Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:57 PM GMT

PDB ID	:	4UDJ
Title	:	Crystal structure of b-1,4-mannopyranosyl-chitobiose phosphorylase at 1.60 Angstrom in complex with beta-D-mannopyranose and inorganic phosphate
Authors	:	Ladeveze, S.; Cioci, G.; Potocki-Veronese, G.; Tranier, S.; Mourey, L.
Deposited on	:	2014-12-10
Resolution	:	1.94 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:

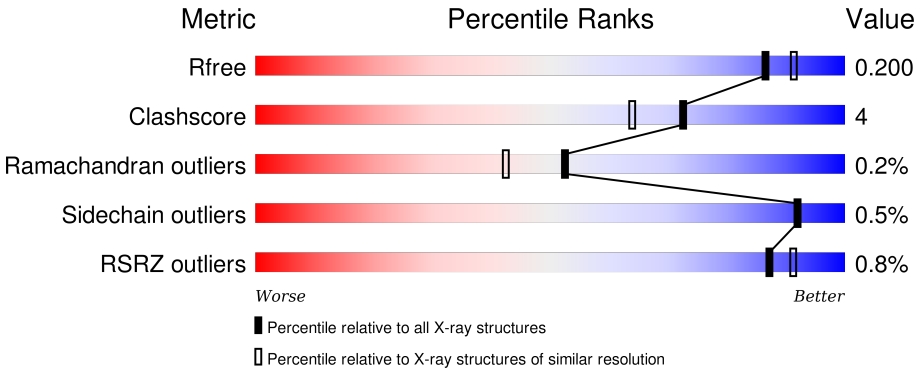
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.94 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	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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	347	82% 10% 8%
1	B	347	% 84% 8% • 7%
1	C	347	% 82% 9% • 8%
1	D	347	% 84% 8% 8%
1	E	347	% 83% 9% • 7%

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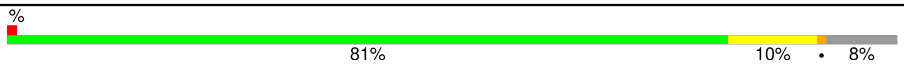
Mol	Chain	Length	Quality of chain
1	F	347	

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	BMA	A	329	-	-	-	X
3	BMA	B	329	-	-	-	X
3	BMA	D	329	-	-	-	X
3	BMA	E	329	-	-	-	X
4	K	A	333	-	-	-	X
4	K	A	606	-	-	-	X
4	K	A	607	-	-	-	X
4	K	B	333	-	-	-	X
4	K	C	333	-	-	-	X
4	K	F	333	-	-	-	X
5	EDO	B	598	-	-	-	X
5	EDO	D	584	-	-	-	X
5	EDO	D	588	-	-	-	X
5	EDO	E	580	-	-	-	X
5	EDO	F	569	-	-	-	X
5	EDO	F	579	-	-	-	X
6	PGE	A	602	-	-	-	X
6	PGE	A	604	-	-	-	X
6	PGE	A	608	-	-	-	X
6	PGE	B	599	-	-	-	X
6	PGE	C	592	-	-	-	X
6	PGE	D	587	-	-	-	X
6	PGE	F	580	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17342 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 UHGB_MP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	13	0
			2669	1722	450	480	17			
1	B	321	Total	C	N	O	S	0	10	0
			2652	1714	444	477	17			
1	C	320	Total	C	N	O	S	0	9	0
			2627	1698	437	475	17			
1	D	320	Total	C	N	O	S	0	12	0
			2666	1719	449	481	17			
1	E	321	Total	C	N	O	S	0	11	0
			2664	1719	448	480	17			
1	F	320	Total	C	N	O	S	0	10	0
			2647	1709	443	478	17			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP D9ZDQ9
A	-18	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
A	-17	SER	-	EXPRESSION TAG	UNP D9ZDQ9
A	-16	SER	-	EXPRESSION TAG	UNP D9ZDQ9
A	-15	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
A	-14	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
A	-13	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
A	-12	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
A	-11	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
A	-10	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
A	-9	SER	-	EXPRESSION TAG	UNP D9ZDQ9
A	-8	SER	-	EXPRESSION TAG	UNP D9ZDQ9
A	-7	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
A	-6	LEU	-	EXPRESSION TAG	UNP D9ZDQ9
A	-5	VAL	-	EXPRESSION TAG	UNP D9ZDQ9
A	-4	PRO	-	EXPRESSION TAG	UNP D9ZDQ9
A	-3	ARG	-	EXPRESSION TAG	UNP D9ZDQ9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
A	-1	SER	-	EXPRESSION TAG	UNP D9ZDQ9
A	0	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
B	-19	MET	-	EXPRESSION TAG	UNP D9ZDQ9
B	-18	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
B	-17	SER	-	EXPRESSION TAG	UNP D9ZDQ9
B	-16	SER	-	EXPRESSION TAG	UNP D9ZDQ9
B	-15	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
B	-14	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
B	-13	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
B	-12	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
B	-11	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
B	-10	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
B	-9	SER	-	EXPRESSION TAG	UNP D9ZDQ9
B	-8	SER	-	EXPRESSION TAG	UNP D9ZDQ9
B	-7	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
B	-6	LEU	-	EXPRESSION TAG	UNP D9ZDQ9
B	-5	VAL	-	EXPRESSION TAG	UNP D9ZDQ9
B	-4	PRO	-	EXPRESSION TAG	UNP D9ZDQ9
B	-3	ARG	-	EXPRESSION TAG	UNP D9ZDQ9
B	-2	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
B	-1	SER	-	EXPRESSION TAG	UNP D9ZDQ9
B	0	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
C	-19	MET	-	EXPRESSION TAG	UNP D9ZDQ9
C	-18	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
C	-17	SER	-	EXPRESSION TAG	UNP D9ZDQ9
C	-16	SER	-	EXPRESSION TAG	UNP D9ZDQ9
C	-15	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
C	-14	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
C	-13	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
C	-12	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
C	-11	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
C	-10	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
C	-9	SER	-	EXPRESSION TAG	UNP D9ZDQ9
C	-8	SER	-	EXPRESSION TAG	UNP D9ZDQ9
C	-7	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
C	-6	LEU	-	EXPRESSION TAG	UNP D9ZDQ9
C	-5	VAL	-	EXPRESSION TAG	UNP D9ZDQ9
C	-4	PRO	-	EXPRESSION TAG	UNP D9ZDQ9
C	-3	ARG	-	EXPRESSION TAG	UNP D9ZDQ9
C	-2	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
C	-1	SER	-	EXPRESSION TAG	UNP D9ZDQ9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
D	-19	MET	-	EXPRESSION TAG	UNP D9ZDQ9
D	-18	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
D	-17	SER	-	EXPRESSION TAG	UNP D9ZDQ9
D	-16	SER	-	EXPRESSION TAG	UNP D9ZDQ9
D	-15	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
D	-14	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
D	-13	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
D	-12	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
D	-11	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
D	-10	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
D	-9	SER	-	EXPRESSION TAG	UNP D9ZDQ9
D	-8	SER	-	EXPRESSION TAG	UNP D9ZDQ9
D	-7	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
D	-6	LEU	-	EXPRESSION TAG	UNP D9ZDQ9
D	-5	VAL	-	EXPRESSION TAG	UNP D9ZDQ9
D	-4	PRO	-	EXPRESSION TAG	UNP D9ZDQ9
D	-3	ARG	-	EXPRESSION TAG	UNP D9ZDQ9
D	-2	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
D	-1	SER	-	EXPRESSION TAG	UNP D9ZDQ9
D	0	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
E	-19	MET	-	EXPRESSION TAG	UNP D9ZDQ9
E	-18	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
E	-17	SER	-	EXPRESSION TAG	UNP D9ZDQ9
E	-16	SER	-	EXPRESSION TAG	UNP D9ZDQ9
E	-15	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
E	-14	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
E	-13	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
E	-12	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
E	-11	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
E	-10	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
E	-9	SER	-	EXPRESSION TAG	UNP D9ZDQ9
E	-8	SER	-	EXPRESSION TAG	UNP D9ZDQ9
E	-7	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
E	-6	LEU	-	EXPRESSION TAG	UNP D9ZDQ9
E	-5	VAL	-	EXPRESSION TAG	UNP D9ZDQ9
E	-4	PRO	-	EXPRESSION TAG	UNP D9ZDQ9
E	-3	ARG	-	EXPRESSION TAG	UNP D9ZDQ9
E	-2	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
E	-1	SER	-	EXPRESSION TAG	UNP D9ZDQ9
E	0	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
F	-19	MET	-	EXPRESSION TAG	UNP D9ZDQ9

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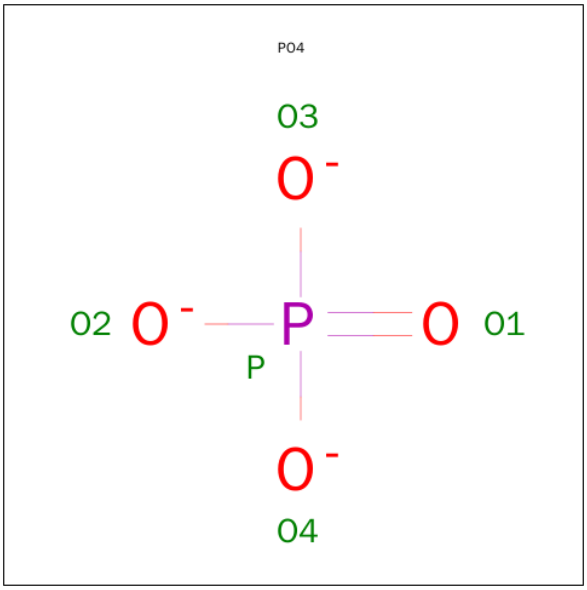
Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
F	-17	SER	-	EXPRESSION TAG	UNP D9ZDQ9
F	-16	SER	-	EXPRESSION TAG	UNP D9ZDQ9
F	-15	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
F	-14	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
F	-13	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
F	-12	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
F	-11	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
F	-10	HIS	-	EXPRESSION TAG	UNP D9ZDQ9
F	-9	SER	-	EXPRESSION TAG	UNP D9ZDQ9
F	-8	SER	-	EXPRESSION TAG	UNP D9ZDQ9
F	-7	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
F	-6	LEU	-	EXPRESSION TAG	UNP D9ZDQ9
F	-5	VAL	-	EXPRESSION TAG	UNP D9ZDQ9
F	-4	PRO	-	EXPRESSION TAG	UNP D9ZDQ9
F	-3	ARG	-	EXPRESSION TAG	UNP D9ZDQ9
F	-2	GLY	-	EXPRESSION TAG	UNP D9ZDQ9
F	-1	SER	-	EXPRESSION TAG	UNP D9ZDQ9
F	0	HIS	-	EXPRESSION TAG	UNP D9ZDQ9

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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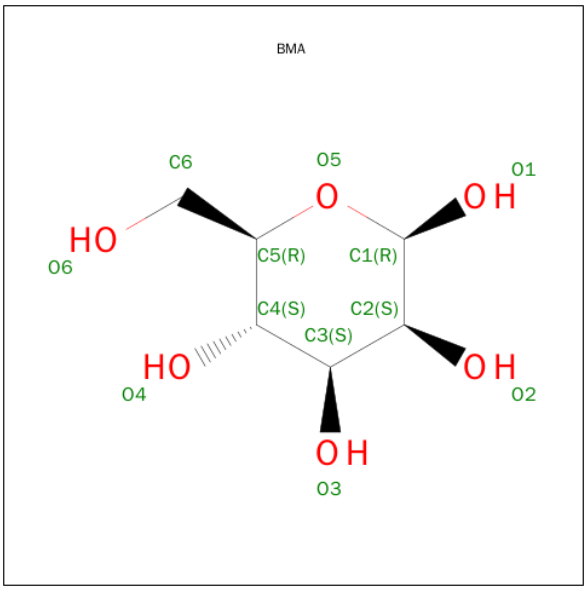
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

- Molecule 3 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula: $C_6H_{12}O_6$).

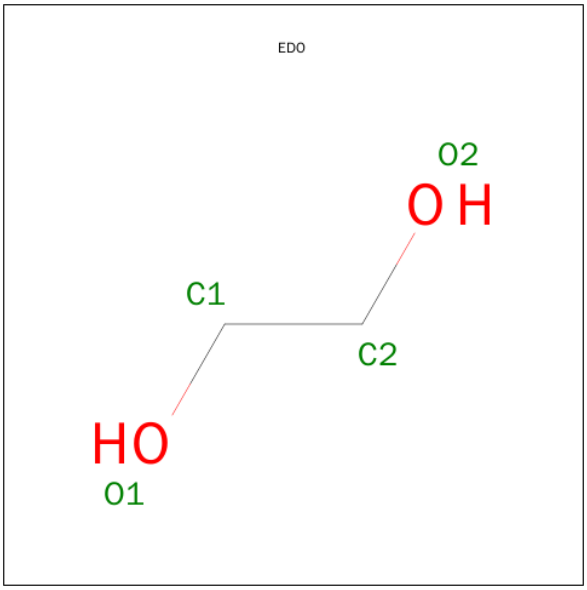


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 6 6	0	0
3	B	1	Total C O 12 6 6	0	0
3	C	1	Total C O 12 6 6	0	0
3	D	1	Total C O 12 6 6	0	0
3	E	1	Total C O 12 6 6	0	0
3	F	1	Total C O 12 6 6	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total K 1 1	0	0
4	E	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0
4	A	3	Total K 3 3	0	0
4	F	1	Total K 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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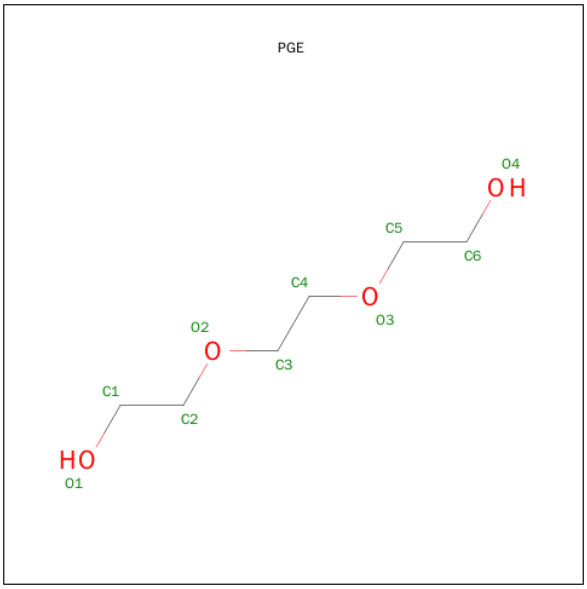
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0

- 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	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

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

- Molecule 7 is water.

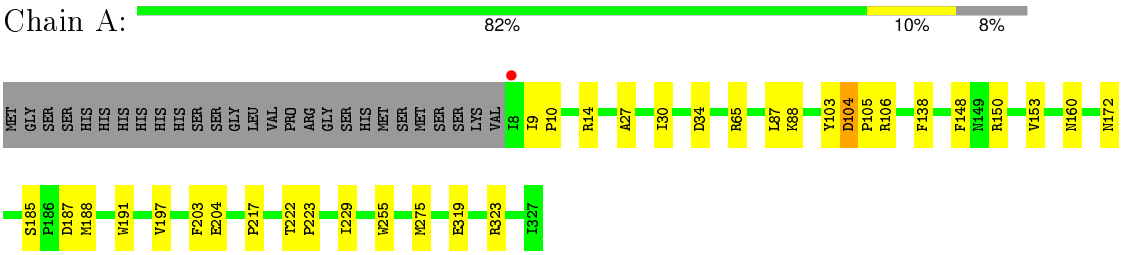
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	205	Total O 205 205	0	0
7	B	222	Total O 222 222	0	0
7	C	225	Total O 225 225	0	0
7	D	172	Total O 172 172	0	0
7	E	207	Total O 207 207	0	0
7	F	142	Total O 142 142	0	0

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.

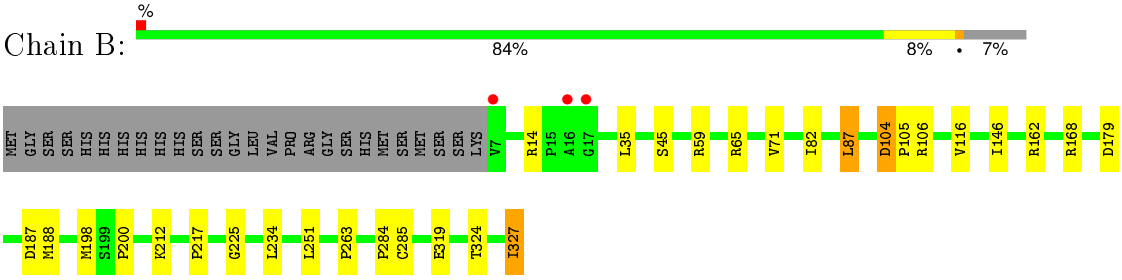
- Molecule 1: UHGB_MP

Chain A:



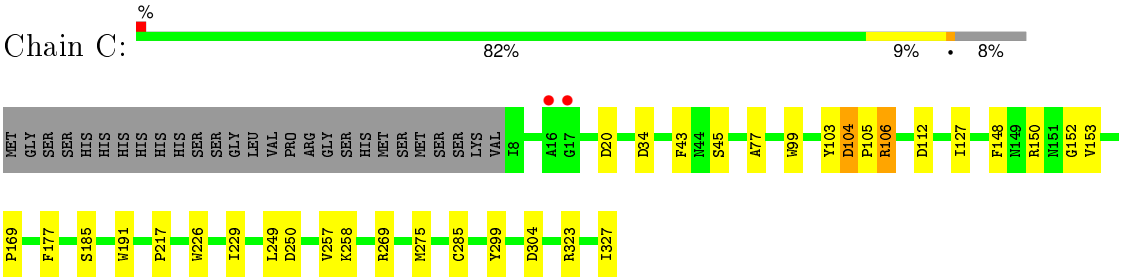
- Molecule 1: UHGB_MP

Chain B:



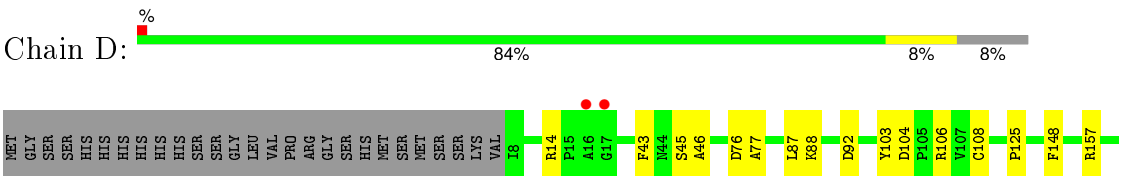
- Molecule 1: UHGB_MP

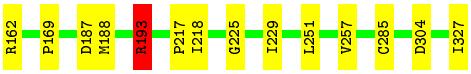
Chain C:



- Molecule 1: UHGB_MP

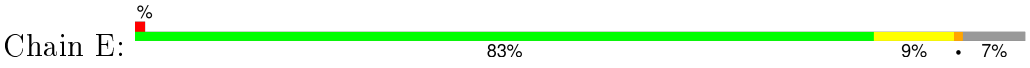
Chain D:

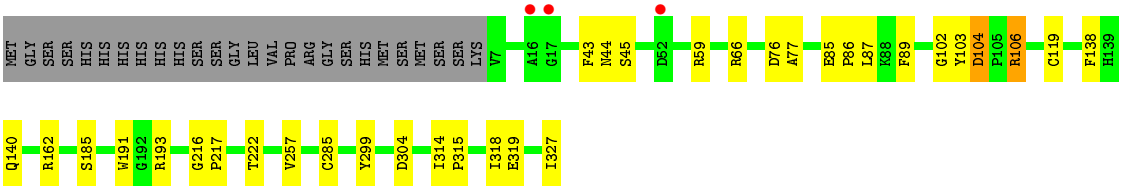




• Molecule 1: UHGB_MP

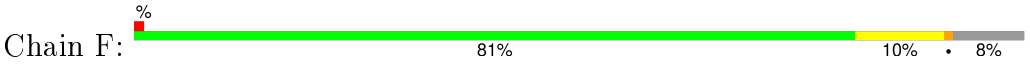
Chain E:

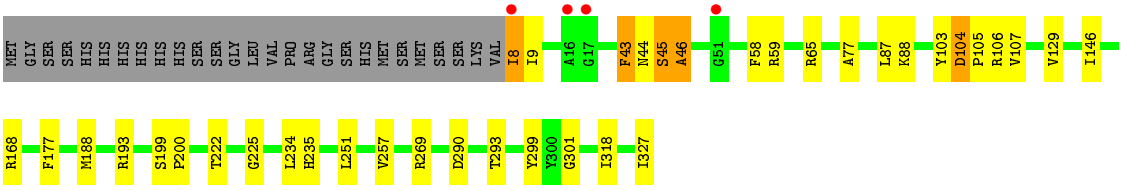




• Molecule 1: UHGB_MP

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.88Å 140.84Å 168.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	108.13 – 1.94 75.11 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.7 (108.13-1.94) 99.7 (75.11-1.94)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.150 , 0.193 0.163 , 0.200	Depositor DCC
R_{free} test set	7405 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	17.2	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 148300 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17342	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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: K, PO4, PGE, EDO, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.02	1/2765 (0.0%)	0.97	6/3768 (0.2%)
1	B	1.01	3/2745 (0.1%)	0.97	6/3742 (0.2%)
1	C	0.99	0/2726	0.95	7/3716 (0.2%)
1	D	0.95	2/2757 (0.1%)	0.93	3/3758 (0.1%)
1	E	0.93	0/2757	0.91	2/3758 (0.1%)
1	F	0.93	0/2740	0.94	7/3735 (0.2%)
All	All	0.97	6/16490 (0.0%)	0.94	31/22477 (0.1%)

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	D	0	3
1	F	0	1
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	87	LEU	C-N	-6.99	1.18	1.34
1	A	204	GLU	CD-OE2	-6.72	1.18	1.25
1	D	45[A]	SER	CB-OG	-5.22	1.35	1.42
1	D	45[B]	SER	CB-OG	-5.22	1.35	1.42
1	B	104[A]	ASP	CB-CG	5.10	1.62	1.51
1	B	104[B]	ASP	CB-CG	5.10	1.62	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	65	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	E	106	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	B	327	ILE	CB-CA-C	-7.07	97.45	111.60
1	D	157	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	65	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	C	106	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	F	193	ARG	CG-CD-NE	-6.42	98.33	111.80
1	A	104[A]	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	104[B]	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	65	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	B	59	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	C	150	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	C	34	ASP	CB-CG-OD1	6.06	123.75	118.30
1	B	162	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	D	193[A]	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	D	193[B]	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	14	ARG	C-N-CD	5.83	140.64	128.40
1	C	104[A]	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	C	104[B]	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	E	66	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	150	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	F	45[A]	SER	N-CA-C	5.61	126.14	111.00
1	F	45[B]	SER	N-CA-C	5.61	126.14	111.00
1	F	43[A]	PHE	N-CA-C	5.54	125.95	111.00
1	F	43[B]	PHE	N-CA-C	5.54	125.95	111.00
1	C	112	ASP	CB-CG-OD2	5.35	123.12	118.30
1	B	65	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	B	179	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	F	65	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	B	198	MET	CG-SD-CE	-5.08	92.08	100.20
1	C	20	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	193[A]	ARG	Mainchain
1	D	193[B]	ARG	Mainchain
1	D	46[A]	ALA	Mainchain
1	F	46[B]	ALA	Mainchain

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	2669	0	2529	22	0
1	B	2652	0	2515	14	0
1	C	2627	0	2485	28	0
1	D	2666	0	2522	18	0
1	E	2664	0	2524	21	0
1	F	2647	0	2504	28	0
2	A	5	0	0	1	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
2	D	5	0	0	1	0
2	E	5	0	0	1	0
2	F	5	0	0	1	0
3	A	12	0	12	1	0
3	B	12	0	12	1	0
3	C	12	0	11	1	0
3	D	12	0	12	1	0
3	E	12	0	12	1	0
3	F	12	0	12	2	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	8	0	12	1	0
5	B	4	0	6	0	0
5	C	4	0	6	1	0
5	D	12	0	18	0	0
5	E	8	0	12	0	0
5	F	8	0	12	0	0
6	A	30	0	42	2	0
6	B	30	0	42	1	0
6	C	10	0	14	0	0
6	D	10	0	14	0	0
6	F	10	0	14	0	0
7	A	205	0	0	1	0
7	B	222	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	225	0	0	3	0
7	D	172	0	0	0	0
7	E	207	0	0	1	0
7	F	142	0	0	3	0
All	All	17342	0	15342	132	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 4.

All (132) 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)
2:C:328:PO4:O4	3:C:329:BMA:H1	1.64	0.96
2:E:328:PO4:O4	3:E:329:BMA:H1	1.69	0.90
2:F:328:PO4:O1	3:F:329:BMA:H1	1.78	0.82
2:B:328:PO4:O3	3:B:329:BMA:H1	1.80	0.81
2:D:328:PO4:O1	3:D:329:BMA:H1	1.80	0.81
2:A:328:PO4:O2	3:A:329:BMA:H1	1.81	0.80
1:F:269:ARG:HD3	7:F:609:HOH:O	1.95	0.67
1:C:45[A]:SER:O	1:C:285[A]:CYS:HB2	1.97	0.64
1:F:222:THR:HG21	1:F:318:ILE:HD11	1.81	0.63
1:A:319:GLU:OE1	1:A:323[B]:ARG:NH1	2.32	0.63
1:D:87:LEU:HD23	1:D:88:LYS:N	2.17	0.60
1:F:104[B]:ASP:OD1	1:F:106:ARG:NH1	2.25	0.60
1:A:275:MET:HE1	1:C:275:MET:CE	2.32	0.60
1:E:319[A]:GLU:HG2	7:E:601:HOH:O	2.01	0.60
1:D:106:ARG:NH1	1:D:285[B]:CYS:SG	2.75	0.59
1:F:8:ILE:O	1:F:8:ILE:HG23	2.01	0.59
1:F:129:VAL:HG11	1:F:188:MET:CE	2.33	0.58
1:B:71:VAL:HG23	1:B:87:LEU:HD12	1.83	0.58
1:E:85:GLU:HG3	1:E:86:PRO:HD2	1.86	0.57
1:F:104[B]:ASP:CG	1:F:106:ARG:HH12	2.08	0.57
1:A:148:PHE:CE1	1:A:172[A]:ASN:HB2	2.40	0.56
1:B:234:LEU:HD23	1:B:234:LEU:C	2.26	0.55
1:A:27:ALA:HB1	6:A:608:PGE:H3	1.89	0.55
1:C:127[B]:ILE:HD13	1:C:152:GLY:HA3	1.89	0.54
1:C:269:ARG:HD3	7:C:639:HOH:O	2.06	0.54
1:F:269:ARG:NH1	7:F:609:HOH:O	2.23	0.54
1:A:160[A]:ASN:HB2	7:A:634:HOH:O	2.07	0.54
1:F:59:ARG:HD2	1:F:103:TYR:HB2	1.91	0.52
1:E:104[B]:ASP:CG	1:E:106:ARG:HH12	2.11	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:TYR:O	1:F:104[B]:ASP:HB3	2.10	0.52
1:C:104[A]:ASP:N	1:C:105:PRO:CD	2.71	0.52
1:F:129:VAL:HG11	1:F:188:MET:HE1	1.90	0.52
1:A:9:ILE:HB	1:A:10:PRO:HD2	1.92	0.52
1:C:323:ARG:NH2	7:C:634:HOH:O	2.28	0.51
1:A:87[B]:LEU:HD11	1:A:138:PHE:CD1	2.46	0.51
1:F:257:VAL:HG12	1:F:327:ILE:HD11	1.94	0.50
1:D:14[B]:ARG:HG3	1:D:14[B]:ARG:HH11	1.77	0.50
1:D:225:GLY:HA2	1:D:251:LEU:HG	1.94	0.49
1:F:225:GLY:HA2	1:F:251:LEU:HD13	1.95	0.49
1:A:34:ASP:O	5:A:348:EDO:H22	2.12	0.49
1:E:45[A]:SER:O	1:E:285[A]:CYS:SG	2.71	0.49
1:D:217:PRO:HD2	1:D:229:ILE:HB	1.94	0.48
1:C:269:ARG:NH1	7:C:639:HOH:O	2.33	0.48
1:D:162:ARG:NH2	1:D:193[B]:ARG:NH1	2.61	0.48
1:D:257:VAL:HG12	1:D:327:ILE:HD11	1.95	0.48
1:B:45[A]:SER:O	1:B:285[A]:CYS:SG	2.71	0.48
1:E:77:ALA:HB1	1:E:299:TYR:OH	2.14	0.48
1:A:275:MET:CE	1:C:275:MET:HE2	2.44	0.47
1:B:146:ILE:CG2	1:D:169:PRO:HG3	2.45	0.47
1:F:77:ALA:HB1	1:F:299:TYR:OH	2.14	0.47
1:A:87[A]:LEU:HD23	1:A:88:LYS:N	2.29	0.47
1:D:76:ASP:O	1:D:77:ALA:HB3	2.14	0.47
1:B:116[B]:VAL:O	1:B:116[B]:VAL:HG13	2.14	0.47
1:F:104[B]:ASP:CG	1:F:106:ARG:NH1	2.68	0.47
1:A:222:THR:HB	1:A:223:PRO:HD2	1.95	0.47
1:F:45[B]:SER:HB2	1:F:58:PHE:CE2	2.50	0.47
1:C:43[A]:PHE:CD2	1:C:304:ASP:HA	2.51	0.46
1:A:106:ARG:HG3	1:A:153:VAL:HG22	1.98	0.46
1:D:162:ARG:NH2	1:D:193[B]:ARG:HH12	2.13	0.46
1:B:104[A]:ASP:N	1:B:105:PRO:CD	2.79	0.46
1:C:104[A]:ASP:N	1:C:105:PRO:HD3	2.31	0.46
1:C:177:PHE:C	1:C:177:PHE:CD1	2.89	0.46
1:C:104[B]:ASP:CG	1:C:106:ARG:HH12	2.20	0.46
1:A:275:MET:HE2	1:C:275:MET:HE2	1.98	0.45
1:E:314:ILE:HB	1:E:315:PRO:HD3	1.98	0.45
1:C:103:TYR:O	1:C:104[B]:ASP:HB3	2.17	0.45
1:C:99:TRP:CG	5:C:594:EDO:H12	2.51	0.45
1:E:257:VAL:HG12	1:E:327:ILE:HD11	1.99	0.45
1:E:85:GLU:HG3	1:E:86:PRO:CD	2.47	0.45
1:D:103:TYR:O	1:D:104[B]:ASP:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ASP:O	1:A:188:MET:HB2	2.17	0.45
1:D:108:CYS:HB3	1:D:218:ILE:HG13	1.98	0.45
1:C:127[B]:ILE:HD13	1:C:152:GLY:CA	2.47	0.45
1:C:106:ARG:HG3	1:C:153:VAL:HG22	1.99	0.45
1:F:199:SER:HB3	1:F:200:PRO:HD2	1.98	0.45
1:F:103:TYR:O	1:F:104[B]:ASP:CB	2.65	0.45
1:B:217:PRO:HD3	1:B:284:PRO:HB2	1.98	0.44
1:B:200:PRO:HG3	1:B:212:LYS:HA	1.98	0.44
1:C:103:TYR:O	1:C:104[B]:ASP:CB	2.62	0.44
1:E:45[A]:SER:O	1:E:285[A]:CYS:HB2	2.17	0.44
1:A:87[A]:LEU:HD23	1:A:87[A]:LEU:C	2.38	0.44
1:A:30:ILE:HA	6:A:608:PGE:H4	1.98	0.44
1:C:217:PRO:HD2	1:C:229[A]:ILE:HB	1.99	0.44
1:E:87:LEU:HD11	1:E:138:PHE:CD1	2.53	0.44
1:D:125:PRO:HD2	1:D:148:PHE:HD1	1.83	0.44
1:F:234[B]:LEU:HD12	1:F:235:HIS:N	2.32	0.44
1:A:275:MET:CE	1:C:275:MET:CE	2.96	0.44
1:C:226:TRP:HB2	1:C:249:LEU:HB2	2.00	0.43
1:A:185:SER:HB2	1:A:191:TRP:CD2	2.53	0.43
1:B:187:ASP:O	1:B:188:MET:HB2	2.18	0.43
1:E:103:TYR:O	1:E:104[B]:ASP:CB	2.64	0.43
1:D:14[B]:ARG:O	1:D:14[B]:ARG:HG2	2.16	0.43
1:D:43[B]:PHE:CD2	1:D:304:ASP:HA	2.54	0.43
1:B:35:LEU:HD23	1:B:82:ILE:HD12	2.00	0.43
1:F:290:ASP:OD2	1:F:293:THR:OG1	2.30	0.43
1:D:257:VAL:HG12	1:D:327:ILE:CD1	2.49	0.43
3:F:329:BMA:O1	7:F:622:HOH:O	2.21	0.43
1:B:106:ARG:NH1	1:B:285[B]:CYS:SG	2.92	0.43
1:E:89:PHE:HB3	1:E:140:GLN:HB2	2.01	0.43
1:F:87:LEU:HD23	1:F:88:LYS:N	2.33	0.42
1:A:217:PRO:HD2	1:A:229[B]:ILE:HB	2.01	0.42
1:C:43[B]:PHE:CD2	1:C:304:ASP:HA	2.55	0.42
1:E:216:GLY:HA3	1:E:217:PRO:HD3	1.84	0.42
1:E:76:ASP:O	1:E:77:ALA:HB3	2.20	0.42
1:E:44[B]:ASN:HB2	1:E:59:ARG:HB3	2.00	0.42
1:C:185:SER:HB2	1:C:191:TRP:CD2	2.55	0.42
1:B:225:GLY:HA2	1:B:251:LEU:HG	2.01	0.42
1:B:263:PRO:HD3	1:B:324:THR:HB	2.02	0.42
1:E:162:ARG:NH2	1:E:193[B]:ARG:CZ	2.83	0.41
1:B:104[A]:ASP:N	1:B:105:PRO:HD3	2.36	0.41
1:C:250:ASP:HA	1:C:258:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46[B]:ALA:CB	1:F:107:VAL:HG23	2.51	0.41
6:B:599:PGE:H6	6:B:599:PGE:H42	1.69	0.41
1:C:77:ALA:HB1	1:C:299:TYR:OH	2.21	0.41
1:A:104[A]:ASP:N	1:A:105:PRO:CD	2.84	0.41
1:F:225:GLY:CA	1:F:251:LEU:HD13	2.50	0.41
1:E:102:GLY:HA2	1:E:119:CYS:O	2.21	0.41
1:A:197:VAL:HG22	1:A:255:TRP:HA	2.03	0.41
1:F:146:ILE:HG21	1:F:146:ILE:HD13	1.75	0.41
1:F:8:ILE:HG13	1:F:8:ILE:O	2.20	0.41
1:E:185:SER:HB2	1:E:191:TRP:CD2	2.56	0.41
1:F:43[A]:PHE:O	1:F:301:GLY:CA	2.69	0.41
1:C:257:VAL:HG12	1:C:327:ILE:HD11	2.02	0.41
1:E:222:THR:HG21	1:E:318:ILE:HD11	2.03	0.41
1:C:148:PHE:HE2	1:F:177:PHE:CE1	2.38	0.41
1:D:187:ASP:O	1:D:188:MET:HB2	2.21	0.41
1:F:105:PRO:O	1:F:106:ARG:HD2	2.21	0.40
1:C:169:PRO:HG3	1:F:146:ILE:HG22	2.04	0.40
1:D:162:ARG:CZ	1:D:193[B]:ARG:NH1	2.85	0.40
1:E:162:ARG:NH2	1:E:193[B]:ARG:NH1	2.69	0.40
1:A:103:TYR:O	1:A:104[B]:ASP:HB3	2.21	0.40
1:E:43[B]:PHE:CD2	1:E:304:ASP:HA	2.56	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	331/347 (95%)	311 (94%)	20 (6%)	0	100	100
1	B	329/347 (95%)	309 (94%)	20 (6%)	0	100	100
1	C	327/347 (94%)	308 (94%)	19 (6%)	0	100	100
1	D	330/347 (95%)	311 (94%)	19 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	330/347 (95%)	313 (95%)	15 (4%)	2 (1%)	30 16
1	F	328/347 (94%)	311 (95%)	13 (4%)	4 (1%)	16 5
All	All	1975/2082 (95%)	1863 (94%)	106 (5%)	6 (0%)	52 35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	44[A]	ASN
1	F	44[B]	ASN
1	F	104[A]	ASP
1	F	104[B]	ASP
1	E	104[A]	ASP
1	E	104[B]	ASP

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	286/298 (96%)	285 (100%)	1 (0%)	94 94
1	B	284/298 (95%)	280 (99%)	4 (1%)	74 68
1	C	281/298 (94%)	281 (100%)	0	100 100
1	D	285/298 (96%)	284 (100%)	1 (0%)	93 93
1	E	285/298 (96%)	285 (100%)	0	100 100
1	F	283/298 (95%)	280 (99%)	3 (1%)	80 76
All	All	1704/1788 (95%)	1695 (100%)	9 (0%)	92 92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	PHE
1	B	14	ARG
1	B	168	ARG
1	B	319	GLU

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Mol	Chain	Res	Type
1	B	327	ILE
1	D	92	ASP
1	F	8	ILE
1	F	9	ILE
1	F	168	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 40 ligands modelled in this entry, 8 are monoatomic - leaving 32 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	PO4	A	328	-	4,4,4	0.67	0	6,6,6	0.28	0
3	BMA	A	329	-	12,12,12	0.99	1 (8%)	17,17,17	2.31	9 (52%)
5	EDO	A	348	-	3,3,3	0.59	0	2,2,2	0.23	0
5	EDO	A	569	-	3,3,3	0.59	0	2,2,2	0.30	0
6	PGE	A	602	-	9,9,9	0.54	0	8,8,8	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	PGE	A	604	-	9,9,9	0.48	0	8,8,8	0.64	0
6	PGE	A	608	-	9,9,9	0.92	0	8,8,8	0.64	0
2	PO4	B	328	-	4,4,4	0.66	0	6,6,6	0.28	0
3	BMA	B	329	-	12,12,12	1.01	1 (8%)	17,17,17	2.44	8 (47%)
6	PGE	B	596	-	9,9,9	0.53	0	8,8,8	0.48	0
5	EDO	B	598	-	3,3,3	0.26	0	2,2,2	0.61	0
6	PGE	B	599	-	9,9,9	0.45	0	8,8,8	0.57	0
6	PGE	B	600	-	9,9,9	0.51	0	8,8,8	0.61	0
2	PO4	C	328	-	4,4,4	1.01	0	6,6,6	0.26	0
3	BMA	C	329	-	12,12,12	1.39	1 (8%)	17,17,17	2.37	6 (35%)
6	PGE	C	592	-	9,9,9	0.49	0	8,8,8	0.71	0
5	EDO	C	594	-	3,3,3	0.59	0	2,2,2	0.62	0
2	PO4	D	328	-	4,4,4	0.83	0	6,6,6	0.31	0
3	BMA	D	329	-	12,12,12	1.11	1 (8%)	17,17,17	2.09	5 (29%)
5	EDO	D	583	-	3,3,3	0.40	0	2,2,2	0.64	0
5	EDO	D	584	-	3,3,3	0.46	0	2,2,2	0.31	0
6	PGE	D	587	-	9,9,9	0.45	0	8,8,8	0.30	0
5	EDO	D	588	-	3,3,3	0.42	0	2,2,2	0.59	0
2	PO4	E	328	-	4,4,4	0.73	0	6,6,6	0.33	0
3	BMA	E	329	-	12,12,12	1.04	2 (16%)	17,17,17	2.13	8 (47%)
5	EDO	E	579	-	3,3,3	0.46	0	2,2,2	0.43	0
5	EDO	E	580	-	3,3,3	0.33	0	2,2,2	0.92	0
2	PO4	F	328	-	4,4,4	0.89	0	6,6,6	0.28	0
3	BMA	F	329	-	12,12,12	0.82	0	17,17,17	1.97	5 (29%)
5	EDO	F	569	-	3,3,3	0.48	0	2,2,2	0.29	0
5	EDO	F	579	-	3,3,3	0.51	0	2,2,2	0.33	0
6	PGE	F	580	-	9,9,9	0.49	0	8,8,8	0.53	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	PO4	A	328	-	-	0/0/0/0	0/0/0/0
3	BMA	A	329	-	-	0/2/22/22	0/1/1/1
5	EDO	A	348	-	-	0/1/1/1	0/0/0/0
5	EDO	A	569	-	-	0/1/1/1	0/0/0/0
6	PGE	A	602	-	-	0/7/7/7	0/0/0/0
6	PGE	A	604	-	-	0/7/7/7	0/0/0/0
6	PGE	A	608	-	-	0/7/7/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	B	328	-	-	0/0/0/0	0/0/0/0
3	BMA	B	329	-	-	0/2/22/22	0/1/1/1
6	PGE	B	596	-	-	0/7/7/7	0/0/0/0
5	EDO	B	598	-	-	0/1/1/1	0/0/0/0
6	PGE	B	599	-	-	0/7/7/7	0/0/0/0
6	PGE	B	600	-	-	0/7/7/7	0/0/0/0
2	PO4	C	328	-	-	0/0/0/0	0/0/0/0
3	BMA	C	329	-	-	0/2/22/22	0/1/1/1
6	PGE	C	592	-	-	0/7/7/7	0/0/0/0
5	EDO	C	594	-	-	0/1/1/1	0/0/0/0
2	PO4	D	328	-	-	0/0/0/0	0/0/0/0
3	BMA	D	329	-	-	0/2/22/22	0/1/1/1
5	EDO	D	583	-	-	0/1/1/1	0/0/0/0
5	EDO	D	584	-	-	0/1/1/1	0/0/0/0
6	PGE	D	587	-	-	0/7/7/7	0/0/0/0
5	EDO	D	588	-	-	0/1/1/1	0/0/0/0
2	PO4	E	328	-	-	0/0/0/0	0/0/0/0
3	BMA	E	329	-	-	0/2/22/22	0/1/1/1
5	EDO	E	579	-	-	0/1/1/1	0/0/0/0
5	EDO	E	580	-	-	0/1/1/1	0/0/0/0
2	PO4	F	328	-	-	0/0/0/0	0/0/0/0
3	BMA	F	329	-	-	0/2/22/22	0/1/1/1
5	EDO	F	569	-	-	0/1/1/1	0/0/0/0
5	EDO	F	579	-	-	0/1/1/1	0/0/0/0
6	PGE	F	580	-	-	0/7/7/7	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	329	BMA	C3-C2	2.01	1.57	1.52
3	E	329	BMA	C1-C2	2.04	1.56	1.52
3	B	329	BMA	C1-C2	2.05	1.56	1.52
3	A	329	BMA	C1-C2	2.46	1.57	1.52
3	D	329	BMA	C1-C2	2.77	1.58	1.52
3	C	329	BMA	C1-C2	3.17	1.59	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	329	BMA	O5-C5-C4	-2.72	104.58	109.68
3	C	329	BMA	O1-C1-O5	-2.55	103.28	110.25
3	E	329	BMA	O5-C5-C4	-2.36	105.26	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	329	BMA	O5-C5-C4	-2.35	105.26	109.68
3	D	329	BMA	O5-C5-C4	-2.25	105.47	109.68
3	B	329	BMA	O3-C3-C4	-2.12	105.56	110.34
3	A	329	BMA	O2-C2-C3	2.07	114.99	110.34
3	E	329	BMA	O5-C5-C6	2.13	111.74	106.36
3	F	329	BMA	O2-C2-C3	2.14	115.16	110.34
3	A	329	BMA	C4-C3-C2	2.18	114.86	110.79
3	A	329	BMA	O1-C1-C2	2.26	115.27	109.21
3	A	329	BMA	O5-C5-C6	2.34	112.28	106.36
3	C	329	BMA	O1-C1-C2	2.37	115.57	109.21
3	A	329	BMA	C3-C4-C5	2.49	114.53	110.20
3	D	329	BMA	O2-C2-C3	2.58	116.15	110.34
3	E	329	BMA	O2-C2-C3	2.58	116.15	110.34
3	C	329	BMA	O2-C2-C3	2.64	116.28	110.34
3	B	329	BMA	O1-C1-C2	2.64	116.29	109.21
3	F	329	BMA	C1-O5-C5	2.84	118.72	113.47
3	B	329	BMA	O5-C5-C6	2.84	113.53	106.36
3	D	329	BMA	C4-C3-C2	2.84	116.10	110.79
3	E	329	BMA	C4-C3-C2	2.88	116.17	110.79
3	C	329	BMA	C4-C3-C2	2.90	116.21	110.79
3	E	329	BMA	O5-C1-C2	2.92	114.46	109.80
3	E	329	BMA	O1-C1-C2	2.95	117.11	109.21
3	F	329	BMA	O2-C2-C1	3.12	116.69	109.82
3	A	329	BMA	O5-C1-C2	3.18	114.87	109.80
3	A	329	BMA	C1-O5-C5	3.23	119.45	113.47
3	E	329	BMA	O2-C2-C1	3.23	116.94	109.82
3	F	329	BMA	C4-C3-C2	3.25	116.86	110.79
3	B	329	BMA	C1-O5-C5	3.37	119.70	113.47
3	E	329	BMA	C1-O5-C5	3.44	119.84	113.47
3	B	329	BMA	O5-C1-C2	3.53	115.43	109.80
3	B	329	BMA	C4-C3-C2	3.68	117.66	110.79
3	F	329	BMA	O5-C1-C2	4.11	116.35	109.80
3	D	329	BMA	O5-C1-C2	4.36	116.75	109.80
3	D	329	BMA	O2-C2-C1	4.37	119.45	109.82
3	C	329	BMA	O2-C2-C1	4.71	120.19	109.82
3	B	329	BMA	O2-C2-C1	4.96	120.74	109.82
3	A	329	BMA	O2-C2-C1	5.21	121.31	109.82
3	C	329	BMA	O5-C1-C2	6.03	119.41	109.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	328	PO4	1	0
3	A	329	BMA	1	0
5	A	348	EDO	1	0
6	A	608	PGE	2	0
2	B	328	PO4	1	0
3	B	329	BMA	1	0
6	B	599	PGE	1	0
2	C	328	PO4	1	0
3	C	329	BMA	1	0
5	C	594	EDO	1	0
2	D	328	PO4	1	0
3	D	329	BMA	1	0
2	E	328	PO4	1	0
3	E	329	BMA	1	0
2	F	328	PO4	1	0
3	F	329	BMA	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	320/347 (92%)	-0.52	1 (0%)	94	96	9, 14, 27, 47	0
1	B	321/347 (92%)	-0.53	3 (0%)	85	89	10, 15, 29, 45	0
1	C	320/347 (92%)	-0.54	2 (0%)	90	93	9, 14, 30, 48	0
1	D	320/347 (92%)	-0.49	2 (0%)	90	93	12, 20, 34, 48	0
1	E	321/347 (92%)	-0.46	3 (0%)	85	89	12, 19, 33, 44	0
1	F	320/347 (92%)	-0.37	4 (1%)	79	84	13, 22, 40, 56	0
All	All	1922/2082 (92%)	-0.49	15 (0%)	87	91	9, 17, 33, 56	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	16	ALA	3.5
1	E	17	GLY	3.4
1	D	16	ALA	3.2
1	F	8	ILE	2.9
1	B	7	VAL	2.7
1	B	16	ALA	2.4
1	E	16	ALA	2.4
1	B	17	GLY	2.3
1	F	17	GLY	2.3
1	D	17	GLY	2.2
1	E	52	ASP	2.2
1	A	8	ILE	2.1
1	F	51	GLY	2.0
1	C	16	ALA	2.0
1	C	17	GLY	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^{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
4	K	A	333	1/1	0.88	0.32	36.99	61,61,61,61	0
4	K	C	333	1/1	0.89	0.32	30.56	60,60,60,60	0
4	K	B	333	1/1	0.93	0.20	21.60	61,61,61,61	0
4	K	F	333	1/1	0.87	0.33	20.67	64,64,64,64	0
6	PGE	B	599	10/10	0.84	0.16	10.15	46,50,60,66	0
6	PGE	F	580	10/10	0.77	0.30	9.75	47,57,60,61	0
6	PGE	C	592	10/10	0.90	0.15	9.38	32,38,43,44	0
5	EDO	E	580	4/4	0.72	0.18	9.17	39,41,47,48	0
6	PGE	A	608	10/10	0.80	0.32	8.51	36,47,54,54	0
4	K	A	607	1/1	0.99	0.19	7.05	44,44,44,44	0
4	K	A	606	1/1	0.99	0.12	6.15	36,36,36,36	0
6	PGE	D	587	10/10	0.83	0.14	5.58	44,45,53,54	0
3	BMA	A	329	12/12	0.92	0.20	5.19	19,23,25,29	0
3	BMA	D	329	12/12	0.89	0.18	4.96	24,28,30,33	0
6	PGE	A	604	10/10	0.90	0.14	4.59	39,43,61,68	0
3	BMA	E	329	12/12	0.93	0.18	4.44	21,24,26,27	0
5	EDO	F	579	4/4	0.88	0.32	3.63	46,48,51,55	0
3	BMA	B	329	12/12	0.89	0.17	3.37	22,30,33,36	0
5	EDO	B	598	4/4	0.84	0.21	2.75	40,44,45,46	0
6	PGE	A	602	10/10	0.91	0.16	2.54	34,42,60,65	0
5	EDO	D	584	4/4	0.76	0.20	2.11	50,52,55,59	0
5	EDO	D	588	4/4	0.88	0.17	2.09	50,51,52,53	0
5	EDO	F	569	4/4	0.86	0.11	2.03	41,44,44,46	0
3	BMA	C	329	12/12	0.95	0.14	1.98	20,21,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	BMA	F	329	12/12	0.91	0.15	1.49	24,30,32,34	0
5	EDO	C	594	4/4	0.86	0.14	1.21	39,42,43,45	0
5	EDO	A	569	4/4	0.91	0.11	0.52	42,43,44,47	0
5	EDO	D	583	4/4	0.94	0.09	0.32	32,35,37,42	0
2	PO4	B	328	5/5	0.99	0.07	-0.47	12,12,14,14	0
2	PO4	F	328	5/5	0.99	0.06	-1.34	13,15,16,16	0
2	PO4	C	328	5/5	0.99	0.07	-1.37	11,12,12,13	0
2	PO4	A	328	5/5	0.99	0.07	-1.75	10,10,11,12	0
2	PO4	D	328	5/5	1.00	0.05	-2.87	14,14,15,16	0
2	PO4	E	328	5/5	1.00	0.05	-3.19	13,13,15,15	0
6	PGE	B	596	10/10	0.66	0.26	-	55,61,70,72	0
6	PGE	B	600	10/10	0.87	0.30	-	49,56,64,65	0
5	EDO	A	348	4/4	0.52	0.31	-	53,56,56,59	0
4	K	E	333	1/1	0.95	0.20	-	57,57,57,57	0
5	EDO	E	579	4/4	0.70	0.16	-	45,47,48,49	0
4	K	D	333	1/1	0.95	0.22	-	56,56,56,56	0

6.5 Other polymers

There are no such residues in this entry.