Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:16 AM GMT

PDB ID	:	2C91
Title	:	MOUSE SUCCINIC SEMIALDEHYDE REDUCTASE, AKR7A5
Authors	:	Zhu, X.; Ellis, E.M.; Lapthorn, A.J.
Deposited on	:	2005-12-08
Resolution	:	2.30 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:

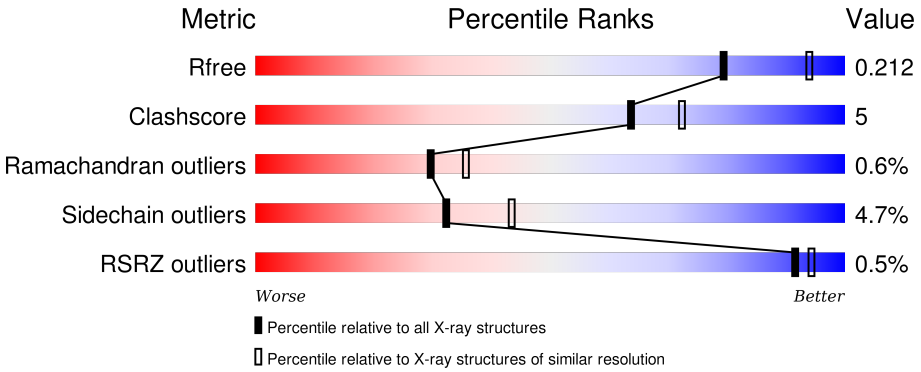
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	338	79% 15%
1	B	338	% 81% 12%
1	C	338	81% 13%
1	D	338	82% 11%
1	E	338	81% 12%

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Mol	Chain	Length	Quality of chain
1	F	338	
1	G	338	
1	H	338	
1	I	338	
1	J	338	

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	TLA	H	360	-	-	-	X
4	GOL	B	361	-	-	-	X
4	GOL	B	362	-	-	-	X
4	GOL	D	363	-	-	-	X
4	GOL	F	361	-	-	-	X
4	GOL	G	363	-	-	-	X
4	GOL	G	364	-	-	X	X
4	GOL	H	362	-	-	-	X
4	GOL	I	361	-	-	-	X
4	GOL	J	363	-	-	-	X
4	GOL	J	364	-	-	-	X
5	PO4	J	367	-	-	-	X
6	MES	B	364	-	-	-	X
6	MES	C	364	-	-	-	X
6	MES	I	363	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28440 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 AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	3	0
			2569	1617	454	480	18			
1	B	324	Total	C	N	O	S	0	0	0
			2545	1603	447	477	18			
1	C	324	Total	C	N	O	S	0	1	0
			2552	1608	447	479	18			
1	D	324	Total	C	N	O	S	0	2	0
			2564	1616	453	477	18			
1	E	324	Total	C	N	O	S	0	1	0
			2556	1611	450	477	18			
1	F	324	Total	C	N	O	S	0	0	0
			2548	1606	447	477	18			
1	G	324	Total	C	N	O	S	0	1	0
			2552	1608	447	479	18			
1	H	324	Total	C	N	O	S	0	1	0
			2538	1601	440	479	18			
1	I	324	Total	C	N	O	S	0	0	0
			2548	1606	447	477	18			
1	J	325	Total	C	N	O	S	0	1	0
			2559	1613	448	480	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	ILE	VAL	CONFLICT	UNP Q8CG76
A	122	CYS	ARG	CONFLICT	UNP Q8CG76
B	87	ILE	VAL	CONFLICT	UNP Q8CG76
B	122	CYS	ARG	CONFLICT	UNP Q8CG76
C	87	ILE	VAL	CONFLICT	UNP Q8CG76
C	122	CYS	ARG	CONFLICT	UNP Q8CG76
D	87	ILE	VAL	CONFLICT	UNP Q8CG76
D	122	CYS	ARG	CONFLICT	UNP Q8CG76
E	87	ILE	VAL	CONFLICT	UNP Q8CG76

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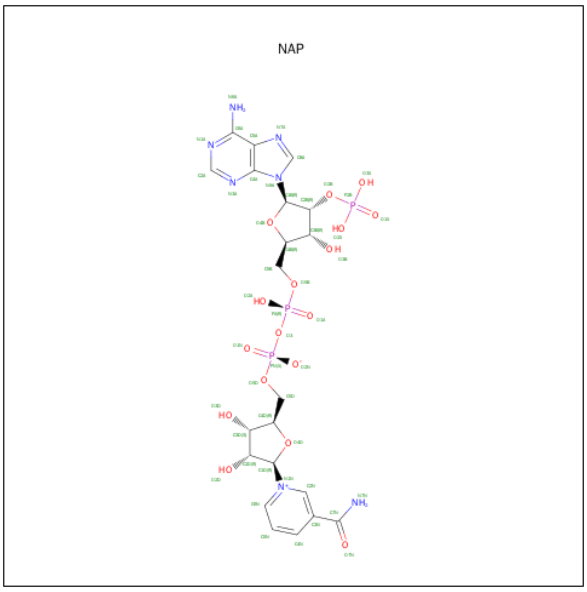
Chain	Residue	Modelled	Actual	Comment	Reference
E	122	CYS	ARG	CONFLICT	UNP Q8CG76
F	87	ILE	VAL	CONFLICT	UNP Q8CG76
F	122	CYS	ARG	CONFLICT	UNP Q8CG76
G	87	ILE	VAL	CONFLICT	UNP Q8CG76
G	122	CYS	ARG	CONFLICT	UNP Q8CG76
H	87	ILE	VAL	CONFLICT	UNP Q8CG76
H	122	CYS	ARG	CONFLICT	UNP Q8CG76
I	87	ILE	VAL	CONFLICT	UNP Q8CG76
I	122	CYS	ARG	CONFLICT	UNP Q8CG76
J	87	ILE	VAL	CONFLICT	UNP Q8CG76
J	122	CYS	ARG	CONFLICT	UNP Q8CG76

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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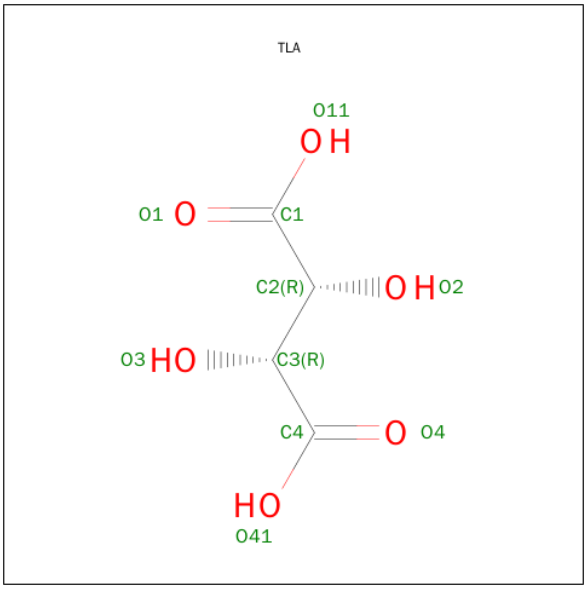
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



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

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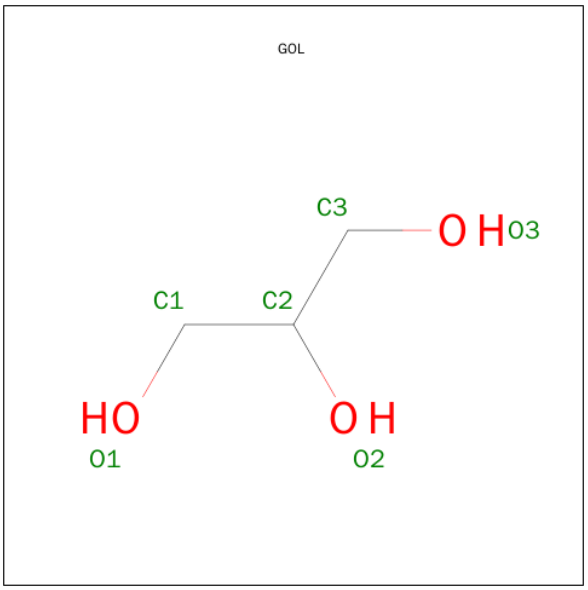
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C O 10 4 6	0	0
3	H	1	Total C O 10 4 6	0	0
3	I	1	Total C O 10 4 6	0	0
3	J	1	Total C O 10 4 6	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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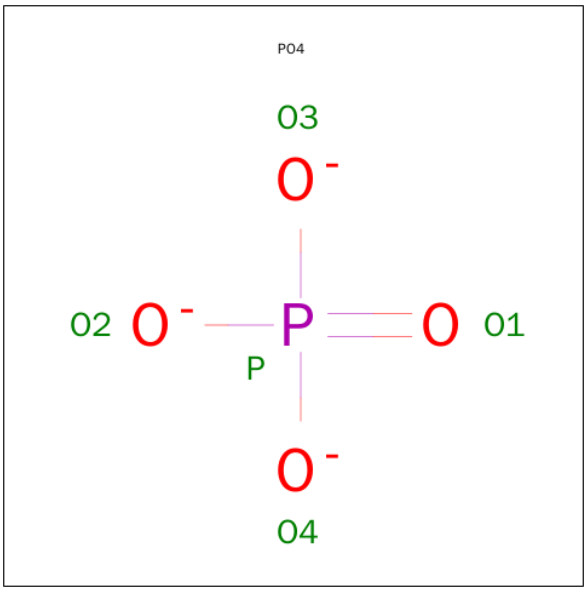
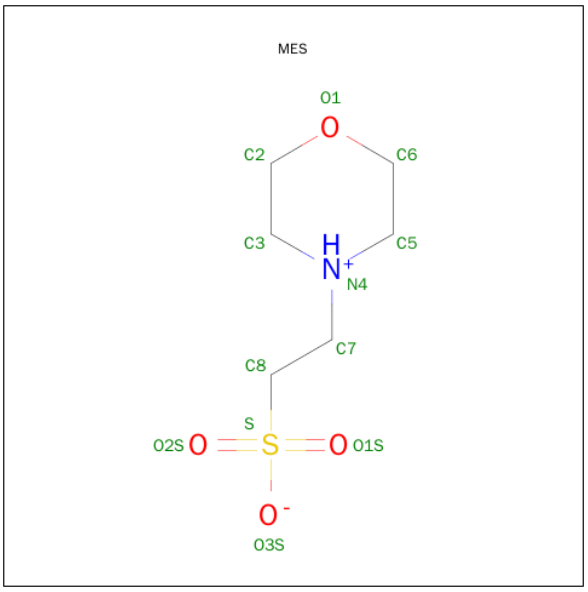
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O S 12 6 1 4 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	I	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	J	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is water.

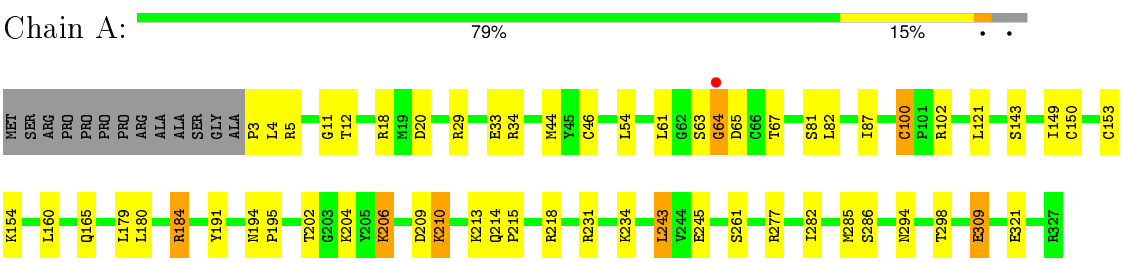
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	223	Total	O	0	0
			223	223		
7	B	131	Total	O	0	0
			131	131		
7	C	225	Total	O	0	0
			225	225		
7	D	272	Total	O	0	0
			272	272		
7	E	262	Total	O	0	0
			262	262		
7	F	214	Total	O	0	0
			214	214		
7	G	257	Total	O	0	0
			257	257		
7	H	159	Total	O	0	0
			159	159		
7	I	164	Total	O	0	0
			164	164		
7	J	202	Total	O	0	0
			202	202		

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.

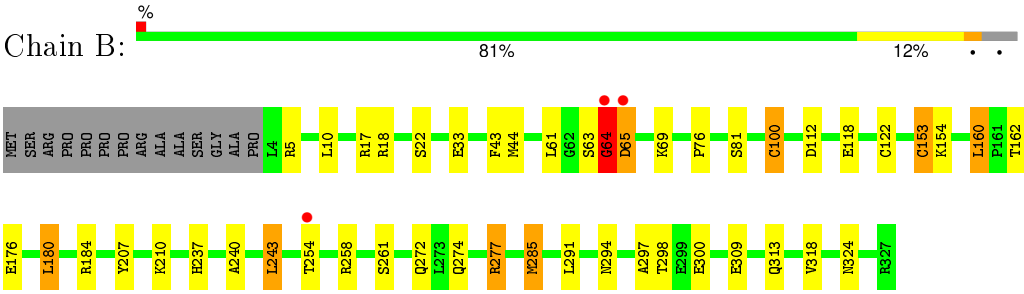
- Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain A:



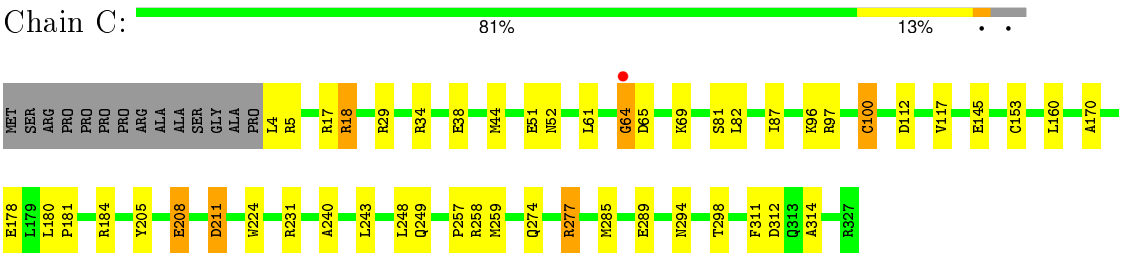
- Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain B:



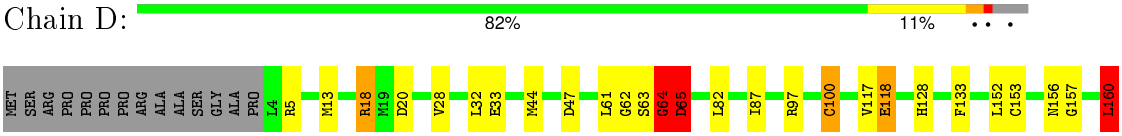
- Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain C:



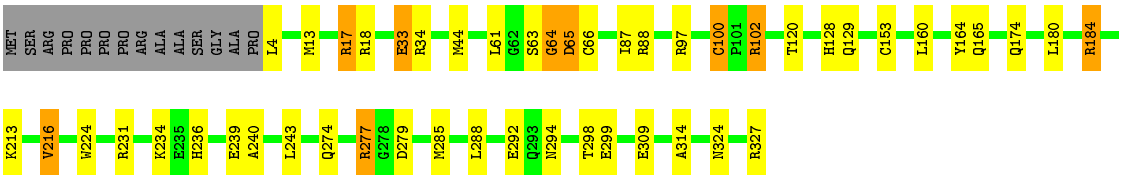
- Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain D:



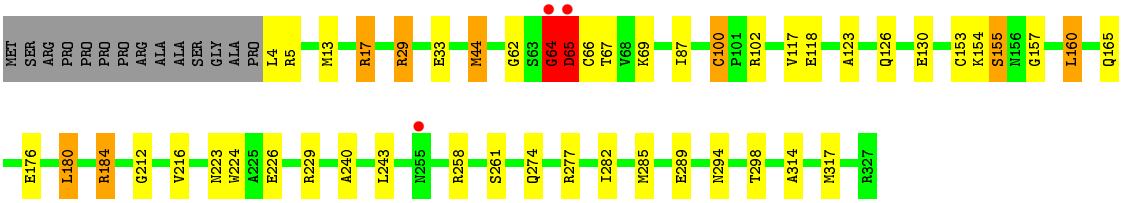
• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain E:



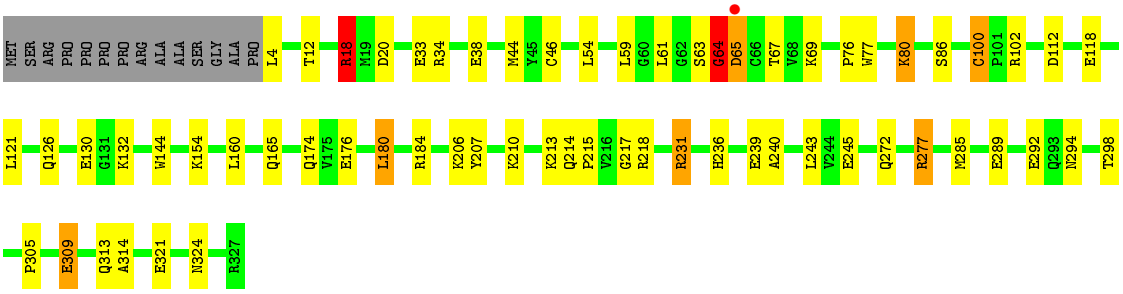
• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain F:



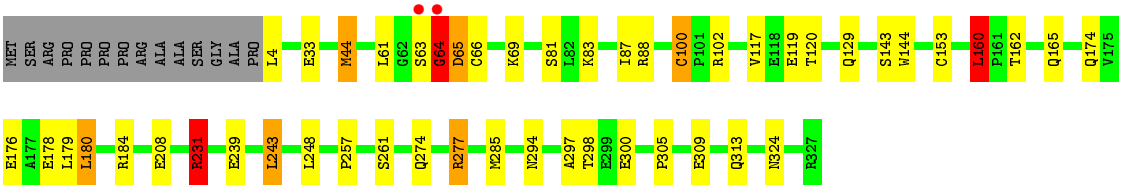
• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain G:



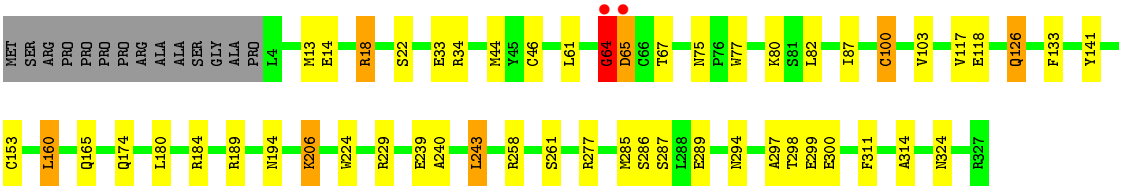
• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain H:



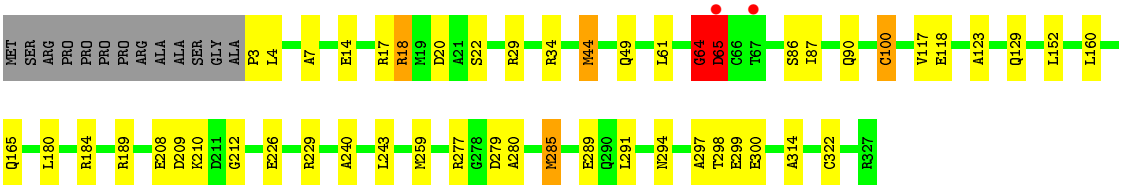
• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain I:



- Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	98.53Å 159.24Å 96.70Å 90.02° 119.40° 78.50°	Depositor
Resolution (Å)	45.00 – 2.30 41.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.8 (45.00-2.30) 86.9 (41.88-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.160 , 0.208 0.170 , 0.212	Depositor DCC
R_{free} test set	9982 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.458 for -h-l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 198863 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	28440	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: GOL, PO4, TLA, NAP, MES

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	1.17	13/2647 (0.5%)	0.98	9/3584 (0.3%)
1	B	1.02	5/2608 (0.2%)	0.89	4/3533 (0.1%)
1	C	1.09	6/2620 (0.2%)	0.95	10/3549 (0.3%)
1	D	1.17	7/2633 (0.3%)	1.03	15/3565 (0.4%)
1	E	1.14	4/2622 (0.2%)	1.05	19/3552 (0.5%)
1	F	1.10	5/2611 (0.2%)	0.97	9/3537 (0.3%)
1	G	1.16	8/2620 (0.3%)	1.00	10/3549 (0.3%)
1	H	1.02	4/2604 (0.2%)	0.88	7/3531 (0.2%)
1	I	1.09	8/2611 (0.3%)	0.94	5/3537 (0.1%)
1	J	1.01	4/2625 (0.2%)	0.94	13/3556 (0.4%)
All	All	1.10	64/26201 (0.2%)	0.96	101/35493 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
All	All	0	10

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	118	GLU	CG-CD	9.15	1.65	1.51
1	D	309	GLU	CG-CD	8.77	1.65	1.51
1	I	100	CYS	CB-SG	-8.64	1.67	1.82
1	F	289	GLU	CG-CD	8.10	1.64	1.51
1	D	18	ARG	CG-CD	8.08	1.72	1.51
1	A	46	CYS	CB-SG	7.77	1.95	1.82
1	F	100	CYS	CB-SG	-7.72	1.69	1.82
1	J	100	CYS	CB-SG	-7.58	1.69	1.82
1	G	33	GLU	CG-CD	7.37	1.63	1.51
1	B	153	CYS	CB-SG	-7.21	1.70	1.82
1	E	309	GLU	CG-CD	7.14	1.62	1.51
1	H	239	GLU	CG-CD	7.12	1.62	1.51
1	H	313	GLN	CG-CD	7.11	1.67	1.51
1	D	309	GLU	CB-CG	6.91	1.65	1.52
1	A	100	CYS	CB-SG	-6.70	1.70	1.82
1	A	206	LYS	CE-NZ	6.68	1.65	1.49
1	F	226	GLU	CB-CG	6.58	1.64	1.52
1	G	100	CYS	CB-SG	-6.52	1.71	1.82
1	A	213	LYS	CE-NZ	6.38	1.65	1.49
1	G	239	GLU	CD-OE1	6.28	1.32	1.25
1	I	33	GLU	CG-CD	6.22	1.61	1.51
1	C	178	GLU	CD-OE1	6.10	1.32	1.25
1	D	118	GLU	CG-CD	6.04	1.61	1.51
1	A	33	GLU	CD-OE1	6.01	1.32	1.25
1	B	33	GLU	CG-CD	6.00	1.60	1.51
1	I	311	PHE	CE2-CZ	5.96	1.48	1.37
1	C	145	GLU	CD-OE1	5.89	1.32	1.25
1	B	313	GLN	CG-CD	5.88	1.64	1.51
1	G	184	ARG	CZ-NH1	5.86	1.40	1.33
1	A	191	TYR	CD2-CE2	-5.78	1.30	1.39
1	G	206	LYS	CE-NZ	5.71	1.63	1.49
1	E	164	TYR	CG-CD2	-5.69	1.31	1.39
1	H	33	GLU	CG-CD	5.69	1.60	1.51
1	E	33	GLU	CG-CD	5.67	1.60	1.51
1	D	18	ARG	CB-CG	5.66	1.67	1.52
1	A	309[A]	GLU	CG-CD	5.58	1.60	1.51
1	A	309[B]	GLU	CG-CD	5.58	1.60	1.51
1	D	5	ARG	CZ-NH2	5.56	1.40	1.33
1	A	321	GLU	CD-OE1	5.54	1.31	1.25
1	C	51	GLU	CB-CG	5.52	1.62	1.52
1	I	206	LYS	CD-CE	5.43	1.64	1.51
1	A	150	CYS	CB-SG	-5.39	1.73	1.81
1	F	184	ARG	CZ-NH2	5.39	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	289	GLU	CB-CG	5.29	1.62	1.52
1	G	289	GLU	CG-CD	5.25	1.59	1.51
1	B	122	CYS	CB-SG	-5.25	1.73	1.81
1	F	154	LYS	CD-CE	5.24	1.64	1.51
1	C	184	ARG	CZ-NH2	5.24	1.39	1.33
1	A	5	ARG	CG-CD	5.22	1.65	1.51
1	B	118	GLU	CG-CD	5.22	1.59	1.51
1	D	117	VAL	CB-CG2	-5.21	1.42	1.52
1	E	213	LYS	CE-NZ	5.21	1.62	1.49
1	J	322	CYS	CB-SG	-5.21	1.73	1.81
1	G	239	GLU	CD-OE2	5.20	1.31	1.25
1	J	289	GLU	CG-CD	5.18	1.59	1.51
1	C	289[A]	GLU	CB-CG	5.15	1.61	1.52
1	C	289[B]	GLU	CB-CG	5.15	1.61	1.52
1	G	46	CYS	CB-SG	5.12	1.91	1.82
1	I	118	GLU	CB-CG	5.11	1.61	1.52
1	I	141	TYR	CD1-CE1	-5.09	1.31	1.39
1	A	154	LYS	CD-CE	5.09	1.64	1.51
1	I	289	GLU	CB-CG	5.07	1.61	1.52
1	A	213	LYS	CD-CE	5.06	1.64	1.51
1	H	208	GLU	CG-CD	5.01	1.59	1.51

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	97	ARG	NE-CZ-NH2	-10.66	114.97	120.30
1	E	184	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	G	80	LYS	CD-CE-NZ	-9.83	89.09	111.70
1	D	97	ARG	NE-CZ-NH1	9.57	125.09	120.30
1	D	18	ARG	NE-CZ-NH1	9.55	125.07	120.30
1	G	18	ARG	NE-CZ-NH1	-9.13	115.73	120.30
1	G	243	LEU	CA-CB-CG	8.98	135.97	115.30
1	B	309	GLU	CB-CA-C	8.74	127.89	110.40
1	C	277	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	E	97	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	E	102	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	J	243	LEU	CA-CB-CG	8.28	134.35	115.30
1	G	231	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	E	97	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	F	184	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	C	97	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	E	216	VAL	CB-CA-C	-7.87	96.44	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	20	ASP	CB-CG-OD1	7.82	125.34	118.30
1	B	243	LEU	CA-CB-CG	7.63	132.86	115.30
1	H	231	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	G	231	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	I	243	LEU	CA-CB-CG	7.41	132.33	115.30
1	D	216	VAL	CB-CA-C	-7.29	97.56	111.40
1	E	184	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	D	5	ARG	NE-CZ-NH2	7.09	123.85	120.30
1	B	44	MET	CG-SD-CE	-7.08	88.87	100.20
1	D	327	ARG	NE-CZ-NH1	-7.07	116.77	120.30
1	D	277	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	D	5	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	J	229	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	F	29	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	H	231	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	I	229	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	E	13	MET	CG-SD-CE	6.81	111.10	100.20
1	A	218	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	A	184[A]	ARG	NE-CZ-NH1	-6.77	116.92	120.30
1	A	184[B]	ARG	NE-CZ-NH1	-6.77	116.92	120.30
1	A	3	PRO	N-CA-CB	6.76	111.41	103.30
1	E	243	LEU	CA-CB-CG	6.75	130.83	115.30
1	C	34	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	J	259	MET	CG-SD-CE	-6.65	89.57	100.20
1	A	243	LEU	CA-CB-CG	6.62	130.53	115.30
1	D	327	ARG	NE-CZ-NH2	6.61	123.60	120.30
1	J	3	PRO	N-CA-CB	6.59	111.21	103.30
1	E	277	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	D	243	LEU	CA-CB-CG	6.51	130.27	115.30
1	E	279	ASP	CB-CG-OD2	-6.47	112.47	118.30
1	G	277	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	E	231	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	J	277	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	F	258	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	E	17	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	E	102	ARG	CG-CD-NE	-6.30	98.57	111.80
1	E	17	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	B	17	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	206	LYS	CD-CE-NZ	6.27	126.11	111.70
1	I	189	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	C	97	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	F	155	SER	CB-CA-C	-6.12	98.47	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	17	ARG	CG-CD-NE	6.08	124.57	111.80
1	I	34	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	J	20	ASP	CB-CG-OD1	5.97	123.67	118.30
1	E	327	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	C	29	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	J	44	MET	CG-SD-CE	-5.81	90.91	100.20
1	A	34	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	H	243	LEU	CA-CB-CG	5.69	128.38	115.30
1	J	189	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	E	327	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	H	44	MET	CG-SD-CE	-5.55	91.32	100.20
1	D	20	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	J	34	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	F	102	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	A	218	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	E	279	ASP	CB-CG-OD1	5.42	123.18	118.30
1	C	258	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	259	MET	CG-SD-CE	-5.38	91.59	100.20
1	F	29	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	J	34	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	I	229	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	E	88	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	F	317	MET	CG-SD-CE	-5.34	91.65	100.20
1	H	88	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	H	277	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	20	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	160	LEU	CA-CB-CG	5.29	127.46	115.30
1	J	29	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	231	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	C	112	ASP	CB-CG-OD1	5.23	123.01	118.30
1	E	234	LYS	CD-CE-NZ	-5.22	99.70	111.70
1	F	229	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	47	ASP	CB-CG-OD1	5.19	122.97	118.30
1	H	160	LEU	CA-CB-CG	5.17	127.20	115.30
1	C	211	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	G	184	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	G	218	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	J	279	ASP	CB-CG-OD1	5.08	122.88	118.30
1	J	209	ASP	CB-CG-OD1	5.08	122.87	118.30
1	G	239	GLU	OE1-CD-OE2	5.02	129.33	123.30
1	D	13	MET	CG-SD-CE	5.02	108.23	100.20
1	G	20	ASP	CB-CG-OD1	5.02	122.81	118.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	64	GLY	Peptide
1	B	64	GLY	Peptide
1	C	64	GLY	Peptide
1	D	64	GLY	Peptide
1	E	64	GLY	Peptide
1	F	64	GLY	Peptide
1	G	64	GLY	Peptide
1	H	64	GLY	Peptide
1	I	64	GLY	Peptide
1	J	64	GLY	Peptide

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	2569	0	2484	35	0
1	B	2545	0	2453	24	0
1	C	2552	0	2464	21	0
1	D	2564	0	2488	21	0
1	E	2556	0	2475	26	0
1	F	2548	0	2462	29	0
1	G	2552	0	2464	37	0
1	H	2538	0	2435	22	0
1	I	2548	0	2462	27	0
1	J	2559	0	2470	20	0
2	A	48	0	25	2	0
2	B	48	0	25	3	0
2	C	48	0	25	0	0
2	D	48	0	25	1	0
2	E	48	0	25	1	0
2	F	48	0	25	3	0
2	G	48	0	24	1	0
2	H	48	0	25	4	0
2	I	48	0	25	3	0
2	J	48	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	0	4	0	0
3	B	10	0	4	2	0
3	C	10	0	4	3	0
3	D	10	0	4	0	0
3	E	10	0	4	1	0
3	F	10	0	4	1	0
3	G	10	0	4	0	0
3	H	10	0	4	2	0
3	I	10	0	4	1	0
3	J	10	0	4	1	0
4	A	12	0	16	2	0
4	B	18	0	24	0	0
4	C	18	0	24	0	0
4	D	18	0	24	0	0
4	E	18	0	24	0	0
4	F	6	0	8	0	0
4	G	18	0	24	5	0
4	H	12	0	16	2	0
4	I	12	0	16	1	0
4	J	18	0	24	0	0
5	A	5	0	0	0	0
5	J	5	0	0	0	0
6	B	12	0	12	0	0
6	C	12	0	12	0	0
6	D	12	0	12	0	0
6	I	12	0	12	0	0
6	J	12	0	12	0	0
7	A	223	0	0	9	0
7	B	131	0	0	3	0
7	C	225	0	0	7	0
7	D	272	0	0	4	0
7	E	262	0	0	7	0
7	F	214	0	0	9	0
7	G	257	0	0	8	0
7	H	159	0	0	2	0
7	I	164	0	0	9	0
7	J	202	0	0	8	0
All	All	28440	0	25206	267	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 5.

All (267) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:CYS:SG	7:E:2088:HOH:O	1.95	1.23
1:C:100:CYS:SG	7:C:2071:HOH:O	2.05	1.10
1:F:44:MET:SD	7:F:2025:HOH:O	2.10	1.08
1:A:100:CYS:SG	7:A:2061:HOH:O	2.10	1.06
1:I:13:MET:HG2	7:I:2008:HOH:O	1.61	0.99
1:E:100:CYS:CB	7:E:2088:HOH:O	2.10	0.95
1:C:100:CYS:CB	7:C:2071:HOH:O	2.18	0.90
1:I:14:GLU:OE1	1:I:18:ARG:HG2	1.75	0.85
1:J:212:GLY:HA3	7:J:2132:HOH:O	1.76	0.85
1:H:87:ILE:HD11	1:H:120:THR:HG23	1.59	0.84
1:E:64:GLY:O	1:E:65:ASP:HB2	1.76	0.84
1:D:118:GLU:HG2	7:D:2104:HOH:O	1.80	0.82
1:D:180:LEU:O	1:D:184[A]:ARG:HG2	1.81	0.81
1:A:29:ARG:NH2	1:F:33:GLU:OE2	2.13	0.79
1:D:245:GLU:OE1	7:D:2181:HOH:O	1.99	0.79
1:I:82:LEU:HD22	1:I:87:ILE:HD11	1.64	0.78
1:E:274:GLN:HE21	1:E:277:ARG:HG3	1.50	0.77
1:B:154:LYS:NZ	7:B:2055:HOH:O	2.17	0.77
1:C:61:LEU:O	1:C:100:CYS:HB2	1.86	0.75
1:H:178:GLU:OE2	7:H:2080:HOH:O	2.04	0.75
1:I:46:CYS:HB3	7:I:2009:HOH:O	1.87	0.75
1:A:102:ARG:O	7:A:2061:HOH:O	2.05	0.74
1:A:309[B]:GLU:OE1	7:A:2198:HOH:O	2.04	0.73
1:E:100:CYS:HB3	7:E:2088:HOH:O	1.82	0.72
1:A:18[B]:ARG:HD3	1:A:286:SER:HB2	1.70	0.72
1:H:305:PRO:O	1:H:309[A]:GLU:HG3	1.90	0.71
1:G:305:PRO:O	1:G:309[A]:GLU:HG3	1.91	0.70
2:H:350:NAP:H4N	3:H:360:TLA:O11	1.91	0.70
1:I:75:ASN:OD1	1:I:80:LYS:NZ	2.24	0.70
1:D:61:LEU:O	1:D:100:CYS:HB2	1.91	0.69
2:B:350:NAP:H4N	3:B:360:TLA:O11	1.93	0.69
1:I:13:MET:CG	7:I:2008:HOH:O	2.31	0.68
1:F:274:GLN:NE2	1:F:277:ARG:HD2	2.08	0.68
1:J:210:LYS:CD	7:J:2130:HOH:O	2.42	0.67
1:D:82:LEU:HD22	1:D:87:ILE:HD11	1.76	0.67
1:I:239:GLU:OE2	7:I:2124:HOH:O	2.13	0.66
1:E:66:CYS:HA	7:E:2054:HOH:O	1.95	0.66
1:F:153:CYS:HB2	1:F:160:LEU:HD22	1.78	0.65
1:H:64:GLY:O	1:H:65:ASP:HB2	1.95	0.65
1:E:61:LEU:O	1:E:100:CYS:HB2	1.97	0.65
1:F:212:GLY:HA3	7:F:2132:HOH:O	1.97	0.64
1:J:64:GLY:O	1:J:65:ASP:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:292:GLU:HG3	7:G:2206:HOH:O	1.97	0.64
1:D:153:CYS:HB2	1:D:160:LEU:HD22	1.79	0.64
1:A:82:LEU:HD22	1:A:87:ILE:HD11	1.80	0.64
1:H:66:CYS:O	1:H:69:LYS:NZ	2.31	0.63
1:J:210:LYS:HD2	7:J:2130:HOH:O	1.99	0.63
1:B:61:LEU:O	1:B:100:CYS:HB2	1.99	0.63
1:B:184:ARG:NH1	7:B:2064:HOH:O	2.32	0.63
1:E:153:CYS:HB2	1:E:160:LEU:HD22	1.81	0.63
1:B:294:ASN:O	1:B:298:THR:HG23	1.99	0.62
1:C:274:GLN:HE21	1:C:277:ARG:HG3	1.64	0.62
1:H:231:ARG:HD2	4:H:361:GOL:O2	1.99	0.62
1:J:129:GLN:HG3	7:J:2089:HOH:O	1.99	0.62
1:C:205:TYR:HB2	7:C:2132:HOH:O	2.00	0.61
1:C:312:ASP:OD1	7:C:2192:HOH:O	2.16	0.61
1:F:153:CYS:CB	1:F:160:LEU:HD22	2.31	0.61
1:D:64:GLY:O	1:D:65:ASP:HB2	2.01	0.61
1:F:44:MET:HG2	7:F:2025:HOH:O	2.00	0.61
1:H:61:LEU:O	1:H:100:CYS:HB2	2.00	0.61
1:A:184[B]:ARG:NH1	1:A:277:ARG:HH11	1.99	0.60
1:I:18:ARG:HG3	1:I:286:SER:HB2	1.83	0.60
1:D:157:GLY:HA2	7:D:2118:HOH:O	2.00	0.60
1:G:294:ASN:O	1:G:298:THR:HG23	2.03	0.58
1:B:153:CYS:CB	1:B:160:LEU:HD22	2.33	0.58
1:E:274:GLN:NE2	1:E:277:ARG:HD2	2.19	0.58
1:I:80:LYS:HE2	7:I:2042:HOH:O	2.02	0.58
1:C:294:ASN:O	1:C:298:THR:HG23	2.04	0.58
1:A:231:ARG:HH11	4:A:361:GOL:H32	1.68	0.58
1:B:274:GLN:NE2	1:B:277:ARG:HD2	2.19	0.57
1:A:153:CYS:HB2	1:A:160:LEU:CD2	2.33	0.57
1:G:77:TRP:O	1:G:80:LYS:HE3	2.05	0.57
1:D:294:ASN:O	1:D:298:THR:HG23	2.05	0.57
1:H:165:GLN:OE1	2:H:350:NAP:H2N	2.04	0.57
1:I:77:TRP:O	1:I:80:LYS:HE3	2.05	0.57
1:B:153:CYS:HB2	1:B:160:LEU:HD22	1.86	0.56
1:G:165:GLN:OE1	2:G:350:NAP:H2N	2.06	0.56
1:F:44:MET:CG	7:F:2025:HOH:O	2.42	0.56
1:G:240:ALA:HB1	1:G:314:ALA:HB1	1.87	0.56
1:I:64:GLY:O	1:I:65:ASP:HB2	2.06	0.56
1:E:294:ASN:O	1:E:298:THR:HG23	2.06	0.56
1:B:165:GLN:OE1	2:B:350:NAP:H2N	2.05	0.55
1:G:34:ARG:HD3	7:G:2028:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:LEU:O	1:E:292:GLU:HG3	2.07	0.55
1:J:165:GLN:OE1	2:J:350:NAP:H2N	2.07	0.54
1:F:126:GLN:O	1:F:130:GLU:HG3	2.07	0.54
1:A:184[B]:ARG:HH11	1:A:277:ARG:NH1	2.05	0.54
1:G:18:ARG:HD2	7:G:2198:HOH:O	2.07	0.54
1:I:184:ARG:NH1	7:I:2102:HOH:O	2.40	0.54
1:B:274:GLN:HE22	1:B:277:ARG:HD2	1.73	0.54
1:A:294:ASN:O	1:A:298:THR:HG23	2.07	0.54
1:A:206:LYS:HE2	1:A:209:ASP:OD1	2.08	0.54
1:D:165:GLN:OE1	2:D:350:NAP:H2N	2.08	0.53
1:G:305:PRO:O	1:G:309[A]:GLU:CG	2.56	0.53
4:G:364:GOL:H31	1:J:226:GLU:HB3	1.91	0.53
1:H:176:GLU:HA	1:H:180:LEU:HD22	1.90	0.53
1:I:294:ASN:O	1:I:298:THR:HG23	2.08	0.53
1:F:157:GLY:HA2	7:F:2102:HOH:O	2.08	0.53
1:D:240:ALA:HB1	1:D:314:ALA:HB1	1.91	0.52
1:A:12:THR:HG21	1:A:54:LEU:HD11	1.91	0.52
1:E:87:ILE:CD1	1:E:120:THR:HG23	2.40	0.52
1:G:64:GLY:O	1:G:65:ASP:HB2	2.10	0.52
1:H:143:SER:HB3	1:H:179:LEU:HA	1.92	0.52
1:H:64:GLY:HA3	7:H:2048:HOH:O	2.09	0.51
1:G:130:GLU:OE1	1:G:132:LYS:HE2	2.10	0.51
1:A:245:GLU:OE1	7:A:2145:HOH:O	2.19	0.51
1:I:153:CYS:HB3	1:I:160:LEU:HD22	1.92	0.51
1:E:33:GLU:HG3	7:E:2020:HOH:O	2.11	0.51
1:F:126:GLN:HB2	7:F:2089:HOH:O	2.10	0.51
1:I:18:ARG:HD3	7:I:2013:HOH:O	2.10	0.51
1:B:277:ARG:HD3	7:B:2064:HOH:O	2.11	0.51
1:A:184[B]:ARG:NH1	1:A:277:ARG:NH1	2.58	0.50
1:G:86:SER:CB	4:G:364:GOL:O2	2.60	0.50
1:A:63:SER:O	1:A:63:SER:OG	2.23	0.50
2:J:350:NAP:H4N	3:J:360:TLA:O11	2.11	0.50
1:G:18:ARG:HH12	1:G:217:GLY:HA2	1.76	0.49
1:D:152:LEU:O	1:D:156:ASN:ND2	2.33	0.49
1:F:87:ILE:HD11	1:F:123:ALA:HB3	1.94	0.49
1:H:294:ASN:O	1:H:298:THR:HG23	2.11	0.49
1:C:38:GLU:HG2	1:C:69:LYS:HB2	1.94	0.49
1:G:64:GLY:N	7:G:2049:HOH:O	2.45	0.49
1:G:214:GLN:N	1:G:215:PRO:CD	2.74	0.49
1:A:277:ARG:NE	7:A:2172:HOH:O	2.45	0.49
1:D:63:SER:O	1:D:63:SER:OG	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:ALA:HB1	1:F:314:ALA:HB1	1.95	0.49
1:A:153:CYS:HB2	1:A:160:LEU:HD22	1.94	0.49
1:F:64:GLY:CA	7:F:2041:HOH:O	2.60	0.49
1:E:236:HIS:CD2	7:E:2182:HOH:O	2.65	0.49
1:H:297:ALA:HA	1:H:300:GLU:OE2	2.13	0.49
1:G:213:LYS:HB3	1:G:215:PRO:HD3	1.94	0.49
1:G:277:ARG:NE	7:G:2195:HOH:O	2.44	0.48
1:I:126:GLN:HG3	7:I:2076:HOH:O	2.11	0.48
1:B:174:GLN:OE1	1:B:324:ASN:HA	2.13	0.48
1:J:61:LEU:O	1:J:100:CYS:HB2	2.13	0.48
1:B:176:GLU:HA	1:B:180:LEU:HD22	1.95	0.48
1:I:153:CYS:CB	1:I:160:LEU:HD22	2.42	0.48
1:D:153:CYS:CB	1:D:160:LEU:HD22	2.44	0.48
1:C:274:GLN:NE2	1:C:277:ARG:HD2	2.29	0.48
1:E:240:ALA:HB1	1:E:314:ALA:HB1	1.95	0.47
1:E:165:GLN:OE1	2:E:350:NAP:H2N	2.13	0.47
1:F:294:ASN:O	1:F:298:THR:HG23	2.13	0.47
1:E:34:ARG:NH1	1:E:299:GLU:OE1	2.47	0.47
1:A:165:GLN:OE1	2:A:350:NAP:H2N	2.14	0.47
1:J:49:GLN:NE2	7:J:2035:HOH:O	2.46	0.47
1:C:82:LEU:HB3	1:C:87:ILE:HD11	1.97	0.47
1:G:176:GLU:HA	1:G:180:LEU:HD22	1.95	0.47
1:B:43:PHE:CZ	1:F:223:ASN:HA	2.49	0.47
1:E:153:CYS:CB	1:E:160:LEU:HD22	2.44	0.47
1:G:80:LYS:HG2	4:G:364:GOL:H2	1.97	0.47
2:H:350:NAP:H8A	2:H:350:NAP:H52A	1.97	0.46
1:H:231:ARG:CD	4:H:361:GOL:O2	2.61	0.46
1:G:144:TRP:HA	1:H:144:TRP:HA	1.97	0.46
1:J:118[B]:GLU:HG3	1:J:152:LEU:HD13	1.97	0.46
1:F:176:GLU:HA	1:F:180:LEU:HD22	1.97	0.46
1:G:61:LEU:O	1:G:100:CYS:HB2	2.15	0.46
1:I:61:LEU:O	1:I:100:CYS:HB2	2.16	0.46
1:F:64:GLY:O	1:F:65:ASP:HB2	2.15	0.46
1:J:49:GLN:HG3	7:J:2004:HOH:O	2.15	0.46
1:A:214:GLN:N	1:A:215:PRO:CD	2.78	0.46
1:C:208:GLU:HG2	7:C:2136:HOH:O	2.15	0.46
1:H:87:ILE:HG21	1:H:87:ILE:HD13	1.57	0.46
1:J:294:ASN:O	1:J:298:THR:HG23	2.16	0.46
1:J:210:LYS:HD3	7:J:2130:HOH:O	2.09	0.46
1:A:214:GLN:N	1:A:215:PRO:HD3	2.31	0.46
1:G:118:GLU:HG2	7:G:2086:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:GLU:CD	1:F:118:GLU:H	2.20	0.45
1:I:13:MET:CE	2:I:350:NAP:C6N	2.94	0.45
1:A:210:LYS:HE2	7:A:2120:HOH:O	2.15	0.45
1:E:128:HIS:HD2	1:E:129:GLN:HE21	1.64	0.45
1:H:174:GLN:OE1	1:H:324:ASN:HA	2.17	0.45
1:B:297:ALA:HA	1:B:300:GLU:OE2	2.17	0.45
1:E:63:SER:O	1:E:63:SER:OG	2.25	0.45
1:J:240:ALA:HB1	1:J:314:ALA:HB1	1.99	0.45
1:B:240:ALA:O	1:B:243:LEU:HB3	2.17	0.45
1:A:202:THR:OG1	1:A:204:LYS:HG2	2.16	0.44
1:G:38:GLU:HG2	1:G:69:LYS:HB2	1.99	0.44
4:I:362:GOL:H11	7:J:2097:HOH:O	2.17	0.44
1:E:239:GLU:OE2	7:E:2182:HOH:O	2.21	0.44
1:C:224:TRP:CH2	3:C:360:TLA:H2	2.53	0.44
1:G:12:THR:HG21	1:G:54:LEU:HD11	1.99	0.44
1:G:309[B]:GLU:HG3	1:G:313:GLN:OE1	2.17	0.44
1:F:13:MET:O	1:F:13:MET:HG2	2.18	0.44
1:E:174:GLN:OE1	1:E:324:ASN:HA	2.18	0.44
1:C:44:MET:CE	3:C:360:TLA:H3	2.47	0.44
1:D:18:ARG:HD3	1:D:286:SER:HB2	2.00	0.44
1:F:282:ILE:HG22	2:F:350:NAP:H4D	1.99	0.44
2:B:350:NAP:H4N	3:B:360:TLA:C1	2.48	0.44
1:I:240:ALA:HB1	1:I:314:ALA:HB1	2.00	0.44
1:A:100:CYS:HB2	7:A:2061:HOH:O	2.18	0.44
1:G:207:TYR:OH	1:G:210:LYS:NZ	2.50	0.43
1:G:174:GLN:OE1	1:G:324:ASN:HA	2.17	0.43
1:E:224:TRP:CZ3	3:E:360:TLA:H2	2.54	0.43
1:G:86:SER:CB	4:G:364:GOL:HO2	2.31	0.43
1:J:86:SER:O	1:J:90:GLN:HG3	2.18	0.43
1:E:100:CYS:SG	1:E:102:ARG:O	2.77	0.43
1:A:231:ARG:HH11	4:A:361:GOL:C3	2.29	0.43
1:G:245:GLU:OE1	7:G:2163:HOH:O	2.21	0.43
1:F:44:MET:CE	1:F:224:TRP:NE1	2.82	0.43
1:H:248:LEU:HD22	1:H:257:PRO:HG2	2.01	0.43
1:I:277:ARG:NH1	7:I:2134:HOH:O	2.50	0.43
1:A:18[B]:ARG:HD3	1:A:286:SER:CB	2.45	0.43
1:I:297:ALA:HA	1:I:300:GLU:OE2	2.19	0.43
1:D:128:HIS:HD2	1:D:133:PHE:O	2.02	0.42
1:I:224:TRP:CH2	3:I:360:TLA:H2	2.55	0.42
1:J:285:MET:HG3	1:J:291:LEU:HB2	2.01	0.42
1:G:86:SER:HA	4:G:364:GOL:O2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLY:HA3	2:A:350:NAP:H4D	2.02	0.42
1:E:63:SER:O	1:E:65:ASP:HB3	2.19	0.42
1:D:63:SER:O	1:D:64:GLY:C	2.58	0.42
1:F:29:ARG:NH2	7:F:2014:HOH:O	2.51	0.42
1:B:76:PRO:HB3	1:B:112:ASP:HB2	1.99	0.42
1:A:143:SER:HB3	1:A:179:LEU:HA	2.02	0.42
1:C:180:LEU:HB2	1:C:181:PRO:HD3	2.02	0.42
1:C:240:ALA:HB1	1:C:314:ALA:HB1	2.02	0.42
1:G:76:PRO:HB3	1:G:112:ASP:HB2	2.01	0.42
1:G:236:HIS:HB2	1:G:321:GLU:OE2	2.19	0.42
1:C:18:ARG:NH2	7:C:2011:HOH:O	2.53	0.42
1:G:126:GLN:HB2	1:G:126:GLN:HE21	1.68	0.42
1:A:121:LEU:HD11	1:A:149:ILE:HG23	2.02	0.42
1:B:285:MET:HG3	1:B:291:LEU:HB2	2.01	0.42
1:G:272:GLN:NE2	7:G:2190:HOH:O	2.47	0.42
1:J:297:ALA:HA	1:J:300:GLU:OE2	2.20	0.42
1:B:237:HIS:HA	1:B:318:VAL:HG11	2.01	0.42
2:H:350:NAP:H4N	3:H:360:TLA:C1	2.48	0.42
1:H:83:LYS:NZ	1:H:119:GLU:OE1	2.48	0.42
1:B:153:CYS:HB3	1:B:160:LEU:HD22	1.99	0.41
1:D:288:LEU:O	1:D:292:GLU:HG3	2.20	0.41
1:D:62:GLY:HA2	7:D:2088:HOH:O	2.20	0.41
1:H:274:GLN:NE2	1:H:277:ARG:HD2	2.35	0.41
1:G:121:LEU:HA	1:G:121:LEU:HD23	1.81	0.41
1:I:103:VAL:O	1:I:133:PHE:HA	2.21	0.41
1:A:100:CYS:CB	7:A:2061:HOH:O	2.57	0.41
1:E:87:ILE:HD12	1:E:120:THR:HG23	2.02	0.41
1:A:194:ASN:N	1:A:195:PRO:CD	2.83	0.41
1:F:62:GLY:HA2	7:F:2073:HOH:O	2.20	0.41
1:B:64:GLY:O	1:B:65:ASP:HB2	2.21	0.41
1:C:170:ALA:HB1	1:C:311:PHE:CD1	2.55	0.41
1:H:63:SER:O	1:H:66:CYS:HB2	2.20	0.41
1:A:153:CYS:CB	1:A:160:LEU:CD2	2.98	0.41
1:C:224:TRP:CZ3	3:C:360:TLA:H2	2.56	0.41
1:I:174:GLN:OE1	1:I:324:ASN:HA	2.20	0.41
1:D:28:VAL:O	1:D:32:LEU:HG	2.20	0.41
1:B:63:SER:O	1:B:63:SER:OG	2.32	0.41
1:G:18:ARG:NH1	1:G:217:GLY:HA2	2.35	0.41
1:F:87:ILE:HG21	1:F:87:ILE:HD13	1.72	0.41
1:B:207:TYR:CZ	1:B:210:LYS:HE3	2.56	0.41
1:A:234:LYS:HE3	7:A:2133:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:SER:O	1:B:64:GLY:C	2.60	0.41
1:D:264:LEU:O	1:D:267:MET:HB2	2.20	0.41
1:I:194:ASN:ND2	2:I:350:NAP:O2N	2.53	0.41
1:H:153:CYS:HB2	1:H:160:LEU:HD22	2.03	0.41
1:I:165:GLN:OE1	2:I:350:NAP:H2N	2.20	0.40
1:F:184:ARG:HG3	1:F:277:ARG:CZ	2.51	0.40
1:C:153:CYS:HB3	1:C:160:LEU:HD22	2.03	0.40
1:C:100:CYS:CA	7:C:2071:HOH:O	2.61	0.40
1:A:195:PRO:HG3	1:A:282:ILE:O	2.22	0.40
1:F:66:CYS:O	1:F:69:LYS:NZ	2.53	0.40
1:F:165:GLN:OE1	2:F:350:NAP:H2N	2.21	0.40
1:B:272:GLN:HE21	1:B:272:GLN:HB3	1.65	0.40
1:J:7:ALA:HB3	1:J:280:ALA:HB2	2.03	0.40
1:F:44:MET:CE	1:F:224:TRP:HE1	2.34	0.40
1:A:61:LEU:O	1:A:100:CYS:HB2	2.21	0.40
1:C:248:LEU:HD22	1:C:257:PRO:HG2	2.03	0.40
1:G:63:SER:O	1:G:64:GLY:C	2.59	0.40
2:F:350:NAP:H4N	3:F:360:TLA:O11	2.22	0.40
1:J:14:GLU:OE1	1:J:18:ARG:HB2	2.21	0.40
1:J:87:ILE:HD11	1:J:123:ALA:HB3	2.04	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	326/338 (96%)	320 (98%)	4 (1%)	2 (1%)	30	36
1	B	322/338 (95%)	314 (98%)	6 (2%)	2 (1%)	30	36
1	C	323/338 (96%)	314 (97%)	7 (2%)	2 (1%)	30	36
1	D	324/338 (96%)	317 (98%)	5 (2%)	2 (1%)	30	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	323/338 (96%)	316 (98%)	6 (2%)	1 (0%)	46	57
1	F	322/338 (95%)	312 (97%)	8 (2%)	2 (1%)	30	36
1	G	323/338 (96%)	316 (98%)	5 (2%)	2 (1%)	30	36
1	H	323/338 (96%)	316 (98%)	5 (2%)	2 (1%)	30	36
1	I	322/338 (95%)	314 (98%)	6 (2%)	2 (1%)	30	36
1	J	324/338 (96%)	313 (97%)	8 (2%)	3 (1%)	21	24
All	All	3232/3380 (96%)	3152 (98%)	60 (2%)	20 (1%)	30	36

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ASP
1	B	65	ASP
1	C	65	ASP
1	D	65	ASP
1	E	65	ASP
1	F	65	ASP
1	G	65	ASP
1	H	65	ASP
1	I	65	ASP
1	J	4	LEU
1	J	65	ASP
1	G	64	GLY
1	I	64	GLY
1	J	64	GLY
1	B	64	GLY
1	A	64	GLY
1	C	64	GLY
1	F	64	GLY
1	H	64	GLY
1	D	64	GLY

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	269/276 (98%)	260 (97%)	9 (3%)	45	61
1	B	265/276 (96%)	250 (94%)	15 (6%)	25	34
1	C	267/276 (97%)	253 (95%)	14 (5%)	29	38
1	D	268/276 (97%)	257 (96%)	11 (4%)	37	50
1	E	267/276 (97%)	258 (97%)	9 (3%)	44	59
1	F	266/276 (96%)	251 (94%)	15 (6%)	26	35
1	G	267/276 (97%)	254 (95%)	13 (5%)	31	41
1	H	264/276 (96%)	249 (94%)	15 (6%)	25	34
1	I	266/276 (96%)	251 (94%)	15 (6%)	26	35
1	J	267/276 (97%)	255 (96%)	12 (4%)	34	46
All	All	2666/2760 (97%)	2538 (95%)	128 (5%)	32	42

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	44	MET
1	A	67	THR
1	A	81	SER
1	A	180	LEU
1	A	210	LYS
1	A	243	LEU
1	A	261	SER
1	A	285	MET
1	B	5	ARG
1	B	10	LEU
1	B	18	ARG
1	B	22	SER
1	B	69	LYS
1	B	81	SER
1	B	100	CYS
1	B	160	LEU
1	B	162	THR
1	B	180	LEU
1	B	254	THR
1	B	258	ARG
1	B	261	SER
1	B	277	ARG
1	B	285	MET

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Mol	Chain	Res	Type
1	C	4	LEU
1	C	5	ARG
1	C	17	ARG
1	C	18	ARG
1	C	52	ASN
1	C	81	SER
1	C	96	LYS
1	C	100	CYS
1	C	117	VAL
1	C	208	GLU
1	C	211	ASP
1	C	243	LEU
1	C	249	GLN
1	C	285	MET
1	D	33	GLU
1	D	44	MET
1	D	65	ASP
1	D	100	CYS
1	D	160	LEU
1	D	184[A]	ARG
1	D	184[B]	ARG
1	D	208	GLU
1	D	216	VAL
1	D	243	LEU
1	D	285	MET
1	E	4	LEU
1	E	17	ARG
1	E	18	ARG
1	E	44	MET
1	E	100	CYS
1	E	180	LEU
1	E	184	ARG
1	E	216	VAL
1	E	285	MET
1	F	4	LEU
1	F	5	ARG
1	F	17	ARG
1	F	44	MET
1	F	65	ASP
1	F	67	THR
1	F	100	CYS
1	F	117	VAL

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Mol	Chain	Res	Type
1	F	155	SER
1	F	160	LEU
1	F	180	LEU
1	F	216	VAL
1	F	243	LEU
1	F	261	SER
1	F	285	MET
1	G	4	LEU
1	G	18	ARG
1	G	44	MET
1	G	59	LEU
1	G	67	THR
1	G	102	ARG
1	G	154	LYS
1	G	160	LEU
1	G	180	LEU
1	G	231	ARG
1	G	285	MET
1	G	309[A]	GLU
1	G	309[B]	GLU
1	H	4	LEU
1	H	44	MET
1	H	81	SER
1	H	100	CYS
1	H	102	ARG
1	H	117	VAL
1	H	129	GLN
1	H	160	LEU
1	H	162	THR
1	H	180	LEU
1	H	184	ARG
1	H	231	ARG
1	H	243	LEU
1	H	261	SER
1	H	285	MET
1	I	18	ARG
1	I	22	SER
1	I	44	MET
1	I	67	THR
1	I	117	VAL
1	I	126	GLN
1	I	160	LEU

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Mol	Chain	Res	Type
1	I	180	LEU
1	I	206	LYS
1	I	243	LEU
1	I	258	ARG
1	I	261	SER
1	I	285	MET
1	I	287	SER
1	I	299	GLU
1	J	17	ARG
1	J	18	ARG
1	J	22	SER
1	J	44	MET
1	J	65	ASP
1	J	117	VAL
1	J	160	LEU
1	J	180	LEU
1	J	184	ARG
1	J	208	GLU
1	J	285	MET
1	J	299	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	52	ASN
1	A	128	HIS
1	A	129	GLN
1	A	272	GLN
1	A	274	GLN
1	A	313	GLN
1	B	49	GLN
1	B	52	ASN
1	B	126	GLN
1	B	129	GLN
1	B	272	GLN
1	B	274	GLN
1	C	49	GLN
1	C	52	ASN
1	C	128	HIS
1	C	274	GLN
1	C	293	GLN

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Mol	Chain	Res	Type
1	D	49	GLN
1	D	52	ASN
1	D	128	HIS
1	D	129	GLN
1	D	274	GLN
1	E	49	GLN
1	E	52	ASN
1	E	129	GLN
1	E	274	GLN
1	F	49	GLN
1	F	52	ASN
1	F	128	HIS
1	F	129	GLN
1	F	272	GLN
1	F	274	GLN
1	F	293	GLN
1	F	313	GLN
1	G	126	GLN
1	G	129	GLN
1	G	236	HIS
1	G	272	GLN
1	G	274	GLN
1	H	129	GLN
1	H	272	GLN
1	H	274	GLN
1	I	49	GLN
1	I	52	ASN
1	I	129	GLN
1	I	272	GLN
1	I	293	GLN
1	J	129	GLN
1	J	272	GLN

5.3.3 RNA (i)

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)

52 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAP	A	350	-	42,52,52	1.84	8 (19%)	54,80,80	1.82	6 (11%)
3	TLA	A	360	-	3,9,9	0.44	0	6,12,12	0.97	0
4	GOL	A	361	-	5,5,5	0.49	0	5,5,5	0.71	0
4	GOL	A	363	-	5,5,5	0.80	0	5,5,5	0.91	0
5	PO4	A	364	-	4,4,4	0.72	0	6,6,6	0.43	0
2	NAP	B	350	-	42,52,52	1.68	7 (16%)	54,80,80	2.63	12 (22%)
3	TLA	B	360	-	3,9,9	2.64	1 (33%)	6,12,12	1.51	2 (33%)
4	GOL	B	361	-	5,5,5	0.53	0	5,5,5	0.57	0
4	GOL	B	362	-	5,5,5	0.73	0	5,5,5	1.28	1 (20%)
4	GOL	B	363	-	5,5,5	0.70	0	5,5,5	0.91	0
6	MES	B	364	-	11,12,12	0.81	0	14,16,16	4.13	9 (64%)
2	NAP	C	350	-	42,52,52	1.49	4 (9%)	54,80,80	1.93	7 (12%)
3	TLA	C	360	-	3,9,9	1.46	1 (33%)	6,12,12	0.91	0
4	GOL	C	361	-	5,5,5	0.66	0	5,5,5	1.35	0
4	GOL	C	362	-	5,5,5	0.52	0	5,5,5	1.17	1 (20%)
4	GOL	C	363	-	5,5,5	0.80	0	5,5,5	1.36	0
6	MES	C	364	-	11,12,12	0.78	0	14,16,16	2.34	7 (50%)
2	NAP	D	350	-	42,52,52	1.62	5 (11%)	54,80,80	1.93	6 (11%)
3	TLA	D	360	-	3,9,9	1.67	1 (33%)	6,12,12	2.12	3 (50%)
4	GOL	D	361	-	5,5,5	0.59	0	5,5,5	0.30	0
4	GOL	D	362	-	5,5,5	0.49	0	5,5,5	0.78	0
4	GOL	D	363	-	5,5,5	1.42	0	5,5,5	1.73	1 (20%)
6	MES	D	364	-	11,12,12	1.06	1 (9%)	14,16,16	3.22	7 (50%)
2	NAP	E	350	-	42,52,52	1.67	5 (11%)	54,80,80	2.43	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	TLA	E	360	-	3,9,9	0.94	0	6,12,12	0.94	0
4	GOL	E	361	-	5,5,5	0.54	0	5,5,5	0.94	0
4	GOL	E	362	-	5,5,5	0.62	0	5,5,5	0.70	0
4	GOL	E	363	-	5,5,5	0.73	0	5,5,5	0.95	0
2	NAP	F	350	-	42,52,52	1.79	4 (9%)	54,80,80	2.15	10 (18%)
3	TLA	F	360	-	3,9,9	0.41	0	6,12,12	1.19	0
4	GOL	F	361	-	5,5,5	0.72	0	5,5,5	1.56	2 (40%)
2	NAP	G	350	-	42,52,52	1.89	9 (21%)	54,80,80	1.88	8 (14%)
3	TLA	G	360	-	3,9,9	1.22	0	6,12,12	1.17	0
4	GOL	G	362	-	5,5,5	0.58	0	5,5,5	1.24	1 (20%)
4	GOL	G	363	-	5,5,5	0.59	0	5,5,5	1.23	1 (20%)
4	GOL	G	364	-	5,5,5	0.95	0	5,5,5	1.58	2 (40%)
2	NAP	H	350	-	42,52,52	1.79	5 (11%)	54,80,80	2.15	14 (25%)
3	TLA	H	360	-	3,9,9	1.59	1 (33%)	6,12,12	1.01	0
4	GOL	H	361	-	5,5,5	0.38	0	5,5,5	0.66	0
4	GOL	H	362	-	5,5,5	0.68	0	5,5,5	1.09	0
2	NAP	I	350	-	42,52,52	1.66	3 (7%)	54,80,80	1.82	9 (16%)
3	TLA	I	360	-	3,9,9	1.97	1 (33%)	6,12,12	1.57	1 (16%)
4	GOL	I	361	-	5,5,5	0.48	0	5,5,5	0.86	0
4	GOL	I	362	-	5,5,5	0.67	0	5,5,5	1.40	1 (20%)
6	MES	I	363	-	11,12,12	1.33	3 (27%)	14,16,16	2.56	5 (35%)
2	NAP	J	350	-	42,52,52	1.52	5 (11%)	54,80,80	2.28	12 (22%)
3	TLA	J	360	-	3,9,9	0.70	0	6,12,12	1.00	0
4	GOL	J	363	-	5,5,5	0.39	0	5,5,5	1.02	0
4	GOL	J	364	-	5,5,5	0.52	0	5,5,5	0.72	0
4	GOL	J	366	-	5,5,5	0.85	0	5,5,5	0.97	0
5	PO4	J	367	-	4,4,4	0.31	0	6,6,6	0.27	0
6	MES	J	368	-	11,12,12	1.08	1 (9%)	14,16,16	2.44	4 (28%)

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	NAP	A	350	-	-	0/27/67/67	0/5/5/5
3	TLA	A	360	-	-	0/4/12/12	0/0/0/0
4	GOL	A	361	-	-	0/4/4/4	0/0/0/0
4	GOL	A	363	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PO4	A	364	-	-	0/0/0/0	0/0/0/0
2	NAP	B	350	-	-	0/27/67/67	0/5/5/5
3	TLA	B	360	-	-	0/4/12/12	0/0/0/0
4	GOL	B	361	-	-	0/4/4/4	0/0/0/0
4	GOL	B	362	-	-	0/4/4/4	0/0/0/0
4	GOL	B	363	-	-	0/4/4/4	0/0/0/0
6	MES	B	364	-	-	0/6/14/14	0/1/1/1
2	NAP	C	350	-	-	0/27/67/67	0/5/5/5
3	TLA	C	360	-	-	0/4/12/12	0/0/0/0
4	GOL	C	361	-	-	0/4/4/4	0/0/0/0
4	GOL	C	362	-	-	0/4/4/4	0/0/0/0
4	GOL	C	363	-	-	0/4/4/4	0/0/0/0
6	MES	C	364	-	-	0/6/14/14	0/1/1/1
2	NAP	D	350	-	-	0/27/67/67	0/5/5/5
3	TLA	D	360	-	-	0/4/12/12	0/0/0/0
4	GOL	D	361	-	-	0/4/4/4	0/0/0/0
4	GOL	D	362	-	-	0/4/4/4	0/0/0/0
4	GOL	D	363	-	-	0/4/4/4	0/0/0/0
6	MES	D	364	-	-	0/6/14/14	0/1/1/1
2	NAP	E	350	-	-	0/27/67/67	0/5/5/5
3	TLA	E	360	-	-	0/4/12/12	0/0/0/0
4	GOL	E	361	-	-	0/4/4/4	0/0/0/0
4	GOL	E	362	-	-	0/4/4/4	0/0/0/0
4	GOL	E	363	-	-	0/4/4/4	0/0/0/0
2	NAP	F	350	-	-	0/27/67/67	0/5/5/5
3	TLA	F	360	-	-	0/4/12/12	0/0/0/0
4	GOL	F	361	-	-	0/4/4/4	0/0/0/0
2	NAP	G	350	-	-	0/27/67/67	0/5/5/5
3	TLA	G	360	-	-	0/4/12/12	0/0/0/0
4	GOL	G	362	-	-	0/4/4/4	0/0/0/0
4	GOL	G	363	-	-	0/4/4/4	0/0/0/0
4	GOL	G	364	-	-	0/4/4/4	0/0/0/0
2	NAP	H	350	-	-	0/27/67/67	0/5/5/5
3	TLA	H	360	-	-	0/4/12/12	0/0/0/0
4	GOL	H	361	-	-	0/4/4/4	0/0/0/0
4	GOL	H	362	-	-	0/4/4/4	0/0/0/0
2	NAP	I	350	-	-	0/27/67/67	0/5/5/5
3	TLA	I	360	-	-	0/4/12/12	0/0/0/0
4	GOL	I	361	-	-	0/4/4/4	0/0/0/0
4	GOL	I	362	-	-	0/4/4/4	0/0/0/0
6	MES	I	363	-	-	0/6/14/14	0/1/1/1
2	NAP	J	350	-	-	0/27/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TLA	J	360	-	-	0/4/12/12	0/0/0/0
4	GOL	J	363	-	-	0/4/4/4	0/0/0/0
4	GOL	J	364	-	-	0/4/4/4	0/0/0/0
4	GOL	J	366	-	-	0/4/4/4	0/0/0/0
5	PO4	J	367	-	-	0/0/0/0	0/0/0/0
6	MES	J	368	-	-	0/6/14/14	0/1/1/1

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	350	NAP	C3N-C7N	-2.83	1.46	1.50
2	G	350	NAP	O4B-C4B	-2.69	1.38	1.45
2	G	350	NAP	O3B-C3B	-2.59	1.36	1.43
2	A	350	NAP	PN-O2N	-2.36	1.44	1.54
2	H	350	NAP	O2B-C2B	-2.27	1.37	1.44
2	G	350	NAP	O2B-C2B	-2.26	1.37	1.44
2	D	350	NAP	PA-O2A	-2.18	1.45	1.54
2	A	350	NAP	O4B-C4B	-2.12	1.40	1.45
2	D	350	NAP	O4B-C4B	-2.07	1.40	1.45
2	J	350	NAP	C3N-C7N	-2.05	1.47	1.50
2	H	350	NAP	PA-O2A	-2.03	1.46	1.54
2	A	350	NAP	O3B-C3B	-2.01	1.38	1.43
2	E	350	NAP	C2A-N3A	2.01	1.35	1.32
6	J	368	MES	O1S-S	2.03	1.51	1.45
3	D	360	TLA	O2-C2	2.06	1.46	1.42
2	J	350	NAP	O4D-C1D	2.07	1.43	1.41
2	B	350	NAP	C2A-N1A	2.10	1.37	1.33
6	I	363	MES	O1S-S	2.11	1.51	1.45
6	I	363	MES	O2S-S	2.12	1.51	1.45
2	B	350	NAP	C2A-N3A	2.15	1.36	1.32
2	D	350	NAP	C2A-N1A	2.16	1.38	1.33
6	I	363	MES	O3S-S	2.22	1.52	1.46
2	B	350	NAP	C2N-C3N	2.23	1.42	1.39
2	E	350	NAP	O4B-C1B	2.27	1.44	1.41
2	B	350	NAP	C3D-C4D	2.30	1.59	1.53
6	D	364	MES	O3S-S	2.33	1.52	1.46
2	H	350	NAP	C2A-N1A	2.38	1.38	1.33
3	C	360	TLA	O3-C3	2.39	1.47	1.42
2	D	350	NAP	C2A-N3A	2.46	1.36	1.32
2	C	350	NAP	C2A-N3A	2.51	1.36	1.32
3	H	360	TLA	O3-C3	2.61	1.48	1.42
2	A	350	NAP	C2A-N1A	2.84	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	350	NAP	O4D-C1D	2.91	1.44	1.41
2	G	350	NAP	C4A-N3A	2.92	1.39	1.35
2	A	350	NAP	O4D-C1D	3.02	1.45	1.41
2	A	350	NAP	C2A-N3A	3.23	1.37	1.32
2	E	350	NAP	O4D-C1D	3.25	1.45	1.41
2	C	350	NAP	C2A-N1A	3.29	1.40	1.33
2	A	350	NAP	O4B-C1B	3.29	1.45	1.41
3	I	360	TLA	O3-C3	3.29	1.49	1.42
2	B	350	NAP	O4B-C1B	3.39	1.45	1.41
2	B	350	NAP	O4D-C1D	3.44	1.45	1.41
2	E	350	NAP	C2A-N1A	3.46	1.40	1.33
2	F	350	NAP	C2A-N1A	3.51	1.40	1.33
2	J	350	NAP	C2A-N3A	3.54	1.38	1.32
2	J	350	NAP	C2A-N1A	3.60	1.40	1.33
2	G	350	NAP	O4D-C1D	4.03	1.46	1.41
2	I	350	NAP	C2A-N1A	4.04	1.41	1.33
2	C	350	NAP	O4D-C1D	4.06	1.46	1.41
2	G	350	NAP	C2A-N3A	4.06	1.39	1.32
2	F	350	NAP	C2A-N3A	4.07	1.39	1.32
2	G	350	NAP	C2A-N1A	4.12	1.41	1.33
3	B	360	TLA	O3-C3	4.22	1.51	1.42
2	H	350	NAP	C2A-N3A	5.00	1.41	1.32
2	I	350	NAP	C2A-N3A	5.08	1.41	1.32
2	C	350	NAP	O7N-C7N	5.98	1.36	1.24
2	G	350	NAP	O7N-C7N	6.36	1.37	1.24
2	J	350	NAP	O7N-C7N	6.43	1.37	1.24
2	I	350	NAP	O7N-C7N	6.53	1.38	1.24
2	B	350	NAP	O7N-C7N	6.76	1.38	1.24
2	E	350	NAP	O7N-C7N	6.89	1.38	1.24
2	D	350	NAP	O7N-C7N	7.41	1.40	1.24
2	H	350	NAP	O7N-C7N	7.76	1.40	1.24
2	A	350	NAP	O7N-C7N	7.79	1.40	1.24
2	F	350	NAP	O7N-C7N	8.05	1.41	1.24

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	350	NAP	N3A-C2A-N1A	-14.64	117.69	128.89
2	E	350	NAP	N3A-C2A-N1A	-14.54	117.76	128.89
2	J	350	NAP	N3A-C2A-N1A	-12.57	119.27	128.89
2	F	350	NAP	N3A-C2A-N1A	-11.90	119.78	128.89
2	D	350	NAP	N3A-C2A-N1A	-11.24	120.29	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	350	NAP	N3A-C2A-N1A	-10.15	121.12	128.89
2	G	350	NAP	N3A-C2A-N1A	-9.64	121.51	128.89
2	H	350	NAP	N3A-C2A-N1A	-9.40	121.70	128.89
2	A	350	NAP	N3A-C2A-N1A	-9.36	121.73	128.89
2	I	350	NAP	N3A-C2A-N1A	-8.16	122.65	128.89
2	H	350	NAP	O7N-C7N-C3N	-5.79	113.27	119.59
6	I	363	MES	C2-C3-N4	-4.42	103.43	110.12
2	B	350	NAP	O2B-P2B-O1X	-4.26	96.47	107.11
2	J	350	NAP	PN-O3-PA	-4.04	121.38	132.73
2	I	350	NAP	O7N-C7N-N7N	-3.57	117.57	122.59
2	F	350	NAP	PN-O3-PA	-3.47	122.99	132.73
2	F	350	NAP	C1B-N9A-C4A	-3.33	121.92	126.94
2	C	350	NAP	C1B-N9A-C4A	-3.30	121.97	126.94
3	D	360	TLA	O2-C2-C1	-3.29	102.90	111.21
2	I	350	NAP	C5N-C4N-C3N	-3.25	116.25	120.33
2	G	350	NAP	O7N-C7N-C3N	-3.21	116.08	119.59
2	J	350	NAP	C5N-C4N-C3N	-3.12	116.41	120.33
2	B	350	NAP	O3B-C3B-C2B	-3.01	102.46	111.16
2	H	350	NAP	O2B-P2B-O1X	-2.97	99.69	107.11
2	J	350	NAP	C1B-N9A-C4A	-2.96	122.48	126.94
2	E	350	NAP	O3-PN-O5D	-2.95	95.10	102.94
6	D	364	MES	O3S-S-O1S	-2.92	104.81	111.61
2	B	350	NAP	C5N-C4N-C3N	-2.92	116.66	120.33
2	H	350	NAP	C5N-C4N-C3N	-2.92	116.67	120.33
2	F	350	NAP	O5D-PN-O1N	-2.73	99.03	109.62
2	G	350	NAP	O2B-P2B-O1X	-2.70	100.37	107.11
2	C	350	NAP	O7N-C7N-C3N	-2.70	116.64	119.59
2	D	350	NAP	O3-PN-O5D	-2.57	96.11	102.94
2	H	350	NAP	C1B-N9A-C4A	-2.53	123.13	126.94
6	C	364	MES	O3S-S-O1S	-2.50	105.78	111.61
3	B	360	TLA	O2-C2-C1	-2.47	104.99	111.21
2	I	350	NAP	O2D-C2D-C3D	-2.44	103.88	111.83
2	D	350	NAP	O4D-C1D-N1N	-2.44	105.45	108.13
2	A	350	NAP	O3-PN-O5D	-2.41	96.54	102.94
6	B	364	MES	O3S-S-O1S	-2.41	106.00	111.61
2	G	350	NAP	C5N-C4N-C3N	-2.40	117.32	120.33
2	H	350	NAP	O5B-PA-O1A	-2.39	100.35	109.62
2	H	350	NAP	O3B-C3B-C2B	-2.35	104.36	111.16
2	J	350	NAP	O7N-C7N-N7N	-2.34	119.30	122.59
2	E	350	NAP	C4D-O4D-C1D	-2.32	107.17	109.72
6	B	364	MES	C6-C5-N4	-2.32	106.61	110.12
2	F	350	NAP	C4A-C5A-N7A	-2.24	107.42	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	350	NAP	O2X-P2B-O1X	-2.22	103.42	110.58
2	J	350	NAP	O4B-C1B-C2B	-2.22	102.59	106.60
3	D	360	TLA	O3-C3-C4	-2.21	105.63	111.21
2	I	350	NAP	O4D-C1D-N1N	-2.15	105.77	108.13
6	I	363	MES	O1S-S-C8	-2.14	105.08	106.91
2	J	350	NAP	C2B-C3B-C4B	-2.09	96.89	101.85
2	C	350	NAP	O2B-P2B-O1X	-2.07	101.94	107.11
2	B	350	NAP	O7N-C7N-C3N	-2.06	117.33	119.59
6	C	364	MES	O3S-S-O2S	-2.06	106.81	111.61
2	F	350	NAP	C5N-C4N-C3N	-2.02	117.80	120.33
4	G	364	GOL	O1-C1-C2	2.01	119.94	110.18
6	B	364	MES	C6-O1-C2	2.01	116.67	109.89
2	B	350	NAP	C3N-C7N-N7N	2.02	120.02	117.82
2	F	350	NAP	O2N-PN-O1N	2.03	123.53	112.53
2	F	350	NAP	C2A-N1A-C6A	2.04	122.41	118.77
2	D	350	NAP	O3-PA-O5B	2.04	108.35	102.94
2	B	350	NAP	P2B-O2B-C2B	2.06	126.49	121.56
2	E	350	NAP	O5D-C5D-C4D	2.06	116.73	109.12
2	E	350	NAP	P2B-O2B-C2B	2.07	126.54	121.56
4	G	364	GOL	O3-C3-C2	2.08	120.25	110.18
4	G	362	GOL	O3-C3-C2	2.08	120.25	110.18
3	B	360	TLA	O2-C2-C3	2.08	114.48	108.61
6	J	368	MES	C2-C3-N4	2.11	113.31	110.12
2	J	350	NAP	O3-PA-O5B	2.11	108.54	102.94
6	C	364	MES	C6-O1-C2	2.12	117.02	109.89
2	I	350	NAP	O2N-PN-O3	2.12	114.70	105.09
2	G	350	NAP	O3X-P2B-O2X	2.13	115.47	107.38
2	J	350	NAP	O4B-C4B-C3B	2.14	109.45	105.15
4	G	363	GOL	C3-C2-C1	2.18	119.66	111.12
4	I	362	GOL	O1-C1-C2	2.20	120.84	110.18
2	H	350	NAP	O2N-PN-O3	2.20	115.09	105.09
2	H	350	NAP	C3N-C7N-N7N	2.22	120.24	117.82
2	B	350	NAP	C6N-C5N-C4N	2.22	122.80	119.44
2	C	350	NAP	C2A-N1A-C6A	2.23	122.74	118.77
4	B	362	GOL	O1-C1-C2	2.23	121.00	110.18
2	D	350	NAP	P2B-O2B-C2B	2.27	127.00	121.56
2	J	350	NAP	C2A-N1A-C6A	2.28	122.84	118.77
2	E	350	NAP	O3D-C3D-C4D	2.31	117.97	111.05
2	E	350	NAP	O4D-C1D-N1N	2.31	110.67	108.13
6	D	364	MES	C7-N4-C5	2.32	117.20	111.27
6	I	363	MES	C7-N4-C5	2.33	117.25	111.27
4	C	362	GOL	O1-C1-C2	2.33	121.50	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	368	MES	C7-N4-C3	2.36	117.31	111.27
4	F	361	GOL	O1-C1-C2	2.36	121.65	110.18
2	G	350	NAP	O7N-C7N-N7N	2.37	125.94	122.59
2	D	350	NAP	O3D-C3D-C4D	2.42	118.32	111.05
2	H	350	NAP	O3D-C3D-C4D	2.43	118.33	111.05
4	F	361	GOL	C3-C2-C1	2.43	120.63	111.12
2	H	350	NAP	C6N-C5N-C4N	2.43	123.11	119.44
6	B	364	MES	C7-N4-C5	2.43	117.49	111.27
6	C	364	MES	O1S-S-C8	2.44	108.98	106.91
2	B	350	NAP	O4D-C1D-N1N	2.52	110.90	108.13
2	A	350	NAP	O4D-C1D-N1N	2.58	110.96	108.13
2	A	350	NAP	C4D-O4D-C1D	2.59	112.56	109.72
2	E	350	NAP	O4D-C4D-C3D	2.63	110.44	105.15
6	J	368	MES	C7-N4-C5	2.67	118.11	111.27
2	B	350	NAP	C2A-N1A-C6A	2.71	123.60	118.77
2	I	350	NAP	O3D-C3D-C4D	2.71	119.18	111.05
6	D	364	MES	C7-N4-C3	2.71	118.23	111.27
2	H	350	NAP	O7N-C7N-N7N	2.75	126.46	122.59
2	C	350	NAP	O3D-C3D-C4D	2.83	119.53	111.05
3	I	360	TLA	O3-C3-C2	2.83	116.59	108.61
6	B	364	MES	O1-C2-C3	2.88	118.43	111.84
3	D	360	TLA	O3-C3-C2	2.97	116.97	108.61
2	A	350	NAP	C2N-C3N-C4N	2.99	121.62	118.29
2	F	350	NAP	C2N-C3N-C4N	3.02	121.65	118.29
6	C	364	MES	C7-N4-C3	3.12	119.26	111.27
6	D	364	MES	O1S-S-C8	3.17	109.61	106.91
6	B	364	MES	C7-N4-C3	3.19	119.45	111.27
6	D	364	MES	C2-C3-N4	3.20	114.97	110.12
2	B	350	NAP	O3D-C3D-C4D	3.21	120.67	111.05
2	J	350	NAP	O7N-C7N-C3N	3.26	123.15	119.59
6	I	363	MES	C7-N4-C3	3.29	119.71	111.27
2	H	350	NAP	P2B-O2B-C2B	3.62	130.25	121.56
4	D	363	GOL	O1-C1-C2	3.63	127.80	110.18
2	I	350	NAP	O7N-C7N-C3N	3.65	123.57	119.59
2	G	350	NAP	C2N-C3N-C4N	3.87	122.60	118.29
2	C	350	NAP	O3-PA-O5B	3.96	113.45	102.94
2	I	350	NAP	C2N-C3N-C4N	4.00	122.74	118.29
2	J	350	NAP	C2N-C3N-C4N	4.10	122.86	118.29
2	A	350	NAP	P2B-O2B-C2B	4.12	131.45	121.56
2	F	350	NAP	O3-PA-O5B	4.18	114.04	102.94
6	C	364	MES	C7-N4-C5	4.22	122.08	111.27
6	C	364	MES	C5-N4-C3	4.43	118.49	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	350	NAP	O3-PA-O5B	4.46	114.78	102.94
2	E	350	NAP	C2A-N1A-C6A	4.54	126.88	118.77
2	B	350	NAP	O3-PA-O5B	6.26	119.55	102.94
6	I	363	MES	C5-N4-C3	6.52	123.03	108.90
6	B	364	MES	C5-N4-C3	6.53	123.05	108.90
6	D	364	MES	O2S-S-C8	6.55	112.50	106.91
6	D	364	MES	C5-N4-C3	7.21	124.52	108.90
6	J	368	MES	C5-N4-C3	7.24	124.58	108.90
6	B	364	MES	O2S-S-C8	7.95	113.69	106.91
6	B	364	MES	O1S-S-C8	9.23	114.78	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	350	NAP	2	0
4	A	361	GOL	2	0
2	B	350	NAP	3	0
3	B	360	TLA	2	0
3	C	360	TLA	3	0
2	D	350	NAP	1	0
2	E	350	NAP	1	0
3	E	360	TLA	1	0
2	F	350	NAP	3	0
3	F	360	TLA	1	0
2	G	350	NAP	1	0
4	G	364	GOL	5	0
2	H	350	NAP	4	0
3	H	360	TLA	2	0
4	H	361	GOL	2	0
2	I	350	NAP	3	0
3	I	360	TLA	1	0
4	I	362	GOL	1	0
2	J	350	NAP	2	0
3	J	360	TLA	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	325/338 (96%)	-0.38	1 (0%) 94 96	30, 36, 47, 72	0
1	B	324/338 (95%)	-0.26	3 (0%) 85 89	29, 36, 47, 71	0
1	C	324/338 (95%)	-0.41	1 (0%) 94 96	30, 36, 47, 72	0
1	D	324/338 (95%)	-0.33	0 100 100	30, 36, 47, 73	0
1	E	324/338 (95%)	-0.38	0 100 100	30, 36, 47, 72	0
1	F	324/338 (95%)	-0.38	3 (0%) 85 89	30, 36, 47, 72	0
1	G	324/338 (95%)	-0.34	1 (0%) 94 96	30, 36, 47, 72	0
1	H	324/338 (95%)	-0.25	2 (0%) 90 93	30, 36, 46, 71	0
1	I	324/338 (95%)	-0.35	2 (0%) 90 93	29, 36, 47, 72	0
1	J	325/338 (96%)	-0.34	2 (0%) 90 93	30, 36, 47, 72	0
All	All	3242/3380 (95%)	-0.34	15 (0%) 91 94	29, 36, 47, 73	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	64	GLY	4.6
1	H	64	GLY	3.9
1	F	65	ASP	3.7
1	A	64	GLY	3.6
1	I	65	ASP	3.1
1	F	64	GLY	3.0
1	B	254	THR	2.7
1	J	67	THR	2.7
1	I	64	GLY	2.7
1	H	63	SER	2.5
1	F	255	ASN	2.5
1	B	65	ASP	2.3
1	J	65	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	65	ASP	2.2
1	B	64	GLY	2.1

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	GOL	D	363	6/6	0.77	0.21	10.37	48,53,55,55	0
4	GOL	H	362	6/6	0.98	0.17	9.65	30,34,36,36	0
6	MES	I	363	12/12	0.96	0.22	8.02	55,60,61,61	0
4	GOL	G	364	6/6	0.88	0.29	6.93	58,62,62,64	0
4	GOL	J	363	6/6	0.95	0.15	5.63	39,42,42,46	0
4	GOL	I	361	6/6	0.97	0.18	4.96	44,47,48,48	0
4	GOL	B	361	6/6	0.97	0.14	4.90	33,40,42,42	0
4	GOL	G	363	6/6	0.98	0.15	3.79	34,36,36,38	0
4	GOL	B	362	6/6	0.91	0.26	3.61	57,61,62,63	0
4	GOL	F	361	6/6	0.97	0.15	3.27	36,39,41,42	0
6	MES	B	364	12/12	0.98	0.15	2.97	50,61,65,65	0
6	MES	C	364	12/12	0.98	0.14	2.77	57,62,64,64	0
3	TLA	H	360	10/10	0.99	0.13	2.64	30,36,41,43	0
5	PO4	J	367	5/5	0.98	0.14	2.62	60,60,65,67	0
4	GOL	J	364	6/6	0.98	0.14	2.29	45,48,49,50	0
6	MES	J	368	12/12	0.97	0.16	1.61	53,57,59,60	0
4	GOL	E	363	6/6	0.98	0.14	1.59	28,31,31,32	0
3	TLA	C	360	10/10	0.97	0.11	1.37	29,33,38,41	0
4	GOL	H	361	6/6	0.96	0.13	1.11	37,44,45,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	E	361	6/6	0.98	0.13	1.05	33,36,36,37	0
4	GOL	E	362	6/6	0.98	0.12	0.74	31,33,36,36	0
4	GOL	A	363	6/6	0.96	0.12	0.58	39,42,42,43	0
4	GOL	C	363	6/6	0.88	0.14	0.44	49,60,61,62	0
4	GOL	J	366	6/6	0.89	0.12	0.38	51,53,53,54	0
4	GOL	I	362	6/6	0.98	0.12	0.28	33,34,36,39	0
3	TLA	F	360	10/10	0.97	0.10	0.14	31,36,39,39	0
5	PO4	A	364	5/5	0.95	0.10	-0.18	59,59,63,65	0
4	GOL	C	361	6/6	0.97	0.10	-0.19	38,45,47,50	0
4	GOL	C	362	6/6	0.98	0.11	-0.36	33,36,39,39	0
4	GOL	A	361	6/6	0.95	0.10	-0.42	37,40,45,46	0
3	TLA	D	360	10/10	0.98	0.10	-0.62	25,31,34,36	0
4	GOL	B	363	6/6	0.98	0.10	-0.85	30,33,34,35	0
2	NAP	B	350	48/48	0.98	0.09	-1.03	27,32,38,43	0
3	TLA	A	360	10/10	0.97	0.09	-1.12	28,33,35,35	0
2	NAP	F	350	48/48	0.99	0.08	-1.21	23,29,34,36	0
3	TLA	I	360	10/10	0.97	0.09	-1.39	27,35,37,40	0
6	MES	D	364	12/12	0.97	0.09	-1.39	48,62,66,67	0
2	NAP	E	350	48/48	0.99	0.08	-1.54	20,27,31,36	0
4	GOL	D	362	6/6	0.97	0.08	-1.55	33,34,35,36	0
2	NAP	D	350	48/48	0.99	0.09	-1.60	20,25,32,37	0
2	NAP	H	350	48/48	0.98	0.08	-1.66	24,33,37,43	0
4	GOL	D	361	6/6	0.96	0.09	-1.75	29,29,33,33	0
3	TLA	B	360	10/10	0.96	0.09	-1.92	34,37,41,42	0
2	NAP	J	350	48/48	0.99	0.07	-1.93	23,30,35,40	0
4	GOL	G	362	6/6	0.97	0.09	-1.99	31,36,37,39	0
2	NAP	I	350	48/48	0.99	0.07	-2.03	22,31,35,36	0
2	NAP	C	350	48/48	0.99	0.07	-2.07	23,29,35,37	0
2	NAP	A	350	48/48	0.99	0.08	-2.15	21,26,31,35	0
3	TLA	G	360	10/10	0.97	0.09	-2.16	31,33,35,35	0
2	NAP	G	350	48/48	0.99	0.08	-2.29	19,27,31,35	0
3	TLA	J	360	10/10	0.98	0.08	-3.12	29,33,34,37	0
3	TLA	E	360	10/10	0.99	0.09	-3.61	26,31,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.