58
1	A	44	GLN	CA-C-N	-6.24	113.89	122.87
1	A	44	GLN	C-N-CA	-6.24	113.89	122.87
1	B	89	GLU	N-CA-C	-6.20	99.65	109.07
1	B	133	LEU	CA-C-N	6.18	126.08	119.28
1	B	133	LEU	C-N-CA	6.18	126.08	119.28
1	A	46	LYS	N-CA-C	-6.14	106.20	113.38
1	B	126	VAL	CG1-CB-CG2	-6.12	97.34	110.80
1	A	133	LEU	CA-C-N	5.76	125.61	119.28
1	A	133	LEU	C-N-CA	5.76	125.61	119.28
1	B	46	LYS	N-CA-C	-5.32	107.15	113.38
1	A	92	VAL	N-CA-C	-5.32	107.94	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	ASP	Peptide

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	1472	0	1468	97	4
1	B	1437	0	1431	65	4
2	A	5	0	0	0	0
2	B	15	0	0	1	0
3	A	36	0	47	41	0
4	A	16	0	10	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	20	0	28	0	0
5	B	23	0	24	2	0
6	B	14	0	20	24	0
7	A	153	0	0	10	0
7	B	167	0	0	10	0
All	All	3358	0	3028	174	4

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 29.

All (174) 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:182:THR:HA	1:A:183:THR:CB	1.47	1.33
1:A:59:ASP:OD1	3:A:2001:12P:H231	1.27	1.30
1:A:69:PHE:HD2	3:A:2001:12P:H91	1.03	1.12
1:A:33:LYS:HD2	3:A:2001:12P:H261	1.18	1.11
1:A:182:THR:CB	1:A:183:THR:HB	1.81	1.10
1:A:182:THR:CA	1:A:183:THR:CB	2.30	1.10
1:A:182:THR:CA	1:A:183:THR:HB	1.80	1.07
1:A:33:LYS:CD	3:A:2001:12P:H261	1.85	1.06
1:A:69:PHE:CD2	3:A:2001:12P:H91	1.91	1.05
1:A:60:GLU:OE2	3:A:2001:12P:H302	1.58	1.03
1:A:182:THR:OG1	1:A:183:THR:HB	1.59	1.02
1:A:59:ASP:OD1	3:A:2001:12P:C23	2.12	0.98
1:A:182:THR:HA	1:A:183:THR:HB	1.35	0.97
1:B:145:HIS:HB2	1:B:150:PRO:HD2	1.46	0.97
1:A:71:ASP:OD2	3:A:2001:12P:H32	1.62	0.96
6:B:2002:ETE:H262	7:B:2100:HOH:O	1.66	0.95
1:B:132:GLY:HA2	1:B:133:LEU:HB2	1.50	0.92
1:B:84:LYS:NZ	7:B:2159:HOH:O	1.85	0.90
4:A:2003[A]:PG4:H82	7:A:2121:HOH:O	1.71	0.90
3:A:2001:12P:H272	7:A:2082:HOH:O	1.73	0.89
1:A:60:GLU:OE2	3:A:2001:12P:C30	2.24	0.85
1:A:71:ASP:CB	3:A:2001:12P:H32	2.08	0.84
1:A:33:LYS:HB3	3:A:2001:12P:H292	1.60	0.84
1:A:4:LEU:HD13	1:A:139:ILE:HG21	1.62	0.80
1:A:71:ASP:CG	3:A:2001:12P:H32	2.05	0.80
1:B:4:LEU:HD13	1:B:139:ILE:HG21	1.64	0.79
1:A:60:GLU:OE2	3:A:2001:12P:H322	1.83	0.79
1:B:99:PRO:HA	6:B:2002:ETE:H242	1.63	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:2002:ETE:H121	5:B:2006:PGE:H42	1.65	0.79
1:B:145:HIS:CB	1:B:150:PRO:HD2	2.12	0.79
1:A:74:TYR:HB2	3:A:2001:12P:H22	1.66	0.77
1:A:43:TRP:HZ3	1:A:90:ARG:HD2	1.49	0.76
1:B:125:ASP:OD1	6:B:2002:ETE:H142	1.84	0.76
1:B:68:TRP:HZ3	1:B:70[B]:LEU:HD22	1.49	0.76
1:A:69:PHE:HD2	3:A:2001:12P:C9	1.95	0.74
1:A:33:LYS:CD	3:A:2001:12P:C26	2.63	0.74
1:A:60:GLU:HG2	3:A:2001:12P:H301	1.67	0.74
1:A:123:ILE:HG22	4:A:2003[B]:PG4:H82	1.71	0.71
1:A:77[A]:ASN:O	1:A:81[A]:MET:HG2	1.91	0.70
1:B:145:HIS:HB2	1:B:150:PRO:CD	2.20	0.70
1:A:59:ASP:OD2	3:A:2001:12P:O10	2.10	0.69
1:A:60:GLU:OE2	3:A:2001:12P:C32	2.41	0.68
6:B:2002:ETE:H231	7:B:2149:HOH:O	1.93	0.68
1:A:72:HIS:HD2	1:A:76:GLU:OE2	1.77	0.67
1:B:99:PRO:CA	6:B:2002:ETE:H242	2.24	0.67
1:B:21:ASP:OD2	7:B:2124:HOH:O	2.13	0.65
1:B:102:HIS:HD2	7:B:2026:HOH:O	1.77	0.65
1:A:33:LYS:HD2	3:A:2001:12P:C26	2.11	0.64
1:A:34:ARG:O	3:A:2001:12P:H291	1.98	0.63
1:B:59:ASP:OD1	7:B:2073:HOH:O	2.16	0.62
1:A:71:ASP:CB	3:A:2001:12P:C3	2.78	0.61
1:A:182:THR:CB	1:A:183:THR:CB	2.67	0.61
1:B:123:ILE:O	6:B:2002:ETE:H261	2.00	0.61
1:B:125:ASP:CG	6:B:2002:ETE:H142	2.26	0.59
3:A:2001:12P:H301	3:A:2001:12P:H262	1.85	0.59
1:B:99:PRO:HA	6:B:2002:ETE:C24	2.33	0.59
1:A:14:LEU:HD12	1:A:18[B]:SER:OG	2.03	0.58
1:B:48:LEU:HD11	1:B:92:VAL:HB	1.84	0.58
1:A:48:LEU:HD11	1:A:92:VAL:HB	1.86	0.58
1:A:71:ASP:HB2	3:A:2001:12P:H32	1.85	0.57
1:B:127:LYS:HG3	6:B:2002:ETE:H132	1.86	0.57
1:A:33:LYS:HD3	3:A:2001:12P:C26	2.35	0.56
1:B:14:LEU:HD12	1:B:18[B]:SER:OG	2.06	0.56
1:B:97:THR:O	6:B:2002:ETE:C24	2.54	0.56
3:A:2001:12P:H51	7:A:2124:HOH:O	2.05	0.56
1:A:21:ASP:OD2	7:A:2085:HOH:O	2.18	0.55
1:B:99:PRO:HA	6:B:2002:ETE:H252	1.88	0.55
1:A:58:PHE:O	3:A:2001:12P:H271	2.07	0.54
1:A:91:ILE:HG22	1:A:116[B]:CYS:SG	2.48	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLY:O	3:A:2001:12P:C36	2.56	0.53
1:B:45:LYS:C	1:B:47:VAL:H	2.17	0.53
1:A:35:VAL:O	1:A:96:HIS:HA	2.10	0.52
1:B:127:LYS:HE3	6:B:2002:ETE:H141	1.91	0.52
1:B:125:ASP:HA	6:B:2002:ETE:H251	1.91	0.52
1:A:26:ILE:HD11	1:A:35:VAL:CG2	2.40	0.52
1:B:9:VAL:O	1:B:160:SER:HA	2.10	0.52
1:B:26:ILE:HD11	1:B:35:VAL:CG2	2.40	0.52
1:A:71:ASP:HB2	3:A:2001:12P:C3	2.39	0.51
1:A:123:ILE:CG2	4:A:2003[B]:PG4:H82	2.39	0.51
1:B:48:LEU:HD11	1:B:92:VAL:CB	2.40	0.51
1:A:132:GLY:HA2	1:A:133:LEU:HB2	1.92	0.51
1:A:44:GLN:HG3	7:A:2089:HOH:O	2.10	0.51
1:B:132:GLY:HA2	1:B:133:LEU:CB	2.30	0.51
1:B:4:LEU:HD13	1:B:139:ILE:CG2	2.38	0.51
1:B:68:TRP:CZ3	1:B:70[B]:LEU:HD22	2.39	0.51
1:A:136:GLU:HG3	2:B:1002:SO4:O3	2.11	0.50
1:B:44:GLN:HG3	7:B:2088:HOH:O	2.11	0.50
1:B:91:ILE:HG22	1:B:116[B]:CYS:SG	2.52	0.50
1:A:48:LEU:HD11	1:A:92:VAL:CB	2.41	0.50
1:A:43:TRP:HZ3	1:A:90:ARG:CD	2.23	0.50
1:B:68:TRP:CH2	1:B:108:ILE:HA	2.47	0.49
1:B:125:ASP:HB2	6:B:2002:ETE:H263	1.92	0.49
1:A:60:GLU:CG	3:A:2001:12P:H301	2.38	0.49
1:A:43:TRP:HZ2	1:A:116[A]:CYS:SG	2.35	0.49
1:A:45:LYS:C	1:A:47:VAL:H	2.20	0.49
1:A:14:LEU:HD12	1:A:18[B]:SER:HG	1.77	0.49
1:A:43:TRP:CZ3	1:A:90:ARG:HD2	2.38	0.49
1:B:125:ASP:CA	6:B:2002:ETE:H251	2.43	0.49
1:A:70[B]:LEU:HD11	1:A:111:LEU:HD22	1.95	0.49
1:A:136:GLU:OE1	4:A:2003[B]:PG4:O5	2.29	0.48
1:B:35:VAL:O	1:B:96:HIS:HA	2.13	0.48
1:B:43:TRP:HZ2	1:B:116[A]:CYS:SG	2.35	0.48
1:B:45:LYS:C	1:B:47:VAL:N	2.71	0.48
1:B:127:LYS:HG3	6:B:2002:ETE:C13	2.43	0.48
3:A:2001:12P:H52	7:A:2135:HOH:O	2.12	0.48
1:A:41:GLY:HA3	1:A:49:ASP:O	2.13	0.47
1:B:99:PRO:HD3	6:B:2002:ETE:H232	1.96	0.47
1:A:71:ASP:OD2	3:A:2001:12P:C3	2.49	0.47
1:B:125:ASP:HA	6:B:2002:ETE:C24	2.45	0.47
4:A:2003[A]:PG4:C8	7:A:2121:HOH:O	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LYS:HA	1:A:116[A]:CYS:O	2.14	0.47
1:A:37:GLY:HA3	1:A:95:TYR:CE2	2.49	0.47
1:A:43:TRP:CZ2	1:A:92:VAL:HG12	2.50	0.47
1:A:125:ASP:OD2	1:A:130:ASP:HB3	2.16	0.46
1:A:159:THR:OG1	1:B:158:VAL:HA	2.15	0.46
1:B:14:LEU:HD12	1:B:18[B]:SER:HG	1.79	0.46
1:B:127:LYS:HE3	6:B:2002:ETE:H131	1.98	0.46
3:A:2001:12P:H82	7:A:2096:HOH:O	2.15	0.46
1:A:39:LEU:HD22	1:A:50:VAL:HG11	1.98	0.46
1:B:37:GLY:HA3	1:B:95:TYR:CE2	2.52	0.45
1:A:113:LYS:HA	1:A:116[B]:CYS:O	2.16	0.45
1:B:58:PHE:HD1	1:B:70[B]:LEU:HB3	1.82	0.44
1:A:123:ILE:CG2	4:A:2003[A]:PG4:H71	2.48	0.44
1:A:94:TRP:CG	1:A:112:MET:HG3	2.53	0.44
1:B:68:TRP:NE1	7:B:2145:HOH:O	2.51	0.44
1:B:156:GLU:HG3	7:B:2091:HOH:O	2.17	0.44
1:A:40:LEU:HA	1:A:90:ARG:O	2.17	0.43
1:A:33:LYS:HB3	3:A:2001:12P:C29	2.40	0.43
1:A:34:ARG:O	3:A:2001:12P:C29	2.64	0.43
1:B:41:GLY:HA3	1:B:49:ASP:O	2.18	0.43
1:A:8:LYS:HG2	1:A:9:VAL:N	2.34	0.43
1:A:45:LYS:C	1:A:47:VAL:N	2.73	0.43
1:A:33:LYS:HD3	3:A:2001:12P:H262	1.99	0.43
1:A:116[B]:CYS:SG	1:A:119:SER:HB2	2.59	0.43
1:B:8:LYS:HG2	1:B:9:VAL:N	2.34	0.43
1:A:59:ASP:CG	3:A:2001:12P:H231	2.24	0.42
1:B:113:LYS:HA	1:B:116[A]:CYS:O	2.19	0.42
1:B:4:LEU:HD11	1:B:156:GLU:CD	2.44	0.42
1:B:125:ASP:OD2	1:B:130:ASP:HB3	2.20	0.42
1:A:4:LEU:HD13	1:A:139:ILE:CG2	2.39	0.42
1:B:76:GLU:OE2	1:B:115:TYR:OH	2.27	0.42
3:A:2001:12P:C5	7:A:2124:HOH:O	2.66	0.42
1:B:125:ASP:HA	6:B:2002:ETE:C14	2.49	0.42
6:B:2002:ETE:H152	7:B:2100:HOH:O	2.19	0.42
1:A:77[B]:ASN:ND2	1:A:81[B]:MET:HE2	2.35	0.42
1:B:43:TRP:CZ2	1:B:92:VAL:HG12	2.54	0.42
1:A:132:GLY:HA2	1:A:133:LEU:CB	2.49	0.42
1:B:142:GLU:HG2	1:B:151:THR:OG1	2.20	0.42
1:B:145:HIS:CG	1:B:150:PRO:HD2	2.53	0.41
1:B:133:LEU:HA	1:B:134:PRO:HD2	1.86	0.41
1:A:33:LYS:HB3	3:A:2001:12P:O31	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LYS:HD3	3:A:2001:12P:O31	2.20	0.41
1:B:125:ASP:HA	6:B:2002:ETE:H241	2.02	0.41
1:A:72:HIS:CD2	1:A:76:GLU:OE2	2.66	0.41
1:A:68:TRP:CH2	1:A:108:ILE:HA	2.55	0.41
1:B:94:TRP:CG	1:B:112:MET:HG3	2.56	0.41
1:B:33:LYS:C	5:B:2006:PGE:H32	2.46	0.40
1:B:127:LYS:HA	1:B:128:PRO:HD3	1.85	0.40
1:B:38:VAL:O	1:B:53:SER:HA	2.22	0.40
1:B:97:THR:O	6:B:2002:ETE:H241	2.21	0.40

All (4) 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:177:ARG:NH1	1:B:145:HIS:O[2_454]	1.29	0.91
1:A:177:ARG:CZ	1:B:145:HIS:O[2_454]	1.68	0.52
1:A:177:ARG:NH1	1:B:145:HIS:C[2_454]	1.88	0.32
1:A:177:ARG:NH2	1:B:145:HIS:O[2_454]	1.99	0.21

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	A	179/187 (96%)	166 (93%)	11 (6%)	2 (1%)	11	4
1	B	174/187 (93%)	166 (95%)	8 (5%)	0	100	100
All	All	353/374 (94%)	332 (94%)	19 (5%)	2 (1%)	21	12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	183	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	168/167 (101%)	156 (93%)	12 (7%)	13	4
1	B	163/167 (98%)	151 (93%)	12 (7%)	13	4
All	All	331/334 (99%)	307 (93%)	24 (7%)	12	4

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	44	GLN
1	A	75	LEU
1	A	88	ARG
1	A	130	ASP
1	A	141	VAL
1	A	142	GLU
1	A	165	GLU
1	A	166	GLU
1	A	175	LEU
1	A	183	THR
1	A	184	VAL
1	B	7	GLN
1	B	14	LEU
1	B	44	GLN
1	B	45	LYS
1	B	75	LEU
1	B	85	VAL
1	B	129	LYS
1	B	130	ASP
1	B	142	GLU
1	B	151	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	165	GLU
1	B	166	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	72	HIS
1	B	7	GLN
1	B	31	ASN
1	B	102	HIS

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](#)

13 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	$\# Z > 2$
5	PGE	B	2005[A]	-	9,9,9	0.42	0	8,8,8	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PG4	A	2003[A]	-	12,12,12	0.70	0	11,11,11	1.12	1 (9%)
2	SO4	A	1001	-	4,4,4	0.33	0	6,6,6	0.41	0
2	SO4	B	1003[A]	-	4,4,4	0.23	0	6,6,6	0.14	0
5	PGE	B	2006	-	9,9,9	0.42	0	8,8,8	0.43	0
5	PGE	B	2005[B]	-	9,9,9	0.43	0	8,8,8	0.27	0
6	ETE	B	2002	-	13,13,13	0.69	0	12,12,12	0.95	0
5	PGE	A	2004	-	9,9,9	0.40	0	8,8,8	0.39	0
5	PGE	A	2007	-	9,9,9	0.46	0	8,8,8	0.58	0
4	PG4	A	2003[B]	-	12,12,12	0.66	0	11,11,11	1.00	0
3	12P	A	2001	-	35,35,36	0.56	0	34,34,35	0.95	3 (8%)
2	SO4	B	1003[B]	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	B	1002	-	4,4,4	0.37	0	6,6,6	0.28	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
5	PGE	B	2005[A]	-	-	5/7/7/7	-
4	PG4	A	2003[A]	-	-	5/10/10/10	-
5	PGE	B	2006	-	-	6/7/7/7	-
5	PGE	B	2005[B]	-	-	5/7/7/7	-
6	ETE	B	2002	-	-	9/11/11/11	-
5	PGE	A	2004	-	-	2/7/7/7	-
5	PGE	A	2007	-	-	5/7/7/7	-
4	PG4	A	2003[B]	-	-	5/10/10/10	-
3	12P	A	2001	-	-	21/33/33/34	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	12P	C35-O34-C33	-2.51	104.24	113.06
3	A	2001	12P	O25-C26-C27	2.31	120.90	110.35
4	A	2003[A]	PG4	O4-C7-C8	2.13	119.48	110.11
3	A	2001	12P	C27-O28-C29	2.04	122.20	113.26

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	12P	C17-C18-O19-C20
6	B	2002	ETE	C24-C14-OH5-C25
6	B	2002	ETE	OH4-C13-C23-OH3
3	A	2001	12P	O28-C29-C30-O31
3	A	2001	12P	O25-C26-C27-O28
3	A	2001	12P	O19-C20-C21-O22
5	B	2006	PGE	O2-C3-C4-O3
3	A	2001	12P	O10-C11-C12-O13
5	B	2005[A]	PGE	O3-C5-C6-O4
5	B	2005[B]	PGE	O3-C5-C6-O4
5	B	2006	PGE	O1-C1-C2-O2
3	A	2001	12P	O4-C5-C6-O7
3	A	2001	12P	C11-C12-O13-C14
4	A	2003[A]	PG4	O2-C3-C4-O3
4	A	2003[B]	PG4	O2-C3-C4-O3
4	A	2003[B]	PG4	O4-C7-C8-O5
5	B	2005[B]	PGE	O1-C1-C2-O2
5	B	2005[A]	PGE	O2-C3-C4-O3
5	B	2005[B]	PGE	O2-C3-C4-O3
6	B	2002	ETE	OH2-C12-C22-OH3
6	B	2002	ETE	C13-C23-OH3-C22
3	A	2001	12P	O22-C23-C24-O25
4	A	2003[A]	PG4	O1-C1-C2-O2
4	A	2003[B]	PG4	O1-C1-C2-O2
5	A	2004	PGE	O3-C5-C6-O4
6	B	2002	ETE	OH6-C15-C25-OH5
5	A	2007	PGE	O1-C1-C2-O2
3	A	2001	12P	C36-C35-O34-C33
5	A	2007	PGE	O2-C3-C4-O3
5	B	2006	PGE	O3-C5-C6-O4
3	A	2001	12P	C2-C3-O4-C5
5	B	2006	PGE	C1-C2-O2-C3
4	A	2003[A]	PG4	C4-C3-O2-C2
4	A	2003[B]	PG4	C4-C3-O2-C2
3	A	2001	12P	C5-C6-O7-C8
4	A	2003[A]	PG4	C8-C7-O4-C6
5	A	2007	PGE	O3-C5-C6-O4
3	A	2001	12P	C20-C21-O22-C23
5	B	2005[A]	PGE	O1-C1-C2-O2
3	A	2001	12P	C24-C23-O22-C21
5	A	2004	PGE	C6-C5-O3-C4
5	A	2007	PGE	C3-C4-O3-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	2006	PGE	C3-C4-O3-C5
6	B	2002	ETE	OH5-C14-C24-OH4
6	B	2002	ETE	C12-C22-OH3-C23
5	B	2005[A]	PGE	C6-C5-O3-C4
5	B	2005[B]	PGE	C6-C5-O3-C4
3	A	2001	12P	C32-C33-O34-C35
5	B	2006	PGE	C4-C3-O2-C2
6	B	2002	ETE	C23-C13-OH4-C24
3	A	2001	12P	C6-C5-O4-C3
3	A	2001	12P	C12-C11-O10-C9
3	A	2001	12P	C27-C26-O25-C24
3	A	2001	12P	C9-C8-O7-C6
5	B	2005[A]	PGE	C1-C2-O2-C3
4	A	2003[A]	PG4	O3-C5-C6-O4
4	A	2003[B]	PG4	O3-C5-C6-O4
3	A	2001	12P	C8-C9-O10-C11
3	A	2001	12P	C23-C24-O25-C26
6	B	2002	ETE	C25-C15-OH6-C26
5	A	2007	PGE	C6-C5-O3-C4
3	A	2001	12P	O13-C14-C15-O16
5	B	2005[B]	PGE	C1-C2-O2-C3

There are no ring outliers.

6 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2003[A]	PG4	3	0
5	B	2006	PGE	2	0
6	B	2002	ETE	24	0
4	A	2003[B]	PG4	3	0
3	A	2001	12P	41	0
2	B	1002	SO4	1	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.

Ligand 12P A 2001	
 Bond lengths	 Bond angles
 Torsions	 Rings

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	179/187 (95%)	-0.99	3 (1%) 69 76	7, 21, 57, 103	25 (13%)
1	B	176/187 (94%)	-1.01	2 (1%) 78 83	9, 21, 61, 99	21 (11%)
All	All	355/374 (94%)	-1.00	5 (1%) 73 79	7, 21, 60, 103	46 (12%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	GLY	4.6
1	A	184	VAL	4.6
1	B	132	GLY	3.9
1	B	144	VAL	2.5
1	A	145	HIS	2.2

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](#)

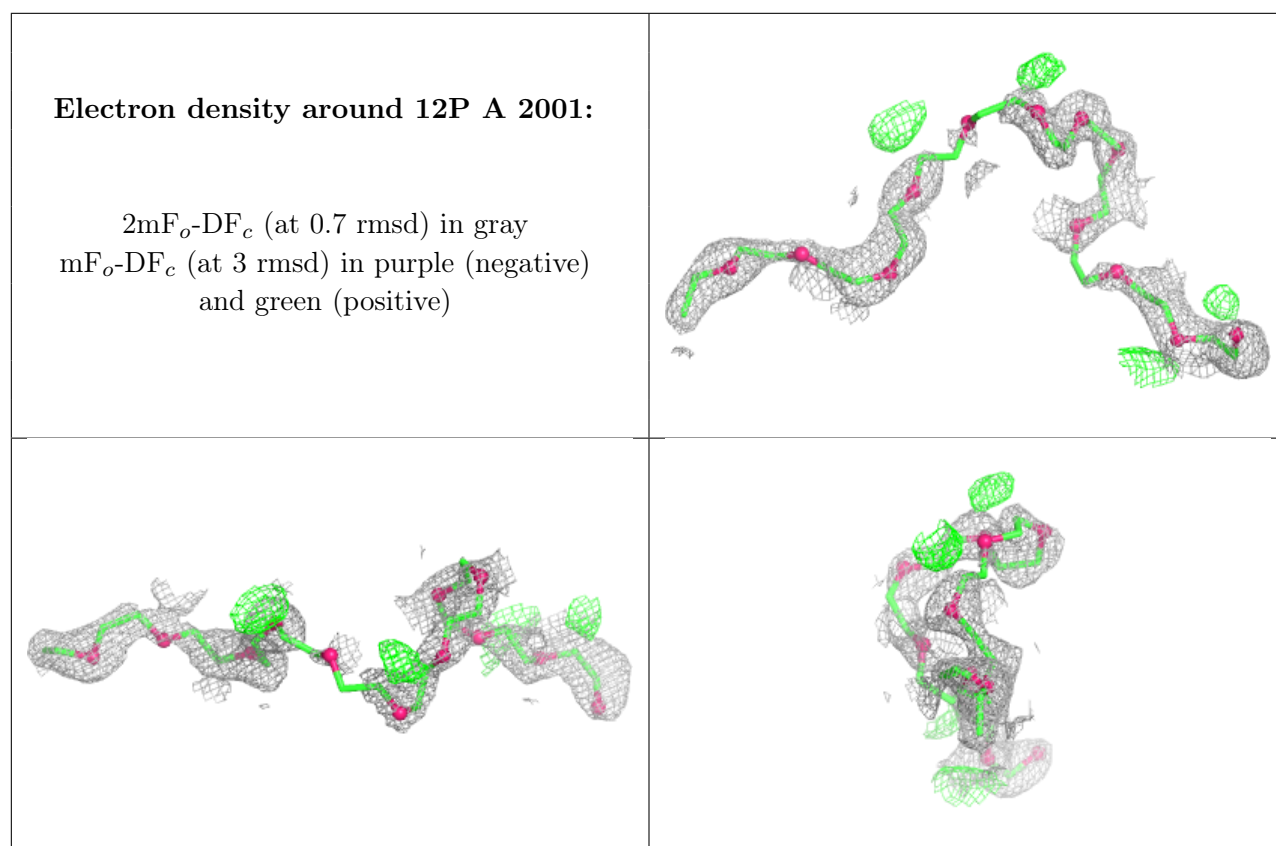
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	1001	5/5	0.98	0.07	33,36,38,38	5
2	SO4	B	1002	5/5	0.98	0.08	36,39,39,40	5
3	12P	A	2001	36/37	0.98	0.07	9,28,36,38	36
4	PG4	A	2003[A]	13/13	0.98	0.06	15,21,29,36	13
4	PG4	A	2003[B]	13/13	0.98	0.06	15,21,29,36	13
5	PGE	A	2004	10/10	0.98	0.06	36,43,47,49	0
5	PGE	A	2007	10/10	0.98	0.05	55,57,60,62	0
5	PGE	B	2006	10/10	0.98	0.06	50,54,55,57	0
6	ETE	B	2002	14/14	0.98	0.06	15,23,35,38	14
5	PGE	B	2005[A]	10/10	0.99	0.03	35,38,47,47	3
5	PGE	B	2005[B]	10/10	0.99	0.03	36,38,47,47	3
2	SO4	B	1003[B]	5/5	0.99	0.05	61,63,63,63	5
2	SO4	B	1003[A]	5/5	0.99	0.05	60,60,61,61	5

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 ⓘ

There are no such residues in this entry.