



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:26 PM GMT

PDB ID : 1OT3  
Title : Crystal structure of Drosophila deoxyribonucleotide kinase complexed with the substrate deoxythymidine  
Authors : Mikkelsen, N.E.; Johansson, K.; Karlsson, A.; Knecht, W.; Andersen, G.; Piskur, J.; Munch-Petersen, B.; Eklund, H.  
Deposited on : 2003-03-21  
Resolution : 2.50 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

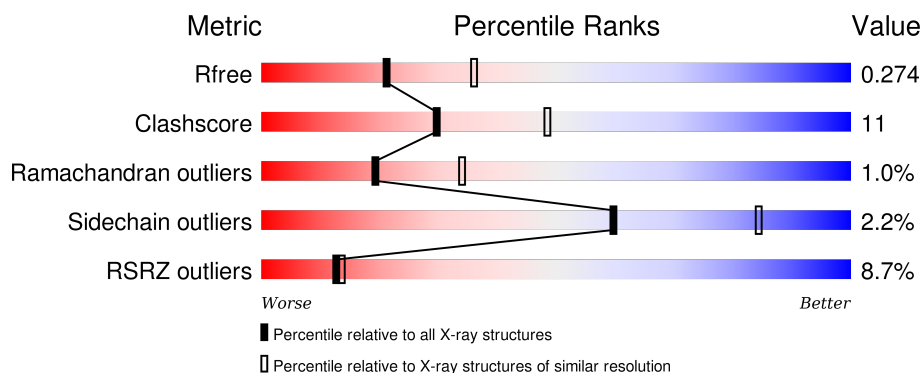
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	250	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>21%</div> <div>•</div> <div>21%</div> </div> </div>
1	B	250	<div> <div>10%</div> <div> <div></div> <div>59%</div> <div>16%</div> <div>•</div> <div>23%</div> </div> </div>
1	C	250	<div> <div>7%</div> <div> <div></div> <div>59%</div> <div>18%</div> <div>•</div> <div>21%</div> </div> </div>
1	D	250	<div> <div>9%</div> <div> <div></div> <div>56%</div> <div>20%</div> <div>•</div> <div>24%</div> </div> </div>
1	E	250	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>19%</div> <div>•</div> <div>23%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	250	
1	G	250	
1	H	250	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13338 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 Deoxyribonucleoside Kinase.

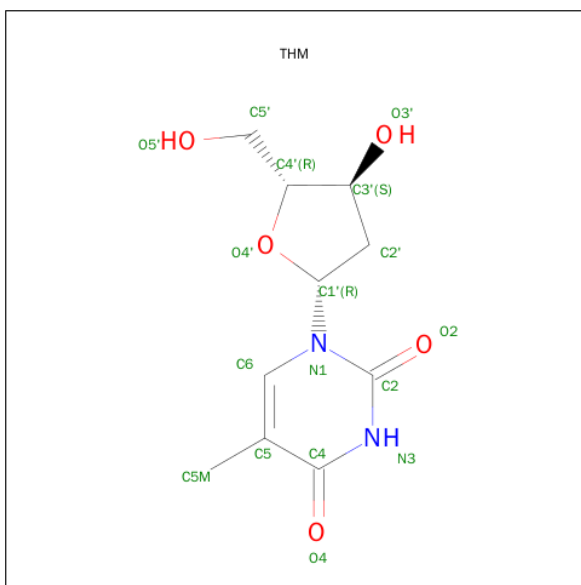
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1640	1046	282	302	10			
1	B	192	Total	C	N	O	S	0	0	0
			1596	1021	270	295	10			
1	C	197	Total	C	N	O	S	0	0	0
			1640	1046	282	302	10			
1	D	191	Total	C	N	O	S	0	0	0
			1587	1016	268	293	10			
1	E	192	Total	C	N	O	S	0	0	0
			1596	1021	270	295	10			
1	F	192	Total	C	N	O	S	0	0	0
			1596	1021	270	295	10			
1	G	192	Total	C	N	O	S	0	0	0
			1596	1021	270	295	10			
1	H	192	Total	C	N	O	S	0	0	0
			1596	1021	270	295	10			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is THYMIDINE (three-letter code: THM) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>2</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	10	2	5		
3	D	1	Total	C	N	O	0	0
			17	10	2	5		
3	E	1	Total	C	N	O	0	0
			17	10	2	5		
3	G	1	Total	C	N	O	0	0
			17	10	2	5		
3	F	1	Total	C	N	O	0	0
			17	10	2	5		
3	C	1	Total	C	N	O	0	0
			17	10	2	5		
3	B	1	Total	C	N	O	0	0
			17	10	2	5		
3	H	1	Total	C	N	O	0	0
			17	10	2	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	112	Total	O	0	0
			112	112		
4	B	30	Total	O	0	0
			30	30		
4	C	25	Total	O	0	0
			25	25		
4	D	17	Total	O	0	0
			17	17		

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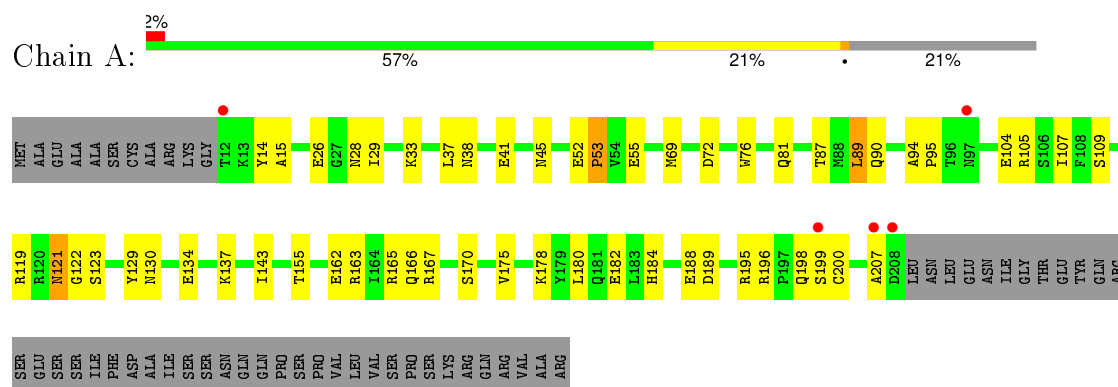
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	27	Total 27	O 27	0	0
4	F	16	Total 16	O 16	0	0
4	G	18	Total 18	O 18	0	0
4	H	65	Total 65	O 65	0	0

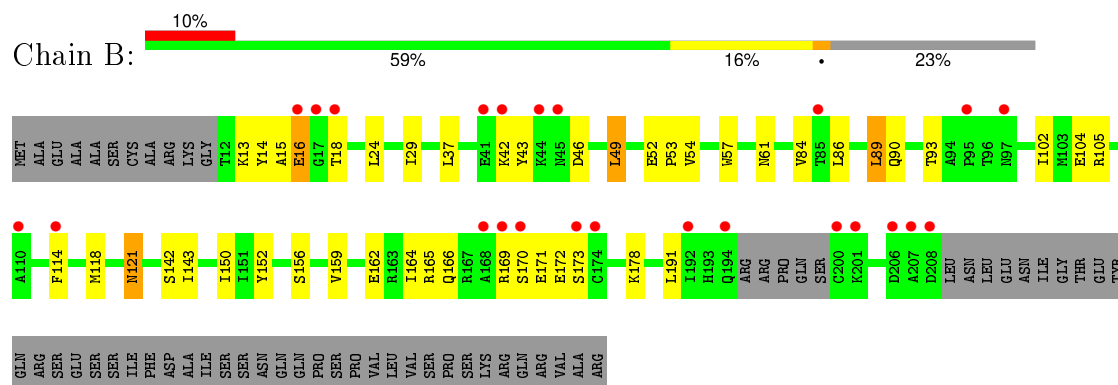
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

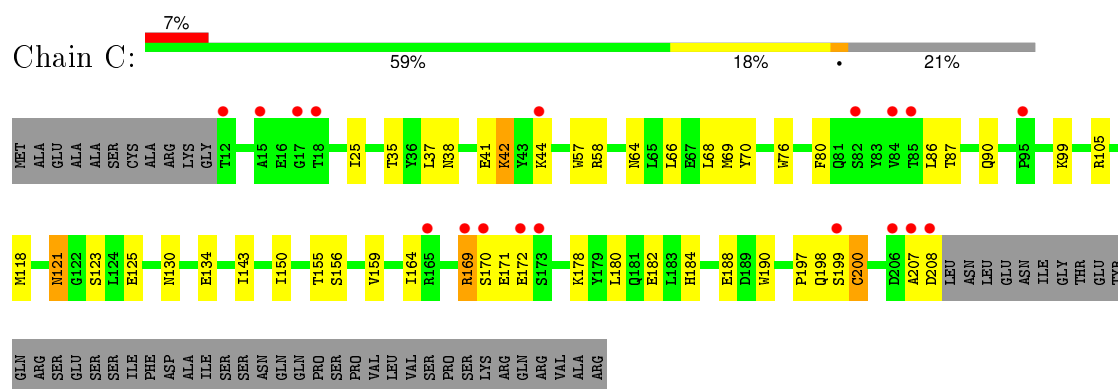
#### • Molecule 1: Deoxyribonucleoside Kinase



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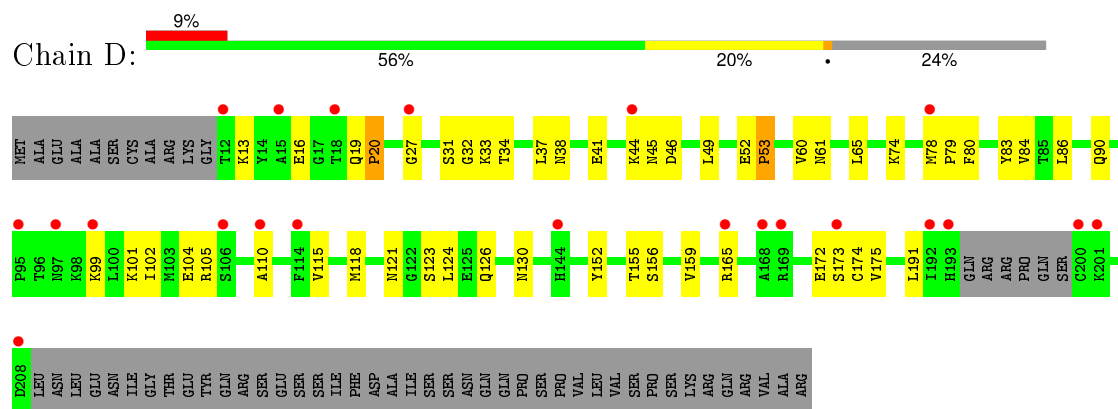


#### • Molecule 1: Deoxyribonucleoside Kinase

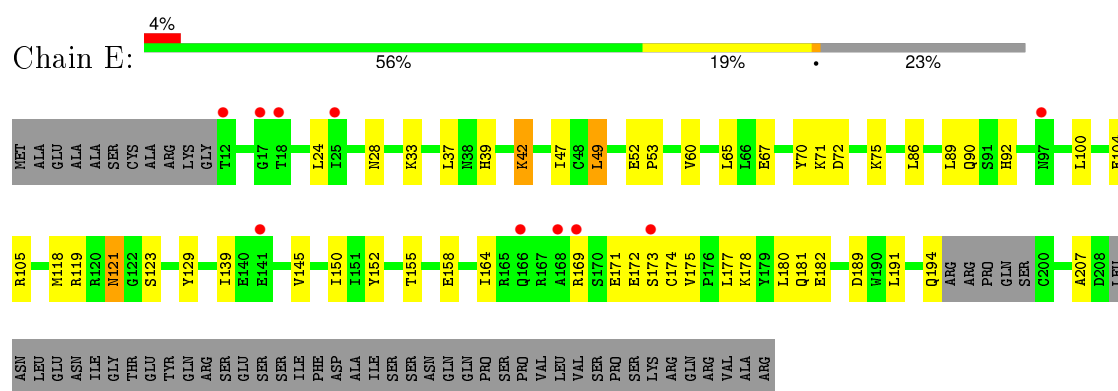




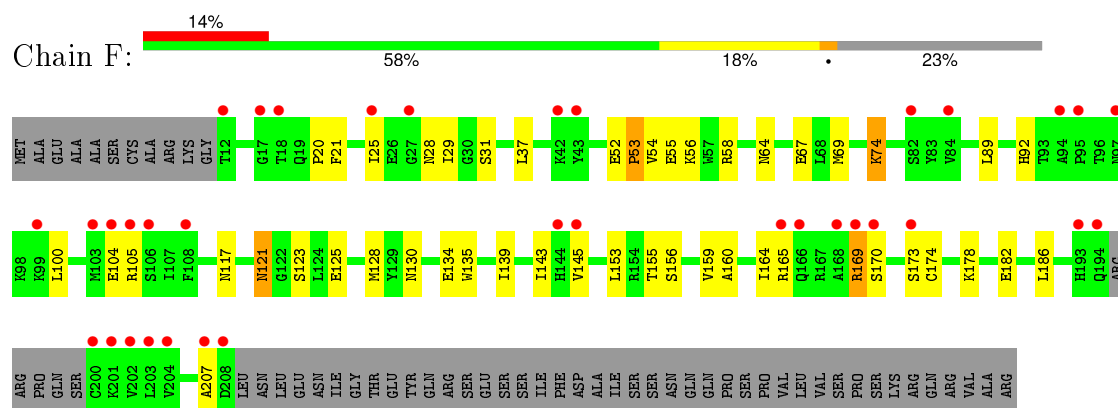
- Molecule 1: Deoxyribonucleoside Kinase



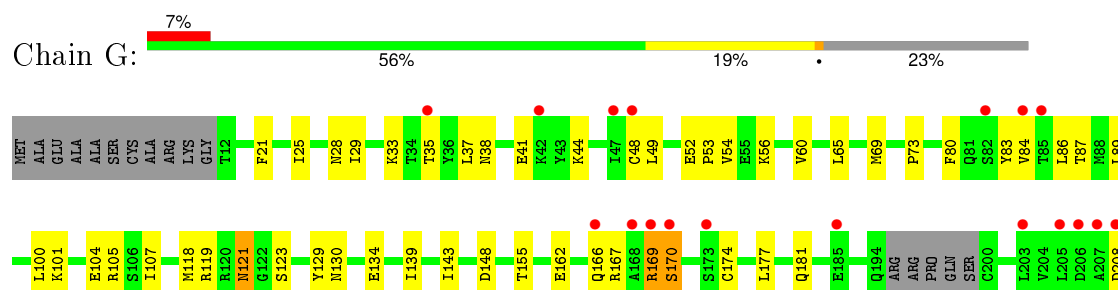
- Molecule 1: Deoxyribonucleoside Kinase



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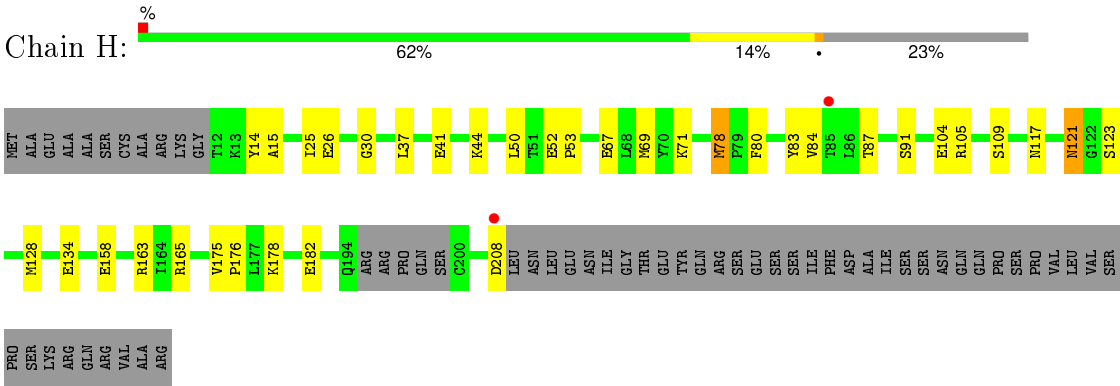


- Molecule 1: Deoxyribonucleoside Kinase



LEU	ASN	LEU	GLU	ASN	ILE	GLY	THR	GLU	TYR	GLN	ARG	SER	GLU	SER	SER	ILE	PHE	ASP	ALA	ILE	SER	SER	ASN	GLN	GLN	PRO	SER	PRO	VAL	LEU	VAL	SER	PRO	SER	SER	LYS	ARG	GLN	ARG	VAL	ALA	ARG
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• Molecule 1: Deoxyribonucleoside Kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.38Å 71.16Å 226.27Å 90.00° 90.59° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 24.89 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.8 (25.00-2.50) 89.9 (24.89-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.38 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.227 , 0.276 0.225 , 0.274	Depositor DCC
$R_{free}$ test set	3560 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.8	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.9	EDS
Estimated twinning fraction	0.000 for -k,-h,-l 0.004 for k,h,-l 0.023 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 70001 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13338	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.69% 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: THM, SO4

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	0.47	0/1678	0.64	0/2268
1	B	0.35	0/1632	0.52	0/2205
1	C	0.33	0/1678	0.50	0/2268
1	D	0.32	0/1623	0.48	0/2193
1	E	0.33	0/1632	0.49	0/2205
1	F	0.30	0/1632	0.46	0/2205
1	G	0.33	0/1632	0.48	0/2205
1	H	0.47	0/1632	0.60	0/2205
All	All	0.37	0/13139	0.52	0/17754

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	1640	0	1629	43	0
1	B	1596	0	1582	34	0
1	C	1640	0	1629	41	0
1	D	1587	0	1574	41	0
1	E	1596	0	1582	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1596	0	1582	35	0
1	G	1596	0	1582	35	0
1	H	1596	0	1582	25	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	17	0	13	0	0
3	B	17	0	14	0	0
3	C	17	0	13	1	0
3	D	17	0	13	1	0
3	E	17	0	13	0	0
3	F	17	0	13	0	0
3	G	17	0	13	0	0
3	H	17	0	14	0	0
4	A	112	0	0	5	0
4	B	30	0	0	1	0
4	C	25	0	0	0	0
4	D	17	0	0	1	0
4	E	27	0	0	1	0
4	F	16	0	0	1	0
4	G	18	0	0	1	0
4	H	65	0	0	2	0
All	All	13338	0	12848	289	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 11.

All (289) 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:G:25:ILE:HG13	1:G:37:LEU:HD21	1.38	1.05
1:H:37:LEU:HD11	1:H:104:GLU:HB2	1.51	0.92
1:F:125:GLU:H	1:F:128:MET:HE3	1.41	0.85
1:D:165:ARG:HA	1:D:165:ARG:HH11	1.47	0.80
1:D:19:GLN:HE22	1:D:101:LYS:NZ	1.81	0.79
1:G:21:PHE:HB3	1:G:100:LEU:HD12	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:LYS:H	1:E:42:LYS:HD3	1.49	0.76
1:A:166:GLN:HG3	4:A:1502:HOH:O	1.86	0.75
1:A:198:GLN:NE2	1:A:199:SER:H	1.86	0.74
1:C:25:ILE:HG13	1:C:37:LEU:HD21	1.70	0.74
1:E:155:THR:HG22	1:E:207:ALA:HB3	1.71	0.73
1:C:35:THR:HA	1:C:38:ASN:HD22	1.53	0.73
1:E:28:ASN:HD21	1:E:180:LEU:HD22	1.53	0.72
1:C:121:ASN:ND2	1:C:123:SER:H	1.88	0.71
1:A:155:THR:HG22	1:A:207:ALA:HB2	1.73	0.70
1:H:121:ASN:C	1:H:121:ASN:HD22	1.96	0.69
1:E:178:LYS:O	1:E:182:GLU:HG3	1.93	0.69
1:C:156:SER:HB3	1:C:159:VAL:HG23	1.76	0.68
1:B:89:LEU:HD21	1:B:143:ILE:HD13	1.76	0.68
1:D:19:GLN:HE22	1:D:101:LYS:HZ1	1.42	0.68
1:D:156:SER:HB3	1:D:159:VAL:HG23	1.76	0.67
1:A:143:ILE:HD12	1:A:143:ILE:H	1.58	0.67
1:G:118:MET:HA	1:G:121:ASN:HD21	1.59	0.66
1:H:121:ASN:ND2	1:H:123:SER:H	1.94	0.66
1:E:47:ILE:HD13	1:E:100:LEU:HD23	1.78	0.66
1:H:25:ILE:HG13	1:H:37:LEU:HD21	1.78	0.66
1:E:42:LYS:HD3	1:E:42:LYS:N	2.09	0.66
1:A:121:ASN:ND2	1:A:123:SER:H	1.94	0.66
1:A:130:ASN:O	1:A:134:GLU:HG2	1.95	0.66
1:G:162:GLU:O	1:G:166:GLN:HG2	1.96	0.66
1:F:37:LEU:HD11	1:F:104:GLU:HB2	1.78	0.64
1:A:189:ASP:HB3	1:A:195:ARG:HD3	1.79	0.64
1:F:156:SER:HB3	1:F:159:VAL:HG23	1.79	0.64
1:C:66:LEU:HG	1:C:171:GLU:HG2	1.80	0.64
1:A:121:ASN:C	1:A:121:ASN:HD22	2.02	0.63
1:A:198:GLN:CD	1:A:199:SER:H	2.01	0.63
1:H:41:GLU:O	1:H:44:LYS:HG3	1.98	0.63
1:H:128:MET:HG3	4:H:1459:HOH:O	1.99	0.63
1:C:42:LYS:H	1:C:42:LYS:HD2	1.63	0.62
1:H:37:LEU:CD1	1:H:104:GLU:HB2	2.28	0.62
1:H:121:ASN:HD22	1:H:123:SER:H	1.46	0.62
1:D:37:LEU:HD11	1:D:49:LEU:HD12	1.82	0.61
1:E:86:LEU:O	1:E:90:GLN:HG3	2.00	0.61
1:C:155:THR:HG22	1:C:207:ALA:HB3	1.82	0.61
1:H:50:LEU:HD13	1:H:91:SER:OG	2.00	0.61
1:F:53:PRO:HB3	1:F:56:LYS:HD3	1.83	0.61
1:D:86:LEU:O	1:D:90:GLN:HG3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LYS:NZ	4:A:1490:HOH:O	2.34	0.60
1:B:169:ARG:HB3	1:B:173:SER:HB3	1.81	0.60
1:D:126:GLN:HE21	1:D:130:ASN:ND2	1.99	0.60
1:H:80:PHE:O	1:H:84:VAL:HG23	2.02	0.60
1:G:89:LEU:HD13	1:G:143:ILE:CD1	2.31	0.60
1:C:150:ILE:HG13	1:C:200:CYS:SG	2.42	0.60
1:B:42:LYS:HE2	1:B:43:TYR:HE1	1.67	0.60
1:H:178:LYS:O	1:H:182:GLU:HG3	2.02	0.59
1:A:95:PRO:HA	4:A:1471:HOH:O	2.02	0.59
1:D:31:SER:HA	1:D:155:THR:HG21	1.84	0.59
1:E:67:GLU:HG2	1:E:71:LYS:HE2	1.83	0.59
1:C:169:ARG:HD3	1:C:170:SER:H	1.68	0.59
1:G:118:MET:HA	1:G:121:ASN:ND2	2.19	0.58
1:F:135:TRP:O	1:F:139:ILE:HG13	2.02	0.58
1:F:64:ASN:ND2	1:F:67:GLU:HB2	2.17	0.58
1:F:121:ASN:C	1:F:121:ASN:HD22	2.07	0.58
1:A:163:ARG:O	1:A:167:ARG:HG3	2.04	0.58
1:A:81:GLN:NE2	1:A:81:GLN:HA	2.20	0.57
1:H:67:GLU:HG3	1:H:71:LYS:HE2	1.87	0.57
1:D:165:ARG:HA	1:D:165:ARG:NH1	2.18	0.57
1:C:198:GLN:NE2	1:C:199:SER:H	2.03	0.57
1:B:89:LEU:HD21	1:B:143:ILE:HG21	1.87	0.56
1:E:42:LYS:CD	1:E:42:LYS:H	2.11	0.56
1:E:121:ASN:ND2	1:E:123:SER:H	2.03	0.56
1:C:99:LYS:HA	1:C:99:LYS:HE2	1.87	0.56
1:F:74:LYS:HD2	1:F:74:LYS:H	1.71	0.56
1:F:178:LYS:O	1:F:182:GLU:HG3	2.07	0.55
1:D:74:LYS:H	1:D:74:LYS:HD2	1.71	0.55
1:F:89:LEU:HD22	1:F:143:ILE:HG21	1.89	0.54
1:E:24:LEU:HB2	1:E:150:ILE:HG12	1.89	0.54
1:G:121:ASN:ND2	1:G:123:SER:H	2.06	0.54
1:D:19:GLN:NE2	1:D:101:LYS:HZ2	2.06	0.54
1:C:156:SER:HB3	1:C:159:VAL:CG2	2.37	0.54
1:A:143:ILE:H	1:A:143:ILE:CD1	2.22	0.53
1:F:121:ASN:ND2	1:F:123:SER:H	2.07	0.53
1:E:118:MET:HB3	1:E:123:SER:HB2	1.91	0.52
1:F:92:HIS:CG	1:F:145:VAL:HG13	2.44	0.52
1:G:53:PRO:HB3	1:G:56:LYS:HD2	1.92	0.52
1:G:155:THR:HG22	1:G:208:ASP:OD2	2.10	0.52
1:E:164:ILE:HD12	1:E:180:LEU:HD11	1.92	0.52
1:C:121:ASN:HD21	1:C:123:SER:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:MET:HA	1:E:121:ASN:HD21	1.75	0.52
1:G:80:PHE:O	1:G:84:VAL:HG23	2.09	0.52
1:E:155:THR:CG2	1:E:207:ALA:HB3	2.39	0.51
1:B:42:LYS:HG3	1:B:43:TYR:CD1	2.45	0.51
1:E:37:LEU:HD23	1:E:49:LEU:HD11	1.91	0.51
1:G:41:GLU:HB3	4:G:1414:HOH:O	2.09	0.51
1:C:58:ARG:HH22	1:C:169:ARG:NH2	2.09	0.51
1:B:114:PHE:O	1:B:118:MET:HG3	2.11	0.51
1:E:104:GLU:O	1:E:105:ARG:HB2	2.11	0.51
1:B:29:ILE:HG22	1:B:164:ILE:HD11	1.93	0.51
1:F:104:GLU:O	1:F:105:ARG:HB2	2.11	0.51
1:G:44:LYS:NZ	1:G:49:LEU:HB3	2.26	0.51
1:B:13:LYS:O	1:B:16:GLU:HG2	2.12	0.50
1:D:49:LEU:HD13	1:D:102:ILE:HB	1.93	0.50
1:B:52:GLU:O	1:B:54:VAL:HG23	2.11	0.50
1:A:69:MET:HA	1:A:76:TRP:HB2	1.92	0.50
1:A:72:ASP:HB3	1:A:76:TRP:HD1	1.77	0.50
1:G:89:LEU:HD11	1:G:139:ILE:HD13	1.94	0.50
1:B:49:LEU:HD22	1:B:102:ILE:HB	1.94	0.50
1:B:152:TYR:HB2	1:B:191:LEU:HD13	1.94	0.49
1:D:118:MET:O	1:D:123:SER:HB2	2.12	0.49
1:E:28:ASN:ND2	1:E:180:LEU:HD22	2.25	0.49
1:B:169:ARG:HH21	1:B:171:GLU:N	2.09	0.49
1:B:42:LYS:HG3	1:B:43:TYR:HD1	1.78	0.49
1:F:25:ILE:HG13	1:F:37:LEU:HD21	1.94	0.49
1:G:86:LEU:HD21	1:H:134:GLU:HB3	1.93	0.49
1:D:13:LYS:HB2	1:D:16:GLU:HB2	1.95	0.49
1:B:37:LEU:HD22	1:B:49:LEU:HD21	1.95	0.49
1:D:27:GLY:O	1:D:33:LYS:HE2	2.12	0.49
1:F:58:ARG:HA	1:F:64:ASN:OD1	2.13	0.49
1:A:87:THR:HA	1:A:90:GLN:OE1	2.13	0.49
1:D:172:GLU:O	1:D:175:VAL:HG22	2.12	0.49
1:H:83:TYR:O	1:H:87:THR:HG23	2.12	0.49
1:D:19:GLN:NE2	1:D:101:LYS:NZ	2.54	0.49
1:D:126:GLN:HE21	1:D:130:ASN:HD21	1.59	0.49
1:A:162:GLU:OE2	1:A:165:ARG:HD3	2.13	0.49
1:A:89:LEU:HD23	1:A:107:ILE:HD12	1.94	0.49
1:B:121:ASN:C	1:B:121:ASN:ND2	2.66	0.49
1:F:169:ARG:HB2	1:F:173:SER:HB3	1.95	0.49
1:F:105:ARG:HD3	4:F:1411:HOH:O	2.12	0.49
1:A:143:ILE:HD12	1:A:143:ILE:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:GLU:O	1:D:105:ARG:HB2	2.13	0.48
1:F:31:SER:HA	1:F:155:THR:HG21	1.95	0.48
1:H:117:ASN:HB3	4:H:1417:HOH:O	2.11	0.48
1:G:35:THR:O	1:G:38:ASN:HB2	2.12	0.48
1:F:52:GLU:C	1:F:54:VAL:H	2.17	0.48
1:C:169:ARG:CD	1:C:170:SER:H	2.26	0.48
1:C:70:TYR:CD1	1:C:171:GLU:HB3	2.49	0.48
1:H:78:MET:HG3	1:H:128:MET:HB3	1.96	0.48
1:G:48:CYS:SG	1:G:101:LYS:HE2	2.54	0.48
1:C:172:GLU:HB3	3:C:1405:THM:O3'	2.13	0.48
1:F:130:ASN:O	1:F:134:GLU:HG2	2.14	0.48
1:A:178:LYS:O	1:A:182:GLU:HG3	2.13	0.48
1:F:69:MET:C	1:F:69:MET:SD	2.92	0.48
1:F:28:ASN:OD1	1:F:29:ILE:N	2.46	0.48
1:B:169:ARG:NE	1:B:172:GLU:HG2	2.29	0.47
1:G:52:GLU:C	1:G:54:VAL:H	2.17	0.47
1:A:14:TYR:CE2	1:B:142:SER:HB3	2.48	0.47
1:C:178:LYS:O	1:C:182:GLU:HG3	2.13	0.47
1:A:121:ASN:C	1:A:121:ASN:ND2	2.65	0.47
1:C:143:ILE:HD12	1:C:143:ILE:H	1.79	0.47
1:C:38:ASN:O	1:C:41:GLU:HB2	2.15	0.47
1:A:119:ARG:HD3	1:A:129:TYR:CD1	2.50	0.47
1:D:80:PHE:O	1:D:84:VAL:HG23	2.15	0.47
1:G:21:PHE:HA	1:G:148:ASP:OD2	2.14	0.47
1:B:104:GLU:O	1:B:105:ARG:HB2	2.14	0.47
1:H:26:GLU:OE2	1:H:109:SER:HB3	2.15	0.47
1:F:54:VAL:CG1	1:F:58:ARG:HH21	2.28	0.47
1:C:35:THR:HA	1:C:38:ASN:ND2	2.27	0.47
1:D:52:GLU:OE2	1:D:105:ARG:HG3	2.15	0.47
1:G:33:LYS:HB2	1:G:33:LYS:NZ	2.30	0.47
1:A:121:ASN:HD22	1:A:123:SER:H	1.63	0.46
1:A:119:ARG:HD3	1:A:129:TYR:CG	2.50	0.46
1:D:110:ALA:O	1:D:115:VAL:HG23	2.16	0.46
1:H:121:ASN:C	1:H:121:ASN:ND2	2.67	0.46
1:F:153:LEU:HD22	1:F:207:ALA:HB2	1.98	0.46
1:B:15:ALA:HB2	1:B:93:THR:HB	1.98	0.46
1:A:184:HIS:O	1:A:188:GLU:HG2	2.16	0.46
1:C:35:THR:O	1:C:38:ASN:HB2	2.16	0.46
1:C:171:GLU:CD	1:C:171:GLU:H	2.19	0.46
1:E:189:ASP:O	1:E:194:GLN:HB2	2.16	0.46
1:G:119:ARG:HG2	1:G:119:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:GLN:CD	1:D:101:LYS:HZ2	2.19	0.46
1:G:69:MET:HG3	1:G:80:PHE:CD2	2.50	0.46
1:E:47:ILE:CD1	1:E:100:LEU:HD23	2.46	0.46
1:E:89:LEU:HD21	1:E:139:ILE:HG21	1.98	0.46
1:E:121:ASN:C	1:E:121:ASN:HD22	2.18	0.45
1:C:41:GLU:O	1:C:44:LYS:HG2	2.16	0.45
1:C:121:ASN:ND2	1:C:121:ASN:C	2.70	0.45
1:G:121:ASN:HD22	1:G:121:ASN:C	2.19	0.45
1:G:119:ARG:HG2	1:G:119:ARG:HH11	1.81	0.45
1:E:177:LEU:O	1:E:181:GLN:HG3	2.16	0.45
1:F:53:PRO:HA	1:F:55:GLU:OE2	2.16	0.45
1:G:89:LEU:HD13	1:G:143:ILE:HD12	1.97	0.45
1:D:41:GLU:OE1	1:D:41:GLU:HA	2.16	0.45
1:D:32:GLY:HA2	4:D:1412:HOH:O	2.16	0.45
1:C:190:TRP:HE1	1:C:198:GLN:HB2	1.82	0.45
1:F:89:LEU:HD21	1:F:139:ILE:HG21	1.97	0.45
1:G:44:LYS:HZ3	1:G:49:LEU:HB3	1.81	0.45
1:A:55:GLU:HB3	4:A:1475:HOH:O	2.16	0.45
1:D:60:VAL:HG21	1:D:65:LEU:HD12	1.98	0.45
1:E:70:TYR:HD1	1:E:171:GLU:HB3	1.80	0.45
1:C:86:LEU:O	1:C:90:GLN:HG3	2.17	0.45
1:H:158:GLU:CD	1:H:158:GLU:H	2.20	0.45
1:D:20:PRO:HB2	1:D:99:LYS:O	2.16	0.45
1:C:130:ASN:O	1:C:134:GLU:HG2	2.17	0.45
1:D:118:MET:HA	1:D:121:ASN:HD21	1.81	0.45
1:A:52:GLU:HA	1:A:53:PRO:HD3	1.76	0.44
1:C:164:ILE:HD12	1:C:180:LEU:HD11	1.99	0.44
1:F:21:PHE:HB3	1:F:100:LEU:HD12	1.99	0.44
1:E:39:HIS:HA	1:E:42:LYS:HE3	1.99	0.44
1:B:86:LEU:O	1:B:90:GLN:HG3	2.17	0.44
1:C:143:ILE:HD12	1:C:143:ILE:N	2.32	0.44
1:B:24:LEU:HB2	1:B:150:ILE:HG12	2.00	0.44
1:E:173:SER:HB3	4:E:1406:HOH:O	2.17	0.44
1:D:44:LYS:C	1:D:46:ASP:H	2.20	0.44
1:F:169:ARG:CB	1:F:173:SER:HB3	2.48	0.44
1:C:159:VAL:HG21	1:C:208:ASP:OD2	2.18	0.44
1:E:158:GLU:H	1:E:158:GLU:CD	2.21	0.44
1:C:64:ASN:O	1:C:68:LEU:HG	2.18	0.44
1:D:60:VAL:HG22	1:D:83:TYR:CE2	2.53	0.44
1:B:162:GLU:O	1:B:166:GLN:HG2	2.18	0.44
1:D:156:SER:HB3	1:D:159:VAL:CG2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:ASN:HD22	1:F:123:SER:H	1.66	0.43
1:G:83:TYR:O	1:G:87:THR:HG23	2.17	0.43
1:A:28:ASN:OD1	1:A:29:ILE:N	2.48	0.43
1:H:30:GLY:O	1:H:163:ARG:HD2	2.19	0.43
1:G:130:ASN:O	1:G:134:GLU:HG2	2.18	0.43
1:F:160:ALA:O	1:F:164:ILE:HG13	2.18	0.43
1:D:172:GLU:C	1:D:174:CYS:H	2.22	0.43
1:G:28:ASN:OD1	1:G:29:ILE:N	2.51	0.43
1:B:169:ARG:NE	1:B:170:SER:H	2.16	0.43
1:C:121:ASN:HD22	1:C:121:ASN:C	2.21	0.43
1:B:57:TRP:CE2	1:B:84:VAL:HG22	2.53	0.43
1:E:52:GLU:HA	1:E:53:PRO:HD3	1.90	0.43
1:G:177:LEU:O	1:G:181:GLN:HG3	2.19	0.43
1:H:52:GLU:HA	1:H:53:PRO:HD3	1.87	0.43
1:D:19:GLN:HE22	1:D:101:LYS:HZ2	1.58	0.42
1:D:52:GLU:OE2	3:D:1401:THM:HM51	2.19	0.42
1:A:38:ASN:O	1:A:41:GLU:HB2	2.19	0.42
1:C:105:ARG:HH11	1:C:105:ARG:HG3	1.83	0.42
1:A:199:SER:O	1:A:200:CYS:HB3	2.18	0.42
1:B:121:ASN:C	1:B:121:ASN:HD22	2.22	0.42
1:B:169:ARG:HH21	1:B:172:GLU:H	1.68	0.42
1:G:69:MET:O	1:G:73:PRO:HG3	2.20	0.42
1:B:118:MET:HA	1:B:121:ASN:OD1	2.20	0.42
1:G:119:ARG:HD3	1:G:129:TYR:CZ	2.54	0.42
1:A:26:GLU:OE2	1:A:109:SER:HB3	2.19	0.42
1:C:118:MET:HA	1:C:121:ASN:ND2	2.34	0.42
1:A:104:GLU:O	1:A:105:ARG:HB2	2.20	0.42
1:A:175:VAL:HG21	1:A:180:LEU:HD21	2.01	0.42
1:H:52:GLU:OE2	1:H:105:ARG:NH1	2.51	0.42
1:E:92:HIS:ND1	1:E:145:VAL:HG13	2.34	0.42
1:A:137:LYS:HE2	4:A:1503:HOH:O	2.20	0.42
1:A:52:GLU:OE2	1:A:105:ARG:HG3	2.20	0.42
1:A:33:LYS:HZ1	1:A:105:ARG:NH2	2.17	0.42
1:F:52:GLU:OE2	1:F:105:ARG:HG3	2.18	0.42
1:B:156:SER:HB3	1:B:159:VAL:HG23	2.02	0.42
1:A:121:ASN:HD22	1:A:122:GLY:N	2.17	0.42
1:E:119:ARG:HD3	1:E:129:TYR:CE1	2.55	0.42
1:A:89:LEU:HD11	1:A:143:ILE:HG12	2.02	0.41
1:E:72:ASP:OD2	1:E:75:LYS:HB3	2.20	0.41
1:D:78:MET:HA	1:D:124:LEU:HD21	2.02	0.41
1:B:53:PRO:HD3	4:B:1433:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:VAL:HG21	1:E:65:LEU:HD12	2.01	0.41
1:H:14:TYR:O	1:H:15:ALA:HB3	2.20	0.41
1:D:52:GLU:HA	1:D:53:PRO:HD3	1.85	0.41
1:G:104:GLU:O	1:G:105:ARG:HB2	2.20	0.41
1:H:69:MET:HG3	1:H:80:PHE:CD2	2.55	0.41
1:B:14:TYR:O	1:B:15:ALA:HB3	2.20	0.41
1:E:175:VAL:O	1:E:175:VAL:HG23	2.21	0.41
1:D:152:TYR:CG	1:D:191:LEU:HD13	2.56	0.41
1:C:69:MET:HG3	1:C:80:PHE:CD2	2.55	0.41
1:G:89:LEU:HD21	1:G:107:ILE:HD12	2.03	0.41
1:G:60:VAL:HG21	1:G:65:LEU:HG	2.03	0.41
1:F:52:GLU:O	1:F:54:VAL:N	2.49	0.41
1:C:198:GLN:HE21	1:C:200:CYS:N	2.18	0.41
1:B:52:GLU:C	1:B:54:VAL:H	2.24	0.41
1:F:155:THR:HG22	1:F:207:ALA:HB3	2.03	0.41
1:F:117:ASN:HB2	1:F:186:LEU:CD1	2.50	0.41
1:C:159:VAL:HG11	1:C:208:ASP:OD2	2.20	0.41
1:F:156:SER:HB3	1:F:159:VAL:CG2	2.48	0.41
1:D:65:LEU:HD13	1:D:80:PHE:HA	2.01	0.41
1:E:169:ARG:HG3	1:E:172:GLU:OE1	2.20	0.41
1:E:152:TYR:HB2	1:E:191:LEU:HD13	2.03	0.41
1:G:169:ARG:HB3	1:G:170:SER:H	1.50	0.41
1:H:175:VAL:HA	1:H:176:PRO:HD3	1.92	0.41
1:D:34:THR:HG22	1:D:38:ASN:HD21	1.85	0.41
1:B:37:LEU:CD2	1:B:49:LEU:HD21	2.51	0.40
1:D:105:ARG:HG3	1:D:105:ARG:HH11	1.84	0.40
1:A:14:TYR:O	1:A:15:ALA:HB3	2.21	0.40
1:C:69:MET:HA	1:C:76:TRP:HB2	2.02	0.40
1:E:33:LYS:NZ	1:E:33:LYS:HB2	2.36	0.40
1:C:57:TRP:HE1	1:C:87:THR:HG21	1.86	0.40
1:E:28:ASN:HD21	1:E:180:LEU:CD2	2.29	0.40
1:E:89:LEU:HD11	1:E:139:ILE:CD1	2.50	0.40
1:C:184:HIS:O	1:C:188:GLU:HG2	2.22	0.40
1:B:178:LYS:HE3	1:B:178:LYS:HB2	1.92	0.40
1:A:14:TYR:CZ	1:B:142:SER:HB3	2.57	0.40
1:D:78:MET:N	1:D:79:PRO:HD2	2.37	0.40
1:A:94:ALA:HA	1:A:95:PRO:HD3	1.80	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	195/250 (78%)	184 (94%)	10 (5%)	1 (0%)	34	55
1	B	188/250 (75%)	158 (84%)	29 (15%)	1 (0%)	34	55
1	C	195/250 (78%)	177 (91%)	17 (9%)	1 (0%)	34	55
1	D	187/250 (75%)	168 (90%)	15 (8%)	4 (2%)	9	14
1	E	188/250 (75%)	171 (91%)	16 (8%)	1 (0%)	34	55
1	F	188/250 (75%)	170 (90%)	14 (7%)	4 (2%)	9	14
1	G	188/250 (75%)	157 (84%)	28 (15%)	3 (2%)	12	21
1	H	188/250 (75%)	173 (92%)	15 (8%)	0	100	100
All	All	1517/2000 (76%)	1358 (90%)	144 (10%)	15 (1%)	19	34

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	174	CYS
1	B	16	GLU
1	D	173	SER
1	E	174	CYS
1	F	20	PRO
1	F	174	CYS
1	G	167	ARG
1	G	170	SER
1	D	45	ASN
1	F	170	SER
1	D	53	PRO
1	A	53	PRO
1	F	53	PRO
1	C	197	PRO
1	D	20	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	182/227 (80%)	176 (97%)	6 (3%)	45	73
1	B	177/227 (78%)	170 (96%)	7 (4%)	38	64
1	C	182/227 (80%)	177 (97%)	5 (3%)	52	79
1	D	176/227 (78%)	175 (99%)	1 (1%)	90	97
1	E	177/227 (78%)	174 (98%)	3 (2%)	68	89
1	F	177/227 (78%)	173 (98%)	4 (2%)	58	83
1	G	177/227 (78%)	175 (99%)	2 (1%)	80	94
1	H	177/227 (78%)	173 (98%)	4 (2%)	58	83
All	All	1425/1816 (78%)	1393 (98%)	32 (2%)	60	84

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	45	ASN
1	A	89	LEU
1	A	121	ASN
1	A	170	SER
1	A	196	ARG
1	B	18	THR
1	B	46	ASP
1	B	49	LEU
1	B	61	ASN
1	B	89	LEU
1	B	121	ASN
1	B	165	ARG
1	C	42	LYS
1	C	121	ASN
1	C	125	GLU
1	C	169	ARG
1	C	200	CYS
1	D	61	ASN

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Mol	Chain	Res	Type
1	E	42	LYS
1	E	49	LEU
1	E	121	ASN
1	F	74	LYS
1	F	121	ASN
1	F	165	ARG
1	F	169	ARG
1	G	121	ASN
1	G	169	ARG
1	H	78	MET
1	H	121	ASN
1	H	165	ARG
1	H	208	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	117	ASN
1	A	121	ASN
1	A	198	GLN
1	B	130	ASN
1	B	194	GLN
1	C	38	ASN
1	C	61	ASN
1	C	117	ASN
1	C	121	ASN
1	C	198	GLN
1	D	19	GLN
1	D	38	ASN
1	D	45	ASN
1	D	61	ASN
1	D	117	ASN
1	D	130	ASN
1	E	28	ASN
1	E	117	ASN
1	E	121	ASN
1	E	130	ASN
1	E	144	HIS
1	F	38	ASN
1	F	117	ASN
1	F	121	ASN

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Mol	Chain	Res	Type
1	F	144	HIS
1	F	193	HIS
1	G	38	ASN
1	G	45	ASN
1	G	117	ASN
1	G	121	ASN
1	H	117	ASN
1	H	121	ASN

### 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](#)

17 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	SO4	A	1300	-	4,4,4	0.43	0	6,6,6	0.29	0
2	SO4	A	1308	-	4,4,4	0.09	0	6,6,6	0.12	0
3	THM	A	1400	-	13,18,18	1.60	2 (15%)	16,26,26	2.90	9 (56%)
2	SO4	B	1306	-	4,4,4	0.18	0	6,6,6	0.07	0
3	THM	B	1406	-	13,18,18	1.46	2 (15%)	16,26,26	2.82	8 (50%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	C	1305	-	4,4,4	0.20	0	6,6,6	0.08	0
3	THM	C	1405	-	13,18,18	1.46	2 (15%)	16,26,26	2.86	8 (50%)
2	SO4	D	1301	-	4,4,4	0.25	0	6,6,6	0.15	0
3	THM	D	1401	-	13,18,18	1.45	2 (15%)	16,26,26	2.96	9 (56%)
2	SO4	E	1302	-	4,4,4	0.38	0	6,6,6	0.10	0
3	THM	E	1402	-	13,18,18	1.53	3 (23%)	16,26,26	2.96	9 (56%)
2	SO4	F	1304	-	4,4,4	0.13	0	6,6,6	0.07	0
3	THM	F	1404	-	13,18,18	1.52	2 (15%)	16,26,26	2.89	9 (56%)
2	SO4	G	1303	-	4,4,4	0.20	0	6,6,6	0.08	0
3	THM	G	1403	-	13,18,18	1.52	2 (15%)	16,26,26	3.02	9 (56%)
2	SO4	H	1307	-	4,4,4	0.07	0	6,6,6	0.32	0
3	THM	H	1407	-	13,18,18	1.76	4 (30%)	16,26,26	2.93	8 (50%)

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	SO4	A	1300	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1308	-	-	0/0/0/0	0/0/0/0
3	THM	A	1400	-	-	0/2/18/18	0/2/2/2
2	SO4	B	1306	-	-	0/0/0/0	0/0/0/0
3	THM	B	1406	-	-	0/2/18/18	0/2/2/2
2	SO4	C	1305	-	-	0/0/0/0	0/0/0/0
3	THM	C	1405	-	-	0/2/18/18	0/2/2/2
2	SO4	D	1301	-	-	0/0/0/0	0/0/0/0
3	THM	D	1401	-	-	0/2/18/18	0/2/2/2
2	SO4	E	1302	-	-	0/0/0/0	0/0/0/0
3	THM	E	1402	-	-	0/2/18/18	0/2/2/2
2	SO4	F	1304	-	-	0/0/0/0	0/0/0/0
3	THM	F	1404	-	-	0/2/18/18	0/2/2/2
2	SO4	G	1303	-	-	0/0/0/0	0/0/0/0
3	THM	G	1403	-	-	0/2/18/18	0/2/2/2
2	SO4	H	1307	-	-	0/0/0/0	0/0/0/0
3	THM	H	1407	-	-	0/2/18/18	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1402	THM	C5'-C4'	2.05	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1407	THM	O3'-C3'	2.16	1.48	1.43
3	H	1407	THM	C5'-C4'	2.26	1.60	1.51
3	A	1400	THM	O4-C4	2.67	1.31	1.24
3	H	1407	THM	O4-C4	2.70	1.31	1.24
3	G	1403	THM	O4-C4	2.82	1.31	1.24
3	C	1405	THM	O4-C4	2.98	1.31	1.24
3	F	1404	THM	O4-C4	2.99	1.31	1.24
3	B	1406	THM	O4-C4	3.01	1.31	1.24
3	E	1402	THM	O4-C4	3.11	1.32	1.24
3	B	1406	THM	O3'-C3'	3.19	1.50	1.43
3	D	1401	THM	O3'-C3'	3.21	1.50	1.43
3	D	1401	THM	O4-C4	3.22	1.32	1.24
3	C	1405	THM	O3'-C3'	3.39	1.51	1.43
3	F	1404	THM	O3'-C3'	3.45	1.51	1.43
3	H	1407	THM	C3'-C4'	3.46	1.62	1.53
3	E	1402	THM	O3'-C3'	3.58	1.51	1.43
3	A	1400	THM	O3'-C3'	3.61	1.51	1.43
3	G	1403	THM	O3'-C3'	3.84	1.52	1.43

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1402	THM	C5-C4-N3	-4.86	119.72	125.14
3	G	1403	THM	C5-C4-N3	-4.80	119.79	125.14
3	C	1405	THM	C5-C4-N3	-4.76	119.83	125.14
3	F	1404	THM	C5-C4-N3	-4.74	119.86	125.14
3	D	1401	THM	C5-C4-N3	-4.72	119.88	125.14
3	B	1406	THM	C5-C4-N3	-4.70	119.91	125.14
3	A	1400	THM	C5-C4-N3	-4.66	119.95	125.14
3	H	1407	THM	C5-C4-N3	-4.39	120.24	125.14
3	H	1407	THM	C2'-C3'-C4'	-3.95	94.59	102.77
3	G	1403	THM	O4'-C4'-C3'	-3.73	96.29	105.67
3	D	1401	THM	C2'-C3'-C4'	-3.62	95.26	102.77
3	G	1403	THM	C2'-C3'-C4'	-3.62	95.27	102.77
3	A	1400	THM	C2'-C3'-C4'	-3.58	95.35	102.77
3	F	1404	THM	C2'-C3'-C4'	-3.57	95.38	102.77
3	B	1406	THM	C2'-C3'-C4'	-3.53	95.46	102.77
3	H	1407	THM	O4'-C4'-C3'	-3.52	96.82	105.67
3	D	1401	THM	O4'-C4'-C3'	-3.52	96.82	105.67
3	E	1402	THM	C2'-C3'-C4'	-3.48	95.56	102.77
3	E	1402	THM	O4'-C4'-C3'	-3.46	96.96	105.67
3	A	1400	THM	O4'-C4'-C3'	-3.46	96.97	105.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1404	THM	O4'-C4'-C3'	-3.46	96.98	105.67
3	C	1405	THM	C2'-C3'-C4'	-3.40	95.73	102.77
3	B	1406	THM	O4'-C4'-C3'	-3.27	97.44	105.67
3	C	1405	THM	O4'-C4'-C3'	-3.18	97.68	105.67
3	E	1402	THM	O4'-C1'-C2'	-2.57	101.14	106.27
3	G	1403	THM	O4'-C1'-C2'	-2.54	101.21	106.27
3	H	1407	THM	O4'-C1'-C2'	-2.47	101.35	106.27
3	D	1401	THM	O4'-C1'-C2'	-2.45	101.39	106.27
3	B	1406	THM	O4'-C1'-C2'	-2.35	101.59	106.27
3	F	1404	THM	O4'-C1'-C2'	-2.26	101.77	106.27
3	C	1405	THM	O4'-C1'-C2'	-2.12	102.04	106.27
3	A	1400	THM	O4'-C1'-C2'	-2.03	102.23	106.27
3	E	1402	THM	C2'-C1'-N1	2.08	119.21	114.16
3	A	1400	THM	O3'-C3'-C4'	2.11	118.57	110.05
3	F	1404	THM	C2'-C1'-N1	2.12	119.30	114.16
3	D	1401	THM	C2'-C1'-N1	2.25	119.64	114.16
3	G	1403	THM	C2'-C1'-N1	2.30	119.74	114.16
3	H	1407	THM	C5'-C4'-C3'	2.39	121.18	114.80
3	B	1406	THM	C5'-C4'-C3'	3.11	123.09	114.80
3	C	1405	THM	O3'-C3'-C2'	3.12	121.08	110.74
3	F	1404	THM	O3'-C3'-C2'	3.13	121.11	110.74
3	E	1402	THM	O3'-C3'-C2'	3.15	121.17	110.74
3	B	1406	THM	O3'-C3'-C2'	3.17	121.25	110.74
3	A	1400	THM	O3'-C3'-C2'	3.19	121.30	110.74
3	D	1401	THM	C5'-C4'-C3'	3.22	123.38	114.80
3	D	1401	THM	O3'-C3'-C2'	3.25	121.50	110.74
3	C	1405	THM	C5'-C4'-C3'	3.26	123.47	114.80
3	F	1404	THM	C5'-C4'-C3'	3.28	123.53	114.80
3	A	1400	THM	C5'-C4'-C3'	3.29	123.57	114.80
3	G	1403	THM	O3'-C3'-C2'	3.32	121.74	110.74
3	H	1407	THM	O3'-C3'-C2'	3.34	121.80	110.74
3	E	1402	THM	C5'-C4'-C3'	3.35	123.72	114.80
3	G	1403	THM	C5'-C4'-C3'	3.49	124.08	114.80
3	B	1406	THM	O4'-C4'-C5'	4.12	118.10	109.17
3	A	1400	THM	O4'-C4'-C5'	4.32	118.53	109.17
3	C	1405	THM	O4'-C4'-C5'	4.41	118.72	109.17
3	F	1404	THM	O4'-C4'-C5'	4.64	119.22	109.17
3	G	1403	THM	O4'-C4'-C5'	4.68	119.31	109.17
3	D	1401	THM	O4'-C4'-C5'	4.73	119.41	109.17
3	H	1407	THM	C4-N3-C2	4.74	119.34	115.25
3	E	1402	THM	O4'-C4'-C5'	4.79	119.54	109.17
3	F	1404	THM	C4-N3-C2	5.05	119.61	115.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1403	THM	C4-N3-C2	5.27	119.80	115.25
3	H	1407	THM	O4'-C4'-C5'	5.38	120.82	109.17
3	E	1402	THM	C4-N3-C2	5.39	119.90	115.25
3	D	1401	THM	C4-N3-C2	5.41	119.92	115.25
3	B	1406	THM	C4-N3-C2	5.42	119.94	115.25
3	C	1405	THM	C4-N3-C2	5.48	119.99	115.25
3	A	1400	THM	C4-N3-C2	5.66	120.14	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1405	THM	1	0
3	D	1401	THM	1	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	197/250 (78%)	0.03	5 (2%) 61 65	20, 37, 59, 97	0
1	B	192/250 (76%)	0.53	24 (12%) 5 5	28, 57, 98, 110	0
1	C	197/250 (78%)	0.49	18 (9%) 11 12	36, 65, 106, 115	0
1	D	191/250 (76%)	0.67	22 (11%) 6 6	41, 72, 103, 114	0
1	E	192/250 (76%)	0.39	10 (5%) 31 35	36, 61, 95, 110	0
1	F	192/250 (76%)	1.00	35 (18%) 2 2	42, 79, 107, 116	0
1	G	192/250 (76%)	0.68	18 (9%) 11 11	32, 69, 108, 123	0
1	H	192/250 (76%)	-0.13	2 (1%) 84 86	21, 35, 55, 71	0
All	All	1545/2000 (77%)	0.46	134 (8%) 13 13	20, 60, 103, 123	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	12	THR	8.0
1	F	168	ALA	5.7
1	F	95	PRO	5.3
1	F	170	SER	5.2
1	G	206	ASP	5.1
1	D	192	ILE	4.9
1	G	207	ALA	4.9
1	F	173	SER	4.8
1	F	18	THR	4.7
1	G	166	GLN	4.6
1	C	169	ARG	4.5
1	G	173	SER	4.5
1	B	170	SER	4.4
1	E	169	ARG	4.2
1	G	169	ARG	4.2
1	C	207	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	169	ARG	4.1
1	C	208	ASP	3.9
1	D	12	THR	3.8
1	C	18	THR	3.8
1	C	172	GLU	3.8
1	B	168	ALA	3.7
1	A	97	ASN	3.6
1	F	145	VAL	3.6
1	E	12	THR	3.5
1	C	199	SER	3.5
1	F	17	GLY	3.5
1	G	170	SER	3.5
1	D	193	HIS	3.4
1	G	168	ALA	3.4
1	A	199	SER	3.4
1	E	166	GLN	3.4
1	D	169	ARG	3.4
1	F	105	ARG	3.4
1	G	203	LEU	3.3
1	G	42	LYS	3.3
1	A	208	ASP	3.2
1	D	95	PRO	3.2
1	A	12	THR	3.2
1	E	168	ALA	3.1
1	E	17	GLY	3.1
1	D	200	CYS	3.1
1	E	18	THR	3.0
1	F	25	ILE	3.0
1	B	110	ALA	3.0
1	D	97	ASN	3.0
1	B	45	ASN	3.0
1	D	114	PHE	2.9
1	F	94	ALA	2.9
1	F	27	GLY	2.9
1	F	208	ASP	2.9
1	B	44	LYS	2.9
1	B	85	THR	2.8
1	C	95	PRO	2.8
1	G	48	CYS	2.8
1	B	201	LYS	2.8
1	F	106	SER	2.8
1	F	82	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	200	CYS	2.8
1	D	15	ALA	2.8
1	F	193	HIS	2.8
1	F	144	HIS	2.8
1	D	165	ARG	2.7
1	F	201	LYS	2.7
1	G	205	LEU	2.7
1	B	173	SER	2.7
1	A	207	ALA	2.7
1	D	27	GLY	2.7
1	F	97	ASN	2.7
1	F	166	GLN	2.7
1	F	165	ARG	2.6
1	F	207	ALA	2.6
1	E	97	ASN	2.6
1	H	85	THR	2.6
1	D	173	SER	2.6
1	D	78	MET	2.6
1	C	17	GLY	2.6
1	G	208	ASP	2.6
1	D	168	ALA	2.6
1	F	203	LEU	2.5
1	G	85	THR	2.5
1	D	144	HIS	2.5
1	F	104	GLU	2.5
1	B	18	THR	2.5
1	B	200	CYS	2.5
1	H	208	ASP	2.5
1	B	17	GLY	2.5
1	D	106	SER	2.5
1	B	192	ILE	2.4
1	F	12	THR	2.4
1	F	194	GLN	2.4
1	F	99	LYS	2.4
1	B	174	CYS	2.4
1	B	194	GLN	2.4
1	B	208	ASP	2.4
1	D	18	THR	2.4
1	F	84	VAL	2.3
1	G	82	SER	2.3
1	B	97	ASN	2.3
1	B	41	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	108	PHE	2.3
1	C	170	SER	2.3
1	G	84	VAL	2.3
1	G	185	GLU	2.3
1	B	16	GLU	2.3
1	E	173	SER	2.3
1	G	47	ILE	2.3
1	B	206	ASP	2.3
1	D	44	LYS	2.2
1	B	95	PRO	2.2
1	C	44	LYS	2.2
1	B	42	LYS	2.2
1	E	25	ILE	2.2
1	F	103	MET	2.2
1	B	169	ARG	2.2
1	D	201	LYS	2.2
1	C	173	SER	2.2
1	C	165	ARG	2.2
1	G	35	THR	2.1
1	B	207	ALA	2.1
1	F	202	VAL	2.1
1	C	82	SER	2.1
1	F	204	VAL	2.1
1	D	99	LYS	2.1
1	C	85	THR	2.1
1	D	110	ALA	2.1
1	D	208	ASP	2.1
1	F	42	LYS	2.1
1	C	15	ALA	2.1
1	B	114	PHE	2.1
1	E	141	GLU	2.0
1	C	84	VAL	2.0
1	C	206	ASP	2.0
1	F	43	TYR	2.0

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

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



### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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( $\text{\AA}^2$ )	Q<0.9
3	THM	G	1403	17/17	0.94	0.28	1.35	66,70,72,73	0
3	THM	C	1405	17/17	0.92	0.27	0.88	55,58,64,65	0
3	THM	D	1401	17/17	0.96	0.26	0.76	48,51,58,60	0
3	THM	B	1406	17/17	0.96	0.23	0.57	29,37,45,45	0
3	THM	H	1407	17/17	0.98	0.18	0.57	16,26,30,31	0
3	THM	A	1400	17/17	0.97	0.20	0.55	27,31,36,38	0
3	THM	E	1402	17/17	0.96	0.19	-0.04	39,44,52,52	0
3	THM	F	1404	17/17	0.96	0.20	-0.36	45,49,56,58	0
2	SO4	F	1304	5/5	0.96	0.16	-0.73	65,67,68,70	0
2	SO4	H	1307	5/5	0.99	0.14	-0.80	30,31,33,34	0
2	SO4	D	1301	5/5	0.95	0.15	-0.96	55,56,60,61	0
2	SO4	C	1305	5/5	0.98	0.11	-1.02	66,67,68,69	0
2	SO4	B	1306	5/5	0.99	0.12	-1.29	43,44,47,50	0
2	SO4	E	1302	5/5	0.99	0.12	-1.44	49,49,51,52	0
2	SO4	G	1303	5/5	0.97	0.12	-1.97	69,69,69,72	0
2	SO4	A	1300	5/5	0.99	0.09	-2.39	29,29,33,35	0
2	SO4	A	1308	5/5	0.99	0.19	-	43,46,49,50	0

### 6.5 Other polymers

There are no such residues in this entry.