



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:48 AM GMT

PDB ID : 2O95  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

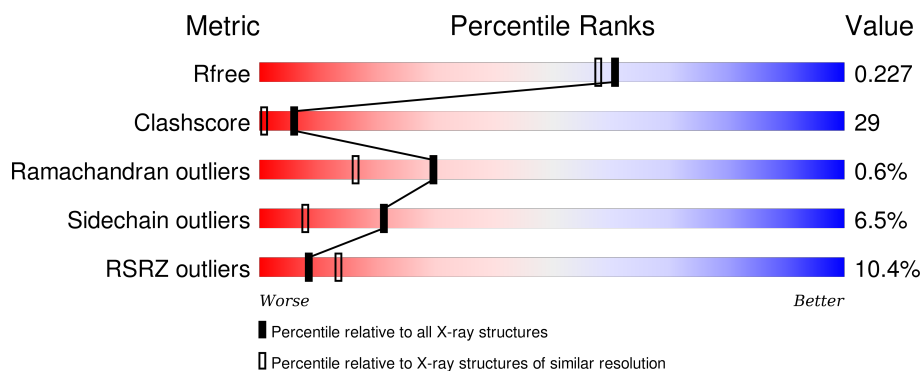
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>11%</div> <div>59%</div> <div>33%</div> <div>.</div> <div>.</div> </div>
1	B	187	<div> <div>9%</div> <div>62%</div> <div>27%</div> <div>5%</div> <div>6%</div> </div>

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
2	SO4	A	1001	-	-	-	X
2	SO4	B	1002	-	-	-	X
3	12P	A	2001	-	-	X	X
4	ETE	B	2002	-	-	X	X
5	PG4	A	2003[A]	-	-	-	X
5	PG4	A	2003[B]	-	-	-	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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



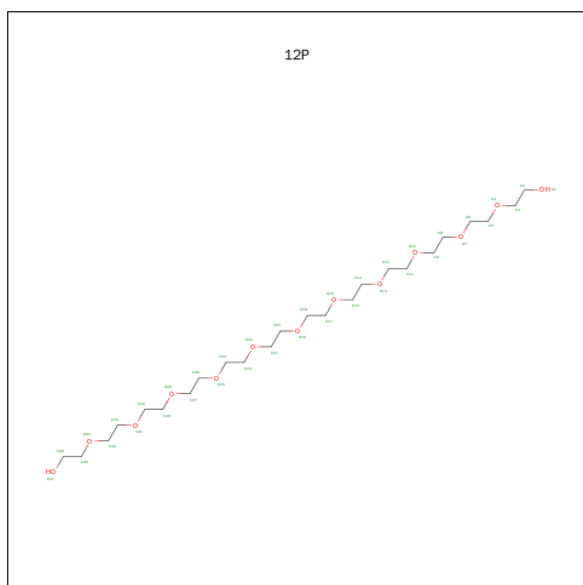
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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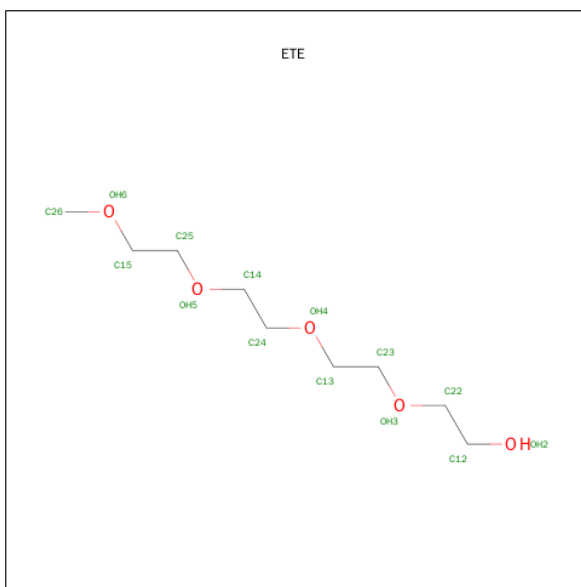
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	1
			10	8	2		

- Molecule 3 is DODECAETHYLENE GLYCOL (three-letter code: 12P) (formula: C<sub>24</sub>H<sub>50</sub>O<sub>13</sub>).



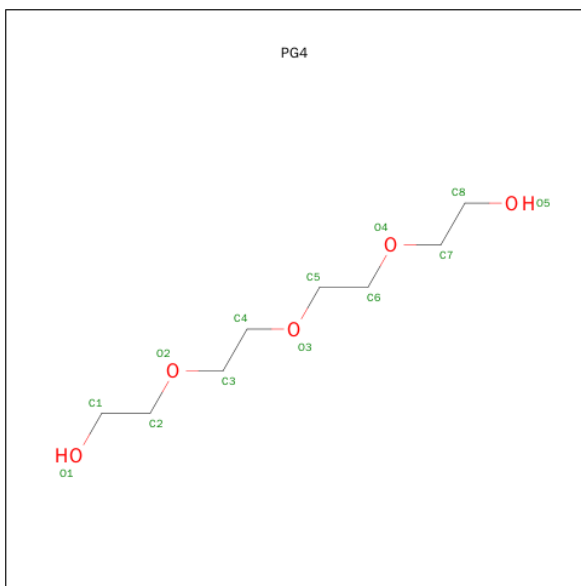
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			36	24	12		

- Molecule 4 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: ETE) (formula: C<sub>9</sub>H<sub>20</sub>O<sub>5</sub>).



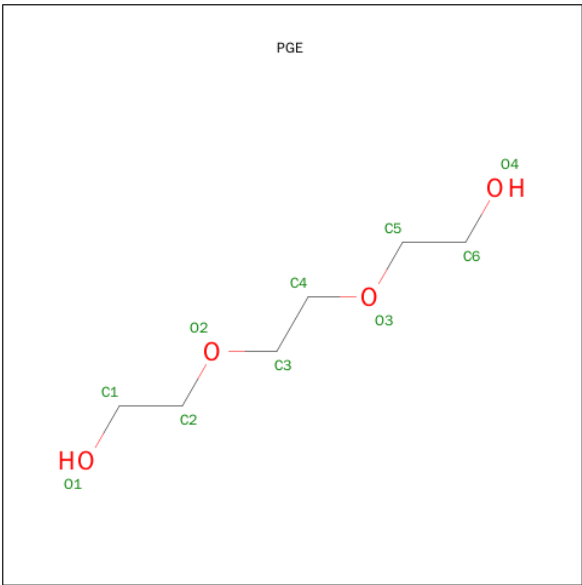
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			14	9	5		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



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

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



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

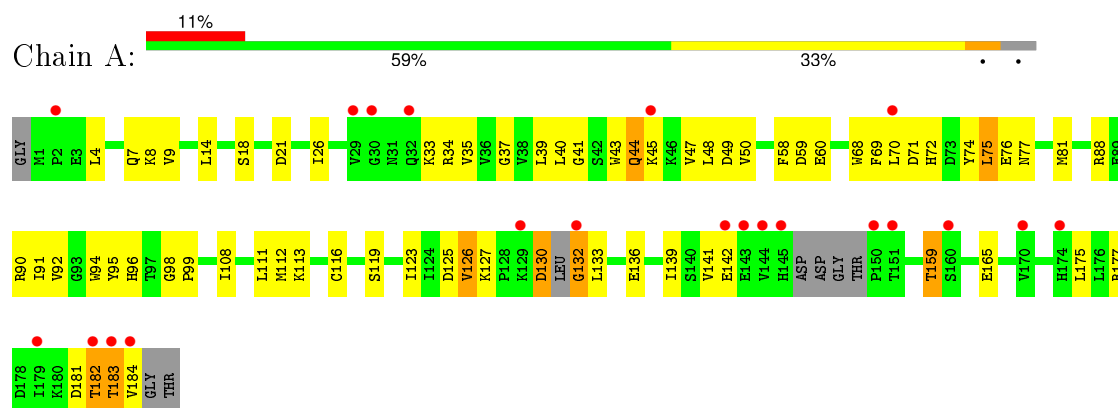
- Molecule 7 is water.

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

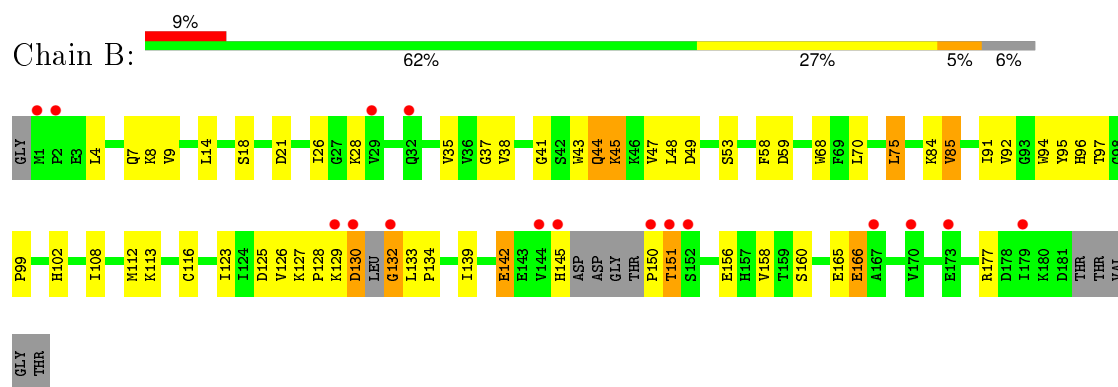
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.201 , 0.240 0.188 , 0.227	Depositor DCC
$R_{free}$ test set	1973 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 65.5	EDS
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
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 39262 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3358	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: 12P, PG4, PGE, SO4, ETE

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	0.97	4/1505 (0.3%)	0.99	3/2038 (0.1%)
1	B	0.97	6/1470 (0.4%)	0.96	4/1990 (0.2%)
All	All	0.97	10/2975 (0.3%)	0.97	7/4028 (0.2%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	28	LYS	CD-CE	-6.67	1.34	1.51
1	A	159	THR	C-O	-6.39	1.11	1.23
1	B	126	VAL	CB-CG2	-6.00	1.40	1.52
1	B	166	GLU	CD-OE2	5.96	1.32	1.25
1	B	126	VAL	CB-CG1	-5.87	1.40	1.52
1	B	177	ARG	CB-CG	-5.84	1.36	1.52
1	A	126	VAL	CB-CG2	-5.81	1.40	1.52
1	B	132	GLY	N-CA	5.45	1.54	1.46
1	A	126	VAL	CB-CG1	-5.22	1.41	1.52
1	A	132	GLY	N-CA	5.21	1.53	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	VAL	CG1-CB-CG2	-9.22	96.15	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	VAL	CG1-CB-CG2	-8.48	97.34	110.90
1	A	75	LEU	CA-CB-CG	7.39	132.30	115.30
1	B	75	LEU	CA-CB-CG	6.42	130.08	115.30
1	B	85	VAL	CG1-CB-CG2	5.86	120.28	110.90
1	A	75	LEU	CB-CG-CD1	5.73	120.74	111.00
1	B	75	LEU	CB-CG-CD1	5.69	120.67	111.00

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	96	4
1	B	1437	0	1431	62	4
2	A	5	0	0	0	0
2	B	15	0	0	1	0
3	A	36	0	47	40	0
4	B	14	0	20	24	0
5	A	16	0	10	6	0
6	A	20	0	28	0	0
6	B	23	0	24	1	0
7	A	153	0	0	10	0
7	B	167	0	0	9	0
All	All	3358	0	3028	170	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 (170) 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:182:THR:CA	1:A:183:THR:HB	1.80	1.11
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: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
4:B:2002:ETE:H262	7:B:2100:HOH:O	1.66	0.95
1:B:84:LYS:NZ	7:B:2159:HOH:O	1.85	0.93
1:B:132:GLY:HA2	1:B:133:LEU:HB2	1.50	0.92
5: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: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	4:B:2002:ETE:H242	1.63	0.79
4:B:2002:ETE:H121	6: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	4: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:71:ASP:CG	3:A:2001:12P:H32	2.05	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	5: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:TRP:HZ2	1:A:116[A]:CYS:HG	1.41	0.68
4: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	4: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:182:THR:CB	1:A:183:THR:CB	2.67	0.61
1:A:71:ASP:CB	3:A:2001:12P:C3	2.78	0.61
1:B:123:ILE:O	4:B:2002:ETE:H261	2.00	0.61
3:A:2001:12P:H301	3:A:2001:12P:H262	1.85	0.59
1:B:99:PRO:HA	4: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	4: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	4:B:2002:ETE:C24	2.54	0.56
3:A:2001:12P:H51	7:A:2124:HOH:O	2.05	0.56
1:B:99:PRO:HA	4:B:2002:ETE:H252	1.88	0.55
1:A:21:ASP:OD2	7:A:2085:HOH:O	2.18	0.55
1:B:125:ASP:CG	4:B:2002:ETE:H142	2.26	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
1:A:98:GLY:O	3:A:2001:12P:C36	2.56	0.53
1:A:35:VAL:O	1:A:96:HIS:HA	2.10	0.52
1:B:127:LYS:HE3	4:B:2002:ETE:H141	1.91	0.52
1:B:125:ASP:HA	4: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:B:43:TRP:HZ2	1:B:116[A]:CYS:HG	1.57	0.51
1:A:123:ILE:CG2	5: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:B:132:GLY:HA2	1:B:133:LEU:CB	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLN:HG3	7:A:2089:HOH:O	2.10	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:125:ASP:HB2	4:B:2002:ETE:H263	1.92	0.49
1:B:68:TRP:CH2	1:B:108:ILE:HA	2.47	0.49
1:A:60:GLU:CG	3:A:2001:12P:H301	2.38	0.49
1:A:43:TRP:CZ3	1:A:90:ARG:HD2	2.38	0.49
1:A:14:LEU:HD12	1:A:18[B]:SER:HG	1.77	0.49
1:B:125:ASP:CA	4: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	5: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:H	2.17	0.48
1:B:127:LYS:HG3	4:B:2002:ETE:C13	2.43	0.48
3:A:2001:12P:H52	7:A:2135:HOH:O	2.12	0.48
1:B:99:PRO:HD3	4:B:2002:ETE:H232	1.96	0.47
1:A:41:GLY:HA3	1:A:49:ASP:O	2.13	0.47
1:A:71:ASP:OD2	3:A:2001:12P:C3	2.49	0.47
1:B:125:ASP:HA	4:B:2002:ETE:C24	2.45	0.47
5:A:2003[A]:PG4:C8	7:A:2121:HOH:O	2.46	0.47
1:A:113:LYS:HA	1:A:116[A]:CYS:O	2.14	0.47
1:A:43:TRP:HZ2	1:A:116[A]:CYS:SG	2.35	0.47
1:A:43:TRP:CZ2	1:A:92:VAL:HG12	2.50	0.47
1:A:37:GLY:HA3	1:A:95:TYR:CE2	2.49	0.47
1:A:125:ASP:OD2	1:A:130:ASP:HB3	2.16	0.46
1:B:127:LYS:HE3	4:B:2002:ETE:H131	1.98	0.46
1:B:14:LEU:HD12	1:B:18[B]:SER:HG	1.79	0.46
1:A:159:THR:OG1	1:B:158:VAL:HA	2.15	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:A:45:LYS:C	1:A:47:VAL:H	2.20	0.45
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	5:A:2003[A]:PG4:H71	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:GLU:HG3	7:B:2091:HOH:O	2.17	0.44
1:A:94:TRP:CG	1:A:112:MET:HG3	2.53	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:45:LYS:C	1:B:47:VAL:N	2.71	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: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:B:113:LYS:HA	1:B:116[A]:CYS:O	2.19	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
3:A:2001:12P:C5	7:A:2124:HOH:O	2.66	0.42
1:B:125:ASP:HA	4:B:2002:ETE:C14	2.49	0.42
4:B:2002:ETE:H152	7:B:2100:HOH:O	2.19	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
1:A:45:LYS:C	1:A:47:VAL:N	2.73	0.41
1:A:33:LYS:HD3	3:A:2001:12P:O31	2.20	0.41
1:B:125:ASP:HA	4:B:2002:ETE:H241	2.02	0.41
1:A:72:HIS:CD2	1:A:76:GLU:OE2	2.66	0.41
1:B:94:TRP:CG	1:B:112:MET:HG3	2.56	0.41
1:A:68:TRP:CH2	1:A:108:ILE:HA	2.55	0.41
1:B:127:LYS:HA	1:B:128:PRO:HD3	1.85	0.40
1:B:97:THR:O	4:B:2002:ETE:H241	2.21	0.40
1:B:38:VAL:O	1:B:53:SER:HA	2.22	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%)	17	6
1	B	174/187 (93%)	166 (95%)	8 (5%)	0	100	100
All	All	353/374 (94%)	332 (94%)	19 (5%)	2 (1%)	30	16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	THR
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%)	158 (94%)	10 (6%)	24	10
1	B	163/167 (98%)	152 (93%)	11 (7%)	20	7
All	All	331/334 (99%)	310 (94%)	21 (6%)	21	8

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	44	GLN
1	A	75	LEU
1	A	88	ARG

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Mol	Chain	Res	Type
1	A	130	ASP
1	A	141	VAL
1	A	142	GLU
1	A	165	GLU
1	A	175	LEU
1	A	184	VAL
1	B	7	GLN
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
1	B	165	GLU
1	B	166	GLU

Some 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 ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	$\# Z  > 2$
2	SO4	A	1001	-	4,4,4	0.38	0	6,6,6	0.25	0
3	12P	A	2001	-	35,35,36	0.57	0	34,34,35	0.93	3 (8%)
5	PG4	A	2003[A]	-	12,12,12	0.70	0	11,11,11	1.09	0
5	PG4	A	2003[B]	-	12,12,12	0.66	0	11,11,11	1.00	0
6	PGE	A	2004	-	9,9,9	0.40	0	8,8,8	0.42	0
6	PGE	A	2007	-	9,9,9	0.46	0	8,8,8	0.56	0
2	SO4	B	1002	-	4,4,4	0.41	0	6,6,6	0.17	0
2	SO4	B	1003[A]	-	4,4,4	0.17	0	6,6,6	0.14	0
2	SO4	B	1003[B]	-	4,4,4	0.14	0	6,6,6	0.09	0
4	ETE	B	2002	-	13,13,13	0.69	0	12,12,12	0.96	0
6	PGE	B	2005[A]	-	9,9,9	0.42	0	8,8,8	0.30	0
6	PGE	B	2005[B]	-	9,9,9	0.43	0	8,8,8	0.28	0
6	PGE	B	2006	-	9,9,9	0.42	0	8,8,8	0.44	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
2	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
3	12P	A	2001	-	-	0/33/33/34	0/0/0/0
5	PG4	A	2003[A]	-	-	0/10/10/10	0/0/0/0
5	PG4	A	2003[B]	-	-	0/10/10/10	0/0/0/0
6	PGE	A	2004	-	-	0/7/7/7	0/0/0/0
6	PGE	A	2007	-	-	0/7/7/7	0/0/0/0
2	SO4	B	1002	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1003[A]	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1003[B]	-	-	0/0/0/0	0/0/0/0
4	ETE	B	2002	-	-	0/11/11/11	0/0/0/0
6	PGE	B	2005[A]	-	-	0/7/7/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PGE	B	2005[B]	-	-	0/7/7/7	0/0/0/0
6	PGE	B	2006	-	-	0/7/7/7	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	12P	C35-O34-C33	-2.23	104.24	112.80
3	A	2001	12P	C27-O28-C29	2.07	122.20	113.31
3	A	2001	12P	O25-C26-C27	2.37	120.90	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	12P	40	0
5	A	2003[A]	PG4	3	0
5	A	2003[B]	PG4	3	0
2	B	1002	SO4	1	0
4	B	2002	ETE	24	0
6	B	2006	PGE	1	0

## 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

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	179/187 (95%)	0.68	21 (11%) <b>6</b> <b>10</b>	10, 23, 64, 103	19 (10%)
1	B	176/187 (94%)	0.59	16 (9%) <b>11</b> <b>18</b>	10, 21, 65, 99	17 (9%)
All	All	355/374 (94%)	0.64	37 (10%) <b>8</b> <b>13</b>	10, 22, 64, 103	36 (10%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	GLY	7.7
1	A	144	VAL	7.5
1	A	184	VAL	7.1
1	B	145	HIS	6.3
1	A	145	HIS	6.3
1	B	144	VAL	6.2
1	B	170	VAL	6.1
1	B	132	GLY	5.7
1	A	2	PRO	5.0
1	B	2	PRO	4.9
1	A	170	VAL	4.7
1	A	182	THR	4.1
1	A	32	GLN	3.9
1	A	183	THR	3.7
1	B	129	LYS	3.6
1	B	151	THR	3.5
1	A	150	PRO	3.5
1	B	167	ALA	3.4
1	B	150	PRO	3.2
1	A	129	LYS	3.1
1	B	130	ASP	3.1
1	B	179	ILE	3.1
1	A	151	THR	3.0
1	B	32	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	29	VAL	3.0
1	A	179	ILE	2.7
1	A	143	GLU	2.7
1	A	174	HIS	2.7
1	A	45	LYS	2.5
1	A	30	GLY	2.5
1	A	29	VAL	2.5
1	B	1	MET	2.3
1	A	70[A]	LEU	2.2
1	B	152	SER	2.2
1	B	173	GLU	2.1
1	A	160[A]	SER	2.1
1	A	142	GLU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	A	1001	5/5	0.85	0.28	6.41	33,36,38,38	5
5	PG4	A	2003[B]	13/13	0.81	0.31	5.34	15,21,29,36	13
5	PG4	A	2003[A]	13/13	0.81	0.31	5.09	15,21,29,36	13
2	SO4	B	1002	5/5	0.83	0.31	3.40	36,39,39,40	5
4	ETE	B	2002	14/14	0.79	0.31	3.00	15,23,35,38	14
3	12P	A	2001	36/37	0.86	0.28	2.23	9,28,36,38	36
6	PGE	B	2006	10/10	0.87	0.30	1.97	50,54,55,57	0
6	PGE	A	2007	10/10	0.85	0.28	1.35	55,57,60,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	1003[A]	5/5	0.89	0.16	1.09	60,60,61,61	5
2	SO4	B	1003[B]	5/5	0.89	0.16	1.00	61,63,63,63	5
6	PGE	A	2004	10/10	0.86	0.17	0.23	36,43,47,49	0
6	PGE	B	2005[A]	10/10	0.89	0.14	-0.23	35,38,47,47	3
6	PGE	B	2005[B]	10/10	0.89	0.14	-0.23	36,38,47,47	3

## 6.5 Other polymers [i](#)

There are no such residues in this entry.