Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:25 PM GMT

PDB ID	:	3R6S
Title	:	Crystal structure of GlxR transcription factor from Corynebacterium glutamicum with cAMP
Authors	:	Jungwirth, B.; Pojer, F.
Deposited on	:	2011-03-22
Resolution	:	2.38 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:

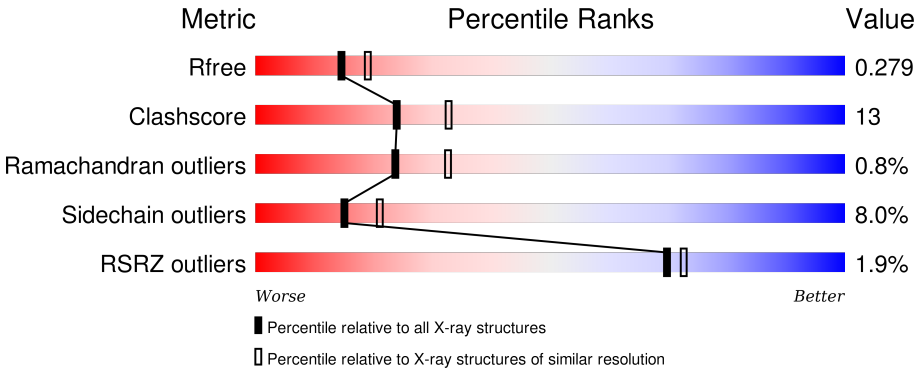
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.38 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	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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	247	73% 17% 9%
1	B	247	2% 64% 23% 9%
1	C	247	60% 26% 9%
1	D	247	4% 69% 21% 9%
1	E	247	70% 19% 9%

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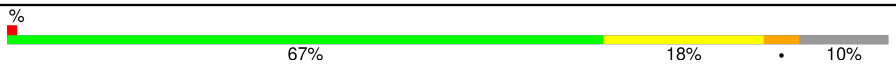
Mol	Chain	Length	Quality of chain
1	F	247	

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	HEZ	D	228	-	-	-	X
3	HEZ	F	228	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10745 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 transcription regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	2	0
			1744	1086	327	325	6			
1	B	225	Total	C	N	O	S	0	2	0
			1754	1092	333	323	6			
1	C	224	Total	C	N	O	S	0	0	0
			1727	1076	323	322	6			
1	D	224	Total	C	N	O	S	0	0	0
			1727	1076	323	322	6			
1	E	225	Total	C	N	O	S	0	1	0
			1745	1087	329	323	6			
1	F	222	Total	C	N	O	S	0	2	0
			1731	1079	326	320	6			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q79VI7
A	-18	GLY	-	EXPRESSION TAG	UNP Q79VI7
A	-17	SER	-	EXPRESSION TAG	UNP Q79VI7
A	-16	SER	-	EXPRESSION TAG	UNP Q79VI7
A	-15	HIS	-	EXPRESSION TAG	UNP Q79VI7
A	-14	HIS	-	EXPRESSION TAG	UNP Q79VI7
A	-13	HIS	-	EXPRESSION TAG	UNP Q79VI7
A	-12	HIS	-	EXPRESSION TAG	UNP Q79VI7
A	-11	HIS	-	EXPRESSION TAG	UNP Q79VI7
A	-10	HIS	-	EXPRESSION TAG	UNP Q79VI7
A	-9	SER	-	EXPRESSION TAG	UNP Q79VI7
A	-8	SER	-	EXPRESSION TAG	UNP Q79VI7
A	-7	GLY	-	EXPRESSION TAG	UNP Q79VI7
A	-6	LEU	-	EXPRESSION TAG	UNP Q79VI7
A	-5	VAL	-	EXPRESSION TAG	UNP Q79VI7
A	-4	PRO	-	EXPRESSION TAG	UNP Q79VI7
A	-3	ARG	-	EXPRESSION TAG	UNP Q79VI7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q79VI7
A	-1	SER	-	EXPRESSION TAG	UNP Q79VI7
A	0	HIS	-	EXPRESSION TAG	UNP Q79VI7
B	-19	MET	-	EXPRESSION TAG	UNP Q79VI7
B	-18	GLY	-	EXPRESSION TAG	UNP Q79VI7
B	-17	SER	-	EXPRESSION TAG	UNP Q79VI7
B	-16	SER	-	EXPRESSION TAG	UNP Q79VI7
B	-15	HIS	-	EXPRESSION TAG	UNP Q79VI7
B	-14	HIS	-	EXPRESSION TAG	UNP Q79VI7
B	-13	HIS	-	EXPRESSION TAG	UNP Q79VI7
B	-12	HIS	-	EXPRESSION TAG	UNP Q79VI7
B	-11	HIS	-	EXPRESSION TAG	UNP Q79VI7
B	-10	HIS	-	EXPRESSION TAG	UNP Q79VI7
B	-9	SER	-	EXPRESSION TAG	UNP Q79VI7
B	-8	SER	-	EXPRESSION TAG	UNP Q79VI7
B	-7	GLY	-	EXPRESSION TAG	UNP Q79VI7
B	-6	LEU	-	EXPRESSION TAG	UNP Q79VI7
B	-5	VAL	-	EXPRESSION TAG	UNP Q79VI7
B	-4	PRO	-	EXPRESSION TAG	UNP Q79VI7
B	-3	ARG	-	EXPRESSION TAG	UNP Q79VI7
B	-2	GLY	-	EXPRESSION TAG	UNP Q79VI7
B	-1	SER	-	EXPRESSION TAG	UNP Q79VI7
B	0	HIS	-	EXPRESSION TAG	UNP Q79VI7
C	-19	MET	-	EXPRESSION TAG	UNP Q79VI7
C	-18	GLY	-	EXPRESSION TAG	UNP Q79VI7
C	-17	SER	-	EXPRESSION TAG	UNP Q79VI7
C	-16	SER	-	EXPRESSION TAG	UNP Q79VI7
C	-15	HIS	-	EXPRESSION TAG	UNP Q79VI7
C	-14	HIS	-	EXPRESSION TAG	UNP Q79VI7
C	-13	HIS	-	EXPRESSION TAG	UNP Q79VI7
C	-12	HIS	-	EXPRESSION TAG	UNP Q79VI7
C	-11	HIS	-	EXPRESSION TAG	UNP Q79VI7
C	-10	HIS	-	EXPRESSION TAG	UNP Q79VI7
C	-9	SER	-	EXPRESSION TAG	UNP Q79VI7
C	-8	SER	-	EXPRESSION TAG	UNP Q79VI7
C	-7	GLY	-	EXPRESSION TAG	UNP Q79VI7
C	-6	LEU	-	EXPRESSION TAG	UNP Q79VI7
C	-5	VAL	-	EXPRESSION TAG	UNP Q79VI7
C	-4	PRO	-	EXPRESSION TAG	UNP Q79VI7
C	-3	ARG	-	EXPRESSION TAG	UNP Q79VI7
C	-2	GLY	-	EXPRESSION TAG	UNP Q79VI7
C	-1	SER	-	EXPRESSION TAG	UNP Q79VI7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	EXPRESSION TAG	UNP Q79VI7
D	-19	MET	-	EXPRESSION TAG	UNP Q79VI7
D	-18	GLY	-	EXPRESSION TAG	UNP Q79VI7
D	-17	SER	-	EXPRESSION TAG	UNP Q79VI7
D	-16	SER	-	EXPRESSION TAG	UNP Q79VI7
D	-15	HIS	-	EXPRESSION TAG	UNP Q79VI7
D	-14	HIS	-	EXPRESSION TAG	UNP Q79VI7
D	-13	HIS	-	EXPRESSION TAG	UNP Q79VI7
D	-12	HIS	-	EXPRESSION TAG	UNP Q79VI7
D	-11	HIS	-	EXPRESSION TAG	UNP Q79VI7
D	-10	HIS	-	EXPRESSION TAG	UNP Q79VI7
D	-9	SER	-	EXPRESSION TAG	UNP Q79VI7
D	-8	SER	-	EXPRESSION TAG	UNP Q79VI7
D	-7	GLY	-	EXPRESSION TAG	UNP Q79VI7
D	-6	LEU	-	EXPRESSION TAG	UNP Q79VI7
D	-5	VAL	-	EXPRESSION TAG	UNP Q79VI7
D	-4	PRO	-	EXPRESSION TAG	UNP Q79VI7
D	-3	ARG	-	EXPRESSION TAG	UNP Q79VI7
D	-2	GLY	-	EXPRESSION TAG	UNP Q79VI7
D	-1	SER	-	EXPRESSION TAG	UNP Q79VI7
D	0	HIS	-	EXPRESSION TAG	UNP Q79VI7
E	-19	MET	-	EXPRESSION TAG	UNP Q79VI7
E	-18	GLY	-	EXPRESSION TAG	UNP Q79VI7
E	-17	SER	-	EXPRESSION TAG	UNP Q79VI7
E	-16	SER	-	EXPRESSION TAG	UNP Q79VI7
E	-15	HIS	-	EXPRESSION TAG	UNP Q79VI7
E	-14	HIS	-	EXPRESSION TAG	UNP Q79VI7
E	-13	HIS	-	EXPRESSION TAG	UNP Q79VI7
E	-12	HIS	-	EXPRESSION TAG	UNP Q79VI7
E	-11	HIS	-	EXPRESSION TAG	UNP Q79VI7
E	-10	HIS	-	EXPRESSION TAG	UNP Q79VI7
E	-9	SER	-	EXPRESSION TAG	UNP Q79VI7
E	-8	SER	-	EXPRESSION TAG	UNP Q79VI7
E	-7	GLY	-	EXPRESSION TAG	UNP Q79VI7
E	-6	LEU	-	EXPRESSION TAG	UNP Q79VI7
E	-5	VAL	-	EXPRESSION TAG	UNP Q79VI7
E	-4	PRO	-	EXPRESSION TAG	UNP Q79VI7
E	-3	ARG	-	EXPRESSION TAG	UNP Q79VI7
E	-2	GLY	-	EXPRESSION TAG	UNP Q79VI7
E	-1	SER	-	EXPRESSION TAG	UNP Q79VI7
E	0	HIS	-	EXPRESSION TAG	UNP Q79VI7
F	-19	MET	-	EXPRESSION TAG	UNP Q79VI7

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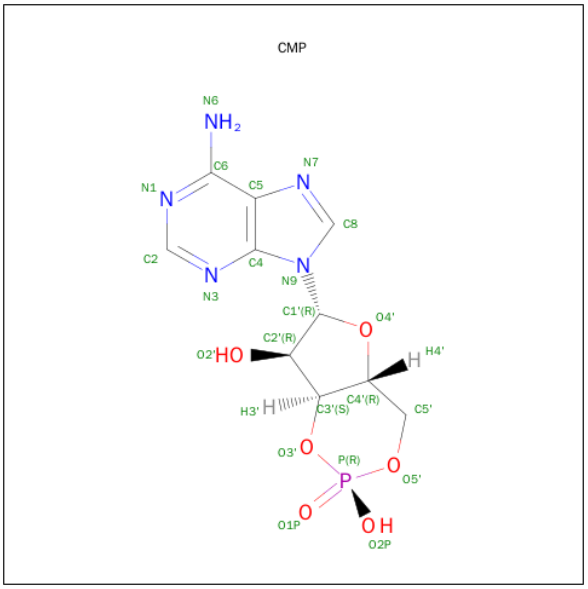
Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	GLY	-	EXPRESSION TAG	UNP Q79VI7
F	-17	SER	-	EXPRESSION TAG	UNP Q79VI7
F	-16	SER	-	EXPRESSION TAG	UNP Q79VI7
F	-15	HIS	-	EXPRESSION TAG	UNP Q79VI7
F	-14	HIS	-	EXPRESSION TAG	UNP Q79VI7
F	-13	HIS	-	EXPRESSION TAG	UNP Q79VI7
F	-12	HIS	-	EXPRESSION TAG	UNP Q79VI7
F	-11	HIS	-	EXPRESSION TAG	UNP Q79VI7
F	-10	HIS	-	EXPRESSION TAG	UNP Q79VI7
F	-9	SER	-	EXPRESSION TAG	UNP Q79VI7
F	-8	SER	-	EXPRESSION TAG	UNP Q79VI7
F	-7	GLY	-	EXPRESSION TAG	UNP Q79VI7
F	-6	LEU	-	EXPRESSION TAG	UNP Q79VI7
F	-5	VAL	-	EXPRESSION TAG	UNP Q79VI7
F	-4	PRO	-	EXPRESSION TAG	UNP Q79VI7
F	-3	ARG	-	EXPRESSION TAG	UNP Q79VI7
F	-2	GLY	-	EXPRESSION TAG	UNP Q79VI7
F	-1	SER	-	EXPRESSION TAG	UNP Q79VI7
F	0	HIS	-	EXPRESSION TAG	UNP Q79VI7

- Molecule 2 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: $C_{10}H_{12}N_5O_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

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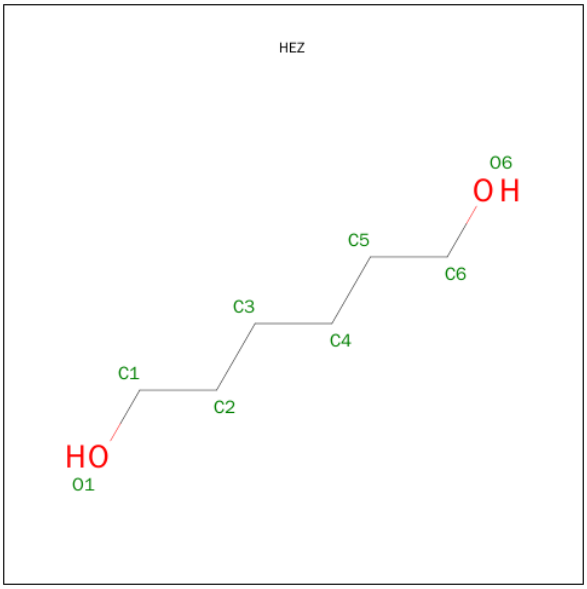
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O P 22 10 5 6 1	0	0
2	C	1	Total C N O P 22 10 5 6 1	0	0
2	D	1	Total C N O P 22 10 5 6 1	0	0
2	E	1	Total C N O P 22 10 5 6 1	0	0
2	F	1	Total C N O P 22 10 5 6 1	0	0

- Molecule 3 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 6 2	0	0
3	D	1	Total C O 8 6 2	0	0
3	F	1	Total C O 8 6 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	32	Total O 32 32	0	0

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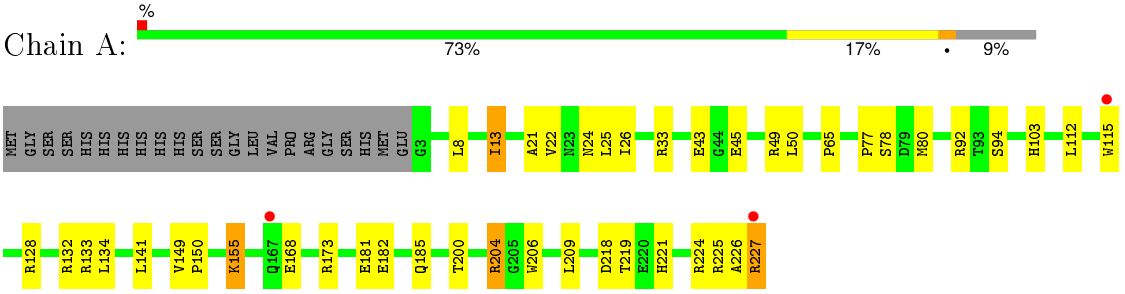
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	18	Total O 18 18	0	0
4	C	30	Total O 30 30	0	0
4	D	14	Total O 14 14	0	0
4	E	45	Total O 45 45	0	0
4	F	22	Total O 22 22	0	0

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.

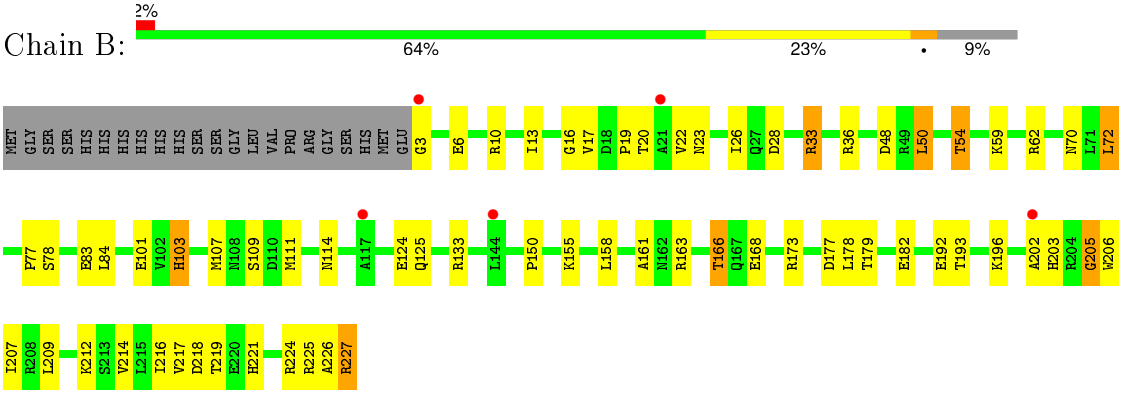
- Molecule 1: transcription regulator

Chain A:



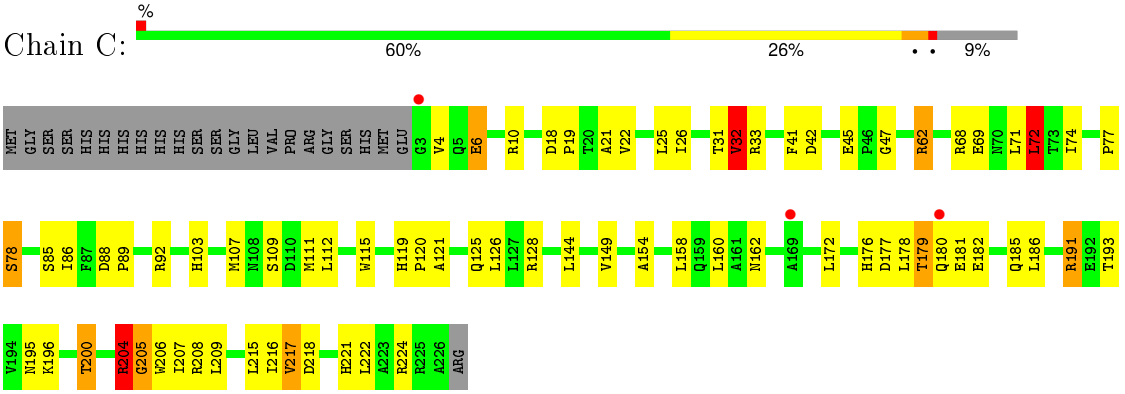
- Molecule 1: transcription regulator

Chain B:



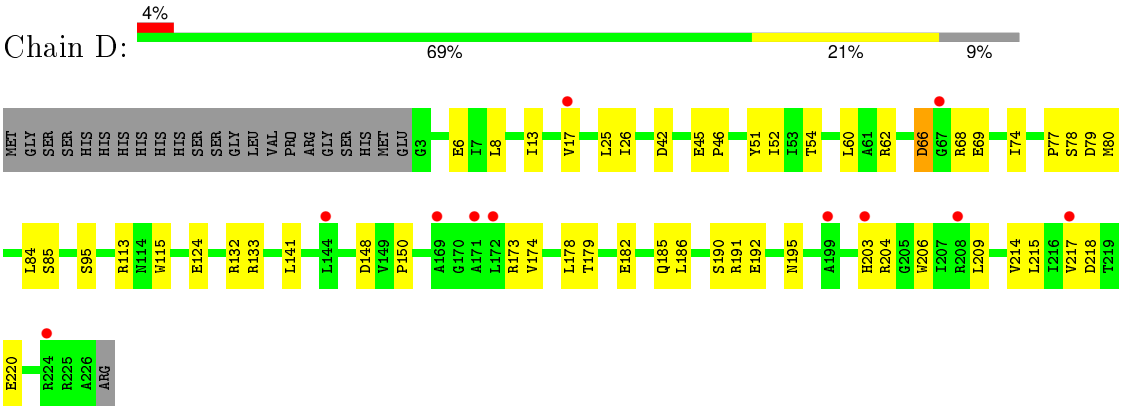
- Molecule 1: transcription regulator

Chain C:



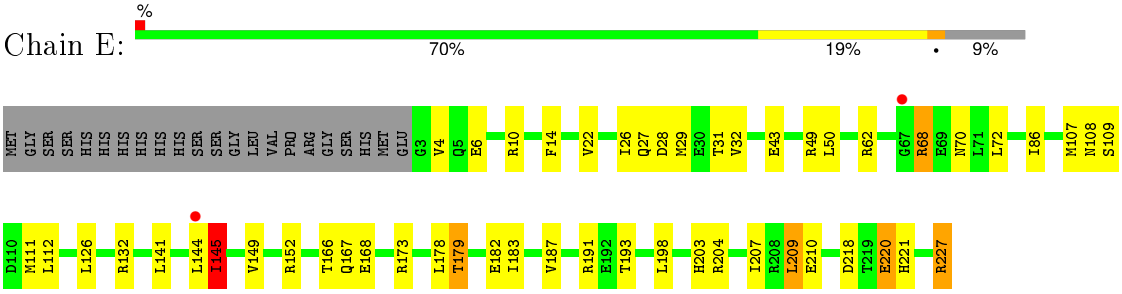
- Molecule 1: transcription regulator

Chain D:



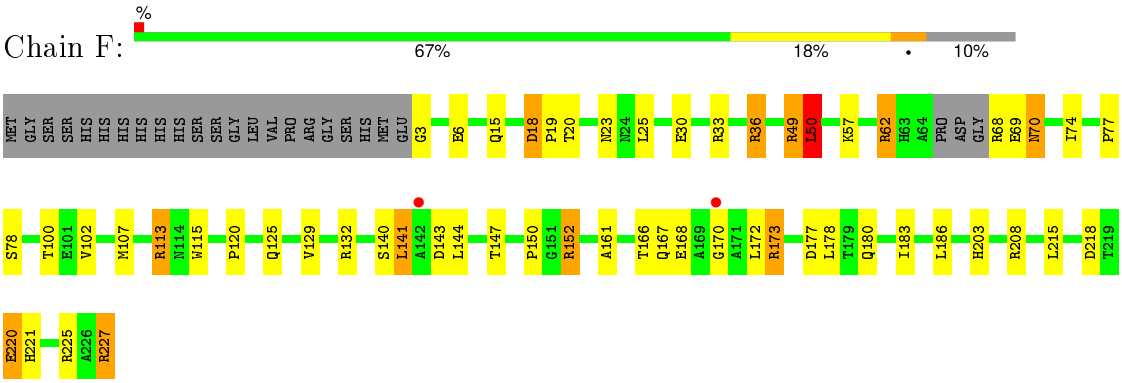
- Molecule 1: transcription regulator

Chain E:



- Molecule 1: transcription regulator

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	111.25Å 111.25Å 186.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	67.09 – 2.38 67.09 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.4 (67.09-2.38) 99.3 (67.09-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.210 , 0.288 0.206 , 0.279	Depositor DCC
R_{free} test set	2742 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	41.6	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.9	EDS
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 53829 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10745	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: HEZ, CMP

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	0.77	0/1774	0.83	0/2403
1	B	0.67	0/1787	0.84	4/2419 (0.2%)
1	C	0.73	0/1754	0.82	2/2377 (0.1%)
1	D	0.74	0/1754	0.82	2/2377 (0.1%)
1	E	0.83	0/1776	0.87	1/2406 (0.0%)
1	F	0.73	0/1763	0.85	2/2386 (0.1%)
All	All	0.75	0/10608	0.84	11/14368 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	133	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	C	32	VAL	CB-CA-C	-6.20	99.62	111.40
1	B	133	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	E	204	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	F	50	LEU	CA-CB-CG	5.95	128.97	115.30
1	B	33	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	133	ARG	CG-CD-NE	-5.59	100.05	111.80
1	C	72	LEU	CA-CB-CG	5.57	128.12	115.30
1	F	227	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	D	113	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	B	33	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	1744	0	1764	37	0
1	B	1754	0	1784	51	0
1	C	1727	0	1745	61	0
1	D	1727	0	1745	34	0
1	E	1745	0	1765	46	0
1	F	1731	0	1754	53	0
2	A	22	0	11	1	0
2	B	22	0	11	2	0
2	C	22	0	11	1	0
2	D	22	0	11	1	0
2	E	22	0	11	1	0
2	F	22	0	11	1	0
3	A	8	0	14	0	0
3	D	8	0	14	0	0
3	F	8	0	14	1	0
4	A	32	0	0	2	0
4	B	18	0	0	0	0
4	C	30	0	0	1	0
4	D	14	0	0	0	0
4	E	45	0	0	2	0
4	F	22	0	0	2	0
All	All	10745	0	10665	279	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 13.

All (279) 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:F:301:CMP:C2	2:F:301:CMP:H2	0.97	1.50
2:B:301:CMP:C2	2:B:301:CMP:H2	0.97	1.49
2:E:301:CMP:H2	2:E:301:CMP:C2	0.97	1.48
2:D:301:CMP:C2	2:D:301:CMP:H2	0.97	1.47
2:A:301:CMP:H2	2:A:301:CMP:C2	0.97	1.46
2:C:301:CMP:C2	2:C:301:CMP:H2	0.97	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:LEU:HA	1:F:143:ASP:H	1.17	1.03
1:E:68:ARG:NH1	1:E:68:ARG:HB2	1.73	1.03
1:C:74:ILE:HD11	1:C:178:LEU:HD11	1.40	0.99
1:F:141:LEU:HA	1:F:143:ASP:N	1.82	0.95
1:D:148:ASP:OD2	1:D:150:PRO:HD2	1.68	0.92
1:B:124:GLU:HB3	1:C:224:ARG:HH22	1.37	0.90
1:D:191:ARG:HE	1:D:195:ASN:ND2	1.70	0.89
1:A:141:LEU:HD23	4:A:309:HOH:O	1.72	0.89
1:C:200:THR:HG22	1:C:204:ARG:HH11	1.36	0.89
1:B:218:ASP:OD2	1:B:221:HIS:HD2	1.57	0.88
1:A:221:HIS:CD2	1:A:224:ARG:NH1	2.43	0.86
1:B:166:THR:HG22	1:B:173:ARG:HB3	1.58	0.85
1:E:68:ARG:HH11	1:E:68:ARG:HB2	1.35	0.84
1:D:191:ARG:HE	1:D:195:ASN:HD21	1.25	0.84
1:F:141:LEU:CA	1:F:143:ASP:H	1.91	0.83
1:F:62:ARG:HG3	1:F:62:ARG:HH11	1.44	0.82
1:C:74:ILE:HD12	1:C:160:LEU:HD21	1.62	0.81
1:C:179:THR:HG22	1:C:182:GLU:H	1.46	0.80
1:B:202:ALA:HA	1:B:207:ILE:O	1.83	0.78
1:F:50:LEU:HD21	1:F:107:MET:HE2	1.67	0.77
1:B:114:ASN:HD21	1:D:203:HIS:CE1	2.03	0.77
1:B:54:THR:HG22	1:B:103:HIS:HB2	1.67	0.77
1:B:36:ARG:HH22	1:B:212:LYS:NZ	1.83	0.76
1:A:226:ALA:O	1:A:227:ARG:HD2	1.86	0.76
1:F:140:SER:C	1:F:143:ASP:HB3	2.06	0.76
1:F:57:LYS:NZ	1:F:177:ASP:OD2	2.19	0.75
1:C:200:THR:HG22	1:C:204:ARG:NH1	2.01	0.75
1:F:218:ASP:OD2	1:F:221:HIS:HD2	1.70	0.75
1:F:125:GLN:O	1:F:129:VAL:HG23	1.87	0.74
1:A:221:HIS:HD2	1:A:224:ARG:HH12	1.34	0.74
1:B:161:ALA:HB2	1:B:216:ILE:HD12	1.69	0.74
1:F:167:GLN:HE22	1:F:170:GLY:H	1.33	0.73
1:C:77:PRO:O	1:C:78:SER:HB2	1.88	0.73
1:B:218:ASP:OD2	1:B:221:HIS:CD2	2.42	0.73
1:B:36:ARG:HH22	1:B:212:LYS:HZ1	1.37	0.73
1:F:50:LEU:HD22	1:F:107:MET:HG2	1.70	0.72
1:F:36:ARG:CG	1:F:36:ARG:HH11	2.01	0.72
1:C:33:ARG:HD3	1:C:103:HIS:NE2	2.05	0.72
1:F:167:GLN:NE2	1:F:170:GLY:H	1.88	0.71
1:C:18:ASP:OD2	1:C:19:PRO:HD2	1.90	0.71
1:B:3:GLY:HA3	1:B:6:GLU:OE1	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ARG:HH11	1:D:215:LEU:HD22	1.55	0.70
1:C:125:GLN:NE2	1:C:128:ARG:HH21	1.88	0.70
1:E:179:THR:CG2	1:E:182:GLU:H	2.05	0.70
1:D:68:ARG:HG2	1:D:69:GLU:H	1.57	0.69
1:B:77:PRO:O	1:B:78:SER:HB2	1.90	0.69
1:E:218:ASP:OD1	1:E:221:HIS:HD2	1.76	0.68
1:A:168:GLU:OE1	1:A:173:ARG:NH2	2.17	0.67
1:E:50:LEU:HD13	1:E:112:LEU:HD22	1.76	0.67
1:B:202:ALA:HB2	1:B:209:LEU:HD13	1.76	0.67
1:C:74:ILE:CD1	1:C:178:LEU:HD11	2.21	0.67
1:A:200:THR:O	1:A:204:ARG:HG2	1.96	0.66
1:F:15:GLN:HA	1:F:15:GLN:OE1	1.96	0.66
1:E:207:ILE:HD12	1:E:209:LEU:HD13	1.78	0.65
1:A:221:HIS:CD2	1:A:224:ARG:HH12	2.07	0.65
1:E:167:GLN:HG3	4:E:323:HOH:O	1.96	0.64
1:A:21:ALA:O	1:A:25:LEU:HG	1.98	0.64
1:B:150:PRO:HB2	1:B:225:ARG:NH2	2.13	0.64
1:E:68:ARG:CZ	1:E:68:ARG:HB2	2.28	0.63
1:B:177:ASP:HA	1:B:212:LYS:HB3	1.81	0.63
1:C:22:VAL:O	1:C:26:ILE:HG12	1.99	0.63
1:B:62[B]:ARG:CZ	1:B:72:LEU:HD22	2.30	0.62
1:C:125:GLN:HE22	1:C:128:ARG:HE	1.48	0.62
1:F:74:ILE:CD1	1:F:178:LEU:HD11	2.29	0.61
1:E:22:VAL:O	1:E:26:ILE:HG12	2.01	0.61
1:E:179:THR:HG22	1:E:182:GLU:CG	2.31	0.61
1:F:74:ILE:HD13	1:F:178:LEU:HD11	1.82	0.61
1:C:111:MET:CE	1:C:115:TRP:HE1	2.14	0.61
1:C:125:GLN:HE21	1:C:128:ARG:HH21	1.48	0.60
1:D:179:THR:HG23	1:D:182:GLU:H	1.66	0.60
1:C:149:VAL:HG11	1:C:193:THR:HB	1.82	0.60
1:A:182:GLU:HA	1:A:185:GLN:HE21	1.66	0.60
1:D:204:ARG:HD3	1:D:206:TRP:CZ2	2.36	0.60
1:E:43:GLU:OE2	1:E:62:ARG:NH1	2.35	0.60
1:E:179:THR:HG22	1:E:182:GLU:HG3	1.83	0.60
1:F:62:ARG:CG	1:F:62:ARG:HH11	2.14	0.59
1:C:207:ILE:HG22	1:C:216:ILE:HG12	1.84	0.59
1:F:30:GLU:OE2	1:F:49:ARG:NH2	2.29	0.59
1:E:207:ILE:HD12	1:E:209:LEU:CD1	2.32	0.59
1:B:50:LEU:HD22	1:B:107:MET:HG2	1.84	0.58
1:E:191:ARG:NH2	1:F:220:GLU:OE1	2.36	0.58
1:B:205:GLY:O	1:B:206:TRP:HD1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ILE:HD11	1:C:186:LEU:HD22	1.84	0.58
1:B:114:ASN:HD21	1:D:203:HIS:HE1	1.48	0.58
1:D:174:VAL:HB	1:D:214:VAL:HG23	1.86	0.58
1:E:145:ILE:O	1:E:145:ILE:CG2	2.51	0.58
1:F:218:ASP:OD2	1:F:221:HIS:CD2	2.54	0.58
1:D:182:GLU:HA	1:D:185:GLN:HE21	1.69	0.58
1:B:6:GLU:O	1:B:10:ARG:HG3	2.03	0.57
1:B:124:GLU:CB	1:C:224:ARG:HH22	2.15	0.57
1:A:132:ARG:HB3	1:A:132:ARG:HH11	1.69	0.57
1:C:191:ARG:HD3	1:C:195:ASN:HD21	1.70	0.57
1:D:66:ASP:OD1	1:D:66:ASP:N	2.30	0.57
1:F:161:ALA:HB1	1:F:172:LEU:HD13	1.87	0.57
1:D:42:ASP:HB2	1:D:45:GLU:HG3	1.86	0.57
1:C:21:ALA:O	1:C:25:LEU:HG	2.05	0.56
1:D:51:TYR:O	1:D:80:MET:HA	2.06	0.56
1:E:179:THR:HG22	1:E:182:GLU:H	1.69	0.56
1:D:25:LEU:HB3	1:D:115:TRP:CZ2	2.40	0.56
1:E:149:VAL:HG11	1:E:193:THR:HG22	1.88	0.56
1:A:22:VAL:O	1:A:26:ILE:HG12	2.06	0.56
1:D:192:GLU:CD	1:D:192:GLU:H	2.08	0.55
1:E:179:THR:HG23	1:E:182:GLU:H	1.71	0.54
1:A:226:ALA:O	1:A:227:ARG:CD	2.55	0.54
1:B:155:LYS:HG3	1:B:226:ALA:HB1	1.89	0.54
1:C:33:ARG:HD3	1:C:103:HIS:CD2	2.43	0.54
1:C:6:GLU:O	1:C:10:ARG:HG3	2.08	0.53
1:C:200:THR:CG2	1:C:204:ARG:NH1	2.70	0.53
1:F:50:LEU:CD2	1:F:107:MET:HE2	2.38	0.53
1:C:206:TRP:HA	1:C:218:ASP:OD1	2.07	0.53
1:A:200:THR:HG22	1:A:204:ARG:HD2	1.89	0.53
1:D:74:ILE:CD1	1:D:178:LEU:HD11	2.39	0.53
1:B:16:GLY:H	1:B:125:GLN:HG3	1.74	0.53
1:D:8:LEU:HD13	1:D:26:ILE:HD12	1.89	0.53
1:B:33:ARG:HD2	1:B:101:GLU:OE2	2.08	0.53
1:F:18:ASP:N	1:F:18:ASP:OD2	2.41	0.52
1:F:68:ARG:HG2	1:F:69:GLU:N	2.25	0.52
1:B:62[B]:ARG:HH21	1:B:70:ASN:ND2	2.07	0.52
1:F:167:GLN:HE22	1:F:170:GLY:N	2.04	0.52
1:D:74:ILE:HD13	1:D:178:LEU:HD11	1.90	0.52
1:B:202:ALA:HB2	1:B:209:LEU:CD1	2.40	0.52
1:B:50:LEU:HD22	1:B:107:MET:CG	2.40	0.52
1:A:80:MET:O	1:A:133:ARG:NH2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:PHE:CE1	1:C:92:ARG:HD2	2.45	0.52
1:D:77:PRO:O	1:D:78:SER:HB2	2.10	0.52
1:C:69:GLU:HB2	1:C:185:GLN:NE2	2.24	0.52
1:A:141:LEU:HD12	1:C:144:LEU:HD12	1.92	0.51
1:F:25:LEU:HD22	1:F:115:TRP:CD1	2.45	0.51
1:F:50:LEU:C	1:F:50:LEU:HD23	2.31	0.51
1:E:29:MET:CE	1:E:107:MET:CE	2.89	0.51
1:E:14:PHE:CE2	1:E:26:ILE:HD11	2.46	0.51
1:A:132:ARG:HB3	1:A:132:ARG:NH1	2.26	0.51
1:B:28:ASP:HB3	1:B:111:MET:SD	2.50	0.50
1:C:77:PRO:O	1:C:78:SER:CB	2.59	0.50
1:B:77:PRO:O	1:B:163[B]:ARG:NH2	2.41	0.50
1:F:141:LEU:HB3	1:F:144:LEU:HB2	1.94	0.50
1:F:36:ARG:HG2	1:F:36:ARG:HH11	1.76	0.50
1:F:168:GLU:OE2	1:F:173:ARG:HD2	2.11	0.50
1:A:141:LEU:HD12	1:C:144:LEU:CD1	2.42	0.50
1:C:111:MET:HE2	1:C:115:TRP:HE1	1.76	0.50
1:A:128:ARG:HH11	1:A:128:ARG:HG2	1.77	0.50
1:A:43:GLU:HB2	1:A:94:SER:HA	1.94	0.50
1:E:68:ARG:CB	1:E:68:ARG:CZ	2.90	0.49
1:A:155:LYS:HG2	1:A:226:ALA:HB1	1.94	0.49
1:C:158:LEU:HD11	1:C:222:LEU:HB3	1.94	0.49
1:E:50:LEU:HB2	1:E:86:ILE:HD12	1.95	0.49
1:E:173:ARG:NH2	1:E:210:GLU:OE1	2.38	0.49
1:C:18:ASP:OD2	1:C:19:PRO:CD	2.61	0.49
1:E:6:GLU:O	1:E:10:ARG:HG3	2.13	0.48
1:B:54:THR:HG22	1:B:103:HIS:CB	2.40	0.48
1:B:72:LEU:N	1:B:72:LEU:HD23	2.28	0.48
1:F:141:LEU:N	1:F:141:LEU:HD23	2.28	0.48
1:C:86:ILE:HG23	1:C:109:SER:HB2	1.95	0.48
1:B:206:TRP:O	1:B:217:VAL:HG22	2.14	0.48
1:A:77:PRO:O	1:A:78:SER:HB2	2.14	0.48
1:F:36:ARG:HG3	1:F:36:ARG:HH11	1.78	0.48
1:E:168:GLU:OE2	1:E:173:ARG:HD2	2.13	0.48
1:A:221:HIS:HA	1:A:224:ARG:HH11	1.80	0.47
1:A:150:PRO:HB2	1:A:225:ARG:NH2	2.29	0.47
1:A:226:ALA:O	1:A:227:ARG:HB3	2.13	0.47
1:B:84:LEU:HB2	2:B:301:CMP:P	2.55	0.47
1:E:152:ARG:HG3	1:E:187:VAL:HG13	1.96	0.47
1:B:62[B]:ARG:HG3	1:B:72:LEU:HD21	1.95	0.47
1:D:206:TRP:N	1:D:206:TRP:CD1	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:ARG:HD3	3:F:228:HEZ:H31	1.96	0.47
1:A:206:TRP:HA	1:A:218:ASP:OD1	2.14	0.47
1:F:77:PRO:O	1:F:78:SER:HB2	2.15	0.47
1:F:143:ASP:O	1:F:152:ARG:NH2	2.47	0.46
1:B:202:ALA:CB	1:B:209:LEU:HD13	2.45	0.46
1:D:25:LEU:HD13	1:D:115:TRP:CD2	2.51	0.46
1:E:29:MET:HE1	1:E:107:MET:CE	2.45	0.46
1:C:42:ASP:O	1:C:45:GLU:HB2	2.15	0.46
1:C:119:HIS:HA	1:C:120:PRO:HD2	1.68	0.46
1:C:191:ARG:HD3	1:C:195:ASN:ND2	2.30	0.46
1:C:71:LEU:HB2	1:C:186:LEU:HA	1.98	0.46
1:C:172:LEU:O	1:C:215:LEU:HD12	2.15	0.46
1:E:29:MET:CE	1:E:107:MET:HE1	2.45	0.46
1:F:77:PRO:O	1:F:78:SER:CB	2.64	0.46
1:F:140:SER:CA	1:F:143:ASP:HB3	2.47	0.45
1:C:224:ARG:HG2	1:C:224:ARG:NH1	2.30	0.45
1:B:22:VAL:O	1:B:26:ILE:HG12	2.16	0.45
1:C:47:GLY:HA3	1:C:92:ARG:CZ	2.47	0.45
1:C:205:GLY:O	1:C:217:VAL:HG22	2.17	0.45
1:C:224:ARG:HG2	1:C:224:ARG:HH11	1.80	0.45
1:A:8:LEU:HB3	1:A:26:ILE:HD12	1.98	0.45
1:D:84:LEU:HD12	1:D:84:LEU:HA	1.68	0.45
1:E:207:ILE:CD1	1:E:209:LEU:HD13	2.46	0.45
1:C:74:ILE:CD1	1:C:186:LEU:HD22	2.47	0.44
1:E:198:LEU:HB3	1:E:209:LEU:HD21	1.98	0.44
1:A:128:ARG:NH1	1:A:128:ARG:HG2	2.32	0.44
1:C:126:LEU:HD23	1:C:126:LEU:HA	1.86	0.44
1:B:205:GLY:O	1:B:206:TRP:CD1	2.68	0.44
1:A:149:VAL:O	1:A:150:PRO:C	2.53	0.44
1:F:150:PRO:HB2	1:F:225:ARG:NH2	2.32	0.44
1:F:74:ILE:CD1	1:F:186:LEU:HD22	2.47	0.44
1:C:6:GLU:HG2	1:C:6:GLU:H	1.44	0.44
1:F:100:THR:O	1:F:102:VAL:HG23	2.17	0.44
1:B:59:LYS:NZ	1:B:182:GLU:OE2	2.41	0.44
1:D:191:ARG:NE	1:D:195:ASN:HD21	2.03	0.44
1:F:19:PRO:O	1:F:23:ASN:ND2	2.50	0.44
1:E:28:ASP:HB3	1:E:111:MET:SD	2.57	0.44
1:E:62:ARG:NH2	4:E:232:HOH:O	2.49	0.44
1:C:86:ILE:HG21	1:C:112:LEU:HD23	1.99	0.44
1:E:178:LEU:HD12	1:E:183:ILE:HD13	1.99	0.44
1:B:48:ASP:OD1	1:B:109:SER:OG	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:HD22	1:A:115:TRP:CD1	2.53	0.44
1:A:13:ILE:HG21	1:A:13:ILE:HD13	1.69	0.44
1:F:3:GLY:N	4:F:231:HOH:O	2.49	0.44
1:E:220:GLU:OE1	1:E:221:HIS:CE1	2.70	0.44
1:C:107:MET:HE1	1:C:115:TRP:CZ3	2.52	0.43
1:E:145:ILE:O	1:E:145:ILE:HG22	2.18	0.43
1:D:74:ILE:CD1	1:D:186:LEU:HD22	2.48	0.43
1:B:179:THR:OG1	1:B:182:GLU:HG3	2.19	0.43
1:E:49:ARG:NH1	1:E:108:ASN:HB3	2.33	0.43
1:F:140:SER:HA	1:F:143:ASP:HB3	2.00	0.43
1:E:191:ARG:HH22	1:F:220:GLU:CD	2.20	0.43
1:F:113:ARG:HE	1:F:113:ARG:HB2	1.29	0.43
1:C:176:HIS:O	1:C:177:ASP:HB2	2.19	0.43
1:C:218:ASP:OD2	1:C:221:HIS:CD2	2.71	0.43
1:B:158:LEU:CD2	1:B:219:THR:HG23	2.49	0.43
1:C:121:ALA:O	1:C:125:GLN:HG2	2.19	0.43
1:D:74:ILE:HD11	1:D:186:LEU:HD22	2.00	0.43
1:A:204:ARG:HB3	1:A:204:ARG:HE	1.45	0.43
1:F:74:ILE:HD11	1:F:178:LEU:HD11	2.00	0.42
1:D:179:THR:HG22	1:D:182:GLU:CD	2.39	0.42
1:D:25:LEU:HD22	1:D:115:TRP:NE1	2.34	0.42
1:A:132:ARG:HH22	1:A:133:ARG:HE	1.67	0.42
1:B:224:ARG:O	1:B:227:ARG:HD3	2.20	0.42
1:D:52:ILE:HA	1:D:79:ASP:O	2.19	0.42
1:F:36:ARG:NH1	4:F:245:HOH:O	2.53	0.42
1:E:70:ASN:OD1	1:E:70:ASN:N	2.46	0.42
1:D:60:LEU:HA	1:D:95:SER:O	2.19	0.42
1:B:178:LEU:HB3	1:B:182:GLU:HB2	2.02	0.42
1:F:208:ARG:HB2	1:F:215:LEU:HB3	2.01	0.42
1:C:62:ARG:HG2	1:C:72:LEU:CD2	2.50	0.42
1:C:179:THR:HG23	1:C:181:GLU:H	1.85	0.42
1:E:179:THR:HG22	1:E:182:GLU:CB	2.50	0.42
1:A:25:LEU:HB3	1:A:115:TRP:CH2	2.55	0.42
1:D:25:LEU:HB3	1:D:115:TRP:CH2	2.55	0.42
1:C:154:ALA:O	1:C:158:LEU:HD12	2.19	0.42
4:C:251:HOH:O	1:E:227:ARG:HD2	2.19	0.42
1:B:125:GLN:HE21	1:C:224:ARG:HH21	1.68	0.42
1:F:183:ILE:HA	1:F:183:ILE:HD13	1.85	0.42
1:B:83:GLU:OE2	1:B:84:LEU:HD13	2.20	0.41
1:B:173:ARG:HA	1:B:173:ARG:HD2	1.73	0.41
1:B:62[B]:ARG:HH21	1:B:70:ASN:HD21	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:THR:HG22	1:D:182:GLU:CG	2.49	0.41
1:A:50:LEU:CD1	1:A:112:LEU:HD22	2.51	0.41
1:B:168:GLU:OE2	1:B:173:ARG:HD3	2.21	0.41
1:E:86:ILE:HG23	1:E:109:SER:CB	2.50	0.41
4:A:309:HOH:O	1:C:62:ARG:NH2	2.52	0.41
1:F:70:ASN:OD1	1:F:70:ASN:C	2.59	0.41
1:C:88:ASP:O	1:C:89:PRO:C	2.58	0.41
1:C:179:THR:CG2	1:C:181:GLU:HB3	2.51	0.41
1:A:33:ARG:HG3	1:A:103:HIS:CD2	2.55	0.41
1:C:181:GLU:HB2	1:C:191:ARG:NH2	2.36	0.41
1:C:111:MET:HE3	1:C:115:TRP:HE1	1.85	0.41
1:E:50:LEU:HB2	1:E:86:ILE:CD1	2.51	0.41
1:B:196:LYS:HE3	1:B:196:LYS:HB2	1.78	0.41
1:A:45:GLU:O	1:A:92:ARG:HG2	2.21	0.41
1:A:25:LEU:HB3	1:A:115:TRP:CZ2	2.56	0.41
1:E:62:ARG:HG3	1:E:72:LEU:HD11	2.03	0.40
1:D:192:GLU:N	1:D:192:GLU:OE1	2.49	0.40
1:B:158:LEU:HD22	1:B:219:THR:HG23	2.03	0.40
1:D:174:VAL:HB	1:D:214:VAL:CG2	2.50	0.40
1:E:144:LEU:O	1:E:145:ILE:HG22	2.21	0.40
1:C:31:THR:HG22	1:C:32:VAL:N	2.36	0.40
1:E:126:LEU:HA	1:E:126:LEU:HD23	1.97	0.40
1:F:140:SER:O	1:F:143:ASP:HB3	2.20	0.40
1:F:107:MET:HE1	1:F:115:TRP:CZ3	2.57	0.40
1:B:62[B]:ARG:NH2	1:B:72:LEU:HD22	2.37	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	224/247 (91%)	213 (95%)	10 (4%)	1 (0%)	39 53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	225/247 (91%)	210 (93%)	11 (5%)	4 (2%)	11 12
1	C	222/247 (90%)	210 (95%)	9 (4%)	3 (1%)	14 17
1	D	222/247 (90%)	210 (95%)	11 (5%)	1 (0%)	34 46
1	E	224/247 (91%)	213 (95%)	10 (4%)	1 (0%)	39 53
1	F	220/247 (89%)	209 (95%)	11 (5%)	0	100 100
All	All	1337/1482 (90%)	1265 (95%)	62 (5%)	10 (1%)	24 36

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	204	ARG
1	B	205	GLY
1	B	203	HIS
1	A	65	PRO
1	D	46	PRO
1	C	78	SER
1	E	145	ILE
1	C	205	GLY
1	B	13	ILE
1	B	19	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	184/202 (91%)	174 (95%)	10 (5%)	27 40
1	B	185/202 (92%)	173 (94%)	12 (6%)	21 30
1	C	182/202 (90%)	165 (91%)	17 (9%)	11 15
1	D	182/202 (90%)	167 (92%)	15 (8%)	14 20
1	E	184/202 (91%)	171 (93%)	13 (7%)	18 26
1	F	183/202 (91%)	163 (89%)	20 (11%)	8 10
All	All	1100/1212 (91%)	1013 (92%)	87 (8%)	15 21

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	24	ASN
1	A	49	ARG
1	A	134	LEU
1	A	155	LYS
1	A	181	GLU
1	A	204	ARG
1	A	209	LEU
1	A	219	THR
1	A	227	ARG
1	B	17	VAL
1	B	20	THR
1	B	23	ASN
1	B	50	LEU
1	B	54	THR
1	B	72	LEU
1	B	103	HIS
1	B	166	THR
1	B	192	GLU
1	B	193	THR
1	B	214	VAL
1	B	227	ARG
1	C	4	VAL
1	C	6	GLU
1	C	32	VAL
1	C	62	ARG
1	C	68	ARG
1	C	72	LEU
1	C	85	SER
1	C	162	ASN
1	C	179	THR
1	C	180	GLN
1	C	191	ARG
1	C	196	LYS
1	C	200	THR
1	C	204	ARG
1	C	208	ARG
1	C	209	LEU
1	C	217	VAL
1	D	6	GLU
1	D	13	ILE
1	D	17	VAL

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Mol	Chain	Res	Type
1	D	54	THR
1	D	62	ARG
1	D	66	ASP
1	D	85	SER
1	D	124	GLU
1	D	132	ARG
1	D	141	LEU
1	D	190	SER
1	D	209	LEU
1	D	217	VAL
1	D	218	ASP
1	D	220	GLU
1	E	4	VAL
1	E	27	GLN
1	E	31	THR
1	E	32	VAL
1	E	68	ARG
1	E	132	ARG
1	E	141	LEU
1	E	145	ILE
1	E	166	THR
1	E	179	THR
1	E	209	LEU
1	E	220	GLU
1	E	227	ARG
1	F	6	GLU
1	F	18	ASP
1	F	20	THR
1	F	33	ARG
1	F	36	ARG
1	F	49	ARG
1	F	50	LEU
1	F	62	ARG
1	F	70	ASN
1	F	113	ARG
1	F	120	PRO
1	F	132	ARG
1	F	141	LEU
1	F	147	THR
1	F	152	ARG
1	F	166	THR
1	F	173	ARG

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Mol	Chain	Res	Type
1	F	180	GLN
1	F	220	GLU
1	F	227	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	185	GLN
1	A	221	HIS
1	B	15	GLN
1	B	24	ASN
1	B	70	ASN
1	B	125	GLN
1	B	180	GLN
1	B	221	HIS
1	C	24	ASN
1	C	63	HIS
1	C	125	GLN
1	C	162	ASN
1	C	167	GLN
1	C	180	GLN
1	C	195	ASN
1	C	221	HIS
1	D	114	ASN
1	D	185	GLN
1	D	195	ASN
1	D	203	HIS
1	E	5	GLN
1	E	63	HIS
1	E	180	GLN
1	E	221	HIS
1	F	24	ASN
1	F	167	GLN
1	F	180	GLN
1	F	185	GLN
1	F	221	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)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEZ	A	228	-	7,7,7	0.43	0	6,6,6	0.75	0
2	CMP	A	301	-	19,25,25	2.13	3 (15%)	18,39,39	3.34	8 (44%)
2	CMP	B	301	-	19,25,25	1.15	1 (5%)	18,39,39	3.54	9 (50%)
2	CMP	C	301	-	19,25,25	1.41	4 (21%)	18,39,39	3.46	9 (50%)
3	HEZ	D	228	-	7,7,7	0.37	0	6,6,6	0.89	0
2	CMP	D	301	-	19,25,25	1.77	3 (15%)	18,39,39	3.43	10 (55%)
2	CMP	E	301	-	19,25,25	2.65	4 (21%)	18,39,39	3.34	7 (38%)
3	HEZ	F	228	-	7,7,7	0.24	0	6,6,6	0.77	0
2	CMP	F	301	-	19,25,25	1.68	3 (15%)	18,39,39	3.90	10 (55%)

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	HEZ	A	228	-	-	0/5/5/5	0/0/0/0
2	CMP	A	301	-	-	0/0/31/31	0/4/4/4
2	CMP	B	301	-	-	0/0/31/31	0/4/4/4
2	CMP	C	301	-	-	0/0/31/31	0/4/4/4
3	HEZ	D	228	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CMP	D	301	-	-	0/0/31/31	0/4/4/4
2	CMP	E	301	-	-	0/0/31/31	0/4/4/4
3	HEZ	F	228	-	-	0/5/5/5	0/0/0/0
2	CMP	F	301	-	-	0/0/31/31	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CMP	O4'-C4'	-3.95	1.35	1.45
2	F	301	CMP	O3'-C3'	-3.83	1.38	1.44
2	B	301	CMP	O5'-C5'	-3.68	1.40	1.46
2	D	301	CMP	O3'-C3'	-3.44	1.39	1.44
2	E	301	CMP	C5'-C4'	-3.35	1.46	1.51
2	C	301	CMP	O3'-C3'	-2.86	1.40	1.44
2	A	301	CMP	C4-N3	-2.27	1.32	1.35
2	E	301	CMP	O3'-C3'	-2.27	1.41	1.44
2	C	301	CMP	P-O2P	-2.15	1.45	1.54
2	C	301	CMP	C5-N7	-2.04	1.32	1.39
2	E	301	CMP	P-O3'	2.23	1.61	1.58
2	F	301	CMP	P-O3'	2.33	1.62	1.58
2	D	301	CMP	P-O3'	3.08	1.63	1.58
2	C	301	CMP	O4'-C1'	3.27	1.45	1.41
2	F	301	CMP	O4'-C1'	4.41	1.46	1.41
2	D	301	CMP	O4'-C1'	4.82	1.47	1.41
2	A	301	CMP	O4'-C1'	7.25	1.50	1.41
2	E	301	CMP	O4'-C1'	9.88	1.53	1.41

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	CMP	N3-C2-N1	-11.40	120.17	128.89
2	B	301	CMP	N3-C2-N1	-10.30	121.00	128.89
2	F	301	CMP	N3-C2-N1	-9.70	121.46	128.89
2	E	301	CMP	N3-C2-N1	-9.41	121.69	128.89
2	D	301	CMP	N3-C2-N1	-9.39	121.71	128.89
2	C	301	CMP	C2'-C1'-N9	-8.09	101.94	114.29
2	C	301	CMP	N3-C2-N1	-7.65	123.04	128.89
2	F	301	CMP	O3'-C3'-C4'	-7.49	104.74	110.72
2	E	301	CMP	O5'-P-O3'	-6.88	95.65	105.75
2	B	301	CMP	C2'-C1'-N9	-6.21	104.80	114.29
2	F	301	CMP	O5'-P-O3'	-5.72	97.35	105.75
2	D	301	CMP	C4'-O4'-C1'	-5.10	104.11	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	CMP	C5'-C4'-C3'	-5.06	101.38	112.62
2	C	301	CMP	O5'-P-O3'	-4.98	98.45	105.75
2	E	301	CMP	O3'-C3'-C4'	-4.30	107.28	110.72
2	D	301	CMP	O5'-P-O3'	-4.30	99.44	105.75
2	B	301	CMP	C4'-O4'-C1'	-4.00	105.32	109.72
2	A	301	CMP	C4-C5-N7	-3.98	105.82	109.48
2	B	301	CMP	O5'-P-O3'	-3.87	100.08	105.75
2	D	301	CMP	C2'-C1'-N9	-3.85	108.41	114.29
2	E	301	CMP	C4'-O4'-C1'	-3.80	105.55	109.72
2	F	301	CMP	C4-C5-N7	-3.76	106.02	109.48
2	D	301	CMP	C5'-C4'-C3'	-3.70	104.41	112.62
2	C	301	CMP	C4-C5-N7	-3.63	106.14	109.48
2	F	301	CMP	C5'-C4'-C3'	-3.51	104.82	112.62
2	F	301	CMP	C1'-N9-C4	-3.48	121.70	126.94
2	B	301	CMP	C5'-C4'-C3'	-3.45	104.95	112.62
2	F	301	CMP	C4'-O4'-C1'	-3.38	106.00	109.72
2	B	301	CMP	O4'-C4'-C3'	-3.10	97.73	104.86
2	A	301	CMP	C2'-C1'-N9	-3.09	109.57	114.29
2	D	301	CMP	C4-C5-N7	-2.99	106.73	109.48
2	D	301	CMP	O3'-C3'-C4'	-2.76	108.52	110.72
2	D	301	CMP	C1'-N9-C4	-2.41	123.30	126.94
2	A	301	CMP	C5'-C4'-C3'	-2.39	107.30	112.62
2	D	301	CMP	O4'-C4'-C3'	-2.39	99.36	104.86
2	A	301	CMP	C4'-O4'-C1'	-2.27	107.23	109.72
2	A	301	CMP	O4'-C4'-C3'	-2.26	99.66	104.86
2	E	301	CMP	C5'-C4'-C3'	-2.20	107.72	112.62
2	B	301	CMP	C2'-C3'-C4'	-2.18	99.21	103.29
2	A	301	CMP	O5'-P-O3'	-2.16	102.58	105.75
2	C	301	CMP	C2'-C3'-C4'	-2.10	99.35	103.29
2	B	301	CMP	C4-C5-N7	-2.06	107.58	109.48
2	C	301	CMP	C4'-O4'-C1'	-2.03	107.49	109.72
2	C	301	CMP	O4'-C4'-C3'	-2.02	100.21	104.86
2	E	301	CMP	C1'-N9-C4	-2.01	123.90	126.94
2	C	301	CMP	O2P-P-O1P	2.58	117.02	108.80
2	F	301	CMP	O2P-P-O1P	2.77	117.63	108.80
2	F	301	CMP	O4'-C4'-C5'	2.87	121.30	112.12
2	D	301	CMP	O2P-P-O1P	3.55	120.11	108.80
2	B	301	CMP	O2P-P-O1P	3.59	120.25	108.80
2	E	301	CMP	O2P-P-O1P	3.73	120.67	108.80
2	A	301	CMP	O2P-P-O1P	3.76	120.79	108.80
2	F	301	CMP	C2'-C1'-N9	4.07	120.51	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	CMP	1	0
2	B	301	CMP	2	0
2	C	301	CMP	1	0
2	D	301	CMP	1	0
2	E	301	CMP	1	0
3	F	228	HEZ	1	0
2	F	301	CMP	1	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	225/247 (91%)	-0.01	3 (1%) 79 81	21, 41, 58, 68	1 (0%)
1	B	225/247 (91%)	0.15	5 (2%) 65 68	29, 44, 66, 77	0
1	C	224/247 (90%)	0.04	3 (1%) 79 81	26, 41, 63, 70	0
1	D	224/247 (90%)	0.24	11 (4%) 33 38	25, 47, 75, 83	0
1	E	225/247 (91%)	-0.06	2 (0%) 85 87	22, 33, 55, 65	0
1	F	222/247 (89%)	0.00	2 (0%) 85 87	23, 40, 58, 67	0
All	All	1345/1482 (90%)	0.06	26 (1%) 70 72	21, 40, 64, 83	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	GLY	5.0
1	D	171	ALA	3.9
1	C	169	ALA	3.4
1	F	142	ALA	3.4
1	D	169	ALA	3.3
1	D	67	GLY	2.9
1	E	144	LEU	2.9
1	D	203	HIS	2.8
1	B	202	ALA	2.8
1	E	67	GLY	2.8
1	A	115	TRP	2.7
1	D	208	ARG	2.6
1	D	144	LEU	2.5
1	B	3	GLY	2.4
1	D	199	ALA	2.4
1	D	217	VAL	2.4
1	D	172	LEU	2.4
1	B	117	ALA	2.3
1	A	227	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	170	GLY	2.2
1	D	224	ARG	2.2
1	C	180	GLN	2.1
1	B	21	ALA	2.1
1	B	144	LEU	2.0
1	A	167	GLN	2.0
1	D	17	VAL	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
3	HEZ	F	228	8/8	0.95	0.22	2.72	37,40,41,42	0
3	HEZ	D	228	8/8	0.94	0.18	2.33	34,37,39,40	0
2	CMP	E	301	22/22	0.97	0.13	0.12	25,31,49,51	0
2	CMP	F	301	22/22	0.97	0.13	-0.10	32,37,54,55	0
2	CMP	A	301	22/22	0.97	0.11	-0.19	22,26,29,31	0
2	CMP	D	301	22/22	0.98	0.12	-0.51	25,28,31,32	0
3	HEZ	A	228	8/8	0.95	0.11	-0.56	29,32,34,37	0
2	CMP	C	301	22/22	0.98	0.10	-0.76	23,27,33,36	0
2	CMP	B	301	22/22	0.98	0.10	-0.85	25,31,35,37	0

6.5 Other polymers (i)

There are no such residues in this entry.