Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:34 PM GMT

PDB ID	:	3ZUK
Title	:	CRYSTAL STRUCTURE OF MYCOBACTERIUM TUBERCULOSIS ZINC METALLOPROTEASE ZMP1 IN COMPLEX WITH INHIBITOR
Authors	:	Ferraris, D.M.; Sbardella, D.; Petrera, A.; Marini, S.; Amstutz, B.; Coletta, M.; Sander, P.; Rizzi, M.
Deposited on	:	2011-07-19
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

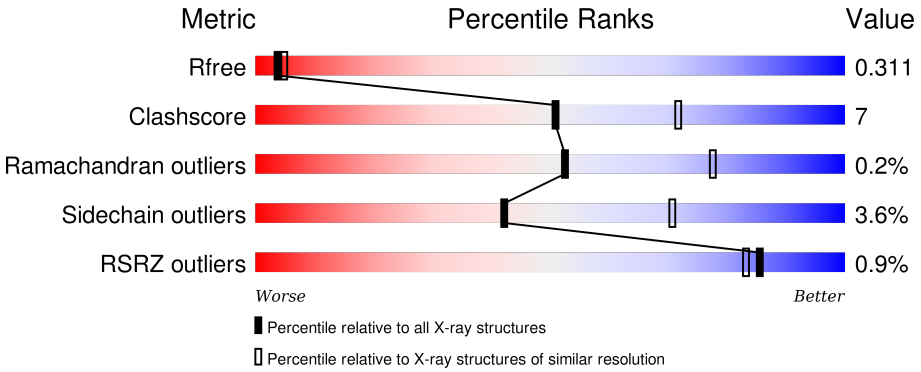
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 <=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	699	% 82% 11% 6%
1	B	699	% 78% 15% • 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
4	211	A	1666	-	-	-	X
5	PEG	A	1667	-	-	-	X
5	PEG	A	1668	-	-	-	X
5	PEG	A	1672	-	-	-	X
5	PEG	A	1673	-	-	-	X
5	PEG	A	1676	-	-	X	X
5	PEG	A	1677	-	-	-	X
5	PEG	A	1678	-	-	-	X
5	PEG	A	1679	-	-	-	X
5	PEG	A	1680	-	-	-	X
5	PEG	A	1681	-	-	-	X
5	PEG	B	1666	-	-	-	X
5	PEG	B	1667	-	-	-	X
5	PEG	B	1668	-	-	-	X
5	PEG	B	1671	-	-	-	X
5	PEG	B	1672	-	-	-	X
5	PEG	B	1673	-	-	-	X
5	PEG	B	1675	-	-	-	X
5	PEG	B	1676	-	-	-	X
5	PEG	B	1677	-	-	-	X
5	PEG	B	1679	-	-	-	X
6	PGE	A	1682	-	-	-	X
6	PGE	A	1683	-	-	-	X
6	PGE	A	1684	-	-	-	X
6	PGE	A	1685	-	-	-	X
6	PGE	A	1686	-	-	-	X
6	PGE	B	1681	-	-	-	X
6	PGE	B	1683	-	-	-	X
7	PG4	A	1687	-	-	-	X
7	PG4	B	1684	-	-	X	X
7	PG4	B	1685	-	-	-	X
7	PG4	B	1686	-	-	-	X
8	ACT	A	1688	-	-	-	X
8	ACT	A	1691	-	-	-	X
8	ACT	A	1692	-	-	-	X
8	ACT	B	1687	-	-	-	X
8	ACT	B	1688	-	-	-	X
8	ACT	B	1689	-	-	-	X
8	ACT	B	1690	-	-	-	X
8	ACT	B	1691	-	-	-	X
8	ACT	B	1692	-	-	X	X
8	ACT	B	1693	-	-	-	X
9	SO4	B	1695	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 11220 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 ENDOPEPTIDASE, PEPTIDASE FAMILY M13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	657	Total	C	N	O	S	0	0	0
			5187	3277	925	976	9			
1	B	657	Total	C	N	O	S	0	0	0
			5187	3277	925	976	9			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	EXPRESSION TAG	UNP O53649
A	-34	ARG	-	EXPRESSION TAG	UNP O53649
A	-33	GLY	-	EXPRESSION TAG	UNP O53649
A	-32	SER	-	EXPRESSION TAG	UNP O53649
A	-31	HIS	-	EXPRESSION TAG	UNP O53649
A	-30	HIS	-	EXPRESSION TAG	UNP O53649
A	-29	HIS	-	EXPRESSION TAG	UNP O53649
A	-28	HIS	-	EXPRESSION TAG	UNP O53649
A	-27	HIS	-	EXPRESSION TAG	UNP O53649
A	-26	HIS	-	EXPRESSION TAG	UNP O53649
A	-25	GLY	-	EXPRESSION TAG	UNP O53649
A	-24	MET	-	EXPRESSION TAG	UNP O53649
A	-23	ALA	-	EXPRESSION TAG	UNP O53649
A	-22	SER	-	EXPRESSION TAG	UNP O53649
A	-21	MET	-	EXPRESSION TAG	UNP O53649
A	-20	THR	-	EXPRESSION TAG	UNP O53649
A	-19	GLY	-	EXPRESSION TAG	UNP O53649
A	-18	GLY	-	EXPRESSION TAG	UNP O53649
A	-17	GLN	-	EXPRESSION TAG	UNP O53649
A	-16	GLN	-	EXPRESSION TAG	UNP O53649
A	-15	MET	-	EXPRESSION TAG	UNP O53649
A	-14	GLY	-	EXPRESSION TAG	UNP O53649
A	-13	ARG	-	EXPRESSION TAG	UNP O53649
A	-12	ASP	-	EXPRESSION TAG	UNP O53649
A	-11	LEU	-	EXPRESSION TAG	UNP O53649

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	TYR	-	EXPRESSION TAG	UNP O53649
A	-9	ASP	-	EXPRESSION TAG	UNP O53649
A	-8	ASP	-	EXPRESSION TAG	UNP O53649
A	-7	ASP	-	EXPRESSION TAG	UNP O53649
A	-6	ASP	-	EXPRESSION TAG	UNP O53649
A	-5	LYS	-	EXPRESSION TAG	UNP O53649
A	-4	ASP	-	EXPRESSION TAG	UNP O53649
A	-3	HIS	-	EXPRESSION TAG	UNP O53649
A	-2	PRO	-	EXPRESSION TAG	UNP O53649
A	-1	PHE	-	EXPRESSION TAG	UNP O53649
A	0	THR	-	EXPRESSION TAG	UNP O53649
B	-35	MET	-	EXPRESSION TAG	UNP O53649
B	-34	ARG	-	EXPRESSION TAG	UNP O53649
B	-33	GLY	-	EXPRESSION TAG	UNP O53649
B	-32	SER	-	EXPRESSION TAG	UNP O53649
B	-31	HIS	-	EXPRESSION TAG	UNP O53649
B	-30	HIS	-	EXPRESSION TAG	UNP O53649
B	-29	HIS	-	EXPRESSION TAG	UNP O53649
B	-28	HIS	-	EXPRESSION TAG	UNP O53649
B	-27	HIS	-	EXPRESSION TAG	UNP O53649
B	-26	HIS	-	EXPRESSION TAG	UNP O53649
B	-25	GLY	-	EXPRESSION TAG	UNP O53649
B	-24	MET	-	EXPRESSION TAG	UNP O53649
B	-23	ALA	-	EXPRESSION TAG	UNP O53649
B	-22	SER	-	EXPRESSION TAG	UNP O53649
B	-21	MET	-	EXPRESSION TAG	UNP O53649
B	-20	THR	-	EXPRESSION TAG	UNP O53649
B	-19	GLY	-	EXPRESSION TAG	UNP O53649
B	-18	GLY	-	EXPRESSION TAG	UNP O53649
B	-17	GLN	-	EXPRESSION TAG	UNP O53649
B	-16	GLN	-	EXPRESSION TAG	UNP O53649
B	-15	MET	-	EXPRESSION TAG	UNP O53649
B	-14	GLY	-	EXPRESSION TAG	UNP O53649
B	-13	ARG	-	EXPRESSION TAG	UNP O53649
B	-12	ASP	-	EXPRESSION TAG	UNP O53649
B	-11	LEU	-	EXPRESSION TAG	UNP O53649
B	-10	TYR	-	EXPRESSION TAG	UNP O53649
B	-9	ASP	-	EXPRESSION TAG	UNP O53649
B	-8	ASP	-	EXPRESSION TAG	UNP O53649
B	-7	ASP	-	EXPRESSION TAG	UNP O53649
B	-6	ASP	-	EXPRESSION TAG	UNP O53649
B	-5	LYS	-	EXPRESSION TAG	UNP O53649

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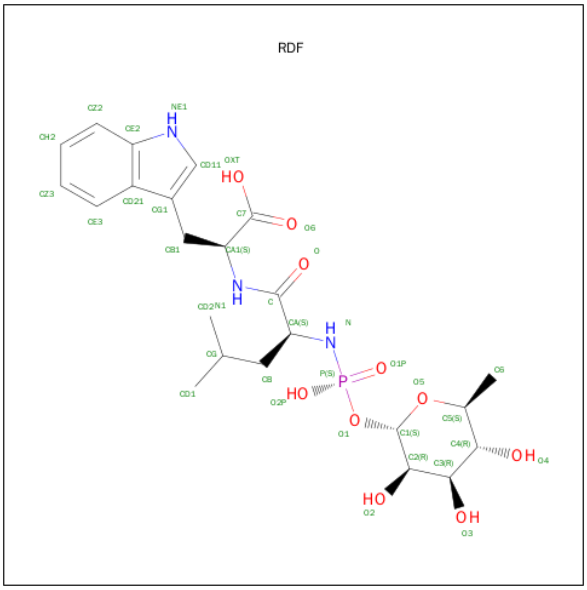
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	ASP	-	EXPRESSION TAG	UNP O53649
B	-3	HIS	-	EXPRESSION TAG	UNP O53649
B	-2	PRO	-	EXPRESSION TAG	UNP O53649
B	-1	PHE	-	EXPRESSION TAG	UNP O53649
B	0	THR	-	EXPRESSION TAG	UNP O53649

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

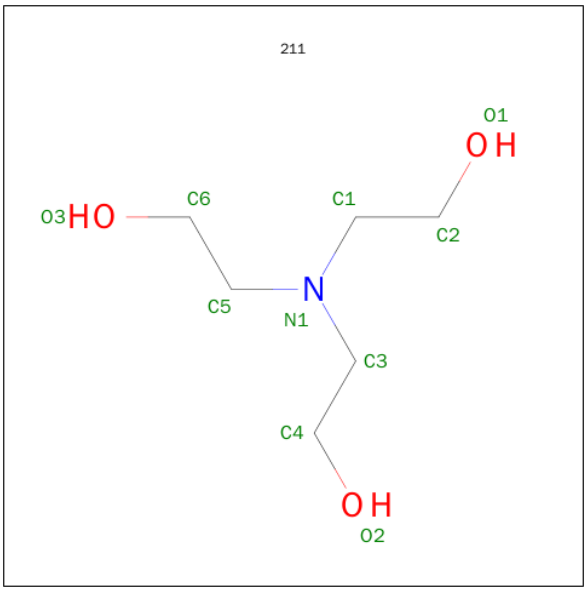
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0

- Molecule 3 is N-ALPHA-L-RHAMNOPYRANOSYLOXY(HYDROXYPHOSPHINYL)-L-LEUCYL-L-TRYPTOPHAN (three-letter code: RDF) (formula: $C_{23}H_{34}N_3O_{10}P$).



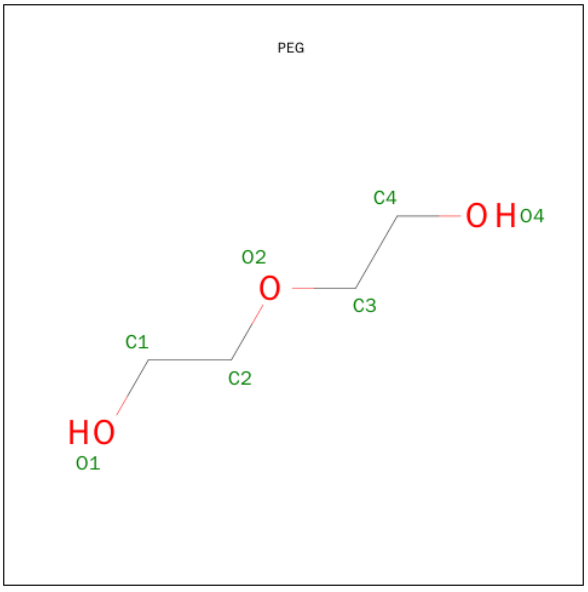
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 37 23 3 10 1	0	0
3	B	1	Total C N O P 37 23 3 10 1	0	0

- Molecule 4 is 2,2',2''-NITRILOTRIETHANOL (three-letter code: 211) (formula: $C_6H_{15}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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

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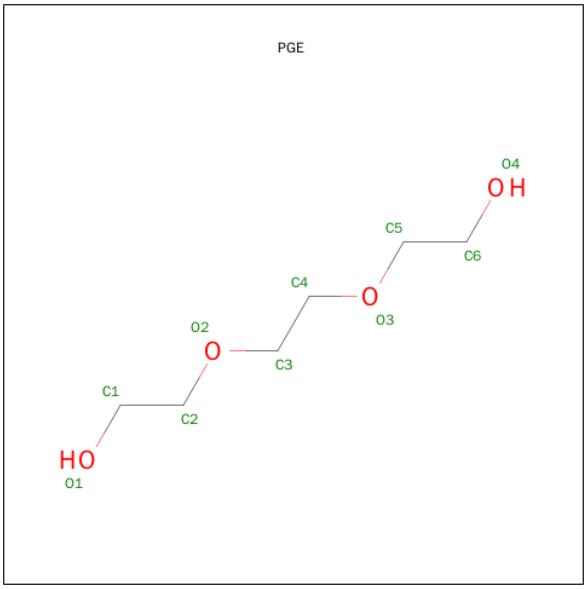
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0

- 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 10 6 4	0	0
6	A	1	Total C O 10 6 4	0	0
6	A	1	Total C O 10 6 4	0	0
6	A	1	Total C O 10 6 4	0	0
6	A	1	Total C O 10 6 4	0	0

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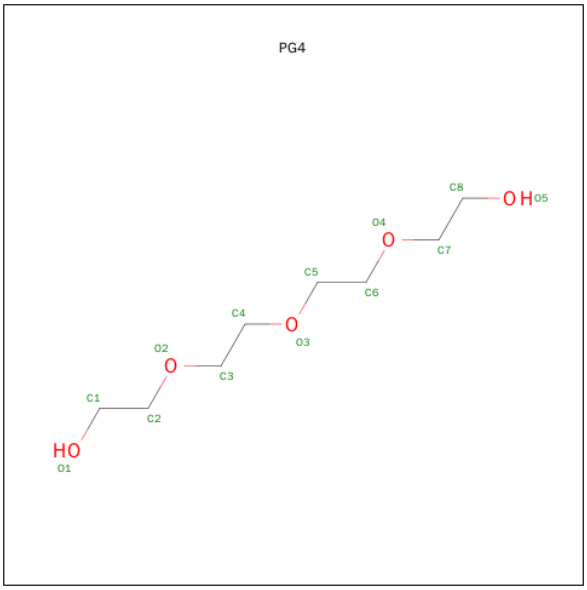
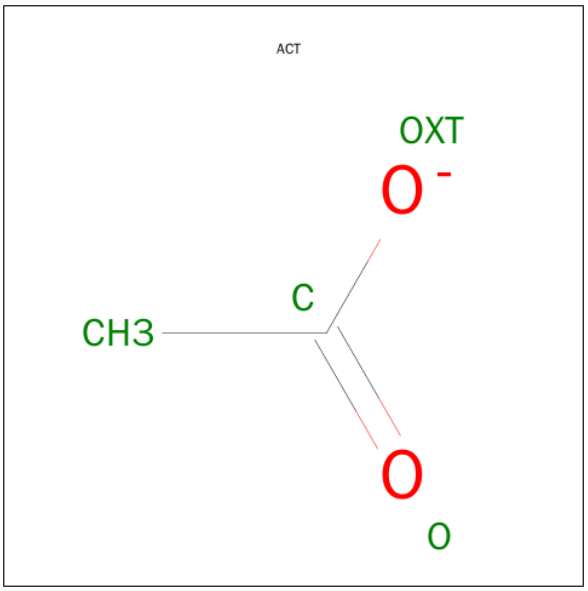
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 10 6 4	0	0
6	B	1	Total C O 10 6 4	0	0
6	B	1	Total C O 10 6 4	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



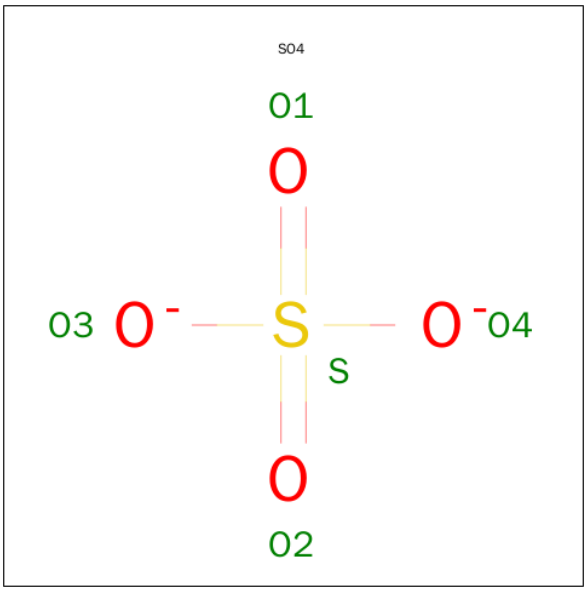
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 13 8 5	0	0
7	B	1	Total C O 13 8 5	0	0
7	B	1	Total C O 13 8 5	0	0
7	B	1	Total C O 13 8 5	0	0

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	2	Total Cl 2 2	0	0
10	A	1	Total Cl 1 1	0	0

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total Ca 1 1	0	0

- Molecule 12 is water.

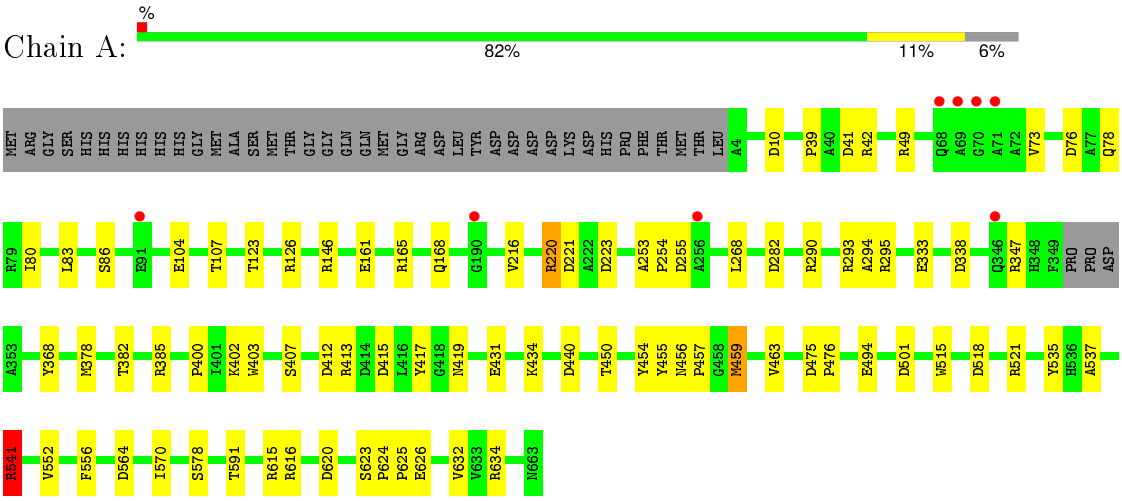
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	159	Total O 159 159	0	0
12	B	173	Total O 173 173	0	0

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.

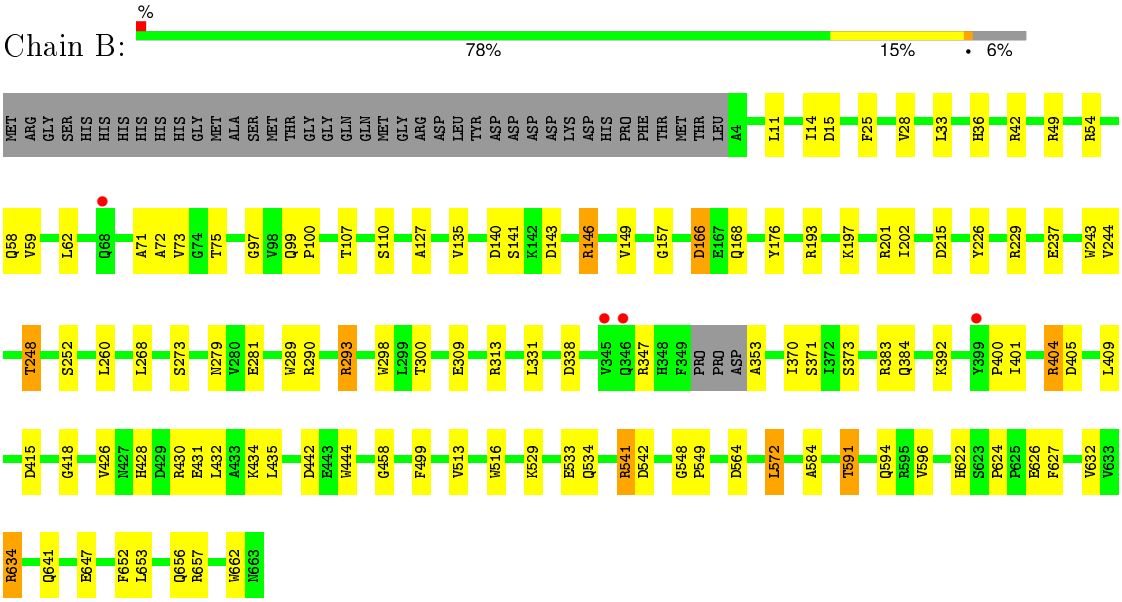
- Molecule 1: ENDOPEPTIDASE, PEPTIDASE FAMILY M13

Chain A:



- Molecule 1: ENDOPEPTIDASE, PEPTIDASE FAMILY M13

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	128.29Å 198.77Å 63.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 54.56 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.8 (30.00-2.60) 76.6 (54.56-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.32 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.175 , 0.250 0.184 , 0.311	Depositor DCC
R_{free} test set	1016 reflections (2.21%)	DCC
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 41.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.37$	Xtriage
Outliers	0 of 72845 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11220	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, PGE, CL, CA, 211, PG4, RDF, SO4, ACT, PEG

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	0.71	0/5317	0.75	2/7236 (0.0%)
1	B	0.73	0/5317	0.75	1/7236 (0.0%)
All	All	0.72	0/10634	0.75	3/14472 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	215	ASP	CB-CG-OD1	5.57	123.32	118.30
1	A	615	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	541	ARG	NE-CZ-NH2	-5.32	117.64	120.30

There are no chirality outliers.

There are no planarity outliers.

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	5187	0	4968	56	0
1	B	5187	0	4968	77	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	37	0	32	8	0
3	B	37	0	32	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	10	0	15	1	0
5	A	105	0	150	14	0
5	B	105	0	150	10	0
6	A	50	0	70	1	0
6	B	30	0	42	2	0
7	A	13	0	18	0	0
7	B	39	0	54	12	0
8	A	20	0	15	0	0
8	B	32	0	24	2	0
9	A	10	0	0	0	0
9	B	20	0	0	0	0
10	A	1	0	0	0	0
10	B	2	0	0	0	0
11	B	1	0	0	0	0
12	A	159	0	0	8	0
12	B	173	0	0	9	0
All	All	11220	0	10538	148	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 7.

All (148) 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:B:1665:RDF:CD11	3:B:1665:RDF:HD1	0.97	1.15
3:A:1665:RDF:HD1	3:A:1665:RDF:CD11	0.97	1.13
1:B:541:ARG:HH11	1:B:541:ARG:HG2	1.16	1.05
1:B:591:THR:HG22	1:B:594:GLN:H	1.29	0.95
1:B:548:GLY:H	5:B:1670:PEG:H31	1.31	0.92
1:B:135:VAL:H	8:B:1692:ACT:H3	1.35	0.89
1:B:42:ARG:HG3	1:B:49:ARG:NH1	1.88	0.89
1:A:417:TYR:HB2	5:A:1669:PEG:H11	1.55	0.89
1:A:333:GLU:HG3	5:A:1668:PEG:H42	1.57	0.87
3:A:1665:RDF:CG1	3:A:1665:RDF:HD1	2.10	0.81
3:B:1665:RDF:HD1	3:B:1665:RDF:CG1	2.10	0.81
1:A:378:MET:CE	1:A:382:THR:HB	2.10	0.81
1:B:542:ASP:HB3	7:B:1684:PG4:H12	1.65	0.78
1:A:624:PRO:HA	5:A:1676:PEG:H32	1.66	0.77
1:A:624:PRO:HG3	5:A:1676:PEG:H22	1.66	0.77
3:A:1665:RDF:CE3	3:A:1665:RDF:CG1	2.57	0.76
3:B:1665:RDF:CE2	3:B:1665:RDF:CE3	2.40	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:ARG:HG2	1:B:430:ARG:CZ	2.19	0.73
7:B:1684:PG4:H11	12:B:2153:HOH:O	1.88	0.71
3:B:1665:RDF:CE3	3:B:1665:RDF:CG1	2.57	0.71
1:A:104:GLU:O	1:A:107:THR:HB	1.90	0.70
3:A:1665:RDF:CE3	3:A:1665:RDF:CE2	2.42	0.69
1:A:41:ASP:OD1	1:A:42:ARG:NH1	2.24	0.69
1:B:624:PRO:HD3	7:B:1684:PG4:H61	1.75	0.68
1:B:127:ALA:HB2	5:B:1671:PEG:H42	1.76	0.67
1:B:541:ARG:NH1	1:B:541:ARG:HG2	1.93	0.66
1:B:309:GLU:OE2	1:B:313:ARG:NH1	2.29	0.66
1:B:634:ARG:HH12	7:B:1686:PG4:H22	1.61	0.66
1:B:36:HIS:CE1	12:B:2012:HOH:O	2.50	0.65
1:B:624:PRO:CD	7:B:1684:PG4:H61	2.27	0.64
1:B:430:ARG:NH1	12:B:2113:HOH:O	2.28	0.63
3:B:1665:RDF:NE1	3:B:1665:RDF:HD1	2.14	0.63
1:B:622:HIS:O	7:B:1684:PG4:H72	1.99	0.62
1:A:413:ARG:CD	12:A:2108:HOH:O	2.47	0.62
1:B:584:ALA:H	6:B:1683:PGE:H2	1.63	0.62
3:A:1665:RDF:NE1	3:A:1665:RDF:HD1	2.15	0.62
1:A:253:ALA:C	1:A:255:ASP:H	2.03	0.61
1:B:627:PHE:CE1	5:B:1676:PEG:H32	2.36	0.60
5:B:1667:PEG:H41	12:B:2051:HOH:O	2.01	0.60
1:B:140:ASP:OD2	1:B:146:ARG:NH1	2.35	0.59
1:A:578:SER:HA	5:A:1681:PEG:H31	1.85	0.59
1:B:42:ARG:HG3	1:B:49:ARG:HH12	1.63	0.59
1:A:10:ASP:HB2	5:A:1667:PEG:H21	1.84	0.58
1:A:413:ARG:HD2	12:A:2108:HOH:O	2.03	0.58
1:B:641:GLN:HG3	12:B:2161:HOH:O	2.03	0.57
1:A:591:THR:HG21	12:A:2154:HOH:O	2.04	0.57
1:B:404:ARG:HG2	1:B:430:ARG:NE	2.21	0.56
1:B:72:ALA:O	1:B:75:THR:HG22	2.07	0.55
1:B:529:LYS:O	1:B:533:GLU:HG3	2.07	0.55
1:A:73:VAL:HA	1:A:78:GLN:HG3	1.88	0.55
1:A:623:SER:C	5:A:1676:PEG:H31	2.27	0.55
1:A:456:ASN:ND2	1:A:459:MET:HG3	2.21	0.54
1:B:647:GLU:HA	1:B:652:PHE:CD2	2.43	0.54
1:B:458:GLY:H	5:B:1673:PEG:H22	1.72	0.54
1:B:624:PRO:HG3	7:B:1684:PG4:H61	1.90	0.54
1:B:157:GLY:HA3	1:B:176:TYR:OH	2.08	0.54
1:A:535:TYR:O	1:A:552:VAL:HB	2.07	0.54
1:B:243:TRP:CZ2	1:B:268:LEU:HD21	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LYS:O	1:B:201:ARG:HG3	2.08	0.54
1:B:428:HIS:HB2	12:B:2114:HOH:O	2.09	0.53
1:B:541:ARG:HG2	1:B:626:GLU:OE2	2.07	0.53
1:A:537:ALA:HB1	1:B:549:PRO:HD3	1.90	0.53
1:A:620:ASP:OD2	5:A:1676:PEG:H41	2.09	0.52
1:B:401:ILE:HD13	1:B:442:ASP:HB3	1.92	0.52
1:B:25:PHE:CE2	1:B:33:LEU:HD11	2.45	0.52
1:A:564:ASP:HB3	1:A:632:VAL:HG21	1.91	0.52
1:A:413:ARG:HD3	12:A:2108:HOH:O	2.08	0.52
1:B:135:VAL:N	8:B:1692:ACT:H3	2.15	0.51
1:A:624:PRO:CA	5:A:1676:PEG:H32	2.37	0.51
1:B:627:PHE:HE1	5:B:1676:PEG:H32	1.76	0.51
1:B:229:ARG:HH12	5:B:1679:PEG:H41	1.76	0.50
1:A:83:LEU:O	1:A:86:SER:HB2	2.12	0.50
1:B:290:ARG:NH1	12:B:2047:HOH:O	2.44	0.49
1:B:401:ILE:H	1:B:401:ILE:HD12	1.77	0.49
1:B:54:ARG:O	1:B:58:GLN:HG3	2.13	0.49
1:B:572:LEU:HD13	1:B:596:VAL:HG11	1.94	0.49
1:A:541:ARG:HD2	1:A:626:GLU:OE1	2.12	0.49
1:B:149:VAL:HG22	1:B:435:LEU:HD11	1.94	0.48
1:A:39:PRO:HG2	1:A:42:ARG:HD2	1.94	0.48
1:A:221:ASP:OD1	1:A:223:ASP:HB2	2.13	0.48
1:A:76:ASP:O	1:A:80:ILE:HD12	2.13	0.48
1:A:378:MET:HE3	1:A:382:THR:HB	1.93	0.48
1:A:253:ALA:C	1:A:255:ASP:N	2.66	0.48
1:A:450:THR:HA	5:A:1668:PEG:H12	1.94	0.48
1:B:624:PRO:CG	7:B:1684:PG4:H61	2.44	0.48
1:B:140:ASP:HB3	1:B:143:ASP:O	2.14	0.47
1:B:564:ASP:HB3	1:B:632:VAL:HG21	1.97	0.47
5:A:1673:PEG:H42	12:A:2117:HOH:O	2.14	0.47
1:B:71:ALA:HB1	1:B:75:THR:HG21	1.95	0.47
1:B:415:ASP:OD2	1:B:418:GLY:HA3	2.15	0.46
1:A:616:ARG:HB2	5:A:1676:PEG:H12	1.96	0.46
1:A:368:TYR:CD2	1:A:570:ILE:HG21	2.50	0.46
1:B:542:ASP:CB	7:B:1684:PG4:H12	2.42	0.46
1:A:385:ARG:NH1	1:A:515:TRP:O	2.45	0.46
1:A:455:TYR:CE2	1:A:457:PRO:HA	2.51	0.46
1:B:431:GLU:HA	1:B:434:LYS:HD2	1.97	0.45
1:B:534:GLN:HE21	7:B:1686:PG4:H62	1.79	0.45
1:A:123:THR:O	1:A:126:ARG:HB3	2.15	0.45
1:A:625:PRO:HG2	12:A:2150:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ILE:O	1:B:373:SER:HB2	2.16	0.45
1:A:290:ARG:NH1	12:A:2082:HOH:O	2.49	0.45
3:A:1665:RDF:H5	6:A:1684:PGE:H12	1.98	0.44
1:A:220:ARG:NH2	1:A:501:ASP:OD2	2.50	0.44
1:B:99:GLN:HB3	1:B:100:PRO:HD3	2.00	0.44
1:B:653:LEU:HG	1:B:657:ARG:HB3	1.98	0.44
1:A:402:LYS:HE3	1:A:440:ASP:OD2	2.18	0.44
3:A:1665:RDF:OXT	4:A:1666:211:H51	2.18	0.43
1:B:400:PRO:HB3	1:B:444:TRP:CD1	2.53	0.43
1:B:11:LEU:HD13	7:B:1685:PG4:H21	2.00	0.43
1:B:298:TRP:CH2	1:B:331:LEU:HD13	2.54	0.43
1:A:294:ALA:HB2	12:A:2029:HOH:O	2.19	0.43
1:B:516:TRP:CD1	6:B:1682:PGE:H6	2.53	0.43
1:B:166:ASP:HB3	1:B:168:GLN:HB2	2.01	0.43
1:B:353:ALA:HB3	5:B:1680:PEG:H22	2.00	0.43
1:A:454:TYR:CZ	1:A:463:VAL:HG21	2.54	0.42
1:B:244:VAL:O	1:B:248:THR:HB	2.19	0.42
1:B:59:VAL:HA	1:B:62:LEU:HD12	2.00	0.42
1:B:392:LYS:HE3	5:B:1678:PEG:H12	2.01	0.42
1:A:412:ASP:HB3	1:A:415:ASP:HB3	2.00	0.42
1:B:97:GLY:HA2	1:B:300:THR:CG2	2.49	0.42
1:A:378:MET:CE	1:A:382:THR:CB	2.92	0.42
1:B:499:PHE:HB3	1:B:662:TRP:CZ2	2.55	0.42
1:B:14:ILE:HD13	1:B:28:VAL:HA	2.02	0.42
1:B:279:ASN:OD1	1:B:281:GLU:HB2	2.20	0.42
1:B:202:ILE:HD13	1:B:289:TRP:HB2	2.01	0.42
1:B:293:ARG:NH1	12:B:2047:HOH:O	2.46	0.41
1:B:409:LEU:HB2	1:B:426:VAL:HG21	2.02	0.41
1:B:15:ASP:C	1:B:15:ASP:OD1	2.58	0.41
1:B:647:GLU:HA	1:B:652:PHE:CG	2.55	0.41
1:A:400:PRO:HD2	1:A:403:TRP:CH2	2.55	0.41
1:B:141:SER:HB2	1:B:226:TYR:CD1	2.55	0.41
1:A:216:VAL:HB	1:A:556:PHE:CE1	2.55	0.41
1:A:475:ASP:HA	1:A:476:PRO:HD2	1.96	0.41
5:B:1668:PEG:H32	12:B:2140:HOH:O	2.21	0.41
1:A:268:LEU:HD12	1:A:268:LEU:HA	1.77	0.41
1:B:401:ILE:N	1:B:401:ILE:HD12	2.36	0.41
1:A:417:TYR:H	5:A:1669:PEG:H22	1.85	0.41
1:B:404:ARG:HD3	1:B:430:ARG:NH1	2.36	0.41
1:A:86:SER:OG	1:A:419:ASN:ND2	2.54	0.41
1:A:385:ARG:HD2	1:A:515:TRP:HB2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ARG:HG3	1:A:417:TYR:OH	2.21	0.40
1:A:42:ARG:HG2	1:A:49:ARG:NH1	2.37	0.40
1:A:39:PRO:CG	1:A:42:ARG:HD2	2.51	0.40
1:A:494:GLU:OE1	3:A:1665:RDF:O2P	2.39	0.40
1:B:634:ARG:NH1	7:B:1686:PG4:H22	2.31	0.40
1:A:415:ASP:HA	5:A:1669:PEG:H32	2.02	0.40
1:B:252:SER:HB2	1:B:432:LEU:HD13	2.02	0.40
1:A:431:GLU:O	1:A:434:LYS:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	653/699 (93%)	624 (96%)	27 (4%)	2 (0%)	46 72
1	B	653/699 (93%)	622 (95%)	31 (5%)	0	100 100
All	All	1306/1398 (93%)	1246 (95%)	58 (4%)	2 (0%)	52 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	A	254	PRO

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	522/558 (94%)	508 (97%)	14 (3%)	52 79
1	B	522/558 (94%)	498 (95%)	24 (5%)	33 61
All	All	1044/1116 (94%)	1006 (96%)	38 (4%)	42 71

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	ARG
1	A	161	GLU
1	A	165	ARG
1	A	220	ARG
1	A	282	ASP
1	A	293	ARG
1	A	338	ASP
1	A	347	ARG
1	A	407	SER
1	A	459	MET
1	A	518	ASP
1	A	521	ARG
1	A	541	ARG
1	A	634	ARG
1	B	73	VAL
1	B	107	THR
1	B	110	SER
1	B	146	ARG
1	B	166	ASP
1	B	193	ARG
1	B	237	GLU
1	B	248	THR
1	B	260	LEU
1	B	273	SER
1	B	293	ARG
1	B	338	ASP
1	B	347	ARG
1	B	371	SER
1	B	383	ARG
1	B	384	GLN
1	B	404	ARG
1	B	405	ASP
1	B	513	VAL
1	B	541	ARG

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Mol	Chain	Res	Type
1	B	572	LEU
1	B	591	THR
1	B	634	ARG
1	B	656	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	GLN
1	B	576	GLN

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

Of 70 ligands modelled in this entry, 6 are monoatomic - leaving 64 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	RDF	A	1665	2	34,39,39	2.25	7 (20%)	40,57,57	2.43	6 (15%)
4	211	A	1666	-	9,9,9	0.79	0	9,9,9	1.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PEG	A	1667	-	6,6,6	0.55	0	5,5,5	1.47	1 (20%)
5	PEG	A	1668	-	6,6,6	0.61	0	5,5,5	1.35	0
5	PEG	A	1669	-	6,6,6	0.55	0	5,5,5	1.59	0
5	PEG	A	1670	-	6,6,6	0.47	0	5,5,5	1.60	0
5	PEG	A	1671	-	6,6,6	0.53	0	5,5,5	1.48	0
5	PEG	A	1672	-	6,6,6	0.66	0	5,5,5	1.36	0
5	PEG	A	1673	-	6,6,6	0.41	0	5,5,5	2.16	3 (60%)
5	PEG	A	1674	-	6,6,6	0.54	0	5,5,5	1.44	0
5	PEG	A	1675	-	6,6,6	0.51	0	5,5,5	1.54	1 (20%)
5	PEG	A	1676	-	6,6,6	0.46	0	5,5,5	2.12	3 (60%)
5	PEG	A	1677	-	6,6,6	0.59	0	5,5,5	1.36	0
5	PEG	A	1678	-	6,6,6	0.45	0	5,5,5	1.84	2 (40%)
5	PEG	A	1679	-	6,6,6	0.58	0	5,5,5	1.49	1 (20%)
5	PEG	A	1680	-	6,6,6	0.58	0	5,5,5	1.36	0
5	PEG	A	1681	-	6,6,6	0.52	0	5,5,5	1.67	1 (20%)
6	PGE	A	1682	-	9,9,9	0.52	0	8,8,8	1.86	4 (50%)
6	PGE	A	1683	-	9,9,9	0.55	0	8,8,8	1.89	3 (37%)
6	PGE	A	1684	-	9,9,9	0.64	0	8,8,8	1.57	1 (12%)
6	PGE	A	1685	-	9,9,9	0.50	0	8,8,8	1.89	3 (37%)
6	PGE	A	1686	-	9,9,9	0.65	0	8,8,8	1.34	0
7	PG4	A	1687	-	12,12,12	1.11	0	11,11,11	1.80	4 (36%)
8	ACT	A	1688	-	1,3,3	1.65	0	0,3,3	0.00	-
8	ACT	A	1689	-	1,3,3	1.90	0	0,3,3	0.00	-
8	ACT	A	1690	-	1,3,3	1.36	0	0,3,3	0.00	-
8	ACT	A	1691	-	1,3,3	0.88	0	0,3,3	0.00	-
8	ACT	A	1692	-	1,3,3	1.77	0	0,3,3	0.00	-
9	SO4	A	1693	-	4,4,4	0.72	0	6,6,6	0.33	0
9	SO4	A	1694	-	4,4,4	0.56	0	6,6,6	0.62	0
3	RDF	B	1665	2	34,39,39	2.28	7 (20%)	40,57,57	2.56	8 (20%)
5	PEG	B	1666	-	6,6,6	0.51	0	5,5,5	1.58	1 (20%)
5	PEG	B	1667	-	6,6,6	0.64	0	5,5,5	1.35	0
5	PEG	B	1668	-	6,6,6	0.58	0	5,5,5	1.55	1 (20%)
5	PEG	B	1669	-	6,6,6	0.56	0	5,5,5	1.32	0
5	PEG	B	1670	-	6,6,6	0.53	0	5,5,5	1.46	1 (20%)
5	PEG	B	1671	-	6,6,6	0.54	0	5,5,5	1.51	0
5	PEG	B	1672	-	6,6,6	0.51	0	5,5,5	1.67	2 (40%)
5	PEG	B	1673	-	6,6,6	0.56	0	5,5,5	1.55	1 (20%)
5	PEG	B	1674	-	6,6,6	0.50	0	5,5,5	1.61	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PEG	B	1675	-	6,6,6	0.57	0	5,5,5	1.62	1 (20%)
5	PEG	B	1676	-	6,6,6	0.54	0	5,5,5	1.83	2 (40%)
5	PEG	B	1677	-	6,6,6	0.47	0	5,5,5	1.69	0
5	PEG	B	1678	-	6,6,6	0.60	0	5,5,5	1.33	0
5	PEG	B	1679	-	6,6,6	0.46	0	5,5,5	1.80	2 (40%)
5	PEG	B	1680	-	6,6,6	0.53	0	5,5,5	1.49	1 (20%)
6	PGE	B	1681	-	9,9,9	0.52	0	8,8,8	1.80	4 (50%)
6	PGE	B	1682	-	9,9,9	0.60	0	8,8,8	1.62	1 (12%)
6	PGE	B	1683	-	9,9,9	0.56	0	8,8,8	1.55	2 (25%)
7	PG4	B	1684	-	12,12,12	1.30	2 (16%)	11,11,11	2.60	10 (90%)
7	PG4	B	1685	-	12,12,12	1.08	1 (8%)	11,11,11	1.69	3 (27%)
7	PG4	B	1686	-	12,12,12	1.10	0	11,11,11	1.71	5 (45%)
8	ACT	B	1687	-	1,3,3	0.56	0	0,3,3	0.00	-
8	ACT	B	1688	-	1,3,3	1.20	0	0,3,3	0.00	-
8	ACT	B	1689	-	1,3,3	1.57	0	0,3,3	0.00	-
8	ACT	B	1690	-	1,3,3	0.90	0	0,3,3	0.00	-
8	ACT	B	1691	-	1,3,3	1.43	0	0,3,3	0.00	-
8	ACT	B	1692	-	1,3,3	0.62	0	0,3,3	0.00	-
8	ACT	B	1693	-	1,3,3	1.49	0	0,3,3	0.00	-
8	ACT	B	1694	-	1,3,3	0.66	0	0,3,3	0.00	-
9	SO4	B	1695	-	4,4,4	0.40	0	6,6,6	0.73	0
9	SO4	B	1696	-	4,4,4	0.98	0	6,6,6	0.56	0
9	SO4	B	1697	-	4,4,4	0.33	0	6,6,6	0.61	0
9	SO4	B	1698	-	4,4,4	0.51	0	6,6,6	0.65	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
3	RDF	A	1665	2	-	0/22/50/50	0/3/3/3
4	211	A	1666	-	-	0/9/9/9	0/0/0/0
5	PEG	A	1667	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1668	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1669	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1670	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1671	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1672	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1673	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	A	1674	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1675	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1676	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1677	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1678	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1679	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1680	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1681	-	-	0/4/4/4	0/0/0/0
6	PGE	A	1682	-	-	0/7/7/7	0/0/0/0
6	PGE	A	1683	-	-	0/7/7/7	0/0/0/0
6	PGE	A	1684	-	-	0/7/7/7	0/0/0/0
6	PGE	A	1685	-	-	0/7/7/7	0/0/0/0
6	PGE	A	1686	-	-	0/7/7/7	0/0/0/0
7	PG4	A	1687	-	-	0/10/10/10	0/0/0/0
8	ACT	A	1688	-	-	0/0/0/0	0/0/0/0
8	ACT	A	1689	-	-	0/0/0/0	0/0/0/0
8	ACT	A	1690	-	-	0/0/0/0	0/0/0/0
8	ACT	A	1691	-	-	0/0/0/0	0/0/0/0
8	ACT	A	1692	-	-	0/0/0/0	0/0/0/0
9	SO4	A	1693	-	-	0/0/0/0	0/0/0/0
9	SO4	A	1694	-	-	0/0/0/0	0/0/0/0
3	RDF	B	1665	2	-	0/22/50/50	0/3/3/3
5	PEG	B	1666	-	-	0/4/4/4	0/0/0/0
5	PEG	B	1667	-	-	0/4/4/4	0/0/0/0
5	PEG	B	1668	-	-	0/4/4/4	0/0/0/0
5	PEG	B	1669	-	-	0/4/4/4	0/0/0/0
5	PEG	B	1670	-	-	0/4/4/4	0/0/0/0
5	PEG	B	1671	-	-	0/4/4/4	0/0/0/0
5	PEG	B	1672	-	-	0/4/4/4	0/0/0/0
5	PEG	B	1673	-	-	0/4/4/4	0/0/0/0
5	PEG	B	1674	-	-	0/4/4/4	0/0/0/0
5	PEG	B	1675	-	-	0/4/4/4	0/0/0/0
5	PEG	B	1676	-	-	0/4/4/4	0/0/0/0
5	PEG	B	1677	-	-	0/4/4/4	0/0/0/0
5	PEG	B	1678	-	-	0/4/4/4	0/0/0/0
5	PEG	B	1679	-	-	0/4/4/4	0/0/0/0
5	PEG	B	1680	-	-	0/4/4/4	0/0/0/0
6	PGE	B	1681	-	-	0/7/7/7	0/0/0/0
6	PGE	B	1682	-	-	0/7/7/7	0/0/0/0
6	PGE	B	1683	-	-	0/7/7/7	0/0/0/0
7	PG4	B	1684	-	-	0/10/10/10	0/0/0/0
7	PG4	B	1685	-	-	0/10/10/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PG4	B	1686	-	-	0/10/10/10	0/0/0/0
8	ACT	B	1687	-	-	0/0/0/0	0/0/0/0
8	ACT	B	1688	-	-	0/0/0/0	0/0/0/0
8	ACT	B	1689	-	-	0/0/0/0	0/0/0/0
8	ACT	B	1690	-	-	0/0/0/0	0/0/0/0
8	ACT	B	1691	-	-	0/0/0/0	0/0/0/0
8	ACT	B	1692	-	-	0/0/0/0	0/0/0/0
8	ACT	B	1693	-	-	0/0/0/0	0/0/0/0
8	ACT	B	1694	-	-	0/0/0/0	0/0/0/0
9	SO4	B	1695	-	-	0/0/0/0	0/0/0/0
9	SO4	B	1696	-	-	0/0/0/0	0/0/0/0
9	SO4	B	1697	-	-	0/0/0/0	0/0/0/0
9	SO4	B	1698	-	-	0/0/0/0	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1665	RDF	C4-C3	-3.61	1.42	1.52
3	A	1665	RDF	C4-C3	-3.44	1.43	1.52
3	A	1665	RDF	C6-C5	-2.02	1.46	1.51
7	B	1685	PG4	O4-C6	-2.02	1.33	1.42
7	B	1684	PG4	O4-C7	2.11	1.51	1.42
3	B	1665	RDF	O5-C5	2.20	1.50	1.44
3	A	1665	RDF	CA1-N1	2.55	1.50	1.46
3	B	1665	RDF	CD11-NE1	2.59	1.41	1.36
7	B	1684	PG4	O5-C8	2.60	1.56	1.42
3	A	1665	RDF	CD11-NE1	3.06	1.42	1.36
3	B	1665	RDF	CA1-N1	3.11	1.51	1.46
3	A	1665	RDF	C-N1	5.17	1.46	1.34
3	B	1665	RDF	C-N1	5.67	1.47	1.34
3	B	1665	RDF	P-N	5.77	1.67	1.61
3	A	1665	RDF	P-N	5.77	1.67	1.61
3	B	1665	RDF	P-O1P	7.30	1.54	1.46
3	A	1665	RDF	P-O1P	7.51	1.54	1.46

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1665	RDF	O1-P-O1P	-9.88	97.48	115.51
3	A	1665	RDF	O1-P-O1P	-9.51	98.16	115.51
3	A	1665	RDF	O1P-P-N	-7.97	98.81	113.08
3	B	1665	RDF	O1P-P-N	-6.51	101.42	113.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1665	RDF	CB1-CG1-CD11	-5.99	120.57	127.97
3	B	1665	RDF	CA1-N1-C	-4.12	117.01	123.43
3	A	1665	RDF	CB1-CG1-CD11	-3.87	123.19	127.97
3	A	1665	RDF	O2-C2-C1	-3.55	102.25	110.02
3	A	1665	RDF	O5-C1-O1	-2.32	108.30	111.36
3	B	1665	RDF	O4-C4-C5	-2.15	104.80	109.84
5	B	1674	PEG	O2-C2-C1	2.00	119.65	110.43
7	B	1685	PG4	O3-C5-C6	2.01	119.30	110.36
7	B	1685	PG4	O2-C3-C4	2.01	119.31	110.36
7	B	1685	PG4	O3-C4-C3	2.01	119.31	110.36
7	B	1686	PG4	O4-C6-C5	2.02	119.33	110.36
5	B	1672	PEG	C3-O2-C2	2.03	122.05	113.31
5	B	1680	PEG	C3-O2-C2	2.03	122.05	113.31
7	A	1687	PG4	O3-C5-C6	2.04	119.41	110.36
6	A	1682	PGE	C5-O3-C4	2.04	122.06	113.31
6	B	1681	PGE	O2-C3-C4	2.04	119.43	110.36
5	A	1667	PEG	O2-C3-C4	2.05	119.88	110.43
5	B	1673	PEG	O2-C2-C1	2.06	119.89	110.43
7	B	1684	PG4	C3-O2-C2	2.06	122.19	113.31
6	B	1681	PGE	C5-O3-C4	2.07	122.19	113.31
7	B	1686	PG4	O3-C4-C3	2.08	119.61	110.36
7	A	1687	PG4	O4-C7-C8	2.08	120.02	110.43
6	A	1685	PGE	O2-C2-C1	2.10	120.11	110.43
5	B	1672	PEG	O2-C3-C4	2.10	120.11	110.43
6	A	1683	PGE	O3-C5-C6	2.11	120.14	110.43
7	A	1687	PG4	O2-C2-C1	2.11	120.16	110.43
5	B	1679	PEG	O2-C2-C1	2.13	120.22	110.43
5	B	1666	PEG	O2-C2-C1	2.13	120.25	110.43
6	A	1684	PGE	O2-C3-C4	2.13	119.85	110.36
5	B	1676	PEG	O2-C2-C1	2.14	120.30	110.43
5	B	1668	PEG	O2-C3-C4	2.16	120.37	110.43
7	B	1684	PG4	O5-C8-C7	2.18	125.47	112.03
6	B	1683	PGE	O3-C5-C6	2.18	120.46	110.43
6	A	1682	PGE	O3-C5-C6	2.20	120.54	110.43
5	A	1679	PEG	O2-C3-C4	2.20	120.57	110.43
7	B	1684	PG4	O2-C2-C1	2.20	120.58	110.43
7	A	1687	PG4	O2-C3-C4	2.21	120.17	110.36
6	B	1682	PGE	O2-C2-C1	2.22	120.65	110.43
5	A	1681	PEG	O2-C3-C4	2.22	120.67	110.43
5	B	1670	PEG	O2-C3-C4	2.23	120.71	110.43
7	B	1686	PG4	C5-O3-C4	2.24	122.92	113.31
5	B	1675	PEG	C3-O2-C2	2.25	122.96	113.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	1686	PG4	O3-C5-C6	2.26	120.42	110.36
6	B	1683	PGE	C3-O2-C2	2.31	123.25	113.31
6	A	1685	PGE	O3-C4-C3	2.32	120.67	110.36
5	A	1673	PEG	O2-C2-C1	2.32	121.13	110.43
7	B	1686	PG4	O2-C3-C4	2.33	120.70	110.36
6	B	1681	PGE	C3-O2-C2	2.33	123.31	113.31
5	A	1678	PEG	O2-C2-C1	2.33	121.16	110.43
5	A	1676	PEG	C3-O2-C2	2.36	123.43	113.31
7	B	1684	PG4	O4-C6-C5	2.36	120.83	110.36
5	A	1678	PEG	O2-C3-C4	2.37	121.36	110.43
6	A	1682	PGE	O3-C4-C3	2.40	121.04	110.36
6	B	1681	PGE	O3-C4-C3	2.43	121.15	110.36
5	A	1675	PEG	O2-C2-C1	2.43	121.61	110.43
5	B	1674	PEG	O2-C3-C4	2.44	121.66	110.43
5	B	1679	PEG	C3-O2-C2	2.47	123.94	113.31
7	B	1684	PG4	C5-O3-C4	2.49	124.00	113.31
5	A	1676	PEG	O2-C2-C1	2.53	122.09	110.43
5	B	1676	PEG	O2-C3-C4	2.56	122.21	110.43
6	A	1682	PGE	O2-C3-C4	2.56	121.76	110.36
6	A	1683	PGE	O2-C3-C4	2.57	121.78	110.36
5	A	1673	PEG	C3-O2-C2	2.59	124.42	113.31
6	A	1685	PGE	O3-C5-C6	2.59	122.36	110.43
5	A	1673	PEG	O2-C3-C4	2.60	122.39	110.43
5	A	1676	PEG	O2-C3-C4	2.75	123.10	110.43
7	B	1684	PG4	O4-C7-C8	2.76	123.16	110.43
7	B	1684	PG4	O3-C4-C3	2.81	122.86	110.36
6	A	1683	PGE	O3-C4-C3	2.92	123.36	110.36
7	B	1684	PG4	O2-C3-C4	2.94	123.45	110.36
7	B	1684	PG4	C7-O4-C6	3.05	126.41	113.31
3	B	1665	RDF	CB1-CA1-N1	3.22	117.78	108.23
7	B	1684	PG4	O3-C5-C6	3.46	125.76	110.36
3	B	1665	RDF	O5-C5-C6	3.75	114.83	106.64
3	A	1665	RDF	O2P-P-O1P	3.79	117.91	110.00
3	B	1665	RDF	O2P-P-O1P	4.21	118.79	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

25 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1665	RDF	8	0
4	A	1666	211	1	0
5	A	1667	PEG	1	0
5	A	1668	PEG	2	0
5	A	1669	PEG	3	0
5	A	1673	PEG	1	0
5	A	1676	PEG	6	0
5	A	1681	PEG	1	0
6	A	1684	PGE	1	0
3	B	1665	RDF	5	0
5	B	1667	PEG	1	0
5	B	1668	PEG	1	0
5	B	1670	PEG	1	0
5	B	1671	PEG	1	0
5	B	1673	PEG	1	0
5	B	1676	PEG	2	0
5	B	1678	PEG	1	0
5	B	1679	PEG	1	0
5	B	1680	PEG	1	0
6	B	1682	PGE	1	0
6	B	1683	PGE	1	0
7	B	1684	PG4	8	0
7	B	1685	PG4	1	0
7	B	1686	PG4	3	0
8	B	1692	ACT	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	657/699 (93%)	-0.37	8 (1%)	81 77	11, 29, 53, 66	0
1	B	657/699 (93%)	-0.55	4 (0%)	90 88	10, 26, 45, 64	0
All	All	1314/1398 (93%)	-0.46	12 (0%)	85 83	10, 27, 51, 66	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	ALA	4.6
1	A	70	GLY	4.5
1	A	346	GLN	3.7
1	A	71	ALA	3.5
1	B	346	GLN	3.2
1	A	68	GLN	2.5
1	B	345	VAL	2.3
1	A	190	GLY	2.3
1	A	69	ALA	2.2
1	B	399	TYR	2.1
1	B	68	GLN	2.1
1	A	91	GLU	2.1

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

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

6.3 Carbohydrates

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^{th} 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^2)	Q<0.9
5	PEG	B	1672	7/7	0.62	0.32	20.25	48,54,55,56	0
5	PEG	B	1667	7/7	0.72	0.36	11.40	56,58,61,62	0
7	PG4	B	1685	13/13	0.50	0.36	10.63	65,78,87,88	0
7	PG4	B	1684	13/13	0.79	0.28	10.35	36,43,47,48	0
5	PEG	A	1676	7/7	0.77	0.34	10.05	46,48,50,51	0
4	211	A	1666	10/10	0.66	0.27	9.84	49,55,57,57	0
8	ACT	B	1687	4/4	0.71	0.29	9.72	71,72,72,72	0
5	PEG	A	1678	7/7	0.74	0.32	9.33	59,65,67,67	0
5	PEG	B	1671	7/7	0.73	0.31	9.14	51,54,57,58	0
8	ACT	B	1691	4/4	0.72	0.24	9.06	53,54,54,54	0
6	PGE	A	1686	10/10	0.76	0.26	8.40	52,53,57,57	0
5	PEG	B	1673	7/7	0.85	0.21	8.01	49,50,53,55	0
5	PEG	A	1668	7/7	0.85	0.23	7.58	46,48,51,51	0
6	PGE	B	1681	10/10	0.74	0.25	7.05	44,49,52,52	0
6	PGE	A	1685	10/10	0.54	0.38	6.93	63,65,70,70	0
5	PEG	A	1677	7/7	0.50	0.28	6.87	68,71,72,72	0
5	PEG	B	1677	7/7	0.57	0.30	6.83	74,74,75,75	0
8	ACT	B	1689	4/4	0.69	0.24	6.06	48,48,48,48	0
5	PEG	B	1666	7/7	0.81	0.25	5.83	49,53,54,54	0
5	PEG	B	1676	7/7	0.66	0.33	5.72	49,53,54,55	0
5	PEG	A	1680	7/7	0.88	0.23	4.47	59,59,60,61	0
5	PEG	B	1668	7/7	0.78	0.26	4.46	47,48,51,52	0
5	PEG	A	1667	7/7	0.79	0.21	4.18	55,56,57,58	0
8	ACT	B	1690	4/4	0.78	0.20	3.99	51,52,52,52	0
9	SO4	B	1695	5/5	0.88	0.22	3.87	91,91,92,92	0
6	PGE	A	1684	10/10	0.90	0.19	3.82	32,40,42,42	0
8	ACT	A	1692	4/4	0.84	0.19	3.69	51,52,52,52	0
5	PEG	B	1679	7/7	0.73	0.21	3.48	55,59,63,63	0
8	ACT	A	1688	4/4	0.82	0.24	3.47	34,35,36,36	0
8	ACT	B	1693	4/4	0.53	0.21	3.31	52,52,53,53	0
8	ACT	B	1692	4/4	0.84	0.21	3.29	48,48,48,48	0
5	PEG	A	1681	7/7	0.73	0.25	3.22	69,70,70,70	0
5	PEG	A	1673	7/7	0.65	0.25	3.16	47,52,54,55	0
6	PGE	B	1683	10/10	0.82	0.21	3.14	45,49,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	PGE	A	1682	10/10	0.76	0.22	3.09	50,56,58,59	0
8	ACT	B	1688	4/4	0.70	0.20	2.97	51,51,51,52	0
5	PEG	B	1675	7/7	0.86	0.21	2.64	53,53,56,56	0
8	ACT	A	1691	4/4	0.60	0.28	2.50	63,63,64,64	0
7	PG4	A	1687	13/13	0.81	0.21	2.25	54,58,59,59	0
5	PEG	A	1679	7/7	0.83	0.18	2.15	41,42,46,48	0
7	PG4	B	1686	13/13	0.83	0.20	2.11	43,53,58,59	0
5	PEG	A	1672	7/7	0.84	0.18	2.03	57,60,63,63	0
6	PGE	A	1683	10/10	0.81	0.21	2.03	41,51,57,57	0
3	RDF	A	1665	37/37	0.95	0.16	1.61	15,19,52,52	0
8	ACT	B	1694	4/4	0.82	0.16	1.56	49,50,50,50	0
3	RDF	B	1665	37/37	0.95	0.16	1.20	16,19,53,53	0
5	PEG	A	1670	7/7	0.68	0.24	1.16	48,54,57,57	0
9	SO4	B	1698	5/5	0.95	0.20	1.14	52,53,55,55	0
5	PEG	A	1674	7/7	0.74	0.17	1.03	50,53,55,55	0
5	PEG	B	1670	7/7	0.84	0.14	0.68	45,46,48,48	0
6	PGE	B	1682	10/10	0.76	0.18	0.66	51,55,57,57	0
5	PEG	B	1669	7/7	0.78	0.17	0.59	48,51,54,55	0
5	PEG	A	1669	7/7	0.80	0.20	0.47	49,52,54,54	0
9	SO4	B	1696	5/5	0.99	0.12	0.39	26,26,28,31	0
5	PEG	B	1674	7/7	0.69	0.22	0.31	58,59,61,61	0
8	ACT	A	1690	4/4	0.75	0.18	0.24	53,53,54,54	0
5	PEG	B	1678	7/7	0.85	0.14	-0.29	50,54,56,57	0
11	CA	B	1700	1/1	1.00	0.12	-0.44	19,19,19,19	0
9	SO4	A	1694	5/5	0.97	0.12	-1.33	51,52,54,54	0
10	CL	B	1699	1/1	0.94	0.09	-1.34	56,56,56,56	0
9	SO4	A	1693	5/5	0.99	0.10	-1.66	24,24,25,26	0
2	ZN	A	1664	1/1	1.00	0.10	-2.08	18,18,18,18	0
5	PEG	A	1671	7/7	0.45	0.37	-	72,76,80,80	0
5	PEG	A	1675	7/7	0.60	0.27	-	61,63,66,67	0
10	CL	A	1695	1/1	0.79	0.09	-	59,59,59,59	0
2	ZN	B	1664	1/1	0.99	0.09	-	16,16,16,16	0
8	ACT	A	1689	4/4	0.74	0.20	-	48,49,49,49	0
10	CL	B	1701	1/1	0.88	0.12	-	57,57,57,57	0
5	PEG	B	1680	7/7	0.50	0.17	-	61,65,68,69	0
9	SO4	B	1697	5/5	0.86	0.19	-	68,69,70,70	0

6.5 Other polymers

There are no such residues in this entry.