



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:15 PM GMT

PDB ID : 3TE1  
Title : Crystal structure of HSC T84A  
Authors : Czyzewski, B.K.; Wang, D-N.  
Deposited on : 2011-08-11  
Resolution : 2.39 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

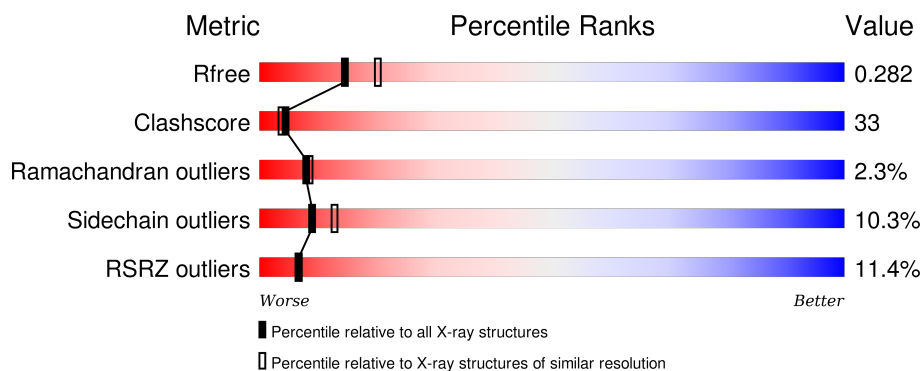
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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>10%</div> <div>54%</div> <div>32%</div> <div>9%</div> <div>.</div> </div>
1	B	268	<div> <div>7%</div> <div>58%</div> <div>32%</div> <div>5%</div> <div>.</div> </div>
1	C	268	<div> <div>22%</div> <div>40%</div> <div>47%</div> <div>11%</div> <div>..</div> </div>
1	D	268	<div> <div>8%</div> <div>62%</div> <div>32%</div> <div>..</div> <div>.</div> </div>
1	E	268	<div> <div>8%</div> <div>56%</div> <div>33%</div> <div>6%</div> <div>.</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	A	266	-	-	X	X
2	PG4	B	266	-	-	X	X
2	PG4	E	267	-	-	X	-
3	BOG	C	269	-	-	X	-
3	BOG	E	266	-	-	X	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9940 atoms, of which 128 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	A	257	Total	C	N	O	S	0	0	0
			1895	1243	299	339	14			
1	B	257	Total	C	N	O	S	0	0	0
			1899	1246	300	339	14			
1	C	266	Total	C	N	O	S	0	0	0
			1967	1289	311	353	14			
1	D	257	Total	C	N	O	S	0	0	0
			1899	1246	300	339	14			
1	E	256	Total	C	N	O	S	0	0	0
			1888	1240	296	338	14			

There are 60 discrepancies between the modelled and reference sequences:

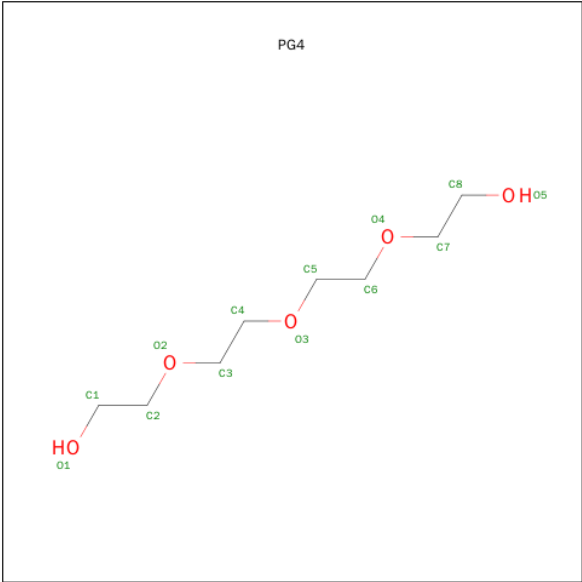
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP Q186B7
A	-1	GLY	-	EXPRESSION TAG	UNP Q186B7
A	0	ARG	-	EXPRESSION TAG	UNP Q186B7
A	1	ALA	-	EXPRESSION TAG	UNP Q186B7
A	84	ALA	THR	ENGINEERED MUTATION	UNP Q186B7
A	259	ALA	-	EXPRESSION TAG	UNP Q186B7
A	260	ALA	-	EXPRESSION TAG	UNP Q186B7
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	84	ALA	THR	ENGINEERED MUTATION	UNP Q186B7
B	259	ALA	-	EXPRESSION TAG	UNP Q186B7
B	260	ALA	-	EXPRESSION TAG	UNP Q186B7

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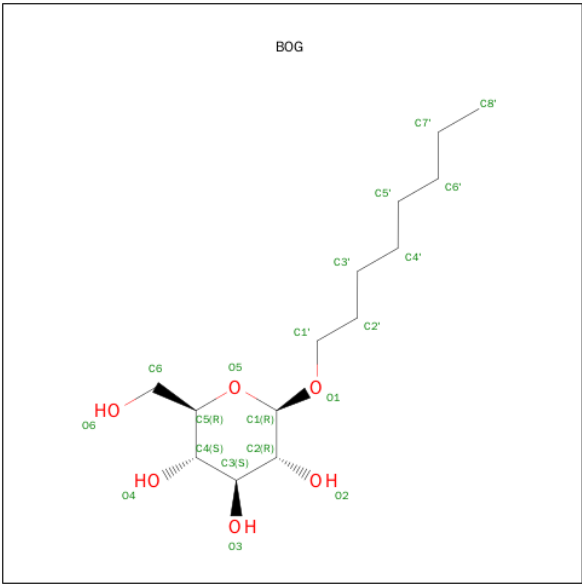
Chain	Residue	Modelled	Actual	Comment	Reference
B	261	ALA	-	EXPRESSION TAG	UNP Q186B7
B	262	GLU	-	EXPRESSION TAG	UNP Q186B7
B	263	ASN	-	EXPRESSION TAG	UNP Q186B7
B	264	LEU	-	EXPRESSION TAG	UNP Q186B7
B	265	TYR	-	EXPRESSION TAG	UNP Q186B7
C	-2	MET	-	EXPRESSION TAG	UNP Q186B7
C	-1	GLY	-	EXPRESSION TAG	UNP Q186B7
C	0	ARG	-	EXPRESSION TAG	UNP Q186B7
C	1	ALA	-	EXPRESSION TAG	UNP Q186B7
C	84	ALA	THR	ENGINEERED MUTATION	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	84	ALA	THR	ENGINEERED MUTATION	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
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	84	ALA	THR	ENGINEERED MUTATION	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

- 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	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		
2	E	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 3 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



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

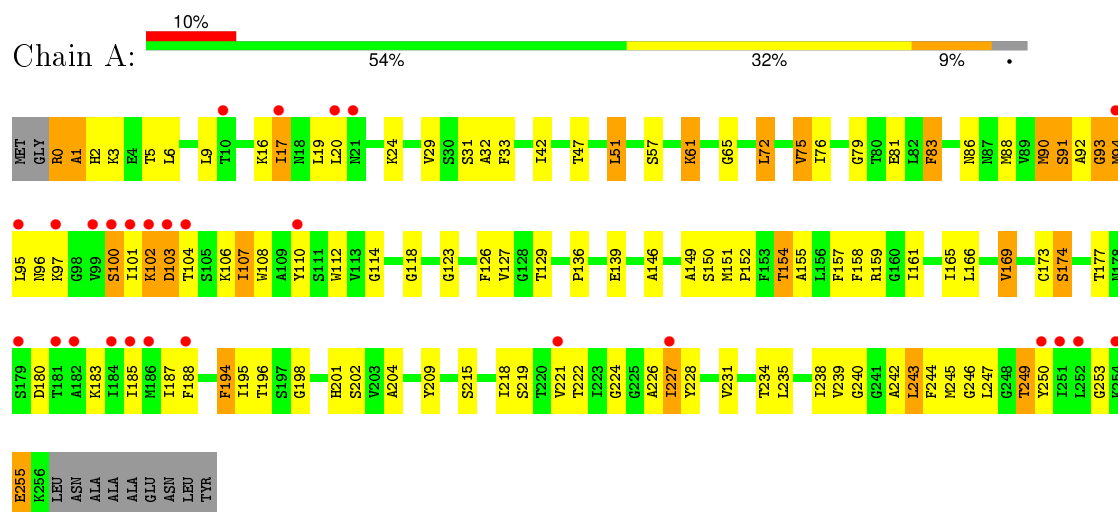
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total	O	0	0
			38	38		
4	B	34	Total	O	0	0
			34	34		
4	C	37	Total	O	0	0
			37	37		
4	D	28	Total	O	0	0
			28	28		
4	E	35	Total	O	0	0
			35	35		

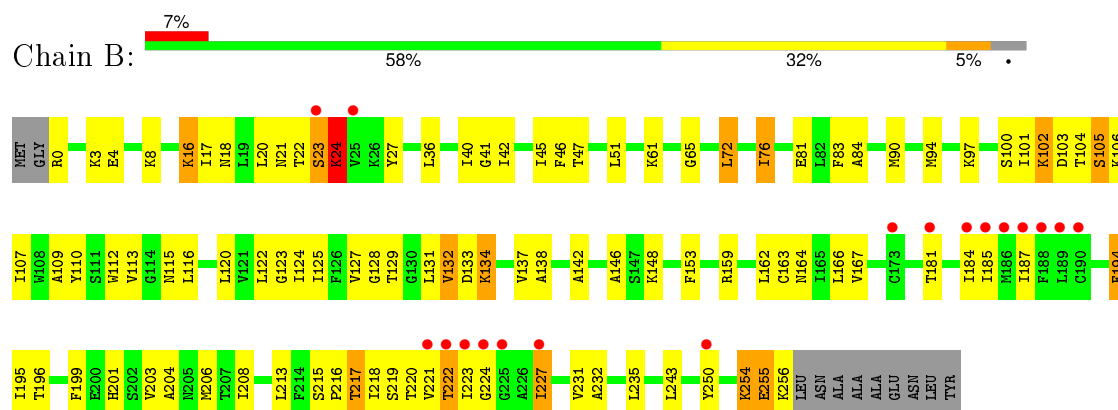
### 3 Residue-property plots

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.

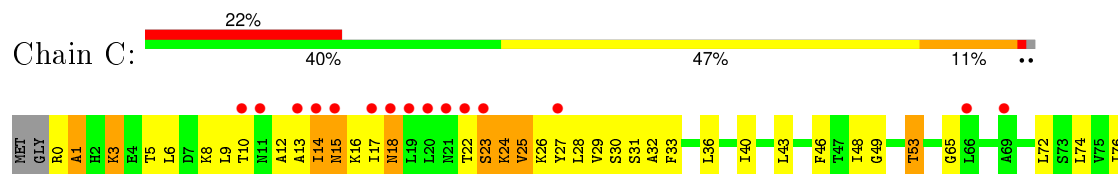
#### • Molecule 1: formate/nitrite transporter



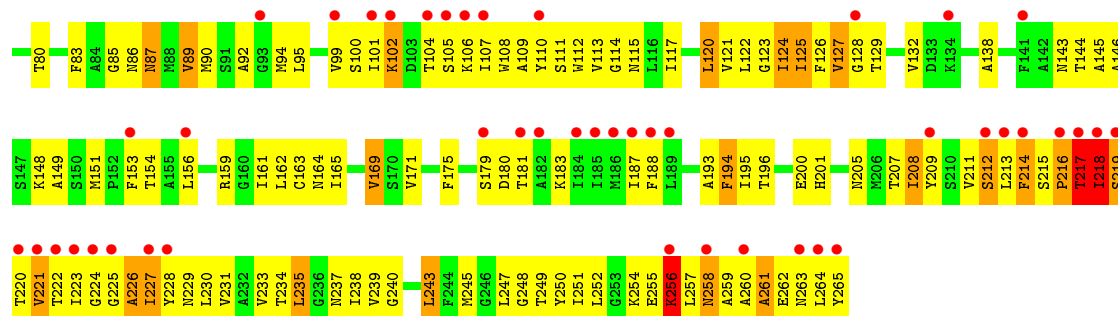
#### • Molecule 1: formate/nitrite transporter



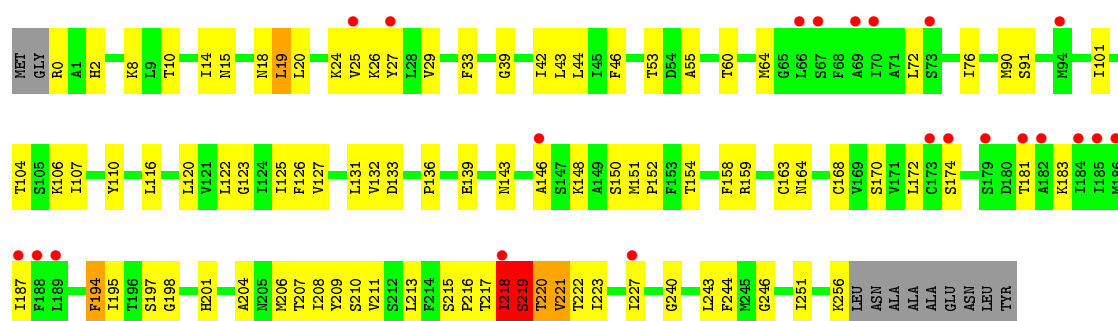
#### • Molecule 1: formate/nitrite transporter



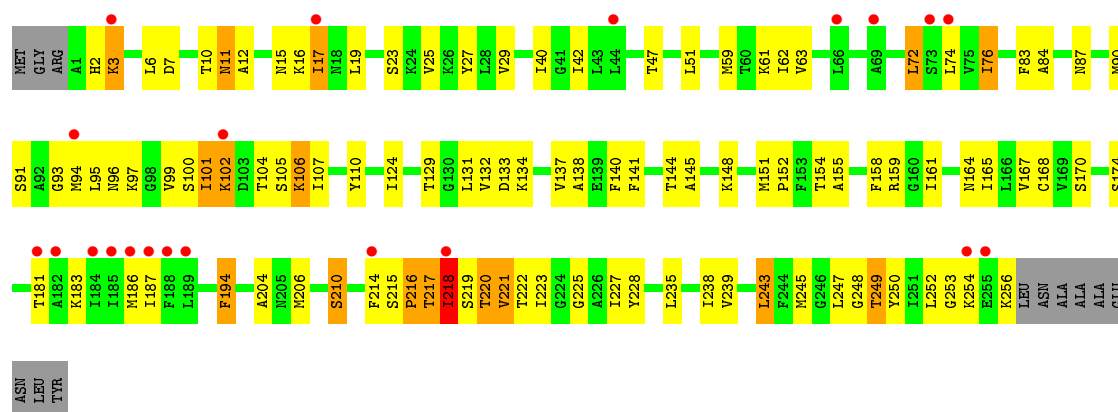




- Molecule 1: formate/nitrite transporter



- 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, $\alpha$ , $\beta$ , $\gamma$	99.04Å 118.41Å 150.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.16 – 2.39 48.16 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.16-2.39) 96.1 (48.16-2.39)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, $R_{free}$	0.213 , 0.275 0.227 , 0.282	Depositor DCC
$R_{free}$ test set	2000 reflections (3.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 70.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 69764 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9940	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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

### 5.1 Standard geometry

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	0.65	0/1927	0.68	0/2612
1	B	0.64	0/1931	0.68	0/2616
1	C	0.54	0/2000	0.68	0/2711
1	D	0.68	1/1931 (0.1%)	0.70	0/2616
1	E	0.65	0/1920	0.69	0/2602
All	All	0.63	1/9709 (0.0%)	0.69	0/13157

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	C	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	146	ALA	CA-CB	5.08	1.63	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	217	THR	Peptide
1	C	218	ILE	Peptide
1	C	256	LYS	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1895	0	1994	115	0
1	B	1899	0	2005	106	1
1	C	1967	0	2069	235	1
1	D	1899	0	2005	91	0
1	E	1888	0	1992	121	1
2	A	13	18	16	7	0
2	B	13	18	17	7	0
2	D	13	18	17	3	0
2	E	13	18	17	7	0
3	C	20	28	28	12	0
3	E	20	28	28	9	0
4	A	38	0	0	2	1
4	B	34	0	0	7	0
4	C	37	0	0	15	0
4	D	28	0	0	5	0
4	E	35	0	0	8	0
All	All	9812	128	10188	646	2

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 33.

All (646) 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:110:TYR:CE1	3:E:266:BOG:H2'1	1.76	1.20
1:C:145:ALA:O	4:C:297:HOH:O	1.63	1.17
1:C:258:ASN:HA	1:C:260:ALA:H	1.07	1.17
1:C:113:VAL:N	4:C:285:HOH:O	1.73	1.16
1:D:223:ILE:HG22	1:D:227:ILE:CD1	1.77	1.14
1:C:181:THR:HG21	3:C:269:BOG:C4'	1.76	1.13
1:C:258:ASN:N	1:C:259:ALA:HB3	1.63	1.12
1:E:124:ILE:HG13	1:E:214:PHE:CE2	1.86	1.09
1:C:181:THR:HG21	3:C:269:BOG:H4'1	1.16	1.09
1:B:222:THR:HG22	1:B:224:GLY:H	1.14	1.09
1:C:132:VAL:HG13	1:C:138:ALA:HA	1.31	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ALA:O	1:B:220:THR:HG21	1.54	1.07
1:A:151:MET:O	1:A:228:TYR:OH	1.69	1.07
1:A:227:ILE:O	1:A:227:ILE:HD12	1.56	1.06
1:A:224:GLY:O	1:A:227:ILE:HG22	1.56	1.03
1:C:23:SER:HB3	1:C:26:LYS:HB2	1.31	1.03
1:C:221:VAL:HG12	1:C:222:THR:N	1.72	1.03
1:C:181:THR:CG2	3:C:269:BOG:H4'1	1.90	1.01
3:C:269:BOG:H5'2	1:E:181:THR:HG21	1.43	1.01
1:C:0:ARG:HG2	1:C:1:ALA:H	1.25	1.01
1:D:223:ILE:CG2	1:D:227:ILE:HD11	1.91	1.00
1:E:110:TYR:CE1	3:E:266:BOG:C2'	2.47	0.96
1:D:223:ILE:HG22	1:D:227:ILE:HD12	1.45	0.96
1:B:227:ILE:HD12	1:B:227:ILE:H	1.29	0.95
1:D:223:ILE:HG22	1:D:227:ILE:HD11	1.48	0.94
1:C:218:ILE:HD12	1:C:219:SER:H	1.31	0.93
1:E:106:LYS:HG3	3:E:266:BOG:O2	1.69	0.92
1:B:148:LYS:HZ2	2:B:266:PG4:H72	1.35	0.92
1:C:219:SER:OG	1:C:220:THR:N	1.97	0.92
1:B:148:LYS:NZ	2:B:266:PG4:H72	1.85	0.91
1:E:223:ILE:O	1:E:227:ILE:HG13	1.71	0.90
1:C:258:ASN:HA	1:C:260:ALA:N	1.87	0.89
1:A:91:SER:HB3	1:A:246:GLY:HA3	1.53	0.89
1:B:213:LEU:HD13	1:B:223:ILE:HG12	1.54	0.89
1:A:79:GLY:O	1:D:0:ARG:HD2	1.72	0.89
1:A:224:GLY:O	1:A:227:ILE:CG2	2.19	0.88
1:C:14:ILE:O	1:C:17:ILE:HG22	1.73	0.88
1:E:90:MET:HE2	1:E:104:THR:HA	1.54	0.88
2:D:266:PG4:O5	4:D:271:HOH:O	1.89	0.88
1:C:258:ASN:ND2	4:C:289:HOH:O	2.07	0.88
1:E:223:ILE:HG22	1:E:227:ILE:HD11	1.55	0.87
1:E:110:TYR:CZ	3:E:266:BOG:H2'1	2.09	0.87
1:C:132:VAL:HG13	1:C:138:ALA:CA	2.07	0.85
1:C:161:ILE:HG23	1:C:240:GLY:HA2	1.59	0.84
1:C:223:ILE:HG22	1:C:227:ILE:HG12	1.59	0.83
1:B:36:LEU:HG	1:B:122:LEU:HD13	1.60	0.83
1:C:254:LYS:NZ	1:C:258:ASN:HB3	1.93	0.83
3:C:269:BOG:H4'2	1:D:181:THR:HG21	1.59	0.83
1:C:218:ILE:CD1	1:C:219:SER:H	1.92	0.83
1:B:222:THR:HG22	1:B:224:GLY:N	1.93	0.83
1:A:101:ILE:H	1:A:101:ILE:HD12	1.42	0.82
1:B:20:LEU:HD11	1:B:110:TYR:CD2	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LYS:NZ	1:B:106:LYS:HE2	1.94	0.81
1:D:143:ASN:ND2	4:D:274:HOH:O	2.07	0.81
1:C:217:THR:O	1:C:218:ILE:HG13	1.81	0.81
1:C:221:VAL:CG1	1:C:222:THR:N	2.44	0.81
1:C:87:ASN:HD22	1:C:87:ASN:N	1.76	0.81
1:A:224:GLY:C	1:A:227:ILE:HG22	2.02	0.80
1:C:239:VAL:HG13	1:C:243:LEU:HD13	1.62	0.80
1:B:250:TYR:CE1	1:B:254:LYS:HG2	2.16	0.80
1:C:49:GLY:O	1:C:53:THR:HB	1.82	0.79
1:E:214:PHE:O	1:E:216:PRO:HD3	1.82	0.79
1:A:234:THR:O	1:A:238:ILE:HG13	1.83	0.79
1:B:102:LYS:HZ1	1:B:106:LYS:HE2	1.46	0.79
1:A:222:THR:OG1	4:A:281:HOH:O	2.01	0.79
1:C:0:ARG:HG2	1:C:1:ALA:N	1.97	0.79
1:B:46:PHE:CZ	1:B:208:ILE:HD11	2.18	0.79
1:B:102:LYS:HA	1:B:105:SER:HB2	1.63	0.79
1:C:86:ASN:HD22	1:C:111:SER:CB	1.95	0.79
1:C:161:ILE:HG23	1:C:240:GLY:CA	2.13	0.78
1:D:223:ILE:CG2	1:D:227:ILE:CD1	2.52	0.78
1:C:46:PHE:HZ	1:C:208:ILE:HD11	1.47	0.78
3:C:269:BOG:C5'	1:E:181:THR:HG21	2.13	0.78
1:C:17:ILE:HG23	1:C:18:ASN:H	1.47	0.78
1:C:194:PHE:C	1:C:194:PHE:CD1	2.57	0.78
1:E:59:MET:O	1:E:63:VAL:HG23	1.83	0.77
1:C:31:SER:HB2	1:C:114:GLY:HA3	1.64	0.77
1:B:42:ILE:HD11	1:B:204:ALA:HB1	1.67	0.77
1:E:2:HIS:O	4:E:287:HOH:O	2.03	0.76
1:C:46:PHE:CZ	1:C:208:ILE:HD11	2.20	0.76
1:C:43:LEU:HD11	1:C:122:LEU:HD11	1.67	0.76
1:D:122:LEU:HD23	1:D:207:THR:HG21	1.66	0.76
1:E:101:ILE:HD12	1:E:101:ILE:H	1.49	0.76
1:A:72:LEU:HD12	1:A:75:VAL:HB	1.66	0.76
1:E:110:TYR:CD1	3:E:266:BOG:H2'1	2.21	0.75
1:C:32:ALA:HA	1:C:114:GLY:O	1.86	0.75
1:C:256:LYS:HE2	1:C:258:ASN:O	1.86	0.75
1:A:227:ILE:HD12	1:A:227:ILE:C	2.07	0.75
1:B:220:THR:HG23	1:B:221:VAL:HG13	1.68	0.74
1:D:133:ASP:HA	1:D:217:THR:HG21	1.69	0.74
1:C:121:VAL:O	1:C:125:ILE:HG13	1.88	0.74
1:B:222:THR:CG2	1:B:223:ILE:N	2.50	0.74
1:E:134:LYS:HD3	1:E:217:THR:HB	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LEU:HA	1:C:9:LEU:CD1	2.19	0.73
1:B:46:PHE:CZ	1:B:208:ILE:CD1	2.71	0.73
1:D:219:SER:OG	1:D:220:THR:N	2.21	0.72
1:A:245:MET:O	1:A:249:THR:OG1	2.07	0.72
1:B:116:LEU:HA	1:B:206:MET:SD	2.29	0.72
1:C:218:ILE:CG1	1:C:219:SER:H	2.01	0.72
1:A:174:SER:HA	1:A:183:LYS:HG2	1.70	0.72
1:C:76:ILE:HG13	1:C:187:ILE:HD11	1.72	0.72
1:C:254:LYS:HZ1	1:C:258:ASN:HB3	1.55	0.72
1:C:225:GLY:O	1:C:226:ALA:O	2.06	0.72
1:C:223:ILE:CG2	1:C:227:ILE:HG12	2.19	0.72
1:E:106:LYS:HE2	3:E:266:BOG:O2	1.90	0.72
1:C:149:ALA:HB1	1:C:225:GLY:HA2	1.70	0.72
1:C:17:ILE:HG23	1:C:18:ASN:N	2.05	0.71
1:C:258:ASN:N	1:C:259:ALA:CB	2.50	0.71
1:D:10:THR:O	1:D:14:ILE:HG13	1.89	0.71
1:C:251:ILE:O	1:D:26:LYS:HE2	1.90	0.71
1:E:133:ASP:O	1:E:134:LYS:HG2	1.89	0.71
1:D:90:MET:HE1	1:D:107:ILE:HG13	1.72	0.70
1:C:123:GLY:O	1:C:127:VAL:HG23	1.90	0.70
1:C:31:SER:CB	1:C:114:GLY:HA3	2.22	0.70
1:D:198:GLY:HA2	2:D:266:PG4:H31	1.73	0.69
1:B:102:LYS:NZ	1:B:102:LYS:HB2	2.07	0.69
1:B:203:VAL:HA	1:B:206:MET:HG3	1.73	0.69
1:C:223:ILE:HG22	1:C:227:ILE:CG1	2.22	0.69
1:C:161:ILE:HG12	1:C:239:VAL:HB	1.74	0.69
1:E:124:ILE:CG1	1:E:214:PHE:CE2	2.72	0.69
1:A:94:MET:O	1:A:97:LYS:N	2.20	0.69
1:C:148:LYS:HB3	1:C:229:ASN:ND2	2.08	0.69
1:E:158:PHE:HD1	1:E:161:ILE:HD12	1.58	0.68
1:A:235:LEU:O	1:A:239:VAL:HG23	1.93	0.68
1:A:151:MET:HG3	1:A:152:PRO:HD2	1.75	0.68
1:C:149:ALA:HB1	1:C:225:GLY:CA	2.23	0.68
1:C:87:ASN:HD22	1:C:87:ASN:H	1.41	0.68
1:E:223:ILE:HG22	1:E:227:ILE:CD1	2.23	0.68
1:A:107:ILE:HG22	1:A:108:TRP:HD1	1.58	0.68
1:E:94:MET:HG2	4:E:292:HOH:O	1.94	0.68
1:E:110:TYR:CZ	3:E:266:BOG:C2'	2.74	0.67
1:B:46:PHE:HZ	1:B:208:ILE:CD1	2.07	0.67
1:A:174:SER:O	1:A:183:LYS:HE2	1.94	0.67
1:D:139:GLU:O	1:D:143:ASN:ND2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:SER:OG	1:A:242:ALA:HA	1.95	0.67
1:B:18:ASN:OD1	4:B:284:HOH:O	2.11	0.67
1:A:91:SER:CB	1:A:246:GLY:HA3	2.24	0.67
1:A:17:ILE:HD13	1:A:103:ASP:HB3	1.77	0.67
1:C:109:ALA:O	4:C:285:HOH:O	2.12	0.66
1:C:129:THR:HB	1:E:159:ARG:HG2	1.77	0.66
1:C:23:SER:CB	1:C:26:LYS:HB2	2.16	0.66
1:C:17:ILE:CG2	1:C:18:ASN:H	2.08	0.66
1:A:185:ILE:HG21	1:B:184:ILE:HG21	1.77	0.66
1:A:240:GLY:O	1:A:244:PHE:HB2	1.94	0.66
1:B:224:GLY:HA2	1:B:227:ILE:HD13	1.77	0.66
1:C:223:ILE:CG2	1:C:227:ILE:CG1	2.73	0.66
3:C:269:BOG:H5'2	1:E:181:THR:CG2	2.22	0.66
1:C:218:ILE:HB	1:C:219:SER:HB3	1.76	0.66
1:A:102:LYS:HG2	1:A:103:ASP:OD1	1.96	0.66
1:E:101:ILE:CD1	1:E:101:ILE:H	2.08	0.66
1:E:215:SER:HB2	1:E:217:THR:HG23	1.78	0.65
1:B:222:THR:HG23	1:B:223:ILE:N	2.11	0.65
1:E:223:ILE:CG2	1:E:227:ILE:HD11	2.27	0.65
1:E:101:ILE:HD12	1:E:101:ILE:N	2.12	0.65
1:C:226:ALA:O	1:C:228:TYR:N	2.30	0.65
1:B:46:PHE:HZ	1:B:208:ILE:HD11	1.61	0.65
1:E:206:MET:O	1:E:210:SER:HB3	1.96	0.65
1:C:221:VAL:HG12	1:C:222:THR:H	1.56	0.65
1:C:86:ASN:ND2	1:C:111:SER:CB	2.59	0.65
1:D:123:GLY:O	1:D:127:VAL:HG23	1.97	0.65
1:A:3:LYS:HG2	1:A:253:GLY:O	1.96	0.64
1:C:0:ARG:NH1	4:C:291:HOH:O	2.29	0.64
1:D:217:THR:O	1:D:218:ILE:HG12	1.97	0.64
1:C:258:ASN:H	1:C:259:ALA:HB3	1.61	0.64
1:E:12:ALA:O	4:E:290:HOH:O	2.15	0.64
1:C:86:ASN:ND2	1:C:111:SER:HB2	2.11	0.64
1:D:25:VAL:O	1:D:29:VAL:HG23	1.97	0.64
1:A:3:LYS:HE3	1:A:255:GLU:OE1	1.97	0.64
1:C:216:PRO:O	1:C:218:ILE:N	2.31	0.64
1:E:155:ALA:O	1:E:159:ARG:HG3	1.98	0.64
1:E:7:ASP:O	1:E:11:ASN:HB2	1.98	0.64
1:B:220:THR:CG2	1:B:221:VAL:HG13	2.27	0.64
1:E:243:LEU:O	1:E:247:LEU:HB3	1.98	0.64
1:C:102:LYS:HB2	1:C:102:LYS:NZ	2.13	0.64
1:C:226:ALA:O	1:C:227:ILE:C	2.36	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:LEU:HD22	1:B:107:ILE:HD13	1.79	0.64
1:D:220:THR:HG23	1:D:220:THR:O	1.98	0.63
1:C:181:THR:HG21	3:C:269:BOG:C3'	2.28	0.63
1:B:222:THR:HG23	1:B:223:ILE:H	1.63	0.63
1:E:102:LYS:NZ	1:E:102:LYS:HB2	2.13	0.63
1:E:95:LEU:O	1:E:97:LYS:HE3	1.98	0.63
1:E:47:THR:HA	1:E:137:VAL:HG22	1.81	0.63
1:D:223:ILE:O	1:D:227:ILE:HD12	1.99	0.62
1:C:256:LYS:HZ3	1:C:262:GLU:C	2.00	0.62
1:A:91:SER:HB3	1:A:246:GLY:CA	2.26	0.62
1:C:124:ILE:HG13	1:C:214:PHE:CE2	2.34	0.62
1:E:158:PHE:CD1	1:E:161:ILE:HD12	2.34	0.62
1:B:146:ALA:HA	1:B:221:VAL:HG12	1.80	0.62
1:C:218:ILE:HD12	1:C:219:SER:N	2.09	0.62
1:C:218:ILE:CG1	1:C:219:SER:N	2.61	0.62
1:C:36:LEU:HG	1:C:122:LEU:HD22	1.82	0.62
1:C:161:ILE:HD13	1:C:239:VAL:HG11	1.81	0.62
1:A:209:TYR:CD1	1:A:226:ALA:HB2	2.35	0.62
1:B:129:THR:OG1	1:B:131:LEU:HD12	1.99	0.62
1:C:14:ILE:HG22	1:C:15:ASN:N	2.15	0.62
1:C:120:LEU:HD23	1:C:214:PHE:CE2	2.35	0.62
1:A:16:LYS:NZ	1:A:86:ASN:OD1	2.25	0.62
1:E:95:LEU:N	4:E:292:HOH:O	2.32	0.61
3:C:269:BOG:C4'	1:D:181:THR:HG21	2.27	0.61
1:A:215:SER:HB3	1:A:218:ILE:HD12	1.80	0.61
1:E:2:HIS:ND1	1:E:252:LEU:HB3	2.16	0.61
1:A:2:HIS:O	1:A:253:GLY:HA3	2.01	0.61
1:E:219:SER:OG	1:E:220:THR:N	2.32	0.61
1:B:109:ALA:O	1:B:113:VAL:HG23	2.00	0.61
1:C:143:ASN:O	1:C:146:ALA:HB3	2.00	0.61
1:C:113:VAL:HG23	4:C:285:HOH:O	2.01	0.60
1:C:230:LEU:O	1:C:234:THR:OG1	2.16	0.60
1:C:254:LYS:HZ2	1:C:258:ASN:HB3	1.66	0.60
1:E:90:MET:CE	1:E:104:THR:HA	2.28	0.60
1:D:90:MET:CE	1:D:107:ILE:HG13	2.31	0.60
1:C:24:LYS:O	1:C:28:LEU:HD12	2.01	0.60
1:C:87:ASN:H	1:C:87:ASN:ND2	1.98	0.60
1:C:258:ASN:CA	1:C:259:ALA:HB3	2.32	0.59
1:A:17:ILE:HD11	1:A:106:LYS:HD3	1.84	0.59
1:C:223:ILE:O	1:C:223:ILE:HG22	2.03	0.59
1:D:0:ARG:HB3	1:D:2:HIS:NE2	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:ILE:HG13	1:D:187:ILE:HD11	1.84	0.59
1:E:221:VAL:HG23	4:E:289:HOH:O	2.02	0.59
1:A:61:LYS:HG2	2:A:266:PG4:H21	1.85	0.59
1:C:132:VAL:HG13	1:C:138:ALA:CB	2.33	0.59
1:A:103:ASP:N	1:A:103:ASP:OD1	2.35	0.59
1:C:226:ALA:O	1:C:229:ASN:N	2.35	0.59
1:C:0:ARG:NH2	4:C:275:HOH:O	2.36	0.59
1:C:87:ASN:ND2	1:C:87:ASN:N	2.46	0.59
1:A:165:ILE:O	1:A:169:VAL:HB	2.03	0.59
1:B:213:LEU:CD1	1:B:223:ILE:HG12	2.30	0.59
1:E:151:MET:HG3	1:E:152:PRO:HD2	1.83	0.59
1:E:72:LEU:HD21	1:E:167:VAL:HG13	1.84	0.58
1:A:243:LEU:O	1:A:247:LEU:HB3	2.02	0.58
1:B:61:LYS:HE2	2:B:266:PG4:H12	1.86	0.58
1:A:6:LEU:HD22	1:A:250:TYR:HA	1.86	0.58
1:A:100:SER:OG	1:A:102:LYS:HB3	2.02	0.58
1:C:112:TRP:N	4:C:285:HOH:O	2.37	0.58
1:C:179:SER:O	1:C:183:LYS:HG3	2.04	0.58
1:B:223:ILE:O	1:B:223:ILE:HG22	2.04	0.58
1:A:157:PHE:CZ	1:A:239:VAL:HG21	2.39	0.58
1:D:122:LEU:HD23	1:D:207:THR:CG2	2.34	0.58
1:C:6:LEU:HA	1:C:9:LEU:HD12	1.84	0.58
1:E:164:ASN:O	1:E:168:CYS:HB2	2.04	0.58
1:B:250:TYR:CZ	1:B:254:LYS:HG2	2.38	0.58
1:B:220:THR:HG23	1:B:221:VAL:CG1	2.33	0.57
1:E:245:MET:O	1:E:249:THR:OG1	2.22	0.57
1:C:223:ILE:CG2	1:C:227:ILE:HD11	2.35	0.57
1:A:92:ALA:O	1:A:94:MET:N	2.37	0.57
1:E:84:ALA:HB1	1:E:164:ASN:OD1	2.05	0.57
1:C:94:MET:HA	1:C:99:VAL:O	2.05	0.57
1:B:215:SER:HB3	1:B:218:ILE:HD12	1.86	0.57
1:E:94:MET:C	4:E:292:HOH:O	2.42	0.57
1:C:248:GLY:O	1:C:252:LEU:HG	2.05	0.57
1:C:3:LYS:HZ3	1:C:255:GLU:HB3	1.69	0.57
1:C:0:ARG:O	1:C:1:ALA:CB	2.52	0.57
1:D:219:SER:OG	1:D:220:THR:HG22	2.05	0.57
1:C:207:THR:O	1:C:211:VAL:HG23	2.04	0.57
1:B:76:ILE:HG12	1:B:187:ILE:HD11	1.86	0.57
1:C:148:LYS:C	1:C:229:ASN:HD22	2.08	0.56
1:D:154:THR:HG23	1:D:158:PHE:HE2	1.69	0.56
1:C:209:TYR:O	1:C:213:LEU:HG	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:THR:HG21	3:C:269:BOG:C5'	2.33	0.56
1:E:61:LYS:CE	2:E:267:PG4:H22	2.36	0.56
1:A:0:ARG:HD3	1:A:1:ALA:N	2.19	0.56
1:E:132:VAL:HA	1:E:138:ALA:HB2	1.88	0.56
1:A:24:LYS:HG2	1:A:110:TYR:CE2	2.40	0.56
1:C:257:LEU:C	1:C:259:ALA:HB3	2.24	0.56
1:D:90:MET:HB3	1:D:104:THR:HG23	1.88	0.56
1:C:17:ILE:CG2	1:C:18:ASN:N	2.68	0.56
1:E:47:THR:O	1:E:51:LEU:HG	2.06	0.56
1:D:116:LEU:HA	1:D:206:MET:SD	2.45	0.56
1:C:225:GLY:O	1:C:226:ALA:C	2.45	0.56
1:D:133:ASP:CA	1:D:217:THR:HG21	2.35	0.56
1:A:166:LEU:HD13	1:A:194:PHE:HB3	1.88	0.56
1:C:250:TYR:CE1	1:C:254:LYS:HD3	2.41	0.55
1:B:146:ALA:HB2	1:B:220:THR:HG23	1.88	0.55
1:C:164:ASN:ND2	1:C:237:ASN:HB3	2.22	0.55
1:C:132:VAL:CG1	1:C:138:ALA:HA	2.21	0.55
1:C:86:ASN:HD22	1:C:111:SER:HB2	1.64	0.55
1:C:149:ALA:N	4:C:297:HOH:O	2.38	0.55
1:E:235:LEU:HA	1:E:238:ILE:HD12	1.89	0.55
1:C:27:TYR:OH	1:C:107:ILE:HG23	2.06	0.55
1:D:194:PHE:CE1	1:D:195:ILE:HD13	2.42	0.55
1:C:148:LYS:HB3	1:C:229:ASN:HD21	1.70	0.55
1:B:181:THR:HG21	3:C:269:BOG:H5'1	1.89	0.55
1:C:9:LEU:H	1:C:9:LEU:HD12	1.70	0.55
1:A:61:LYS:HG2	2:A:266:PG4:H12	1.89	0.55
1:B:61:LYS:HE2	2:B:266:PG4:C2	2.37	0.55
1:E:94:MET:SD	1:E:101:ILE:HA	2.47	0.55
1:D:154:THR:HG23	1:D:158:PHE:CE2	2.42	0.55
1:E:76:ILE:HG12	1:E:187:ILE:HD11	1.89	0.55
1:B:132:VAL:HG12	1:B:138:ALA:HA	1.88	0.54
1:C:159:ARG:HB3	1:C:200:GLU:HG2	1.89	0.54
1:E:218:ILE:HG13	1:E:218:ILE:O	2.07	0.54
1:C:143:ASN:O	1:C:146:ALA:N	2.40	0.54
1:A:173:CYS:O	1:A:177:THR:HG22	2.07	0.54
1:B:116:LEU:CA	1:B:206:MET:SD	2.96	0.54
1:A:123:GLY:O	1:A:127:VAL:HG23	2.06	0.54
1:A:24:LYS:HG2	1:A:110:TYR:HE2	1.72	0.54
1:E:42:ILE:HD11	1:E:204:ALA:HB1	1.89	0.54
1:E:11:ASN:O	1:E:15:ASN:ND2	2.40	0.54
1:A:157:PHE:HZ	1:A:239:VAL:HG21	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:SER:OG	1:D:246:GLY:HA3	2.08	0.54
1:B:94:MET:SD	1:B:101:ILE:HG12	2.48	0.54
1:C:227:ILE:O	1:C:231:VAL:HG23	2.08	0.54
1:B:227:ILE:H	1:B:227:ILE:CD1	2.03	0.54
1:D:207:THR:O	1:D:211:VAL:HG23	2.08	0.54
1:D:218:ILE:HA	4:D:269:HOH:O	2.07	0.54
1:A:79:GLY:HA2	1:D:0:ARG:HH21	1.73	0.53
1:E:215:SER:HB2	1:E:217:THR:CG2	2.38	0.53
1:A:2:HIS:O	1:A:253:GLY:CA	2.56	0.53
1:D:194:PHE:CD1	1:D:194:PHE:C	2.80	0.53
1:C:30:SER:O	1:C:80:THR:HB	2.07	0.53
1:D:76:ILE:CG1	1:D:187:ILE:HD11	2.37	0.53
1:B:194:PHE:C	1:B:194:PHE:CD1	2.81	0.53
1:C:16:LYS:HB3	1:C:107:ILE:HD12	1.89	0.53
1:A:227:ILE:CD1	1:A:231:VAL:HG23	2.39	0.53
1:E:61:LYS:HG2	2:E:267:PG4:H31	1.91	0.53
1:C:243:LEU:O	1:C:247:LEU:HB3	2.09	0.53
1:A:42:ILE:HD11	1:A:204:ALA:HB1	1.90	0.53
1:B:124:ILE:HG22	1:B:125:ILE:N	2.22	0.53
1:C:109:ALA:O	1:C:113:VAL:HG23	2.08	0.53
1:C:85:GLY:O	1:C:89:VAL:HG23	2.09	0.53
1:E:61:LYS:HE2	2:E:267:PG4:H22	1.89	0.53
1:D:0:ARG:H1	1:D:0:ARG:HD3	1.74	0.53
1:E:221:VAL:C	1:E:222:THR:HG23	2.30	0.53
1:C:225:GLY:O	1:C:228:TYR:HB3	2.09	0.52
1:C:256:LYS:HG3	1:C:259:ALA:N	2.24	0.52
1:E:133:ASP:O	1:E:134:LYS:CG	2.56	0.52
1:D:151:MET:HG3	1:D:152:PRO:HD2	1.90	0.52
1:A:227:ILE:CD1	1:A:227:ILE:C	2.77	0.52
1:E:87:ASN:O	1:E:91:SER:HB3	2.09	0.52
1:C:121:VAL:HA	1:C:124:ILE:CD1	2.39	0.52
1:A:108:TRP:O	1:A:112:TRP:HB2	2.08	0.52
1:C:13:ALA:HB1	1:C:90:MET:HE1	1.91	0.52
1:C:194:PHE:CE1	1:C:195:ILE:HD13	2.45	0.52
1:B:36:LEU:HD12	1:B:122:LEU:HB2	1.91	0.52
1:E:144:THR:CG2	1:E:148:LYS:HE2	2.40	0.52
1:C:46:PHE:CZ	1:C:208:ILE:CD1	2.91	0.52
1:A:157:PHE:CE2	1:A:161:ILE:HD11	2.43	0.52
1:B:90:MET:HB3	1:B:104:THR:HG23	1.91	0.52
1:C:121:VAL:HA	1:C:124:ILE:HD12	1.91	0.52
1:A:6:LEU:O	1:A:6:LEU:HD12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ILE:HG23	1:E:62:ILE:HD11	1.92	0.51
1:A:76:ILE:HG13	1:A:187:ILE:HD11	1.91	0.51
1:D:216:PRO:O	1:D:218:ILE:HG23	2.11	0.51
1:B:133:ASP:O	1:B:134:LYS:HB3	2.11	0.51
1:A:151:MET:O	1:A:228:TYR:CZ	2.61	0.51
1:A:227:ILE:HD11	1:A:231:VAL:HG23	1.92	0.51
1:C:180:ASP:HA	1:C:183:LYS:HG3	1.93	0.51
1:C:105:SER:HA	1:C:108:TRP:HB2	1.93	0.51
1:B:102:LYS:O	1:B:106:LYS:HG2	2.11	0.51
1:D:8:LYS:HE2	4:D:290:HOH:O	2.09	0.51
1:C:101:ILE:HD12	1:C:101:ILE:H	1.76	0.50
1:B:163:CYS:SG	1:B:201:HIS:HB2	2.50	0.50
1:A:151:MET:CG	1:A:152:PRO:HD2	2.40	0.50
1:C:216:PRO:C	1:C:218:ILE:H	2.13	0.50
1:C:161:ILE:CD1	1:C:239:VAL:HG11	2.42	0.50
1:C:239:VAL:O	1:C:243:LEU:HB2	2.11	0.50
1:D:53:THR:C	1:D:55:ALA:H	2.15	0.50
1:C:256:LYS:NZ	1:C:262:GLU:O	2.34	0.50
1:B:148:LYS:HZ1	2:B:266:PG4:H72	1.69	0.50
1:C:102:LYS:O	1:C:106:LYS:HB2	2.12	0.50
1:C:208:ILE:O	1:C:212:SER:OG	2.29	0.50
1:B:146:ALA:HB2	1:B:220:THR:CG2	2.42	0.50
1:E:133:ASP:C	1:E:134:LYS:HG2	2.32	0.50
1:B:115:ASN:HB3	1:B:203:VAL:HG13	1.93	0.50
1:A:88:MET:HA	1:A:91:SER:HB2	1.94	0.49
1:C:194:PHE:O	1:C:194:PHE:HD1	1.95	0.49
1:E:72:LEU:HB3	1:E:187:ILE:HG23	1.93	0.49
1:D:15:ASN:O	1:D:19:LEU:HB2	2.12	0.49
1:C:209:TYR:CE2	1:C:226:ALA:HA	2.47	0.49
1:E:10:THR:HA	1:E:93:GLY:HA2	1.94	0.49
1:B:181:THR:O	1:B:185:ILE:HG13	2.12	0.49
1:C:127:VAL:HG11	1:C:215:SER:HA	1.95	0.49
1:C:163:CYS:SG	1:C:201:HIS:HB2	2.53	0.49
1:C:5:THR:HG22	1:C:9:LEU:HD11	1.95	0.49
1:E:215:SER:C	1:E:217:THR:H	2.16	0.49
1:C:36:LEU:CD1	1:C:122:LEU:HB2	2.43	0.49
1:C:217:THR:C	1:C:218:ILE:HG13	2.33	0.48
1:E:102:LYS:HZ1	1:E:102:LYS:HB2	1.76	0.48
1:D:101:ILE:N	1:D:101:ILE:HD12	2.28	0.48
1:B:102:LYS:HZ2	1:B:106:LYS:HE2	1.74	0.48
1:D:164:ASN:O	1:D:168:CYS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:GLY:O	1:B:127:VAL:HG23	2.12	0.48
1:E:148:LYS:NZ	2:E:267:PG4:O5	2.32	0.48
1:E:174:SER:HA	1:E:183:LYS:HG2	1.94	0.48
1:C:72:LEU:O	1:C:76:ILE:HG12	2.14	0.48
1:C:164:ASN:HD22	1:C:237:ASN:HB3	1.79	0.48
1:A:224:GLY:CA	1:A:227:ILE:HG22	2.43	0.48
1:A:72:LEU:CD1	1:A:75:VAL:HB	2.40	0.48
1:B:47:THR:O	1:B:51:LEU:HG	2.14	0.48
1:C:223:ILE:CG2	1:C:227:ILE:CD1	2.91	0.48
1:C:217:THR:C	1:C:218:ILE:CG1	2.81	0.48
1:C:247:LEU:O	1:C:247:LEU:HD12	2.13	0.48
1:B:24:LYS:O	1:B:27:TYR:N	2.47	0.48
1:C:74:LEU:HD23	1:E:186:MET:CE	2.44	0.48
1:C:251:ILE:O	1:D:26:LYS:CE	2.61	0.48
1:A:83:PHE:CD1	1:A:112:TRP:HB2	2.49	0.48
1:A:166:LEU:O	1:A:169:VAL:HG12	2.14	0.48
1:C:245:MET:O	1:C:249:THR:OG1	2.19	0.48
1:E:17:ILE:HD12	1:E:17:ILE:O	2.14	0.48
1:C:151:MET:O	1:C:228:TYR:OH	2.17	0.48
1:A:227:ILE:HG23	1:A:228:TYR:N	2.29	0.48
1:A:126:PHE:O	1:A:129:THR:OG1	2.22	0.48
1:A:154:THR:CG2	1:A:155:ALA:N	2.75	0.48
1:A:90:MET:HB2	1:A:108:TRP:HE1	1.78	0.47
1:E:10:THR:HG22	1:E:11:ASN:N	2.29	0.47
1:E:72:LEU:HB3	1:E:187:ILE:CG2	2.44	0.47
1:E:248:GLY:O	1:E:252:LEU:HG	2.14	0.47
1:C:87:ASN:OD1	1:C:238:ILE:HA	2.14	0.47
1:B:231:VAL:HG12	1:B:232:ALA:N	2.29	0.47
1:D:107:ILE:HD13	1:D:107:ILE:HA	1.73	0.47
1:A:90:MET:HG3	1:A:104:THR:OG1	2.14	0.47
1:C:159:ARG:HB3	1:C:200:GLU:CG	2.45	0.47
1:B:203:VAL:CA	1:B:206:MET:HG3	2.44	0.47
1:E:221:VAL:O	1:E:222:THR:HG23	2.14	0.47
1:B:215:SER:HA	1:B:216:PRO:HD3	1.76	0.47
1:C:259:ALA:C	1:C:261:ALA:H	2.18	0.47
1:E:10:THR:OG1	1:E:96:ASN:HB3	2.14	0.47
1:E:218:ILE:C	1:E:218:ILE:HD12	2.34	0.47
1:A:61:LYS:HG2	2:A:266:PG4:C1	2.45	0.47
1:B:65:GLY:HA3	1:B:196:THR:OG1	2.13	0.47
1:B:61:LYS:HE2	2:B:266:PG4:C1	2.44	0.47
1:E:3:LYS:HE3	1:E:7:ASP:OD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LYS:HZ3	1:B:102:LYS:HB2	1.78	0.47
1:A:159:ARG:CG	1:B:129:THR:HB	2.45	0.46
1:E:219:SER:OG	1:E:221:VAL:HG22	2.14	0.46
1:D:72:LEU:HB3	1:D:187:ILE:CG2	2.45	0.46
1:A:92:ALA:O	1:A:93:GLY:C	2.52	0.46
1:C:143:ASN:ND2	4:C:296:HOH:O	2.18	0.46
1:A:166:LEU:HD21	1:B:40:ILE:HG21	1.98	0.46
1:C:222:THR:C	1:C:224:GLY:N	2.69	0.46
1:A:17:ILE:HD13	1:A:103:ASP:CB	2.44	0.46
1:B:0:ARG:N	4:B:291:HOH:O	2.48	0.46
1:C:148:LYS:O	1:C:229:ASN:ND2	2.39	0.46
1:A:47:THR:HG22	1:A:51:LEU:CD1	2.46	0.46
1:D:223:ILE:C	1:D:227:ILE:HD12	2.36	0.46
1:A:16:LYS:O	1:A:19:LEU:HB3	2.16	0.46
1:B:116:LEU:O	1:B:120:LEU:HG	2.16	0.46
1:A:195:ILE:HD12	2:A:266:PG4:H62	1.97	0.46
1:C:22:THR:O	1:C:22:THR:HG22	2.13	0.46
1:C:223:ILE:HG21	1:C:227:ILE:HD11	1.96	0.46
1:D:133:ASP:HA	1:D:217:THR:CG2	2.41	0.46
1:E:3:LYS:HA	1:E:253:GLY:O	2.14	0.46
1:C:149:ALA:CB	1:C:225:GLY:CA	2.94	0.46
1:B:250:TYR:O	1:B:254:LYS:HB2	2.16	0.46
1:C:106:LYS:O	1:C:110:TYR:N	2.43	0.46
1:E:222:THR:N	4:E:289:HOH:O	2.05	0.46
1:C:146:ALA:HB3	4:C:287:HOH:O	2.16	0.46
1:E:87:ASN:O	1:E:91:SER:CB	2.64	0.46
1:C:104:THR:HG22	1:C:105:SER:N	2.30	0.46
1:E:124:ILE:HG13	1:E:214:PHE:CD2	2.46	0.46
1:A:17:ILE:HD13	1:A:103:ASP:CA	2.46	0.46
1:D:53:THR:C	1:D:55:ALA:N	2.70	0.46
1:A:29:VAL:HG21	1:D:251:ILE:HG21	1.98	0.46
1:B:166:LEU:HD23	1:B:166:LEU:HA	1.81	0.46
1:A:185:ILE:CG2	1:B:184:ILE:HG21	2.44	0.46
1:B:16:LYS:HD3	1:B:81:GLU:OE1	2.16	0.46
1:C:162:LEU:HD21	1:D:125:ILE:HG21	1.97	0.45
1:E:194:PHE:CD1	1:E:194:PHE:C	2.89	0.45
1:B:199:PHE:CD1	1:B:199:PHE:N	2.83	0.45
1:B:72:LEU:HD21	1:B:167:VAL:HG13	1.99	0.45
1:A:91:SER:HG	1:A:242:ALA:HA	1.79	0.45
1:E:239:VAL:O	1:E:243:LEU:HB3	2.16	0.45
1:E:223:ILE:HG22	1:E:227:ILE:CG1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:THR:HG22	1:E:148:LYS:HE2	1.97	0.45
1:A:47:THR:O	1:A:51:LEU:HD12	2.15	0.45
1:C:227:ILE:HD13	1:C:227:ILE:H	1.81	0.45
1:E:132:VAL:O	1:E:217:THR:HG21	2.17	0.45
1:D:14:ILE:HG22	1:D:18:ASN:ND2	2.32	0.45
1:D:72:LEU:HD12	1:D:72:LEU:HA	1.64	0.45
1:A:61:LYS:HE2	2:A:266:PG4:H11	1.99	0.45
1:E:104:THR:O	1:E:104:THR:HG22	2.17	0.45
1:E:132:VAL:CA	1:E:138:ALA:HB2	2.46	0.45
1:A:0:ARG:HD3	1:A:0:ARG:C	2.37	0.45
1:C:3:LYS:NZ	1:C:255:GLU:HB3	2.32	0.45
1:B:222:THR:HG22	1:B:223:ILE:N	2.29	0.45
1:D:126:PHE:CE2	1:D:132:VAL:HG13	2.51	0.45
1:C:65:GLY:HA3	1:C:196:THR:OG1	2.17	0.45
1:E:6:LEU:HD22	1:E:250:TYR:HA	1.99	0.45
1:C:201:HIS:HB3	4:C:268:HOH:O	2.16	0.45
1:C:25:VAL:O	1:C:29:VAL:HG23	2.17	0.45
1:C:153:PHE:C	1:C:153:PHE:CD1	2.89	0.45
1:B:100:SER:HB3	1:B:103:ASP:CG	2.36	0.45
1:C:10:THR:C	1:C:12:ALA:H	2.20	0.45
1:B:102:LYS:HZ2	1:B:102:LYS:HB2	1.81	0.45
1:B:254:LYS:HD2	1:B:255:GLU:N	2.32	0.45
1:C:36:LEU:O	1:C:40:ILE:HG13	2.17	0.45
1:C:164:ASN:HD22	1:C:237:ASN:C	2.20	0.45
1:A:20:LEU:O	1:A:20:LEU:HD12	2.17	0.45
1:D:60:THR:O	1:D:64:MET:HG3	2.17	0.45
1:C:258:ASN:H	1:C:259:ALA:CB	2.23	0.45
1:C:222:THR:C	1:C:224:GLY:H	2.19	0.45
1:B:133:ASP:O	1:B:217:THR:HG21	2.17	0.45
1:D:223:ILE:H	1:D:223:ILE:HD12	1.82	0.44
1:C:126:PHE:CE2	1:C:132:VAL:CG2	3.00	0.44
1:A:101:ILE:CD1	1:A:101:ILE:H	2.16	0.44
1:E:16:LYS:O	1:E:19:LEU:HB3	2.17	0.44
1:E:129:THR:OG1	1:E:131:LEU:HD12	2.17	0.44
1:C:234:THR:O	1:C:235:LEU:C	2.54	0.44
1:B:224:GLY:CA	1:B:227:ILE:HD13	2.45	0.44
1:C:132:VAL:O	1:C:132:VAL:HG12	2.17	0.44
1:D:136:PRO:HA	1:D:139:GLU:HB2	1.99	0.44
1:C:30:SER:HB2	1:E:252:LEU:HD22	1.99	0.44
1:C:46:PHE:CZ	1:C:144:THR:HG21	2.53	0.44
1:C:205:ASN:HA	1:C:208:ILE:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:PRO:HB2	1:C:217:THR:H	1.64	0.44
1:B:61:LYS:HE2	2:B:266:PG4:H21	2.00	0.44
1:D:201:HIS:ND1	1:D:204:ALA:HB2	2.33	0.44
1:E:110:TYR:CZ	3:E:266:BOG:H2'2	2.53	0.44
1:A:107:ILE:HG22	1:A:108:TRP:CD1	2.47	0.44
1:B:153:PHE:CD2	1:B:232:ALA:HB2	2.53	0.44
1:C:46:PHE:HZ	1:C:208:ILE:CD1	2.24	0.44
1:B:61:LYS:NZ	4:B:301:HOH:O	2.50	0.44
1:C:17:ILE:HA	1:C:107:ILE:HD11	1.99	0.44
1:D:120:LEU:HA	1:D:210:SER:OG	2.18	0.44
1:D:221:VAL:C	1:D:222:THR:HG23	2.38	0.44
1:C:256:LYS:C	1:C:259:ALA:HB2	2.38	0.43
1:C:126:PHE:CE2	1:C:132:VAL:HG23	2.53	0.43
1:C:257:LEU:CA	1:C:259:ALA:HB3	2.46	0.43
1:C:262:GLU:HG3	1:C:263:ASN:N	2.32	0.43
1:C:0:ARG:CG	1:C:1:ALA:N	2.68	0.43
1:E:217:THR:O	1:E:217:THR:OG1	2.31	0.43
1:A:180:ASP:HA	1:A:183:LYS:HD2	2.00	0.43
1:B:137:VAL:HB	4:B:297:HOH:O	2.19	0.43
1:C:258:ASN:CA	1:C:260:ALA:H	2.00	0.43
1:A:151:MET:HA	1:A:152:PRO:HD3	1.90	0.43
1:A:94:MET:C	1:A:96:ASN:N	2.71	0.43
1:A:136:PRO:HA	1:A:139:GLU:HB2	2.00	0.43
1:C:83:PHE:CE2	1:C:234:THR:HG23	2.53	0.43
1:A:79:GLY:CA	1:D:0:ARG:HH21	2.31	0.43
1:B:65:GLY:HA2	1:B:195:ILE:HB	2.01	0.43
1:D:46:PHE:CZ	1:D:208:ILE:CD1	3.01	0.43
1:D:209:TYR:O	1:D:213:LEU:HG	2.19	0.43
1:C:216:PRO:C	1:C:218:ILE:N	2.71	0.43
1:C:194:PHE:O	1:C:194:PHE:CD1	2.71	0.43
1:A:102:LYS:HG2	1:A:103:ASP:N	2.32	0.43
1:E:61:LYS:NZ	2:E:267:PG4:H22	2.34	0.43
1:C:171:VAL:O	1:C:175:PHE:HD2	2.00	0.43
1:C:83:PHE:N	1:C:115:ASN:OD1	2.43	0.43
1:D:46:PHE:CZ	1:D:208:ILE:HD11	2.54	0.43
1:B:8:LYS:HD3	4:B:287:HOH:O	2.19	0.43
1:D:240:GLY:O	1:D:244:PHE:HB2	2.18	0.43
1:C:3:LYS:HZ3	1:C:255:GLU:CB	2.30	0.43
1:C:32:ALA:CA	1:C:114:GLY:O	2.64	0.43
1:A:247:LEU:HD12	1:A:247:LEU:O	2.19	0.43
1:D:42:ILE:O	1:D:46:PHE:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:O	1:A:72:LEU:HD12	2.18	0.42
1:C:121:VAL:O	1:C:125:ILE:CG1	2.64	0.42
1:C:5:THR:O	1:C:8:LYS:N	2.51	0.42
1:E:110:TYR:CE1	3:E:266:BOG:C1'	3.02	0.42
1:D:223:ILE:HD12	1:D:223:ILE:N	2.34	0.42
1:A:224:GLY:HA2	1:A:227:ILE:HG22	2.02	0.42
1:C:12:ALA:O	1:C:16:LYS:HG3	2.18	0.42
1:A:61:LYS:HG2	2:A:266:PG4:C2	2.48	0.42
1:A:32:ALA:O	1:A:118:GLY:HA3	2.19	0.42
4:A:291:HOH:O	1:D:172:LEU:HD21	2.18	0.42
1:E:218:ILE:HD12	1:E:219:SER:N	2.34	0.42
1:E:235:LEU:O	1:E:238:ILE:HB	2.19	0.42
1:C:162:LEU:O	1:C:163:CYS:C	2.58	0.42
1:D:27:TYR:OH	1:D:107:ILE:HD12	2.20	0.42
1:C:16:LYS:CB	1:C:107:ILE:HD12	2.50	0.42
1:D:39:GLY:HA3	1:D:122:LEU:CD2	2.50	0.42
1:A:159:ARG:HG3	1:B:129:THR:HB	2.01	0.42
1:E:140:PHE:O	1:E:141:PHE:C	2.58	0.42
1:B:97:LYS:HA	1:B:97:LYS:HD3	1.83	0.42
1:C:149:ALA:O	1:C:228:TYR:HE2	2.03	0.42
1:A:151:MET:HG3	1:A:152:PRO:CD	2.47	0.42
1:C:17:ILE:HD12	1:C:17:ILE:HA	1.87	0.42
1:C:121:VAL:O	1:C:124:ILE:HD12	2.20	0.42
1:E:102:LYS:O	1:E:102:LYS:HE3	2.20	0.42
1:A:195:ILE:HD13	1:A:195:ILE:HA	1.81	0.42
1:E:61:LYS:HD3	2:E:267:PG4:O1	2.20	0.42
1:E:104:THR:O	1:E:104:THR:CG2	2.68	0.42
1:C:72:LEU:HD12	1:C:72:LEU:HA	1.86	0.42
1:C:148:LYS:HB2	4:C:297:HOH:O	2.20	0.42
1:C:208:ILE:HG22	1:C:209:TYR:N	2.34	0.42
1:E:15:ASN:HB2	4:E:290:HOH:O	2.19	0.42
1:D:174:SER:HA	1:D:183:LYS:HG2	2.02	0.42
1:C:149:ALA:C	1:C:151:MET:H	2.23	0.41
1:C:36:LEU:HD23	1:C:36:LEU:C	2.40	0.41
1:C:128:GLY:HA3	1:E:158:PHE:CD2	2.55	0.41
1:B:76:ILE:HA	1:B:76:ILE:HD12	1.94	0.41
1:A:65:GLY:HA3	1:A:196:THR:OG1	2.20	0.41
1:A:31:SER:HA	1:A:81:GLU:O	2.20	0.41
1:E:90:MET:HE3	1:E:99:VAL:HG21	2.01	0.41
1:A:76:ILE:CG1	1:A:187:ILE:HD11	2.50	0.41
1:C:251:ILE:HG21	1:D:29:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:MET:HE2	1:A:107:ILE:HG12	2.02	0.41
1:A:146:ALA:O	1:A:149:ALA:N	2.48	0.41
1:A:238:ILE:O	1:A:242:ALA:HB3	2.21	0.41
1:C:86:ASN:ND2	1:C:111:SER:HB3	2.33	0.41
1:D:154:THR:O	1:D:158:PHE:HD2	2.03	0.41
1:E:74:LEU:HD23	1:E:74:LEU:HA	1.88	0.41
1:E:61:LYS:HE2	2:E:267:PG4:H31	2.02	0.41
1:C:92:ALA:HA	1:C:95:LEU:HD12	2.01	0.41
1:C:255:GLU:O	1:C:257:LEU:N	2.54	0.41
3:C:269:BOG:H1	4:C:270:HOH:O	2.21	0.41
1:A:158:PHE:CD2	1:B:128:GLY:HA3	2.55	0.41
1:D:106:LYS:O	1:D:110:TYR:HB2	2.21	0.41
1:C:0:ARG:O	1:C:1:ALA:HB2	2.20	0.41
1:C:16:LYS:NZ	1:C:86:ASN:OD1	2.30	0.41
1:C:161:ILE:HD13	1:C:239:VAL:CG1	2.49	0.41
1:A:108:TRP:O	1:A:112:TRP:CB	2.68	0.41
1:D:151:MET:SD	1:D:159:ARG:NH1	2.94	0.41
1:A:158:PHE:HD2	1:B:128:GLY:O	2.04	0.41
1:A:5:THR:O	1:A:9:LEU:HG	2.21	0.41
1:C:229:ASN:O	1:C:233:VAL:HG23	2.20	0.41
1:C:217:THR:O	1:C:218:ILE:CG1	2.61	0.41
1:D:72:LEU:HB3	1:D:187:ILE:HG23	2.02	0.41
1:D:163:CYS:SG	1:D:201:HIS:HB2	2.61	0.41
1:C:165:ILE:O	1:C:169:VAL:HB	2.20	0.41
1:E:215:SER:CB	1:E:217:THR:HG23	2.50	0.41
1:C:151:MET:HG2	1:C:156:LEU:HG	2.04	0.40
1:D:148:LYS:HE3	2:D:266:PG4:H81	2.02	0.40
1:E:145:ALA:HB1	1:E:221:VAL:HG11	2.03	0.40
1:C:193:ALA:HA	1:D:44:LEU:HD13	2.04	0.40
1:C:10:THR:C	1:C:12:ALA:N	2.73	0.40
1:B:46:PHE:HZ	1:B:208:ILE:HD13	1.82	0.40
1:A:198:GLY:HA2	2:A:266:PG4:O1	2.21	0.40
1:D:126:PHE:CE2	1:D:132:VAL:CG1	3.05	0.40
1:B:159:ARG:NH1	1:E:131:LEU:HD21	2.36	0.40
1:B:41:GLY:O	1:B:45:ILE:HG23	2.22	0.40
1:B:219:SER:HA	4:B:296:HOH:O	2.21	0.40
1:C:46:PHE:CE2	1:C:208:ILE:HG12	2.56	0.40
1:D:76:ILE:HG12	1:D:187:ILE:CD1	2.51	0.40
1:B:132:VAL:HG23	4:B:278:HOH:O	2.22	0.40
1:D:42:ILE:HD11	1:D:204:ALA:HB1	2.04	0.40
1:A:31:SER:HB2	1:A:114:GLY:HA3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:LEU:HD11	1:D:110:TYR:CD2	2.57	0.40
1:E:27:TYR:CZ	1:E:107:ILE:HD12	2.56	0.40
1:B:84:ALA:HB1	1:B:164:ASN:OD1	2.21	0.40
1:B:17:ILE:HG13	1:B:21:ASN:ND2	2.36	0.40
1:E:225:GLY:O	1:E:228:TYR:HB3	2.21	0.40
1:E:25:VAL:O	1:E:29:VAL:HG23	2.21	0.40
1:B:83:PHE:CD1	1:B:112:TRP:HB2	2.57	0.40
1:C:209:TYR:CD2	1:C:230:LEU:HD21	2.56	0.40
1:C:209:TYR:HD2	1:C:230:LEU:HD21	1.86	0.40
1:C:262:GLU:HG3	1:C:263:ASN:H	1.86	0.40
1:C:113:VAL:CB	4:C:285:HOH:O	2.69	0.40
1:C:252:LEU:HD21	1:D:29:VAL:HG12	2.03	0.40
1:E:47:THR:HA	1:E:137:VAL:CG2	2.51	0.40
1:E:72:LEU:HD12	1:E:76:ILE:HD13	2.03	0.40
1:C:159:ARG:NH2	1:D:131:LEU:HG	2.37	0.40
1:B:94:MET:SD	1:B:101:ILE:CG1	3.09	0.40
1:B:22:THR:O	1:B:23:SER:HB2	2.22	0.40
1:B:162:LEU:HD23	1:B:162:LEU:HA	1.85	0.40
1:D:207:THR:OG1	4:D:285:HOH:O	2.22	0.40
1:D:43:LEU:HD13	1:D:126:PHE:CD1	2.55	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:ALA:O	1:E:100:SER:OG[3_645]	1.82	0.38
1:B:4:GLU:OE2	4:A:281:HOH:O[4_555]	2.07	0.13

## 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%)	230 (90%)	20 (8%)	5 (2%)	9	11
1	B	255/268 (95%)	242 (95%)	10 (4%)	3 (1%)	16	23
1	C	264/268 (98%)	212 (80%)	38 (14%)	14 (5%)	2	1
1	D	255/268 (95%)	242 (95%)	10 (4%)	3 (1%)	16	23
1	E	254/268 (95%)	233 (92%)	16 (6%)	5 (2%)	9	11
All	All	1283/1340 (96%)	1159 (90%)	94 (7%)	30 (2%)	8	8

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1	ALA
1	C	14	ILE
1	C	214	PHE
1	C	217	THR
1	C	226	ALA
1	C	227	ILE
1	D	218	ILE
1	D	219	SER
1	D	220	THR
1	E	218	ILE
1	E	220	THR
1	A	93	GLY
1	A	95	LEU
1	B	23	SER
1	C	18	ASN
1	C	216	PRO
1	C	218	ILE
1	C	235	LEU
1	C	258	ASN
1	C	261	ALA
1	E	83	PHE
1	A	1	ALA
1	B	24	LYS
1	E	243	LEU
1	A	83	PHE
1	B	134	LYS
1	C	15	ASN
1	A	75	VAL
1	C	221	VAL
1	E	216	PRO

### 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	205/213 (96%)	177 (86%)	28 (14%)	4	5
1	B	206/213 (97%)	189 (92%)	17 (8%)	14	21
1	C	212/213 (100%)	186 (88%)	26 (12%)	6	7
1	D	206/213 (97%)	193 (94%)	13 (6%)	22	35
1	E	205/213 (96%)	183 (89%)	22 (11%)	8	11
All	All	1034/1065 (97%)	928 (90%)	106 (10%)	9	13

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	ARG
1	A	17	ILE
1	A	33	PHE
1	A	51	LEU
1	A	57	SER
1	A	61	LYS
1	A	72	LEU
1	A	90	MET
1	A	91	SER
1	A	94	MET
1	A	100	SER
1	A	102	LYS
1	A	103	ASP
1	A	107	ILE
1	A	150	SER
1	A	154	THR
1	A	169	VAL
1	A	174	SER
1	A	188	PHE
1	A	194	PHE
1	A	201	HIS
1	A	202	SER
1	A	219	SER

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Mol	Chain	Res	Type
1	A	221	VAL
1	A	227	ILE
1	A	243	LEU
1	A	249	THR
1	A	255	GLU
1	B	3	LYS
1	B	16	LYS
1	B	24	LYS
1	B	72	LEU
1	B	76	ILE
1	B	102	LYS
1	B	105	SER
1	B	132	VAL
1	B	194	PHE
1	B	217	THR
1	B	222	THR
1	B	227	ILE
1	B	235	LEU
1	B	243	LEU
1	B	254	LYS
1	B	255	GLU
1	B	256	LYS
1	C	3	LYS
1	C	23	SER
1	C	24	LYS
1	C	25	VAL
1	C	33	PHE
1	C	53	THR
1	C	87	ASN
1	C	89	VAL
1	C	100	SER
1	C	102	LYS
1	C	117	ILE
1	C	120	LEU
1	C	124	ILE
1	C	125	ILE
1	C	127	VAL
1	C	154	THR
1	C	169	VAL
1	C	188	PHE
1	C	194	PHE
1	C	208	ILE

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Mol	Chain	Res	Type
1	C	212	SER
1	C	219	SER
1	C	243	LEU
1	C	256	LYS
1	C	264	LEU
1	C	265	TYR
1	D	19	LEU
1	D	24	LYS
1	D	33	PHE
1	D	150	SER
1	D	170	SER
1	D	194	PHE
1	D	197	SER
1	D	215	SER
1	D	218	ILE
1	D	219	SER
1	D	221	VAL
1	D	243	LEU
1	D	256	LYS
1	E	3	LYS
1	E	11	ASN
1	E	17	ILE
1	E	23	SER
1	E	40	ILE
1	E	72	LEU
1	E	76	ILE
1	E	101	ILE
1	E	102	LYS
1	E	105	SER
1	E	106	LYS
1	E	154	THR
1	E	165	ILE
1	E	170	SER
1	E	194	PHE
1	E	210	SER
1	E	217	THR
1	E	218	ILE
1	E	221	VAL
1	E	249	THR
1	E	254	LYS
1	E	256	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such



sidechains are listed below:

Mol	Chain	Res	Type
1	B	21	ASN
1	C	87	ASN
1	C	164	ASN
1	D	143	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 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	266	-	12,12,12	1.08	0	11,11,11	1.48	2 (18%)
2	PG4	B	266	-	12,12,12	1.08	0	11,11,11	1.68	3 (27%)
3	BOG	C	269	-	20,20,20	0.46	0	25,25,25	0.62	0
2	PG4	D	266	-	12,12,12	1.02	0	11,11,11	1.24	2 (18%)
3	BOG	E	266	-	20,20,20	0.45	0	25,25,25	0.63	0
2	PG4	E	267	-	12,12,12	1.04	0	11,11,11	1.55	3 (27%)

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	266	-	-	0/10/10/10	0/0/0/0
2	PG4	B	266	-	-	0/10/10/10	0/0/0/0
3	BOG	C	269	-	-	0/11/31/31	0/1/1/1
2	PG4	D	266	-	-	0/10/10/10	0/0/0/0
3	BOG	E	266	-	-	0/11/31/31	0/1/1/1
2	PG4	E	267	-	-	0/10/10/10	0/0/0/0

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	266	PG4	C3-O2-C2	2.08	122.27	113.31
2	A	266	PG4	C5-O3-C4	2.38	123.55	113.31
2	E	267	PG4	C3-O2-C2	2.53	124.20	113.31
2	E	267	PG4	C7-O4-C6	2.62	124.56	113.31
2	D	266	PG4	C7-O4-C6	2.83	125.48	113.31
2	B	266	PG4	C7-O4-C6	2.90	125.77	113.31
2	B	266	PG4	C3-O2-C2	2.91	125.81	113.31
2	E	267	PG4	C5-O3-C4	3.24	127.25	113.31
2	B	266	PG4	C5-O3-C4	3.59	128.73	113.31
2	A	266	PG4	C7-O4-C6	3.61	128.83	113.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	266	PG4	7	0
2	B	266	PG4	7	0
3	C	269	BOG	12	0
2	D	266	PG4	3	0
3	E	266	BOG	9	0
2	E	267	PG4	7	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<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%)	0.51	27 (10%) 8 8	31, 60, 88, 115	0
1	B	257/268 (95%)	0.38	18 (7%) 19 19	26, 55, 85, 107	0
1	C	266/268 (99%)	1.19	60 (22%) 1 1	33, 75, 115, 186	0
1	D	257/268 (95%)	0.53	22 (8%) 13 13	29, 55, 89, 167	0
1	E	256/268 (95%)	0.43	21 (8%) 14 14	29, 57, 89, 120	0
All	All	1293/1340 (96%)	0.61	148 (11%) 7 7	26, 59, 96, 186	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	220	THR	8.1
1	A	250	TYR	7.3
1	C	102	LYS	7.2
1	C	219	SER	6.3
1	C	227	ILE	6.0
1	C	19	LEU	5.8
1	A	101	ILE	5.6
1	C	216	PRO	5.5
1	A	95	LEU	5.3
1	C	14	ILE	5.3
1	C	22	THR	5.2
1	C	93	GLY	5.0
1	B	185	ILE	4.9
1	C	221	VAL	4.8
1	A	102	LYS	4.7
1	D	185	ILE	4.7
1	C	17	ILE	4.7
1	C	10	THR	4.7
1	B	225	GLY	4.5
1	E	188	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	181	THR	4.4
1	C	265	TYR	4.4
1	C	13	ALA	4.4
1	A	181	THR	4.4
1	C	185	ILE	4.4
1	A	94	MET	4.3
1	E	181	THR	4.2
1	E	185	ILE	4.2
1	D	218	ILE	4.1
1	C	21	ASN	4.1
1	C	212	SER	4.0
1	C	15	ASN	4.0
1	C	11	ASN	3.9
1	C	264	LEU	3.9
1	A	99	VAL	3.9
1	B	181	THR	3.8
1	C	107	ILE	3.8
1	C	222	THR	3.8
1	A	182	ALA	3.8
1	C	223	ILE	3.8
1	A	254	LYS	3.7
1	C	214	PHE	3.7
1	B	25	VAL	3.7
1	B	224	GLY	3.7
1	C	213	LEU	3.7
1	C	99	VAL	3.6
1	D	188	PHE	3.5
1	A	17	ILE	3.5
1	C	188	PHE	3.4
1	B	188	PHE	3.4
1	E	73	SER	3.4
1	C	66	LEU	3.3
1	C	184	ILE	3.3
1	C	258	ASN	3.3
1	C	224	GLY	3.3
1	B	250	TYR	3.2
1	C	27	TYR	3.2
1	C	23	SER	3.2
1	C	181	THR	3.2
1	B	227	ILE	3.2
1	D	227	ILE	3.2
1	B	222	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	189	LEU	3.1
1	D	184	ILE	3.1
1	C	104	THR	3.1
1	D	25	VAL	3.1
1	B	189	LEU	3.1
1	E	17	ILE	3.0
1	E	214	PHE	3.0
1	A	103	ASP	3.0
1	E	182	ALA	3.0
1	A	184	ILE	3.0
1	C	217	THR	3.0
1	A	221	VAL	3.0
1	D	182	ALA	3.0
1	D	189	LEU	3.0
1	E	3	LYS	2.9
1	C	260	ALA	2.9
1	A	97	LYS	2.8
1	E	187	ILE	2.8
1	C	18	ASN	2.8
1	A	100	SER	2.8
1	B	184	ILE	2.8
1	C	187	ILE	2.8
1	C	228	TYR	2.7
1	B	23	SER	2.7
1	C	156	LEU	2.7
1	E	218	ILE	2.7
1	C	182	ALA	2.7
1	E	255	GLU	2.7
1	C	110	TYR	2.7
1	A	185	ILE	2.6
1	B	187	ILE	2.6
1	D	73	SER	2.6
1	D	173	CYS	2.6
1	A	252	LEU	2.6
1	D	94	MET	2.6
1	A	110	TYR	2.6
1	C	189	LEU	2.6
1	C	186	MET	2.6
1	A	20	LEU	2.5
1	A	104	THR	2.5
1	E	74	LEU	2.5
1	B	190	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	184	ILE	2.5
1	C	218	ILE	2.5
1	C	153	PHE	2.5
1	E	44	LEU	2.4
1	A	251	ILE	2.4
1	D	66	LEU	2.4
1	C	256	LYS	2.4
1	B	223	ILE	2.4
1	D	67	SER	2.4
1	B	186	MET	2.4
1	E	94	MET	2.4
1	C	263	ASN	2.4
1	E	102	LYS	2.4
1	C	209	TYR	2.4
1	C	106	LYS	2.3
1	E	69	ALA	2.3
1	D	187	ILE	2.3
1	A	188	PHE	2.3
1	B	173	CYS	2.3
1	C	69	ALA	2.3
1	E	66	LEU	2.3
1	C	128	GLY	2.2
1	A	227	ILE	2.2
1	D	27	TYR	2.2
1	C	20	LEU	2.2
1	E	186	MET	2.2
1	D	70	ILE	2.2
1	C	141	PHE	2.1
1	D	179	SER	2.1
1	D	69	ALA	2.1
1	D	146	ALA	2.1
1	A	10	THR	2.1
1	C	225	GLY	2.1
1	C	179	SER	2.1
1	D	186	MET	2.1
1	C	134	LYS	2.1
1	A	21	ASN	2.1
1	A	186	MET	2.1
1	C	105	SER	2.1
1	C	101	ILE	2.1
1	D	174	SER	2.0
1	B	221	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	254	LYS	2.0
1	A	179	SER	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	E	266	20/20	0.75	0.60	5.73	10,10,10,10	0
2	PG4	B	266	13/13	0.91	0.21	2.75	48,77,99,102	0
2	PG4	A	266	13/13	0.89	0.18	2.55	38,67,154,159	0
3	BOG	C	269	20/20	0.69	0.38	1.28	10,10,10,10	0
2	PG4	E	267	13/13	0.81	0.17	1.05	70,91,126,140	0
2	PG4	D	266	13/13	0.89	0.14	-0.50	45,72,116,121	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.