



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:15 PM GMT

PDB ID : 3TDS  
Title : Crystal structure of HSC F194I  
Authors : Czyzewski, B.K.; Wang, D-N.  
Deposited on : 2011-08-11  
Resolution : 1.98 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

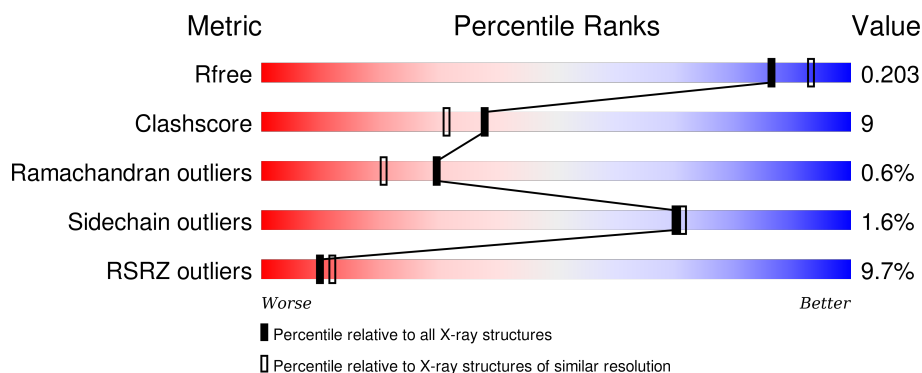
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	268	<div> <div>12%</div> <div>87% 7% . .</div> </div>
1	B	268	<div> <div>10%</div> <div>87% 9% .</div> </div>
1	C	268	<div> <div>14%</div> <div>83% 13% . .</div> </div>
1	D	268	<div> <div>7%</div> <div>84% 10% . .</div> </div>
1	E	268	<div> <div>4%</div> <div>87% 7% . .</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PG4	B	301	-	-	-	X
2	PG4	D	301	-	-	-	X
2	PG4	E	301	-	-	-	X
3	BOG	A	302	-	-	-	X
3	BOG	A	303	-	-	-	X
3	BOG	B	302	-	-	-	X
3	BOG	D	302	-	-	-	X
3	BOG	E	302	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10211 atoms, of which 212 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 formate/nitrite transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	256	Total	C	N	O	S	0	0	0
			1887	1238	296	339	14			
1	A	257	Total	C	N	O	S	0	0	0
			1894	1241	299	340	14			
1	B	257	Total	C	N	O	S	0	0	0
			1898	1244	300	340	14			
1	C	266	Total	C	N	O	S	0	0	0
			1966	1287	311	354	14			
1	D	257	Total	C	N	O	S	0	0	0
			1898	1244	300	340	14			

There are 60 discrepancies between the modelled and reference sequences:

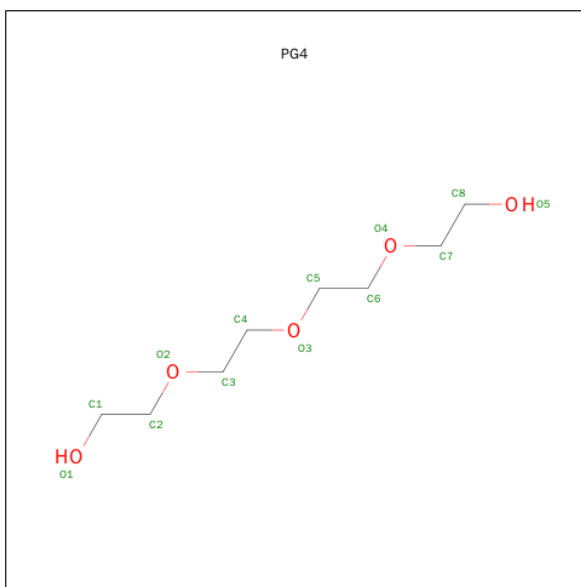
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	MET	-	EXPRESSION TAG	UNP Q186B7
E	-1	GLY	-	EXPRESSION TAG	UNP Q186B7
E	0	ARG	-	EXPRESSION TAG	UNP Q186B7
E	1	ALA	-	EXPRESSION TAG	UNP Q186B7
E	194	ILE	PHE	CONFLICT	UNP Q186B7
E	259	ALA	-	EXPRESSION TAG	UNP Q186B7
E	260	ALA	-	EXPRESSION TAG	UNP Q186B7
E	261	ALA	-	EXPRESSION TAG	UNP Q186B7
E	262	GLU	-	EXPRESSION TAG	UNP Q186B7
E	263	ASN	-	EXPRESSION TAG	UNP Q186B7
E	264	LEU	-	EXPRESSION TAG	UNP Q186B7
E	265	TYR	-	EXPRESSION TAG	UNP Q186B7
A	-2	MET	-	EXPRESSION TAG	UNP Q186B7
A	-1	GLY	-	EXPRESSION TAG	UNP Q186B7
A	0	ARG	-	EXPRESSION TAG	UNP Q186B7
A	1	ALA	-	EXPRESSION TAG	UNP Q186B7
A	194	ILE	PHE	CONFLICT	UNP Q186B7
A	259	ALA	-	EXPRESSION TAG	UNP Q186B7
A	260	ALA	-	EXPRESSION TAG	UNP Q186B7

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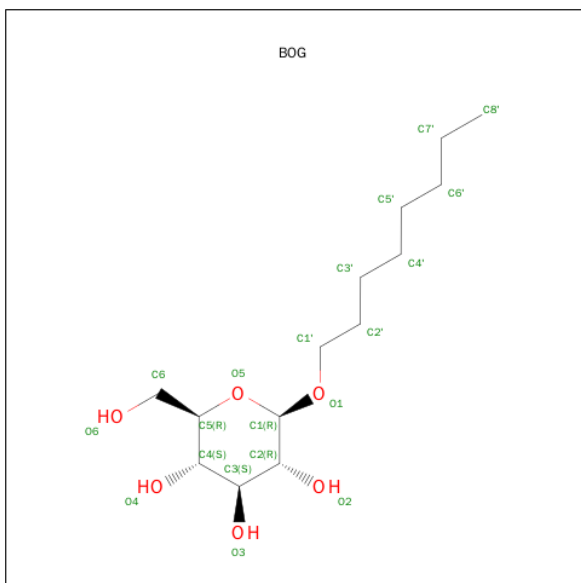
Chain	Residue	Modelled	Actual	Comment	Reference
A	261	ALA	-	EXPRESSION TAG	UNP Q186B7
A	262	GLU	-	EXPRESSION TAG	UNP Q186B7
A	263	ASN	-	EXPRESSION TAG	UNP Q186B7
A	264	LEU	-	EXPRESSION TAG	UNP Q186B7
A	265	TYR	-	EXPRESSION TAG	UNP Q186B7
B	-2	MET	-	EXPRESSION TAG	UNP Q186B7
B	-1	GLY	-	EXPRESSION TAG	UNP Q186B7
B	0	ARG	-	EXPRESSION TAG	UNP Q186B7
B	1	ALA	-	EXPRESSION TAG	UNP Q186B7
B	194	ILE	PHE	CONFLICT	UNP Q186B7
B	259	ALA	-	EXPRESSION TAG	UNP Q186B7
B	260	ALA	-	EXPRESSION TAG	UNP Q186B7
B	261	ALA	-	EXPRESSION TAG	UNP Q186B7
B	262	GLU	-	EXPRESSION TAG	UNP Q186B7
B	263	ASN	-	EXPRESSION TAG	UNP Q186B7
B	264	LEU	-	EXPRESSION TAG	UNP Q186B7
B	265	TYR	-	EXPRESSION TAG	UNP Q186B7
C	-2	MET	-	EXPRESSION TAG	UNP Q186B7
C	-1	GLY	-	EXPRESSION TAG	UNP Q186B7
C	0	ARG	-	EXPRESSION TAG	UNP Q186B7
C	1	ALA	-	EXPRESSION TAG	UNP Q186B7
C	194	ILE	PHE	CONFLICT	UNP Q186B7
C	259	ALA	-	EXPRESSION TAG	UNP Q186B7
C	260	ALA	-	EXPRESSION TAG	UNP Q186B7
C	261	ALA	-	EXPRESSION TAG	UNP Q186B7
C	262	GLU	-	EXPRESSION TAG	UNP Q186B7
C	263	ASN	-	EXPRESSION TAG	UNP Q186B7
C	264	LEU	-	EXPRESSION TAG	UNP Q186B7
C	265	TYR	-	EXPRESSION TAG	UNP Q186B7
D	-2	MET	-	EXPRESSION TAG	UNP Q186B7
D	-1	GLY	-	EXPRESSION TAG	UNP Q186B7
D	0	ARG	-	EXPRESSION TAG	UNP Q186B7
D	1	ALA	-	EXPRESSION TAG	UNP Q186B7
D	194	ILE	PHE	CONFLICT	UNP Q186B7
D	259	ALA	-	EXPRESSION TAG	UNP Q186B7
D	260	ALA	-	EXPRESSION TAG	UNP Q186B7
D	261	ALA	-	EXPRESSION TAG	UNP Q186B7
D	262	GLU	-	EXPRESSION TAG	UNP Q186B7
D	263	ASN	-	EXPRESSION TAG	UNP Q186B7
D	264	LEU	-	EXPRESSION TAG	UNP Q186B7
D	265	TYR	-	EXPRESSION TAG	UNP Q186B7

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	H	O	0	0
			31	8	18	5		
2	A	1	Total	C	H	O	0	0
			31	8	18	5		
2	B	1	Total	C	H	O	0	0
			31	8	18	5		
2	D	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 3 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula:  $C_{14}H_{28}O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	H	O	0	0
			48	14	28	6		
3	A	1	Total	C	H	O	0	0
			48	14	28	6		
3	A	1	Total	C	H	O	0	0
			48	14	28	6		
3	B	1	Total	C	H	O	0	0
			48	14	28	6		
3	D	1	Total	C	H	O	0	0
			48	14	28	6		

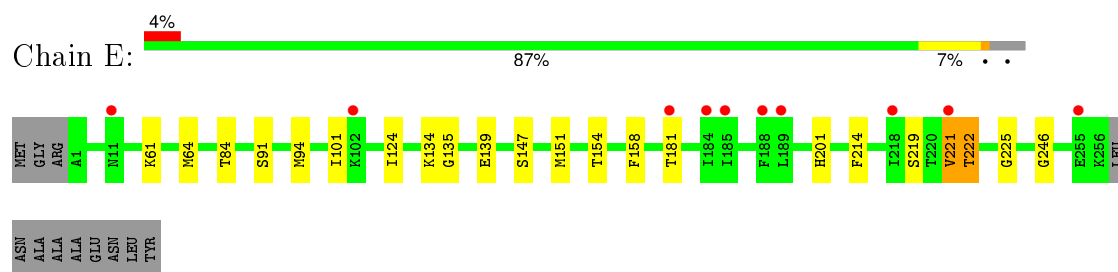
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	55	Total	O	0	0
			55	55		
4	A	71	Total	O	0	0
			71	71		
4	B	84	Total	O	0	0
			84	84		
4	C	30	Total	O	0	0
			30	30		
4	D	64	Total	O	0	0
			64	64		

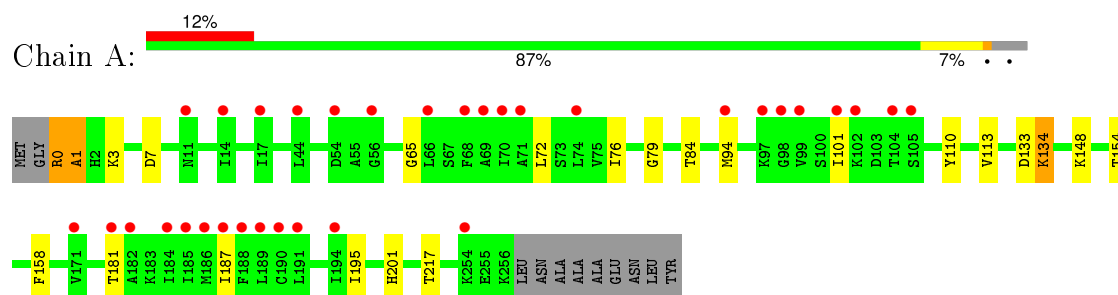
### 3 Residue-property plots

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.

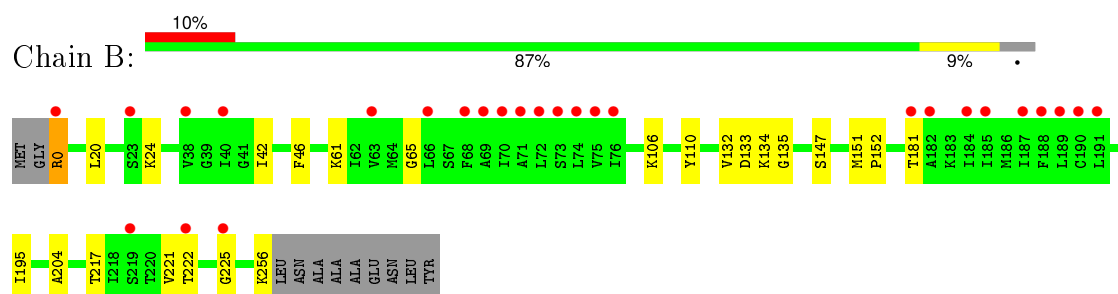
- Molecule 1: formate/nitrite transporter



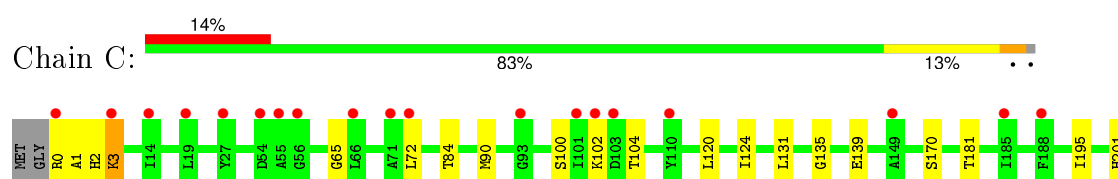
- Molecule 1: formate/nitrite transporter



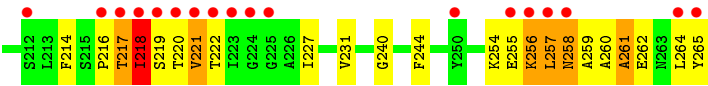
- Molecule 1: formate/nitrite transporter



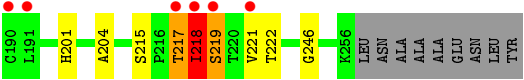
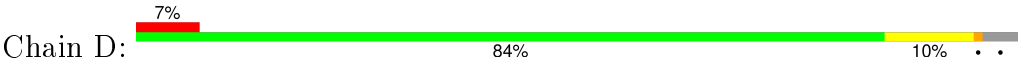
- Molecule 1: formate/nitrite transporter







● Molecule 1: formate/nitrite transporter



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.61Å 118.05Å 150.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.97 – 1.98 41.97 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.4 (41.97-1.98) 95.2 (41.97-1.98)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 1.98Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.177 , 0.205 0.175 , 0.203	Depositor DCC
$R_{free}$ test set	6086 reflections (5.47%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.6	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 73.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 121099 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10211	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, BOG

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	0.39	0/1925	0.48	0/2610
1	B	0.39	0/1929	0.47	0/2614
1	C	0.29	0/1998	0.44	0/2709
1	D	0.36	0/1929	0.46	0/2614
1	E	0.36	0/1918	0.46	0/2600
All	All	0.36	0/9699	0.46	0/13147

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1894	0	1998	20	0
1	B	1898	0	2009	23	0
1	C	1966	0	2073	78	0
1	D	1898	0	2009	37	0
1	E	1887	0	1996	23	0
2	A	13	18	18	2	0
2	B	13	18	18	5	0
2	D	13	18	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	13	18	18	4	0
3	A	40	56	56	2	0
3	B	20	28	28	0	0
3	D	20	28	28	2	0
3	E	20	28	28	10	0
4	A	71	0	0	0	0
4	B	84	0	0	0	0
4	C	30	0	0	4	0
4	D	64	0	0	7	0
4	E	55	0	0	1	0
All	All	9999	212	10297	183	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 9.

All (183) 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:C:256:LYS:HG2	1:C:264:LEU:CD1	1.69	1.21
1:D:3:LYS:HD3	1:D:3:LYS:N	1.59	1.16
1:C:258:ASN:N	1:C:259:ALA:HB3	1.60	1.16
1:C:258:ASN:HA	1:C:260:ALA:H	0.98	1.09
1:D:3:LYS:H	1:D:3:LYS:CD	1.62	1.09
1:C:219:SER:O	1:C:220:THR:HG22	1.58	1.03
1:C:0:ARG:CB	1:C:1:ALA:HA	1.89	1.03
3:E:302:BOG:H2'2	1:D:181:THR:HG21	1.39	1.02
1:C:0:ARG:HB3	1:C:1:ALA:CA	1.89	1.01
1:C:258:ASN:HA	1:C:260:ALA:N	1.76	1.00
1:C:256:LYS:CG	1:C:264:LEU:HD12	1.91	1.00
1:B:133:ASP:O	1:B:217:THR:HG21	1.61	1.00
1:C:258:ASN:H	1:C:259:ALA:HB3	0.83	0.98
1:C:0:ARG:HB3	1:C:1:ALA:HA	0.98	0.98
1:E:134:LYS:HD2	1:E:135:GLY:H	1.32	0.94
1:C:256:LYS:HG2	1:C:264:LEU:HD12	0.95	0.93
1:C:258:ASN:H	1:C:259:ALA:CB	1.80	0.92
3:E:302:BOG:H2'1	1:C:181:THR:HG21	1.53	0.91
1:D:3:LYS:HD3	1:D:3:LYS:H	0.77	0.91
1:C:264:LEU:O	1:C:265:TYR:HB3	1.73	0.89
1:A:0:ARG:HD3	1:A:1:ALA:N	1.89	0.88
1:C:218:ILE:HD12	1:C:219:SER:H	1.40	0.86
2:D:301:PG4:O1	4:D:463:HOH:O	1.92	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:LYS:CG	1:C:264:LEU:CD1	2.52	0.86
1:B:61:LYS:HE2	2:B:301:PG4:H42	1.58	0.85
1:E:221:VAL:O	1:E:222:THR:HG22	1.76	0.85
1:C:227:ILE:O	1:C:231:VAL:HG23	1.77	0.84
1:E:181:THR:HG21	3:E:302:BOG:H3'2	1.59	0.84
1:D:217:THR:O	1:D:217:THR:HG22	1.76	0.84
1:B:61:LYS:HD3	2:B:301:PG4:H31	1.58	0.84
1:C:258:ASN:O	4:C:329:HOH:O	1.96	0.83
1:C:221:VAL:O	1:C:222:THR:OG1	1.99	0.81
1:C:258:ASN:CA	1:C:260:ALA:H	1.87	0.79
1:C:0:ARG:HH22	1:C:3:LYS:HB3	1.47	0.78
1:C:256:LYS:CD	1:C:264:LEU:HD11	2.16	0.76
3:E:302:BOG:H3'1	1:B:181:THR:HG21	1.68	0.76
1:D:218:ILE:HG22	1:D:219:SER:N	2.01	0.76
1:D:127:VAL:O	4:D:455:HOH:O	2.03	0.75
1:D:3:LYS:HG2	4:D:423:HOH:O	1.86	0.74
1:C:256:LYS:NZ	1:C:264:LEU:HD21	2.03	0.74
3:E:302:BOG:C2'	1:C:181:THR:HG21	2.18	0.73
1:C:218:ILE:CG1	1:C:219:SER:N	2.51	0.72
3:E:302:BOG:C3'	1:B:181:THR:HG21	2.23	0.68
1:C:218:ILE:HG13	1:C:219:SER:N	2.07	0.68
1:C:260:ALA:O	1:C:261:ALA:CB	2.43	0.67
1:C:256:LYS:HE3	4:C:329:HOH:O	1.94	0.67
1:B:61:LYS:CE	2:B:301:PG4:H42	2.26	0.66
1:E:222:THR:HG23	1:E:225:GLY:H	1.60	0.66
1:D:217:THR:O	1:D:217:THR:CG2	2.42	0.66
1:E:61:LYS:HE2	2:E:301:PG4:H42	1.77	0.66
1:E:134:LYS:HD2	1:E:135:GLY:N	2.08	0.66
1:B:222:THR:HG23	1:B:225:GLY:H	1.61	0.65
1:B:134:LYS:HG3	1:B:135:GLY:N	2.11	0.65
1:C:256:LYS:HE2	1:C:264:LEU:HG	1.79	0.65
1:C:219:SER:O	1:C:220:THR:CG2	2.40	0.65
1:D:0:ARG:N	1:D:0:ARG:HD3	2.11	0.65
1:C:258:ASN:N	1:C:259:ALA:CB	2.49	0.64
1:C:218:ILE:CD1	1:C:219:SER:H	2.09	0.64
1:C:256:LYS:HZ1	1:C:264:LEU:HD21	1.62	0.64
1:C:84:THR:HG21	1:C:201:HIS:CD2	2.34	0.62
1:D:151:MET:HE1	1:D:159:ARG:CZ	2.30	0.61
1:C:256:LYS:HZ3	1:C:264:LEU:HD11	1.66	0.60
1:C:257:LEU:O	1:C:258:ASN:CB	2.50	0.59
1:E:134:LYS:CD	1:E:135:GLY:H	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:ILE:HD12	1:C:219:SER:N	2.13	0.59
1:D:151:MET:CE	1:D:159:ARG:CZ	2.81	0.59
1:D:215:SER:O	4:D:462:HOH:O	2.17	0.58
1:C:256:LYS:HD3	1:C:264:LEU:HD11	1.85	0.58
2:E:301:PG4:H11	1:C:131:LEU:HD22	1.84	0.58
3:E:302:BOG:H1'2	3:E:302:BOG:H61	1.85	0.58
1:D:218:ILE:HD13	1:D:218:ILE:H	1.68	0.58
1:E:221:VAL:HG12	1:E:222:THR:N	2.17	0.57
1:E:222:THR:CG2	1:E:225:GLY:H	2.16	0.57
1:B:221:VAL:HG22	1:B:222:THR:N	2.20	0.57
1:C:2:HIS:HD2	4:C:307:HOH:O	1.87	0.57
1:C:135:GLY:O	1:C:139:GLU:HG3	2.04	0.57
1:A:76:ILE:HG13	1:A:187:ILE:HD11	1.87	0.56
1:C:256:LYS:CD	1:C:264:LEU:CD1	2.83	0.56
1:C:216:PRO:O	1:C:218:ILE:N	2.34	0.56
1:C:256:LYS:CE	1:C:264:LEU:HD11	2.36	0.56
1:A:133:ASP:O	1:A:134:LYS:HB2	2.06	0.55
1:D:151:MET:HE1	1:D:159:ARG:NE	2.21	0.55
1:A:148:LYS:NZ	2:A:301:PG4:H72	2.21	0.55
1:E:219:SER:OG	1:E:221:VAL:HG23	2.07	0.55
1:C:218:ILE:CD1	1:C:219:SER:N	2.69	0.55
1:E:61:LYS:HD3	2:E:301:PG4:H31	1.87	0.55
3:E:302:BOG:H3'1	1:A:181:THR:HG21	1.88	0.55
1:D:42:ILE:HD11	1:D:204:ALA:HB1	1.89	0.54
1:C:216:PRO:C	1:C:218:ILE:H	2.11	0.54
1:A:0:ARG:HD3	1:A:0:ARG:C	2.28	0.54
1:C:3:LYS:HE2	1:C:255:GLU:OE1	2.07	0.54
1:E:151:MET:HG2	4:E:452:HOH:O	2.08	0.53
1:C:217:THR:O	1:C:217:THR:HG23	2.09	0.53
1:D:151:MET:HE1	1:D:159:ARG:CD	2.39	0.52
1:E:221:VAL:O	1:E:222:THR:CG2	2.53	0.52
1:D:84:THR:HG21	1:D:201:HIS:CD2	2.44	0.52
1:D:221:VAL:O	1:D:222:THR:OG1	2.18	0.52
1:D:0:ARG:HD3	1:D:0:ARG:H1	1.74	0.52
1:A:148:LYS:HZ2	2:A:301:PG4:H72	1.74	0.52
1:C:256:LYS:HZ3	1:C:264:LEU:HD21	1.75	0.51
1:C:240:GLY:O	1:C:244:PHE:HB2	2.11	0.51
1:D:134:LYS:HG2	1:D:135:GLY:N	2.26	0.51
1:B:20:LEU:HD21	1:B:106:LYS:HG2	1.93	0.51
1:A:79:GLY:O	1:D:0:ARG:HD2	2.12	0.50
1:D:151:MET:HE1	1:D:159:ARG:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:0:ARG:O	4:D:434:HOH:O	2.19	0.50
1:C:257:LEU:O	1:C:258:ASN:HB3	2.11	0.50
1:D:113:VAL:HG11	3:D:302:BOG:H5'2	1.92	0.50
1:A:133:ASP:O	1:A:217:THR:CG2	2.60	0.50
1:A:133:ASP:O	1:A:217:THR:HG21	2.12	0.49
1:C:0:ARG:HH12	1:C:3:LYS:H	1.59	0.49
1:E:84:THR:HG21	1:E:201:HIS:CD2	2.48	0.49
1:D:218:ILE:CD1	1:D:218:ILE:H	2.26	0.49
1:C:102:LYS:N	1:C:102:LYS:HD2	2.28	0.49
1:C:256:LYS:CG	1:C:264:LEU:HD11	2.37	0.48
1:A:3:LYS:HE2	1:A:7:ASP:OD2	2.12	0.48
1:C:258:ASN:CA	1:C:259:ALA:HB3	2.41	0.48
1:A:0:ARG:O	1:A:1:ALA:HB2	2.13	0.48
1:B:65:GLY:HA2	1:B:195:ILE:HB	1.95	0.48
1:C:216:PRO:C	1:C:218:ILE:N	2.68	0.48
1:C:256:LYS:HE3	1:C:262:GLU:OE1	2.15	0.47
1:D:217:THR:O	1:D:218:ILE:C	2.52	0.47
1:B:42:ILE:HD11	1:B:204:ALA:HB1	1.96	0.47
1:E:134:LYS:CG	1:E:135:GLY:N	2.77	0.47
1:B:134:LYS:CG	1:B:135:GLY:N	2.78	0.47
1:C:124:ILE:CG1	1:C:214:PHE:CE2	2.98	0.47
1:C:2:HIS:HE1	4:D:416:HOH:O	1.97	0.47
1:C:258:ASN:CA	1:C:260:ALA:N	2.63	0.47
1:C:256:LYS:NZ	1:C:264:LEU:HD11	2.29	0.47
1:E:94:MET:SD	1:E:101:ILE:HG12	2.54	0.46
1:C:264:LEU:O	1:C:265:TYR:CB	2.53	0.46
1:B:61:LYS:HD3	2:B:301:PG4:C3	2.36	0.46
1:D:25:VAL:O	1:D:29:VAL:HG23	2.15	0.46
1:A:94:MET:SD	1:A:101:ILE:HG12	2.55	0.46
1:A:84:THR:HG21	1:A:201:HIS:CD2	2.51	0.46
1:C:65:GLY:HA2	1:C:195:ILE:HB	1.97	0.46
1:C:3:LYS:HZ1	1:C:255:GLU:CD	2.18	0.46
1:C:218:ILE:CG1	1:C:219:SER:H	2.26	0.46
1:C:260:ALA:O	1:C:261:ALA:HB3	2.14	0.45
1:D:138:ALA:HB1	1:D:217:THR:HG21	1.97	0.45
1:D:217:THR:O	1:D:219:SER:OG	2.32	0.45
1:D:110:TYR:CE1	3:D:302:BOG:H2'1	2.52	0.45
1:C:256:LYS:HD2	1:C:256:LYS:HA	1.55	0.44
1:D:43:LEU:HD13	1:D:126:PHE:CD1	2.52	0.44
1:C:124:ILE:HG12	1:C:214:PHE:CE2	2.52	0.44
1:A:154:THR:HG23	1:A:158:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:LEU:O	1:C:124:ILE:HG13	2.18	0.44
1:C:90:MET:HB3	1:C:104:THR:HG23	1.99	0.44
3:E:302:BOG:H61	3:E:302:BOG:C1'	2.47	0.44
1:B:147:SER:O	1:B:151:MET:HG2	2.17	0.44
3:E:302:BOG:H3'2	1:B:181:THR:HG21	2.00	0.44
1:D:120:LEU:O	1:D:124:ILE:HG13	2.18	0.43
1:D:91:SER:OG	1:D:246:GLY:HA3	2.17	0.43
1:B:221:VAL:HG22	1:B:222:THR:H	1.82	0.43
1:E:91:SER:OG	1:E:246:GLY:HA3	2.18	0.43
1:E:135:GLY:O	1:E:139:GLU:HG3	2.19	0.43
1:B:134:LYS:HG3	1:B:135:GLY:H	1.80	0.43
1:E:124:ILE:HG13	1:E:214:PHE:CE2	2.53	0.42
1:D:151:MET:HE3	1:D:159:ARG:CZ	2.48	0.42
1:C:254:LYS:HE2	4:C:330:HOH:O	2.17	0.42
1:C:260:ALA:O	1:C:261:ALA:HB2	2.17	0.42
1:C:256:LYS:O	1:C:259:ALA:HB2	2.19	0.42
1:A:65:GLY:HA2	1:A:195:ILE:HB	1.99	0.42
1:C:72:LEU:CD2	1:C:170:SER:OG	2.68	0.42
1:A:113:VAL:HG11	3:A:302:BOG:H5'1	2.02	0.42
1:E:64:MET:CE	2:E:301:PG4:H61	2.49	0.42
1:C:0:ARG:CB	1:C:1:ALA:CA	2.69	0.42
1:E:134:LYS:CD	1:E:135:GLY:N	2.74	0.42
1:E:134:LYS:HG3	1:E:135:GLY:N	2.35	0.42
1:C:256:LYS:CE	1:C:264:LEU:CD1	2.99	0.41
1:B:46:PHE:CE1	2:B:301:PG4:H72	2.55	0.41
1:A:110:TYR:CE1	3:A:302:BOG:H2'1	2.54	0.41
1:B:151:MET:HE3	1:B:152:PRO:HD2	2.01	0.41
1:A:217:THR:HG22	1:A:217:THR:O	2.20	0.41
1:C:0:ARG:NH1	1:C:3:LYS:H	2.17	0.41
1:A:72:LEU:HB3	1:A:187:ILE:HG23	2.03	0.41
1:B:20:LEU:CD2	1:B:106:LYS:HG2	2.50	0.41
1:E:154:THR:HG23	1:E:158:PHE:HE2	1.85	0.41
1:B:24:LYS:HE3	1:B:110:TYR:OH	2.21	0.41
1:B:0:ARG:HA	1:B:0:ARG:HD2	1.89	0.41
1:C:3:LYS:CE	1:C:255:GLU:HB2	2.50	0.40
1:D:147:SER:O	1:D:151:MET:HG3	2.21	0.40
1:D:97:LYS:NZ	4:D:461:HOH:O	2.54	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	255/268 (95%)	249 (98%)	5 (2%)	1 (0%)	39	31
1	B	255/268 (95%)	253 (99%)	2 (1%)	0	100	100
1	C	264/268 (98%)	252 (96%)	8 (3%)	4 (2%)	13	5
1	D	255/268 (95%)	246 (96%)	7 (3%)	2 (1%)	24	14
1	E	254/268 (95%)	251 (99%)	2 (1%)	1 (0%)	39	31
All	All	1283/1340 (96%)	1251 (98%)	24 (2%)	8 (1%)	30	21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	221	VAL
1	A	1	ALA
1	C	258	ASN
1	D	218	ILE
1	C	218	ILE
1	C	261	ALA
1	C	217	THR
1	D	219	SER

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/214 (96%)	204 (99%)	2 (1%)	82	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	207/214 (97%)	204 (99%)	3 (1%)	74	75
1	C	213/214 (100%)	207 (97%)	6 (3%)	51	48
1	D	207/214 (97%)	203 (98%)	4 (2%)	65	65
1	E	206/214 (96%)	204 (99%)	2 (1%)	82	84
All	All	1039/1070 (97%)	1022 (98%)	17 (2%)	70	71

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	147	SER
1	E	222	THR
1	A	0	ARG
1	A	134	LYS
1	B	0	ARG
1	B	132	VAL
1	B	256	LYS
1	C	3	LYS
1	C	100	SER
1	C	218	ILE
1	C	221	VAL
1	C	256	LYS
1	C	257	LEU
1	D	3	LYS
1	D	33	PHE
1	D	217	THR
1	D	218	ILE

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [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$
2	PG4	A	301	-	12,12,12	0.62	0	11,11,11	1.65	2 (18%)
3	BOG	A	302	-	20,20,20	1.34	3 (15%)	25,25,25	1.52	2 (8%)
3	BOG	A	303	-	20,20,20	1.45	4 (20%)	25,25,25	2.22	8 (32%)
2	PG4	B	301	-	12,12,12	0.62	0	11,11,11	1.67	2 (18%)
3	BOG	B	302	-	20,20,20	1.28	2 (10%)	25,25,25	1.84	4 (16%)
2	PG4	D	301	-	12,12,12	0.67	0	11,11,11	1.54	0
3	BOG	D	302	-	20,20,20	1.38	3 (15%)	25,25,25	1.46	2 (8%)
2	PG4	E	301	-	12,12,12	0.60	0	11,11,11	1.68	2 (18%)
3	BOG	E	302	-	20,20,20	1.36	2 (10%)	25,25,25	2.02	6 (24%)

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	PG4	A	301	-	-	0/10/10/10	0/0/0/0
3	BOG	A	302	-	-	0/11/31/31	0/1/1/1
3	BOG	A	303	-	-	0/11/31/31	0/1/1/1
2	PG4	B	301	-	-	0/10/10/10	0/0/0/0
3	BOG	B	302	-	-	0/11/31/31	0/1/1/1
2	PG4	D	301	-	-	0/10/10/10	0/0/0/0
3	BOG	D	302	-	-	0/11/31/31	0/1/1/1
2	PG4	E	301	-	-	0/10/10/10	0/0/0/0
3	BOG	E	302	-	-	0/11/31/31	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	BOG	C3-C2	-4.02	1.41	1.52
3	E	302	BOG	C3-C2	-3.85	1.42	1.52
3	A	302	BOG	C3-C2	-3.84	1.42	1.52
3	B	302	BOG	C3-C2	-3.77	1.42	1.52
3	A	303	BOG	C3-C2	-3.58	1.43	1.52
3	A	303	BOG	C4-C3	-2.31	1.46	1.52
3	D	302	BOG	C4-C3	-2.25	1.46	1.52
3	A	302	BOG	C4-C3	-2.19	1.46	1.52
3	A	303	BOG	O1-C1	2.46	1.44	1.40
3	B	302	BOG	O5-C1	2.74	1.48	1.41
3	A	302	BOG	O5-C1	3.06	1.49	1.41
3	D	302	BOG	O5-C1	3.13	1.49	1.41
3	E	302	BOG	O5-C1	3.14	1.49	1.41
3	A	303	BOG	O5-C1	3.52	1.50	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	302	BOG	O3-C3-C2	-2.61	104.45	110.34
3	A	303	BOG	O2-C2-C1	-2.48	104.59	110.02
3	B	302	BOG	C1-O5-C5	-2.37	109.15	113.75
3	B	302	BOG	O3-C3-C2	-2.16	105.48	110.34
2	E	301	PG4	O3-C4-C3	2.03	119.41	110.36
2	E	301	PG4	O3-C5-C6	2.05	119.49	110.36
3	E	302	BOG	O1-C1'-C2'	2.06	118.08	109.88
2	A	301	PG4	C3-O2-C2	2.19	122.72	113.31
2	B	301	PG4	C3-O2-C2	2.33	123.32	113.31
2	A	301	PG4	O4-C6-C5	2.35	120.80	110.36
3	A	303	BOG	O5-C1-C2	2.35	115.10	110.28
3	A	303	BOG	O1-C1'-C2'	2.39	119.38	109.88
3	E	302	BOG	O5-C5-C6	2.46	112.56	106.36
3	E	302	BOG	O6-C6-C5	2.46	119.47	111.33
3	A	303	BOG	O6-C6-C5	2.54	119.72	111.33
2	B	301	PG4	O3-C4-C3	2.54	121.64	110.36
3	A	303	BOG	O5-C1-O1	2.84	116.89	110.05
3	D	302	BOG	O1-C1-C2	2.91	111.71	108.04
3	E	302	BOG	C1'-O1-C1	3.16	119.47	113.94
3	A	303	BOG	O5-C5-C6	3.47	115.13	106.36
3	A	303	BOG	C1-C2-C3	3.67	117.20	109.97
3	A	302	BOG	O1-C1-C2	3.79	112.82	108.04
3	D	302	BOG	C1'-O1-C1	4.09	121.09	113.94
3	A	302	BOG	C1'-O1-C1	4.15	121.20	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	BOG	O1-C1-C2	4.60	113.84	108.04
3	B	302	BOG	C1'-O1-C1	4.79	122.31	113.94
3	E	302	BOG	O1-C1-C2	6.65	116.44	108.04
3	A	303	BOG	C1'-O1-C1	6.90	126.00	113.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	PG4	2	0
3	A	302	BOG	2	0
2	B	301	PG4	5	0
2	D	301	PG4	1	0
3	D	302	BOG	2	0
2	E	301	PG4	4	0
3	E	302	BOG	10	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	257/268 (95%)	0.57	33 (12%) 5 6	27, 40, 63, 106	0
1	B	257/268 (95%)	0.36	27 (10%) 8 10	27, 39, 63, 87	0
1	C	266/268 (99%)	0.77	37 (13%) 4 5	32, 60, 96, 152	0
1	D	257/268 (95%)	0.35	18 (7%) 19 23	28, 44, 75, 118	0
1	E	256/268 (95%)	0.15	10 (3%) 43 47	29, 44, 67, 111	0
All	All	1293/1340 (96%)	0.44	125 (9%) 10 12	27, 45, 77, 152	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	219	SER	11.4
1	C	218	ILE	8.4
1	D	218	ILE	8.3
1	C	265	TYR	6.7
1	C	220	THR	5.7
1	B	185	ILE	5.5
1	A	185	ILE	5.1
1	E	218	ILE	4.6
1	A	184	ILE	4.6
1	B	184	ILE	4.3
1	D	185	ILE	4.3
1	C	3	LYS	4.2
1	C	217	THR	4.2
1	B	219	SER	4.2
1	A	17	ILE	4.2
1	A	188	PHE	4.1
1	B	188	PHE	4.0
1	B	187	ILE	3.9
1	A	189	LEU	3.9
1	A	101	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	224	GLY	3.8
1	C	110	TYR	3.8
1	C	222	THR	3.8
1	D	184	ILE	3.8
1	C	221	VAL	3.8
1	D	189	LEU	3.6
1	C	264	LEU	3.6
1	C	258	ASN	3.6
1	C	66	LEU	3.6
1	A	14	ILE	3.6
1	C	212	SER	3.5
1	D	182	ALA	3.4
1	B	189	LEU	3.4
1	C	223	ILE	3.4
1	D	186	MET	3.4
1	D	217	THR	3.4
1	B	69	ALA	3.3
1	E	184	ILE	3.2
1	A	187	ILE	3.2
1	B	76	ILE	3.2
1	B	66	LEU	3.2
1	B	70	ILE	3.2
1	D	188	PHE	3.2
1	C	56	GLY	3.2
1	A	191	LEU	3.1
1	A	181	THR	3.1
1	A	74	LEU	3.0
1	A	56	GLY	3.0
1	C	149	ALA	2.9
1	E	188	PHE	2.9
1	A	102	LYS	2.9
1	C	257	LEU	2.9
1	C	102	LYS	2.9
1	A	254	LYS	2.9
1	C	256	LYS	2.8
1	A	66	LEU	2.8
1	A	69	ALA	2.8
1	C	185	ILE	2.8
1	C	255	GLU	2.8
1	E	185	ILE	2.7
1	A	68	PHE	2.7
1	C	19	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	104	THR	2.7
1	C	93	GLY	2.7
1	C	14	ILE	2.6
1	D	181	THR	2.6
1	A	190	CYS	2.6
1	B	71	ALA	2.6
1	D	69	ALA	2.6
1	C	225	GLY	2.6
1	E	255	GLU	2.6
1	B	73	SER	2.6
1	C	101	ILE	2.6
1	C	188	PHE	2.5
1	C	216	PRO	2.5
1	C	55	ALA	2.5
1	B	182	ALA	2.5
1	A	99	VAL	2.5
1	E	181	THR	2.5
1	B	72	LEU	2.5
1	B	222	THR	2.5
1	B	191	LEU	2.4
1	B	75	VAL	2.4
1	B	74	LEU	2.4
1	E	221	VAL	2.4
1	A	171	VAL	2.4
1	A	105	SER	2.3
1	D	219	SER	2.3
1	B	181	THR	2.3
1	E	11	ASN	2.3
1	B	23	SER	2.3
1	A	71	ALA	2.3
1	B	63	VAL	2.3
1	A	194	ILE	2.3
1	E	189	LEU	2.3
1	A	44	LEU	2.3
1	E	102	LYS	2.3
1	A	98	GLY	2.3
1	A	182	ALA	2.3
1	C	27	TYR	2.3
1	B	190	CYS	2.2
1	A	97	LYS	2.2
1	C	72	LEU	2.2
1	C	0	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	66	LEU	2.2
1	B	68	PHE	2.2
1	D	0	ARG	2.2
1	B	225	GLY	2.2
1	D	99	VAL	2.2
1	D	221	VAL	2.2
1	A	94	MET	2.2
1	A	186	MET	2.2
1	D	191	LEU	2.1
1	D	190	CYS	2.1
1	B	38	VAL	2.1
1	A	70	ILE	2.1
1	A	54	ASP	2.1
1	A	11	ASN	2.1
1	C	71	ALA	2.0
1	B	40	ILE	2.0
1	D	17	ILE	2.0
1	C	250	TYR	2.0
1	B	0	ARG	2.0
1	C	54	ASP	2.0
1	C	103	ASP	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	BOG	A	303	20/20	0.85	0.23	9.08	49,70,104,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PG4	E	301	13/13	0.60	0.25	6.20	62,94,114,114	0
2	PG4	D	301	13/13	0.77	0.23	5.49	61,87,110,115	0
2	PG4	B	301	13/13	0.73	0.24	3.81	60,83,109,110	0
3	BOG	B	302	20/20	0.84	0.27	3.07	72,100,143,147	0
3	BOG	D	302	20/20	0.86	0.26	2.93	92,111,124,127	0
3	BOG	A	302	20/20	0.89	0.35	2.21	79,101,128,130	0
3	BOG	E	302	20/20	0.63	0.32	1.75	43,86,109,115	0
2	PG4	A	301	13/13	0.87	0.16	1.44	40,72,95,99	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.