



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:18 AM GMT

PDB ID : 2WHI
Title : CRYSTAL STRUCTURE OF MYCOBACTERIUM TUBERCULOSIS GLUTAMINE SYNTHETASE IN COMPLEX WITH A PURINE ANALOGUE INHIBITOR AND L-METHIONINE-S-SULFOXIMINE PHOSPHATE.
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Deposited on : 2009-05-05
Resolution : 2.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

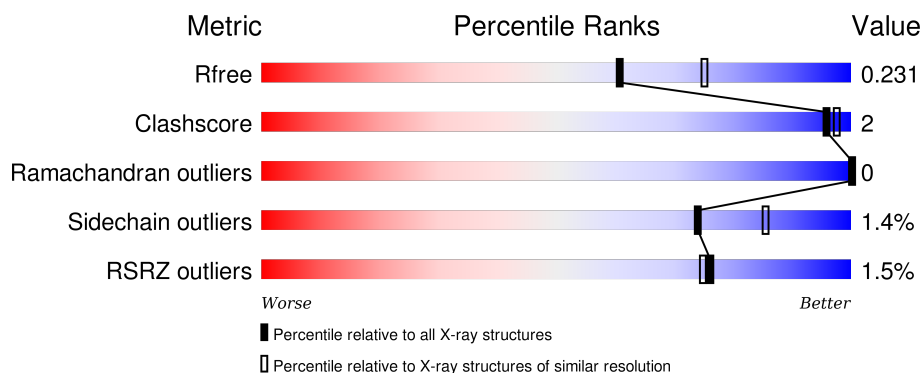
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 ≥ 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	486	<div> <div>2%</div> <div>95%</div> <div>..</div> </div>
1	B	486	<div> <div>%</div> <div>95%</div> <div>..</div> </div>
1	C	486	<div> <div>2%</div> <div>95%</div> <div>..</div> </div>
1	D	486	<div> <div>%</div> <div>95%</div> <div>..</div> </div>
1	E	486	<div> <div>95%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	486	<div> <div></div> <div>%</div> <div>96%</div> <div></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
3	MG	E	502	-	-	-	X
7	1PE	A	508	-	-	X	-
7	1PE	B	508	-	-	X	X
7	1PE	C	508	-	-	X	X
7	1PE	D	508	-	-	X	X
7	1PE	E	508	-	-	X	X
7	1PE	F	508	-	-	X	X

2 Entry composition [i](#)

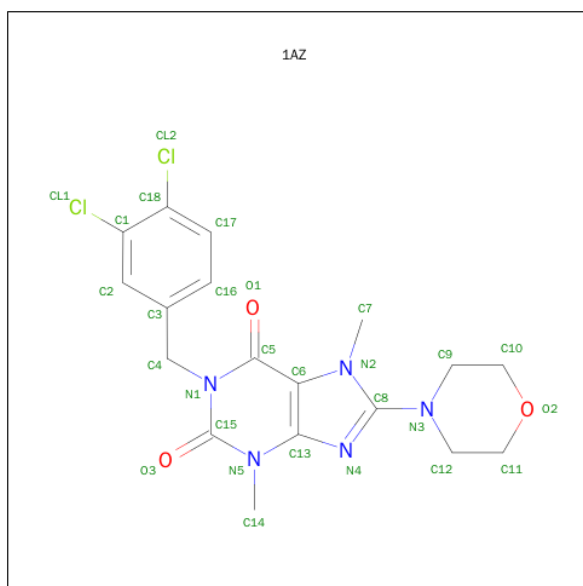
There are 8 unique types of molecules in this entry. The entry contains 24683 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUTAMINE SYNTHETASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3771	2402	632	725	12			
1	B	476	Total	C	N	O	S	0	0	0
			3771	2402	632	725	12			
1	C	476	Total	C	N	O	S	0	0	0
			3771	2402	632	725	12			
1	D	476	Total	C	N	O	S	0	0	0
			3771	2402	632	725	12			
1	E	476	Total	C	N	O	S	0	0	0
			3771	2402	632	725	12			
1	F	476	Total	C	N	O	S	0	0	0
			3771	2402	632	725	12			

- Molecule 2 is 1-(3,4-DICHLOROBENZYL)-3,7-DIMETHYL-8-MORPHOLIN-4-YL-3,7-DIHYDRO-1H-PURINE-2,6-DIONE (three-letter code: 1AZ) (formula: C₁₈H₁₉Cl₂N₅O₃).

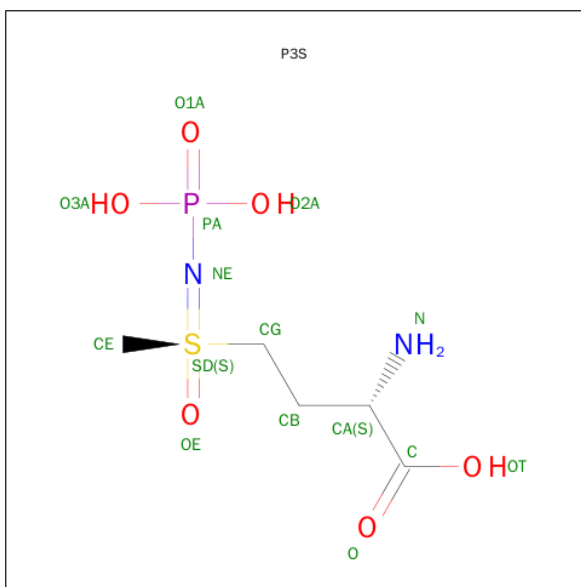


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	B	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	C	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	D	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	E	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	F	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	3	Total	Mg	0	0
			3	3		
3	E	3	Total	Mg	0	0
			3	3		
3	B	3	Total	Mg	0	0
			3	3		
3	C	3	Total	Mg	0	0
			3	3		
3	A	3	Total	Mg	0	0
			3	3		
3	F	3	Total	Mg	0	0
			3	3		

- Molecule 4 is L-METHIONINE-S-SULFOXIMINE PHOSPHATE (three-letter code: P3S) (formula: C₅H₁₃N₂O₆PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
4	B	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
4	C	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
4	D	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
4	E	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
4	F	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

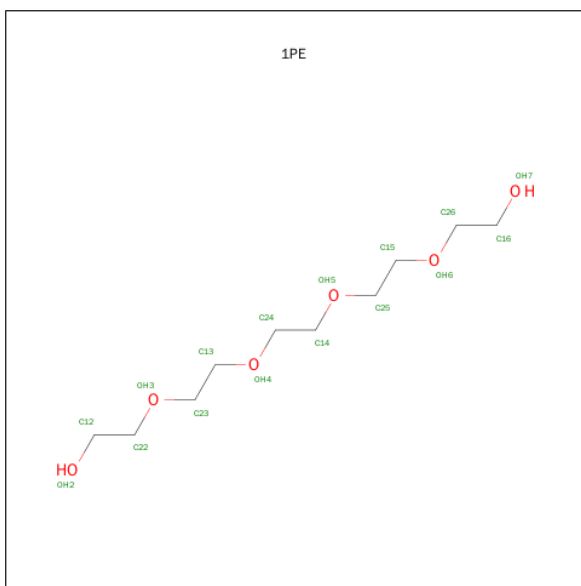


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Cl	0	0
			1	1		
6	E	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		
6	C	1	Total	Cl	0	0
			1	1		
6	A	1	Total	Cl	0	0
			1	1		
6	F	1	Total	Cl	0	0
			1	1		

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			16	10	6		
7	B	1	Total	C	O	0	0
			16	10	6		
7	C	1	Total	C	O	0	0
			16	10	6		
7	D	1	Total	C	O	0	0
			16	10	6		
7	E	1	Total	C	O	0	0
			16	10	6		
7	F	1	Total	C	O	0	0
			16	10	6		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	276	Total	O	0	0
			276	276		
8	B	276	Total	O	0	0
			276	276		
8	C	274	Total	O	0	0
			274	274		
8	D	279	Total	O	0	0
			279	279		
8	E	275	Total	O	0	0
			275	275		

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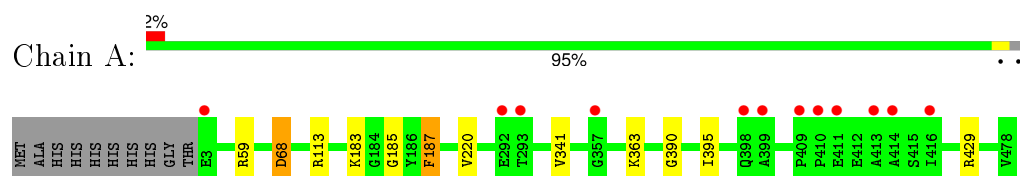
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	269	Total 269	O 269	0	0

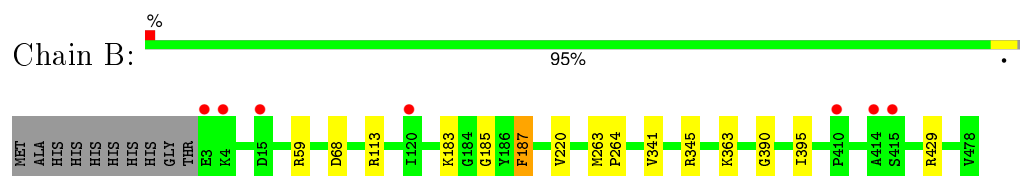
3 Residue-property plots [i](#)

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.

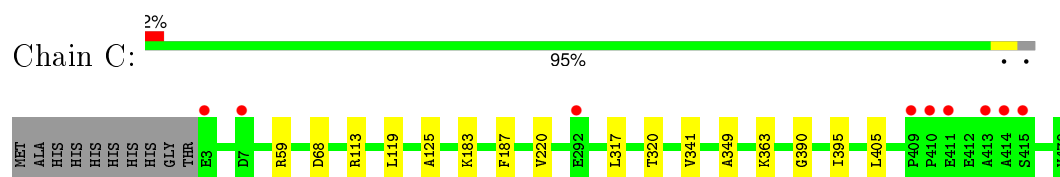
• Molecule 1: GLUTAMINE SYNTHETASE 1



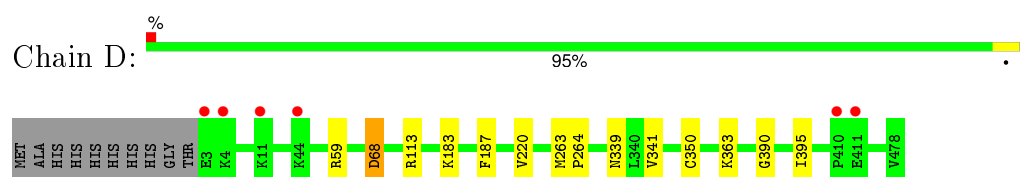
• Molecule 1: GLUTAMINE SYNTHETASE 1



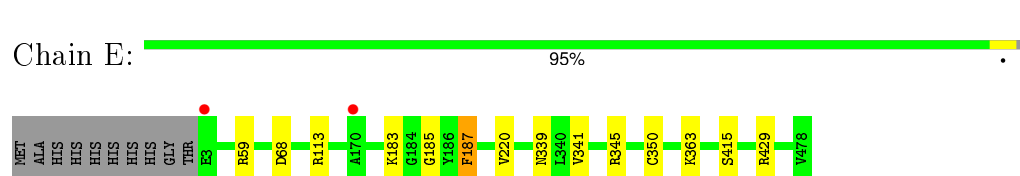
• Molecule 1: GLUTAMINE SYNTHETASE 1



• Molecule 1: GLUTAMINE SYNTHETASE 1



• Molecule 1: GLUTAMINE SYNTHETASE 1



• Molecule 1: GLUTAMINE SYNTHETASE 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	133.21Å 228.76Å 202.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.81 – 2.20 39.80 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (39.81-2.20) 98.1 (39.80-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.231 0.212 , 0.231	Depositor DCC
R_{free} test set	7666 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.8	EDS
Estimated twinning fraction	0.036 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.044 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 153001 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24683	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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, 0.375 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: MG, CL, PO4, 1PE, P3S, 1AZ

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	0.45	0/3877	0.55	0/5269
1	B	0.45	0/3877	0.54	0/5269
1	C	0.45	0/3877	0.54	0/5269
1	D	0.44	0/3877	0.54	0/5269
1	E	0.45	0/3877	0.55	0/5269
1	F	0.44	0/3877	0.55	0/5269
All	All	0.45	0/23262	0.54	0/31614

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	3771	0	3597	11	0
1	B	3771	0	3597	11	0
1	C	3771	0	3597	12	0
1	D	3771	0	3597	12	0
1	E	3771	0	3597	11	0
1	F	3771	0	3597	8	0
2	A	28	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	28	0	19	0	0
2	C	28	0	19	0	0
2	D	28	0	19	0	0
2	E	28	0	19	0	0
2	F	28	0	19	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
4	A	15	0	10	0	0
4	B	15	0	10	0	0
4	C	15	0	10	0	0
4	D	15	0	10	0	0
4	E	15	0	10	0	0
4	F	15	0	10	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	A	16	0	22	8	0
7	B	16	0	22	7	0
7	C	16	0	22	8	0
7	D	16	0	22	8	0
7	E	16	0	22	7	0
7	F	16	0	22	8	0
8	A	276	0	0	1	0
8	B	276	0	0	1	0
8	C	274	0	0	1	0
8	D	279	0	0	1	0
8	E	275	0	0	2	0
8	F	269	0	0	1	0
All	All	24683	0	21888	69	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 2.

All (69) 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:F:59:ARG:HH12	7:F:508:1PE:H121	1.22	1.01
1:B:59:ARG:HH12	7:B:508:1PE:H121	1.25	0.99
1:E:59:ARG:HH12	7:E:508:1PE:H121	1.26	0.99
1:C:59:ARG:HH12	7:C:508:1PE:H121	1.28	0.96
1:F:59:ARG:HH11	7:F:508:1PE:H131	1.31	0.95
1:C:59:ARG:HH11	7:C:508:1PE:H131	1.30	0.94
1:B:59:ARG:HH11	7:B:508:1PE:H131	1.31	0.94
1:D:59:ARG:HH12	7:D:508:1PE:H121	1.30	0.93
1:E:59:ARG:HH11	7:E:508:1PE:H131	1.30	0.93
1:D:59:ARG:HH11	7:D:508:1PE:H131	1.33	0.92
1:A:59:ARG:HH12	7:A:508:1PE:H121	1.34	0.91
1:A:59:ARG:HH11	7:A:508:1PE:H131	1.34	0.88
1:B:59:ARG:NH1	7:B:508:1PE:H131	1.91	0.85
1:A:59:ARG:NH1	7:A:508:1PE:H131	1.93	0.83
1:C:59:ARG:NH1	7:C:508:1PE:H131	1.93	0.83
1:D:59:ARG:NH1	7:D:508:1PE:H131	1.93	0.82
1:F:59:ARG:NH1	7:F:508:1PE:H131	1.96	0.81
1:E:59:ARG:NH1	7:E:508:1PE:H131	1.96	0.80
1:F:59:ARG:NH1	7:F:508:1PE:H121	1.99	0.76
1:E:59:ARG:NH1	7:E:508:1PE:H121	2.03	0.72
1:B:59:ARG:NH1	7:B:508:1PE:H121	2.04	0.69
1:D:59:ARG:NH1	7:D:508:1PE:H121	2.07	0.67
1:C:59:ARG:NH1	7:C:508:1PE:H121	2.05	0.66
1:E:59:ARG:HH12	7:E:508:1PE:C12	2.07	0.61
1:C:59:ARG:HH12	7:C:508:1PE:C12	2.10	0.59
1:D:59:ARG:HH12	7:D:508:1PE:C12	2.11	0.57
1:F:59:ARG:HH12	7:F:508:1PE:C12	2.04	0.57
1:A:59:ARG:NH1	7:A:508:1PE:H121	2.12	0.56
1:A:59:ARG:HH12	7:A:508:1PE:C12	2.14	0.52
1:E:415:SER:HB3	8:E:2229:HOH:O	2.09	0.52
7:E:508:1PE:H122	8:E:2275:HOH:O	2.11	0.51
1:D:59:ARG:HG2	7:D:508:1PE:H162	1.93	0.51
1:A:59:ARG:HG2	7:A:508:1PE:H162	1.93	0.50
1:B:59:ARG:HH12	7:B:508:1PE:C12	2.10	0.50
7:A:508:1PE:H122	8:A:2276:HOH:O	2.11	0.50
7:B:508:1PE:H122	8:B:2277:HOH:O	2.12	0.49
7:D:508:1PE:H122	8:D:2279:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ARG:HG2	7:C:508:IPE:H162	1.95	0.48
1:B:59:ARG:HG2	7:B:508:IPE:H162	1.96	0.48
1:F:59:ARG:HG2	7:F:508:IPE:H162	1.96	0.47
7:F:508:IPE:H122	8:F:2269:HOH:O	2.15	0.47
1:D:183:LYS:HA	1:D:220:VAL:HG12	1.96	0.46
7:C:508:IPE:H122	8:C:2274:HOH:O	2.14	0.46
1:D:59:ARG:CG	7:D:508:IPE:H162	2.46	0.46
1:A:59:ARG:CG	7:A:508:IPE:H162	2.46	0.45
1:D:68:ASP:HB2	1:E:345:ARG:HG3	1.99	0.45
1:C:349:ALA:HA	1:C:405:LEU:HD12	1.99	0.45
1:E:183:LYS:HA	1:E:220:VAL:HG12	1.99	0.45
1:A:183:LYS:HA	1:A:220:VAL:HG12	1.99	0.45
1:F:59:ARG:CG	7:F:508:IPE:H162	2.48	0.44
1:F:183:LYS:HA	1:F:220:VAL:HG12	2.00	0.44
1:C:390:GLY:HA2	1:C:395:ILE:HD12	2.00	0.44
1:C:119:LEU:HD11	1:C:125:ALA:HB3	2.00	0.43
1:B:183:LYS:HA	1:B:220:VAL:HG12	2.00	0.43
1:B:390:GLY:HA2	1:B:395:ILE:HD12	2.00	0.43
1:B:263:MET:HA	1:B:264:PRO:HD3	1.93	0.43
1:C:183:LYS:HA	1:C:220:VAL:HG12	1.99	0.43
1:E:59:ARG:CG	7:E:508:IPE:H162	2.48	0.42
1:B:185:GLY:O	1:B:187:PHE:HA	2.19	0.42
1:A:68:ASP:HB2	1:B:345:ARG:HG3	2.02	0.42
1:E:339:ASN:O	1:E:350:CYS:HB2	2.20	0.42
1:A:390:GLY:HA2	1:A:395:ILE:HD12	2.01	0.41
1:C:59:ARG:CG	7:C:508:IPE:H162	2.49	0.41
1:D:339:ASN:O	1:D:350:CYS:HB2	2.21	0.41
1:D:390:GLY:HA2	1:D:395:ILE:HD12	2.02	0.41
1:E:185:GLY:O	1:E:187:PHE:HA	2.22	0.40
1:A:185:GLY:O	1:A:187:PHE:HA	2.20	0.40
1:D:263:MET:HA	1:D:264:PRO:HD3	1.94	0.40
1:C:317:LEU:HA	1:C:320:THR:OG1	2.22	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	A	474/486 (98%)	464 (98%)	10 (2%)	0	100	100
1	B	474/486 (98%)	466 (98%)	8 (2%)	0	100	100
1	C	474/486 (98%)	469 (99%)	5 (1%)	0	100	100
1	D	474/486 (98%)	466 (98%)	8 (2%)	0	100	100
1	E	474/486 (98%)	466 (98%)	8 (2%)	0	100	100
1	F	474/486 (98%)	467 (98%)	7 (2%)	0	100	100
All	All	2844/2916 (98%)	2798 (98%)	46 (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	A	403/411 (98%)	397 (98%)	6 (2%)	72	84
1	B	403/411 (98%)	397 (98%)	6 (2%)	72	84
1	C	403/411 (98%)	398 (99%)	5 (1%)	78	88
1	D	403/411 (98%)	398 (99%)	5 (1%)	78	88
1	E	403/411 (98%)	397 (98%)	6 (2%)	72	84
1	F	403/411 (98%)	397 (98%)	6 (2%)	72	84
All	All	2418/2466 (98%)	2384 (99%)	34 (1%)	74	85

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ASP
1	A	113	ARG
1	A	187	PHE

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Mol	Chain	Res	Type
1	A	341	VAL
1	A	363	LYS
1	A	429	ARG
1	B	68	ASP
1	B	113	ARG
1	B	187	PHE
1	B	341	VAL
1	B	363	LYS
1	B	429	ARG
1	C	68	ASP
1	C	113	ARG
1	C	187	PHE
1	C	341	VAL
1	C	363	LYS
1	D	68	ASP
1	D	113	ARG
1	D	187	PHE
1	D	341	VAL
1	D	363	LYS
1	E	68	ASP
1	E	113	ARG
1	E	187	PHE
1	E	341	VAL
1	E	363	LYS
1	E	429	ARG
1	F	68	ASP
1	F	113	ARG
1	F	187	PHE
1	F	341	VAL
1	F	363	LYS
1	F	429	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	65	HIS

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 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	$\# Z > 2$
2	1AZ	A	501	-	24,31,31	1.31	4 (16%)	25,46,46	1.40	3 (12%)
4	P3S	A	505	3	10,14,14	3.46	3 (30%)	6,21,21	1.37	1 (16%)
5	PO4	A	506	3	4,4,4	0.35	0	6,6,6	0.29	0
7	1PE	A	508	-	15,15,15	0.62	0	14,14,14	0.38	0
2	1AZ	B	501	-	24,31,31	1.27	5 (20%)	25,46,46	1.35	3 (12%)
4	P3S	B	505	3	10,14,14	3.40	3 (30%)	6,21,21	1.26	1 (16%)
5	PO4	B	506	3	4,4,4	0.28	0	6,6,6	0.28	0
7	1PE	B	508	-	15,15,15	0.62	0	14,14,14	0.32	0
2	1AZ	C	501	-	24,31,31	1.24	4 (16%)	25,46,46	1.41	4 (16%)
4	P3S	C	505	3	10,14,14	3.32	3 (30%)	6,21,21	1.08	1 (16%)
5	PO4	C	506	3	4,4,4	0.41	0	6,6,6	0.29	0
7	1PE	C	508	-	15,15,15	0.66	0	14,14,14	0.34	0
2	1AZ	D	501	-	24,31,31	1.24	3 (12%)	25,46,46	1.36	3 (12%)
4	P3S	D	505	3	10,14,14	3.56	3 (30%)	6,21,21	0.46	0
5	PO4	D	506	3	4,4,4	0.51	0	6,6,6	0.29	0
7	1PE	D	508	-	15,15,15	0.64	0	14,14,14	0.36	0
2	1AZ	E	501	-	24,31,31	1.27	3 (12%)	25,46,46	1.37	4 (16%)
4	P3S	E	505	3	10,14,14	3.51	3 (30%)	6,21,21	1.53	1 (16%)
5	PO4	E	506	3	4,4,4	0.48	0	6,6,6	0.28	0
7	1PE	E	508	-	15,15,15	0.64	0	14,14,14	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1AZ	F	501	-	24,31,31	1.30	5 (20%)	25,46,46	1.42	3 (12%)
4	P3S	F	505	3	10,14,14	3.69	3 (30%)	6,21,21	0.55	0
5	PO4	F	506	3	4,4,4	0.52	0	6,6,6	0.29	0
7	1PE	F	508	-	15,15,15	0.62	0	14,14,14	0.34	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	1AZ	A	501	-	-	0/4/16/16	0/4/4/4
4	P3S	A	505	3	-	0/5/16/16	0/0/0/0
5	PO4	A	506	3	-	0/0/0/0	0/0/0/0
7	1PE	A	508	-	-	0/13/13/13	0/0/0/0
2	1AZ	B	501	-	-	0/4/16/16	0/4/4/4
4	P3S	B	505	3	-	0/5/16/16	0/0/0/0
5	PO4	B	506	3	-	0/0/0/0	0/0/0/0
7	1PE	B	508	-	-	0/13/13/13	0/0/0/0
2	1AZ	C	501	-	-	0/4/16/16	0/4/4/4
4	P3S	C	505	3	-	0/5/16/16	0/0/0/0
5	PO4	C	506	3	-	0/0/0/0	0/0/0/0
7	1PE	C	508	-	-	0/13/13/13	0/0/0/0
2	1AZ	D	501	-	-	0/4/16/16	0/4/4/4
4	P3S	D	505	3	-	0/5/16/16	0/0/0/0
5	PO4	D	506	3	-	0/0/0/0	0/0/0/0
7	1PE	D	508	-	-	0/13/13/13	0/0/0/0
2	1AZ	E	501	-	-	0/4/16/16	0/4/4/4
4	P3S	E	505	3	-	0/5/16/16	0/0/0/0
5	PO4	E	506	3	-	0/0/0/0	0/0/0/0
7	1PE	E	508	-	-	0/13/13/13	0/0/0/0
2	1AZ	F	501	-	-	0/4/16/16	0/4/4/4
4	P3S	F	505	3	-	0/5/16/16	0/0/0/0
5	PO4	F	506	3	-	0/0/0/0	0/0/0/0
7	1PE	F	508	-	-	0/13/13/13	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	505	P3S	CG-SD	-10.76	1.67	1.79
4	D	505	P3S	CG-SD	-10.25	1.67	1.79
4	E	505	P3S	CG-SD	-9.96	1.68	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	505	P3S	CG-SD	-9.89	1.68	1.79
4	B	505	P3S	CG-SD	-9.65	1.68	1.79
4	C	505	P3S	CG-SD	-9.19	1.68	1.79
2	A	501	1AZ	C13-N5	-3.63	1.34	1.39
2	B	501	1AZ	C13-N5	-3.60	1.35	1.39
2	E	501	1AZ	C13-N5	-3.46	1.35	1.39
2	F	501	1AZ	C13-N5	-3.31	1.35	1.39
2	C	501	1AZ	C13-N5	-3.19	1.35	1.39
2	D	501	1AZ	C13-N5	-3.09	1.35	1.39
2	F	501	1AZ	C5-N1	-2.29	1.34	1.38
2	B	501	1AZ	C5-N1	-2.20	1.35	1.38
2	A	501	1AZ	C5-N1	-2.16	1.35	1.38
4	F	505	P3S	PA-NE	2.08	1.68	1.59
2	B	501	1AZ	C13-N4	2.09	1.35	1.33
2	F	501	1AZ	C13-N4	2.15	1.35	1.33
2	B	501	1AZ	C1-CL1	2.22	1.79	1.73
2	C	501	1AZ	C18-CL2	2.24	1.79	1.73
2	E	501	1AZ	C1-CL1	2.25	1.79	1.73
2	D	501	1AZ	C1-CL1	2.26	1.79	1.73
2	C	501	1AZ	C13-N4	2.26	1.35	1.33
4	E	505	P3S	PA-NE	2.29	1.68	1.59
4	D	505	P3S	PA-NE	2.31	1.68	1.59
4	B	505	P3S	PA-NE	2.37	1.69	1.59
2	A	501	1AZ	C1-CL1	2.42	1.79	1.73
4	A	505	P3S	PA-O1A	2.43	1.50	1.46
2	B	501	1AZ	C18-CL2	2.44	1.79	1.73
4	C	505	P3S	PA-NE	2.49	1.69	1.59
2	F	501	1AZ	C1-CL1	2.51	1.79	1.73
4	A	505	P3S	PA-NE	2.51	1.69	1.59
2	C	501	1AZ	C1-CL1	2.56	1.79	1.73
4	F	505	P3S	PA-O1A	2.63	1.51	1.46
2	F	501	1AZ	C18-CL2	2.64	1.80	1.73
2	A	501	1AZ	C18-CL2	2.76	1.80	1.73
4	B	505	P3S	PA-O1A	2.79	1.51	1.46
2	D	501	1AZ	C18-CL2	2.98	1.80	1.73
2	E	501	1AZ	C18-CL2	3.06	1.81	1.73
4	D	505	P3S	PA-O1A	3.21	1.52	1.46
4	E	505	P3S	PA-O1A	3.22	1.52	1.46
4	C	505	P3S	PA-O1A	3.71	1.52	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	1AZ	C10-C9-N3	-3.47	103.90	110.02
2	E	501	1AZ	C11-C12-N3	-3.46	103.93	110.02
2	C	501	1AZ	C10-C9-N3	-3.42	104.00	110.02
2	B	501	1AZ	C10-C9-N3	-3.26	104.27	110.02
2	F	501	1AZ	C11-C12-N3	-3.25	104.30	110.02
2	F	501	1AZ	C10-C9-N3	-3.21	104.36	110.02
2	C	501	1AZ	C11-C12-N3	-3.15	104.47	110.02
2	D	501	1AZ	C10-C9-N3	-3.12	104.53	110.02
2	D	501	1AZ	C11-C12-N3	-3.06	104.63	110.02
2	A	501	1AZ	C11-C12-N3	-3.05	104.64	110.02
2	E	501	1AZ	C10-C9-N3	-2.93	104.86	110.02
2	B	501	1AZ	C11-C12-N3	-2.89	104.92	110.02
2	A	501	1AZ	C1-C2-C3	-2.36	118.84	120.36
2	C	501	1AZ	C6-C5-N1	-2.34	119.14	120.52
2	B	501	1AZ	C1-C2-C3	-2.18	118.96	120.36
2	D	501	1AZ	C6-C13-N4	-2.11	106.75	110.83
2	E	501	1AZ	C1-C2-C3	-2.10	119.00	120.36
2	C	501	1AZ	C6-C13-N4	-2.10	106.77	110.83
2	F	501	1AZ	C6-C13-N4	-2.09	106.79	110.83
2	E	501	1AZ	C6-C13-N4	-2.06	106.83	110.83
4	C	505	P3S	OE-SD-CG	2.20	109.75	108.23
4	B	505	P3S	OE-SD-CG	2.91	110.25	108.23
4	A	505	P3S	OE-SD-CG	2.99	110.30	108.23
4	E	505	P3S	OE-SD-CG	3.60	110.72	108.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	508	1PE	8	0
7	B	508	1PE	7	0
7	C	508	1PE	8	0
7	D	508	1PE	8	0
7	E	508	1PE	7	0
7	F	508	1PE	8	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, 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	476/486 (97%)	-0.07	12 (2%) 61 60	18, 26, 39, 57	0
1	B	476/486 (97%)	-0.04	7 (1%) 76 75	18, 26, 39, 57	0
1	C	476/486 (97%)	-0.05	9 (1%) 70 68	18, 26, 39, 57	0
1	D	476/486 (97%)	-0.07	6 (1%) 79 78	18, 26, 39, 57	0
1	E	476/486 (97%)	-0.17	2 (0%) 93 93	18, 26, 37, 57	0
1	F	476/486 (97%)	-0.06	6 (1%) 79 78	18, 26, 38, 57	0
All	All	2856/2916 (97%)	-0.08	42 (1%) 76 75	18, 26, 39, 57	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	GLU	5.7
1	A	410	PRO	4.8
1	C	3	GLU	4.4
1	A	409	PRO	4.2
1	D	3	GLU	3.9
1	C	409	PRO	3.9
1	B	410	PRO	3.5
1	E	3	GLU	3.5
1	C	414	ALA	3.5
1	A	414	ALA	3.3
1	A	357	GLY	3.2
1	C	410	PRO	3.1
1	B	414	ALA	3.1
1	D	410	PRO	3.0
1	F	3	GLU	2.9
1	B	4	LYS	2.9
1	D	4	LYS	2.9
1	A	292	GLU	2.8
1	C	411	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	411	GLU	2.7
1	B	415	SER	2.6
1	F	414	ALA	2.6
1	A	413	ALA	2.6
1	F	411	GLU	2.5
1	C	292	GLU	2.4
1	A	293	THR	2.4
1	E	170	ALA	2.4
1	A	3	GLU	2.3
1	D	44	LYS	2.3
1	C	7	ASP	2.3
1	B	15	ASP	2.2
1	A	416	ILE	2.2
1	A	398	GLN	2.2
1	A	399	ALA	2.2
1	F	44	LYS	2.2
1	A	411	GLU	2.2
1	D	11	LYS	2.2
1	C	413	ALA	2.1
1	F	7	ASP	2.1
1	C	415	SER	2.0
1	B	120	ILE	2.0
1	F	409	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 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
7	1PE	B	508	16/16	0.73	0.26	5.92	30,32,37,38	0
3	MG	E	502	1/1	0.98	0.23	5.08	24,24,24,24	0
7	1PE	F	508	16/16	0.75	0.23	4.04	30,32,37,38	0
7	1PE	C	508	16/16	0.73	0.24	3.79	31,32,37,38	0
7	1PE	E	508	16/16	0.78	0.24	3.69	30,32,37,38	0
7	1PE	D	508	16/16	0.73	0.24	3.64	30,32,37,38	0
5	PO4	C	506	5/5	0.93	0.16	1.81	37,37,39,39	0
5	PO4	B	506	5/5	0.88	0.19	1.74	37,37,39,39	0
7	1PE	A	508	16/16	0.82	0.17	1.37	30,32,37,38	0
2	1AZ	E	501	28/28	0.88	0.16	0.77	37,38,40,41	0
4	P3S	E	505	15/15	0.97	0.16	0.55	24,24,24,25	0
4	P3S	F	505	15/15	0.99	0.17	0.53	24,24,25,25	0
5	PO4	D	506	5/5	0.96	0.16	0.51	37,37,39,39	0
2	1AZ	B	501	28/28	0.89	0.14	0.35	37,38,40,41	0
3	MG	D	503	1/1	0.97	0.16	0.33	27,27,27,27	0
3	MG	D	502	1/1	0.95	0.17	0.27	25,25,25,25	0
2	1AZ	A	501	28/28	0.88	0.14	0.22	37,38,40,41	0
2	1AZ	D	501	28/28	0.88	0.14	0.14	37,38,40,41	0
3	MG	B	503	1/1	0.96	0.14	0.07	27,27,27,27	0
2	1AZ	C	501	28/28	0.88	0.14	-0.07	37,38,40,41	0
4	P3S	D	505	15/15	0.98	0.14	-0.21	24,24,25,25	0
5	PO4	A	506	5/5	0.94	0.13	-0.23	37,37,39,39	0
3	MG	C	502	1/1	0.98	0.14	-0.36	25,25,25,25	0
2	1AZ	F	501	28/28	0.91	0.13	-0.41	37,38,40,41	0
3	MG	A	502	1/1	0.90	0.13	-0.45	25,25,25,25	0
4	P3S	B	505	15/15	0.98	0.11	-0.70	24,24,25,25	0
3	MG	F	502	1/1	0.94	0.17	-0.70	25,25,25,25	0
5	PO4	F	506	5/5	0.96	0.14	-0.76	37,37,39,39	0
4	P3S	A	505	15/15	0.97	0.10	-0.87	24,24,25,25	0
4	P3S	C	505	15/15	0.97	0.10	-0.96	24,24,25,25	0
5	PO4	E	506	5/5	0.97	0.12	-1.27	37,37,39,39	0
3	MG	B	502	1/1	0.97	0.12	-1.44	25,25,25,25	0
3	MG	E	503	1/1	0.98	0.09	-2.01	27,27,27,27	0
3	MG	F	503	1/1	0.95	0.09	-2.36	26,26,26,26	0
6	CL	E	507	1/1	0.99	0.04	-2.57	28,28,28,28	0
6	CL	B	507	1/1	0.98	0.03	-2.84	28,28,28,28	0
6	CL	F	507	1/1	0.99	0.03	-3.09	28,28,28,28	0
6	CL	C	507	1/1	0.98	0.05	-3.40	28,28,28,28	0
6	CL	A	507	1/1	0.99	0.04	-3.56	28,28,28,28	0
6	CL	D	507	1/1	0.99	0.04	-4.26	28,28,28,28	0
3	MG	C	503	1/1	0.97	0.06	-4.85	27,27,27,27	0
3	MG	A	503	1/1	0.94	0.04	-6.63	27,27,27,27	0
3	MG	A	504	1/1	0.95	0.06	-	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	C	504	1/1	0.98	0.11	-	24,24,24,24	0
3	MG	D	504	1/1	0.97	0.15	-	25,25,25,25	0
3	MG	F	504	1/1	0.96	0.15	-	24,24,24,24	0
3	MG	E	504	1/1	0.96	0.17	-	24,24,24,24	0
3	MG	B	504	1/1	0.92	0.11	-	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.