Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2023 – 12:16 PM EDT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

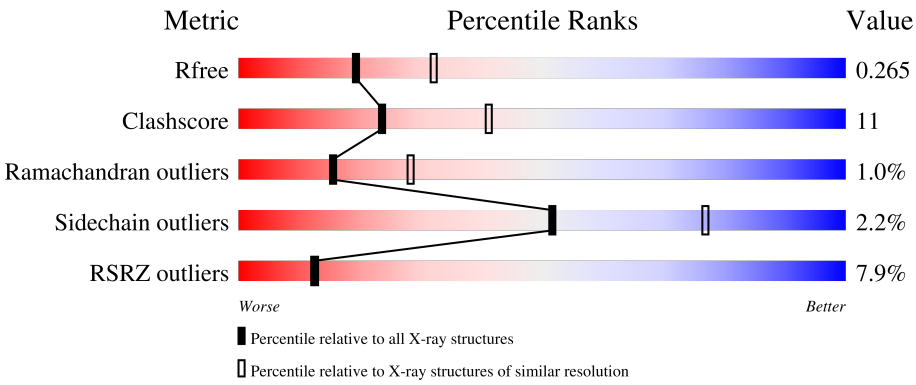
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	2%, 57%, 21%, •, 21%
1	B	250	9%, 59%, 16%, •, 23%
1	C	250	6%, 59%, 18%, •, 21%
1	D	250	8%, 56%, 20%, •, 24%
1	E	250	4%, 56%, 19%, •, 23%

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Mol	Chain	Length	Quality of chain
1	F	250	13% 58% 18% 23%
1	G	250	7% 56% 19% 23%
1	H	250	% 62% 14% 23%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	THM	H	1407	-	X	-	-

2 Entry composition (i)

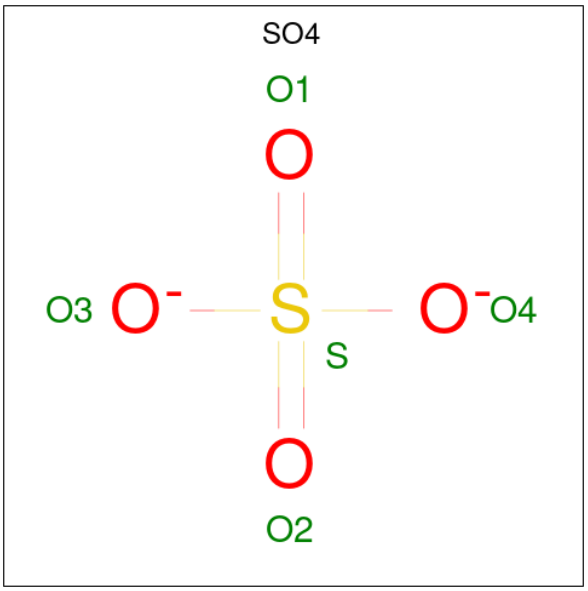
There are 4 unique types of molecules in this entry. The entry contains 13338 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

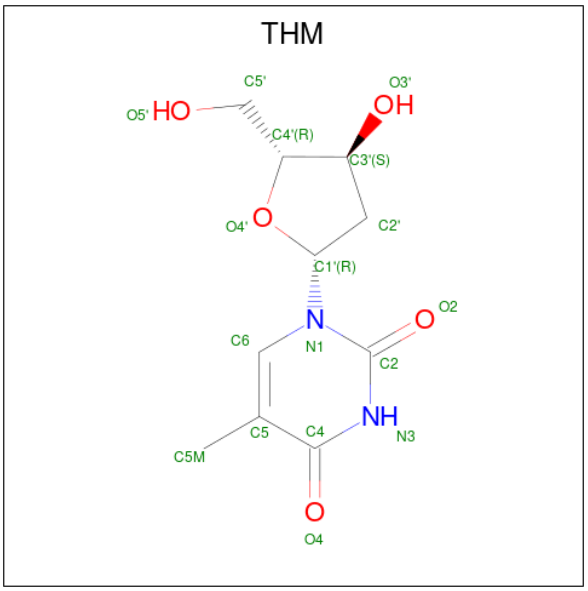
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	197	1640	1046	282	302	10	0	0	0
1	B	192	1596	1021	270	295	10	0	0	0
1	C	197	1640	1046	282	302	10	0	0	0
1	D	191	1587	1016	268	293	10	0	0	0
1	E	192	1596	1021	270	295	10	0	0	0
1	F	192	1596	1021	270	295	10	0	0	0
1	G	192	1596	1021	270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

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is THYMIDINE (three-letter code: THM) (formula: $C_{10}H_{14}N_2O_5$).



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

- Molecule 4 is water.

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

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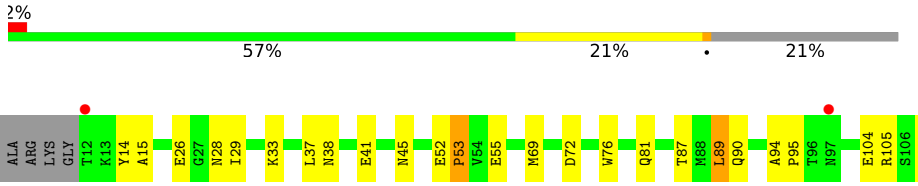
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	E	27	27	27	0	0
			Total	O		
4	F	16	16	16	0	0
			Total	O		
4	G	18	18	18	0	0
			Total	O		
4	H	65	65	65	0	0

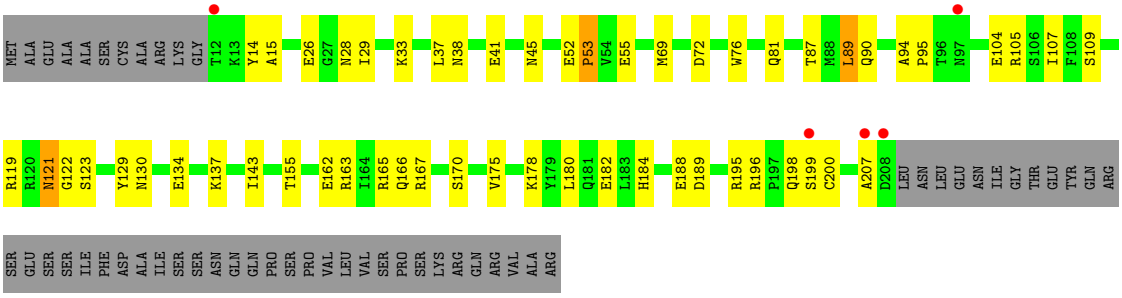
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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

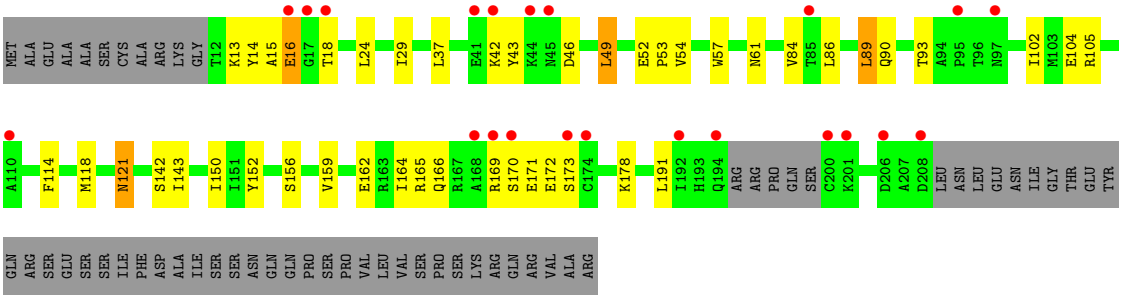
Chain A:





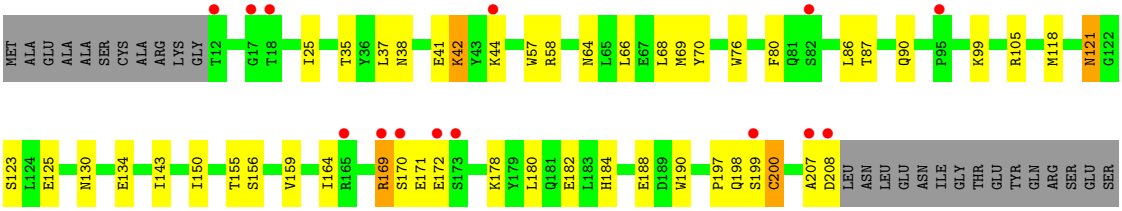
• Molecule 1: Deoxyribonucleoside Kinase

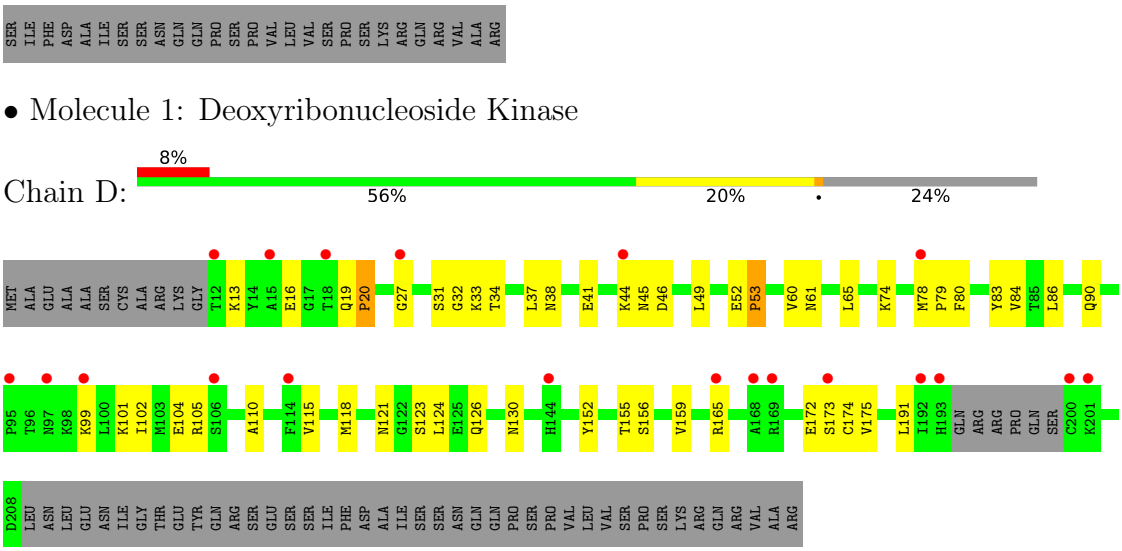
Chain B:

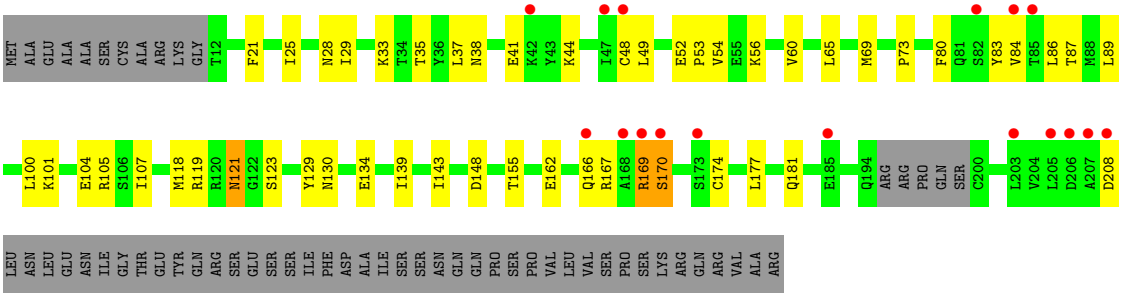


• Molecule 1: Deoxyribonucleoside Kinase

Chain C:

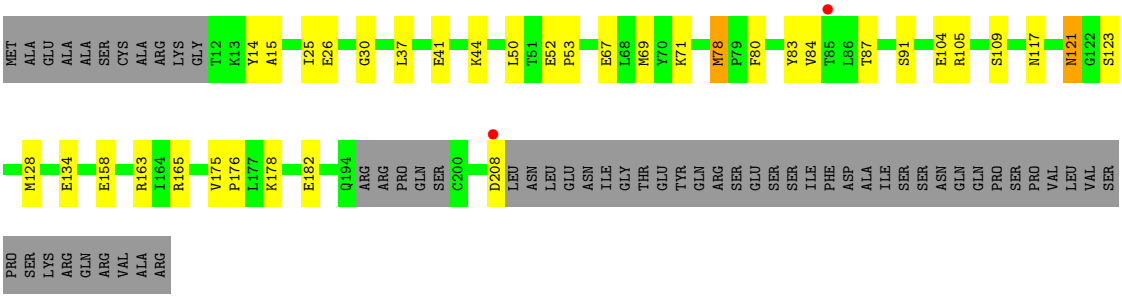



SER ILE PHE ASP ALA ILE SER SER ASN GLN GLN PRO SER PRO VAL LEU VAL SER PRO SER LYS ARG GLN ARG VAL ALA ARG
• Molecule 1: Deoxyribonucleoside Kinase
Chain D:
8%
56%
20%
24%
MET ALA GLU ALA ALA SER CYS ALA ARG LYS GLY T12 K13 Y14 A15 E16 G17 T18 Q19 P20 G27 S31 G32 K33 T34 L37 N38 E41 K44 N45 D46 L49 E52 P53 V60 N61 L65 K74 M78 P79 F80 Y83 V84 T85 L86 Q90
P95 T96 N97 K98 K99 L100 K101 I102 M103 E104 R105 S106 A110 F114 V115 M118 N121 G122 S123 L124 E125 Q126 N130 H144 Y152 T155 S156 V159 R165 A168 R169 E172 S173 C174 V175 L191 I192 H193 GLN ARG ARG PRO GLN SER C200 K201
D208 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 LYS ARG GLN ARG VAL ALA ARG
• Molecule 1: Deoxyribonucleoside Kinase
Chain E:
4%
56%
19%
23%
MET ALA GLU ALA ALA SER CYS ALA ARG LYS GLY T12 G17 T18 L24 I25 N28 K33 L37 N38 H39 K42 I47 C48 L49 E52 P53 V60 L65 L66 E67 Y70 K71 D72 K75 L86 L89 Q90 S91 H92 N97 L100 E104
R105 M118 R119 R120 N121 G122 S123 Y129 I139 V145 I150 I151 Y152 T155 E158 I164 R165 Q166 R167 A168 R169 S170 E171 E172 S173 C174 V175 P176 L177 K178 Y179 L180 Q181 E182 D189 W190 L191 Q194 ARG ARG PRO GLN SER C200 A207 D208 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 LYS ARG GLN ARG VAL ALA ARG
• Molecule 1: Deoxyribonucleoside Kinase
Chain F:
13%
58%
18%
23%
MET ALA GLU ALA ALA SER CYS ALA ARG LYS GLY T12 G17 T18 Q19 P20 F21 I25 E26 G27 N28 I29 G30 S31 L37 K42 E52 P53 V54 E55 K56 W57 R58 N64 E67 L68 M69 K74 S82 Y83 V84 L89 H92 T93 A94 P95 T96 N97 K98
K99 L100 M103 E104 R105 S106 I107 F108 N117 N121 G122 S123 L124 E125 M128 Y129 N130 E134 W135 I139 I143 H144 V145 L153 R154 T155 S156 V159 A160 I164 R165 Q166 R167 A168 R169 S170 S173 C174 K178 E182 L186 H193 Q194 ARG ARG
PRO GLN SER C200 K201 V202 L203 A207 D208 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 LYS ARG GLN ARG VAL ALA ARG
• Molecule 1: Deoxyribonucleoside Kinase
Chain G:
7%
56%
19%
23%



- Molecule 1: Deoxyribonucleoside Kinase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	3.38 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.276 0.219 , 0.265	Depositor DCC
R_{free} test set	3560 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	46.8	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l 0.004 for k,h,-l 0.023 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13338	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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:H	1:A:143:ILE:HD12	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:E:42:LYS:HD3	1:E:42:LYS:N	2.09	0.66
1:H:25:ILE:HG13	1:H:37:LEU:HD21	1.78	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:A:33:LYS:NZ	4:A:1490:HOH:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ARG:HB3	1:B:173:SER:HB3	1.81	0.60
1:D:86:LEU:O	1:D:90:GLN:HG3	2.00	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:C:150:ILE:HG13	1:C:200:CYS:SG	2.42	0.60
1:G:89:LEU:HD13	1:G:143:ILE:CD1	2.31	0.60
1:B:42:LYS:HE2	1:B:43:TYR:HE1	1.67	0.60
1:A:95:PRO:HA	4:A:1471:HOH:O	2.02	0.59
1:H:178:LYS:O	1:H:182:GLU:HG3	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:F:135:TRP:O	1:F:139:ILE:HG13	2.02	0.58
1:G:118:MET:HA	1:G:121:ASN:ND2	2.19	0.58
1:F:64:ASN:ND2	1:F:67:GLU:HB2	2.17	0.58
1:A:163:ARG:O	1:A:167:ARG:HG3	2.04	0.58
1:F:121:ASN:C	1:F:121:ASN:HD22	2.07	0.58
1:A:81:GLN:HA	1:A:81:GLN:NE2	2.20	0.57
1:H:67:GLU:HG3	1:H:71:LYS:HE2	1.87	0.57
1:C:198:GLN:NE2	1:C:199:SER:H	2.03	0.57
1:D:165:ARG:HA	1:D:165:ARG:NH1	2.18	0.57
1:B:89:LEU:HD21	1:B:143:ILE:HG21	1.87	0.56
1:C:99:LYS:HE2	1:C:99:LYS:HA	1.87	0.56
1:E:42:LYS:H	1:E:42:LYS:CD	2.11	0.56
1:E:121:ASN:ND2	1:E:123:SER:H	2.03	0.56
1:F:74:LYS:H	1:F:74:LYS:HD2	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:C:121:ASN:HD21	1:C:123:SER:HB2	1.75	0.52
1:E:118:MET:HA	1:E:121:ASN:HD21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:ILE:HD12	1:E:180:LEU:HD11	1.92	0.52
1:G:80:PHE:O	1:G:84:VAL:HG23	2.09	0.52
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:E:155:THR:CG2	1:E:207:ALA:HB3	2.39	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:A:69:MET:HA	1:A:76:TRP:HB2	1.92	0.50
1:B:52:GLU:O	1:B:54:VAL:HG23	2.11	0.50
1:D:49:LEU:HD13	1:D:102:ILE:HB	1.93	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:B:169:ARG:HH21	1:B:171:GLU:N	2.09	0.49
1:E:28:ASN:ND2	1:E:180:LEU:HD22	2.25	0.49
1:B:42:LYS:HG3	1:B:43:TYR:HD1	1.78	0.49
1:D:13:LYS:HB2	1:D:16:GLU:HB2	1.95	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: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: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:F:58:ARG:HA	1:F:64:ASN:OD1	2.13	0.49
1:H:83:TYR:O	1:H:87:THR:HG23	2.12	0.49
1:A:162:GLU:OE2	1:A:165:ARG:HD3	2.13	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: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:G:35:THR:O	1:G:38:ASN:HB2	2.12	0.48
1:H:117:ASN:HB3	4:H:1417:HOH:O	2.11	0.48
1:C:169:ARG:CD	1:C:170:SER:H	2.26	0.48
1:F:52:GLU:C	1:F:54:VAL:H	2.17	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: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:G:48:CYS:SG	1:G:101:LYS:HE2	2.54	0.48
1:A:178:LYS:O	1:A:182:GLU:HG3	2.13	0.48
1:F:28:ASN:OD1	1:F:29:ILE:N	2.46	0.48
1:F:69:MET:SD	1:F:69:MET:C	2.92	0.48
1:A:14:TYR:CE2	1:B:142:SER:HB3	2.48	0.47
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:C:178:LYS:O	1:C:182:GLU:HG3	2.13	0.47
1:A:121:ASN:ND2	1:A:121:ASN:C	2.65	0.47
1:C:143:ILE:HD12	1:C:143:ILE:H	1.79	0.47
1:A:119:ARG:HD3	1:A:129:TYR:CD1	2.50	0.47
1:C:38:ASN:O	1:C:41:GLU:HB2	2.15	0.47
1:D:80:PHE:O	1:D:84:VAL:HG23	2.15	0.47
1:B:104:GLU:O	1:B:105:ARG:HB2	2.14	0.47
1:G:21:PHE:HA	1:G:148:ASP:OD2	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:F:153:LEU:HD22	1:F:207:ALA:HB2	1.98	0.46
1:H:121:ASN:C	1:H:121:ASN:ND2	2.67	0.46
1:A:184:HIS:O	1:A:188:GLU:HG2	2.16	0.46
1:B:15:ALA:HB2	1:B:93:THR:HB	1.98	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:NH1	1:G:119:ARG:HG2	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:C	1:G:121:ASN:HD22	2.19	0.45
1:E:177:LEU:O	1:E:181:GLN:HG3	2.16	0.45
1:G:119:ARG:HG2	1:G:119:ARG:HH11	1.81	0.45
1:D:32:GLY:HA2	4:D:1412:HOH:O	2.16	0.45
1:D:41:GLU:OE1	1:D:41:GLU:HA	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: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:C:86:LEU:O	1:C:90:GLN:HG3	2.17	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:130:ASN:O	1:C:134:GLU:HG2	2.17	0.45
1:D:20:PRO:HB2	1:D:99:LYS:O	2.16	0.45
1:H:158:GLU:H	1:H:158:GLU:CD	2.20	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:B:24:LEU:HB2	1:B:150:ILE:HG12	2.00	0.44
1:C:143:ILE:HD12	1:C:143:ILE:N	2.32	0.44
1:D:44:LYS:C	1:D:46:ASP:H	2.20	0.44
1:E:173:SER:HB3	4:E:1406:HOH:O	2.17	0.44
1:F:169:ARG:CB	1:F:173:SER:HB3	2.48	0.44
1:C:64:ASN:O	1:C:68:LEU:HG	2.18	0.44
1:C:159:VAL:HG21	1:C:208:ASP:OD2	2.18	0.44
1:E:158:GLU:CD	1:E:158:GLU:H	2.21	0.44
1:B:162:GLU:O	1:B:166:GLN:HG2	2.18	0.44
1:D:60:VAL:HG22	1:D:83:TYR:CE2	2.53	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:A:28:ASN:OD1	1:A:29:ILE:N	2.48	0.43
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:H:30:GLY:O	1:H:163:ARG:HD2	2.19	0.43
1:F:160:ALA:O	1:F:164:ILE:HG13	2.18	0.43
1:G:130:ASN:O	1:G:134:GLU:HG2	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:B:57:TRP:CE2	1:B:84:VAL:HG22	2.53	0.43
1:C:121:ASN:C	1:C:121:ASN:HD22	2.21	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:A:38:ASN:O	1:A:41:GLU:HB2	2.19	0.42
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:C:105:ARG:HG3	1:C:105:ARG:HH11	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:A:26:GLU:OE2	1:A:109:SER:HB3	2.19	0.42
1:B:118:MET:HA	1:B:121:ASN:OD1	2.20	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:G:119:ARG:HD3	1:G:129:TYR:CZ	2.54	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:C:118:MET:HA	1:C:121:ASN:ND2	2.34	0.42
1:A:137:LYS:HE2	4:A:1503:HOH:O	2.20	0.42
1:E:92:HIS:ND1	1:E:145:VAL:HG13	2.34	0.42
1:H:52:GLU:OE2	1:H:105:ARG:NH1	2.51	0.42
1:A:33:LYS:HZ1	1:A:105:ARG:NH2	2.17	0.42
1:A:52:GLU:OE2	1:A:105:ARG:HG3	2.20	0.42
1:B:156:SER:HB3	1:B:159:VAL:HG23	2.02	0.42
1:F:52:GLU:OE2	1:F:105:ARG:HG3	2.18	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:D:78:MET:HA	1:D:124:LEU:HD21	2.02	0.41
1:E:72:ASP:OD2	1:E:75:LYS:HB3	2.20	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: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:H:69:MET:HG3	1:H:80:PHE:CD2	2.55	0.41
1:C:69:MET:HG3	1:C:80:PHE:CD2	2.55	0.41
1:D:152:TYR:CG	1:D:191:LEU:HD13	2.56	0.41
1:G:60:VAL:HG21	1:G:65:LEU:HG	2.03	0.41
1:G:89:LEU:HD21	1:G:107:ILE:HD12	2.03	0.41
1:B:52:GLU:C	1:B:54:VAL:H	2.24	0.41
1:C:198:GLN:HE21	1:C:200:CYS:N	2.18	0.41
1:F:52:GLU:O	1:F:54:VAL:N	2.49	0.41
1:F:117:ASN:HB2	1:F:186:LEU:CD1	2.50	0.41
1:F:155:THR:HG22	1:F:207:ALA:HB3	2.03	0.41
1:C:159:VAL:HG11	1:C:208:ASP:OD2	2.20	0.41
1:D:65:LEU:HD13	1:D:80:PHE:HA	2.01	0.41
1:E:152:TYR:HB2	1:E:191:LEU:HD13	2.03	0.41
1:E:169:ARG:HG3	1:E:172:GLU:OE1	2.20	0.41
1:F:156:SER:HB3	1:F:159:VAL:CG2	2.48	0.41
1:G:169:ARG:HB3	1:G:170:SER:H	1.50	0.41
1:D:34:THR:HG22	1:D:38:ASN:HD21	1.85	0.41
1:H:175:VAL:HA	1:H:176:PRO:HD3	1.92	0.41
1:A:14:TYR:O	1:A:15:ALA:HB3	2.21	0.40
1:B:37:LEU:CD2	1:B:49:LEU:HD21	2.51	0.40
1:C:57:TRP:HE1	1:C:87:THR:HG21	1.86	0.40
1:C:69:MET:HA	1:C:76:TRP:HB2	2.02	0.40
1:D:105:ARG:HG3	1:D:105:ARG:HH11	1.84	0.40
1:E:33:LYS:HB2	1:E:33:LYS:NZ	2.36	0.40
1:B:178:LYS:HE3	1:B:178:LYS:HB2	1.92	0.40
1:C:184:HIS:O	1:C:188:GLU:HG2	2.22	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: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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	195/250 (78%)	184 (94%)	10 (5%)	1 (0%)	29	48
1	B	188/250 (75%)	158 (84%)	29 (15%)	1 (0%)	29	48
1	C	195/250 (78%)	177 (91%)	17 (9%)	1 (0%)	29	48
1	D	187/250 (75%)	168 (90%)	15 (8%)	4 (2%)	7	11
1	E	188/250 (75%)	171 (91%)	16 (8%)	1 (0%)	29	48
1	F	188/250 (75%)	170 (90%)	14 (7%)	4 (2%)	7	11
1	G	188/250 (75%)	157 (84%)	28 (15%)	3 (2%)	9	17
1	H	188/250 (75%)	173 (92%)	15 (8%)	0	100	100
All	All	1517/2000 (76%)	1358 (90%)	144 (10%)	15 (1%)	15	28

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	182/227 (80%)	176 (97%)	6 (3%)	38	64
1	B	177/227 (78%)	170 (96%)	7 (4%)	31	56
1	C	182/227 (80%)	177 (97%)	5 (3%)	44	71
1	D	176/227 (78%)	175 (99%)	1 (1%)	86	95
1	E	177/227 (78%)	174 (98%)	3 (2%)	60	82
1	F	177/227 (78%)	173 (98%)	4 (2%)	50	76
1	G	177/227 (78%)	175 (99%)	2 (1%)	73	89
1	H	177/227 (78%)	173 (98%)	4 (2%)	50	76
All	All	1425/1816 (78%)	1393 (98%)	32 (2%)	52	77

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

Sometimes 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 monosaccharides 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	G	1303	-	4,4,4	0.26	0	6,6,6	0.06	0
3	THM	C	1405	-	18,18,18	2.10	5 (27%)	26,26,26	3.01	16 (61%)
3	THM	H	1407	-	18,18,18	2.47	9 (50%)	26,26,26	3.20	15 (57%)
2	SO4	A	1300	-	4,4,4	0.33	0	6,6,6	0.15	0
2	SO4	H	1307	-	4,4,4	0.18	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	C	1305	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	A	1308	-	4,4,4	0.16	0	6,6,6	0.09	0
2	SO4	D	1301	-	4,4,4	0.28	0	6,6,6	0.10	0
3	THM	B	1406	-	18,18,18	2.30	6 (33%)	26,26,26	3.04	13 (50%)
3	THM	D	1401	-	18,18,18	2.16	6 (33%)	26,26,26	3.08	15 (57%)
3	THM	E	1402	-	18,18,18	2.21	6 (33%)	26,26,26	3.06	16 (61%)
3	THM	F	1404	-	18,18,18	2.21	7 (38%)	26,26,26	3.10	15 (57%)
3	THM	A	1400	-	18,18,18	2.27	7 (38%)	26,26,26	3.06	14 (53%)
3	THM	G	1403	-	18,18,18	2.15	5 (27%)	26,26,26	3.14	15 (57%)
2	SO4	B	1306	-	4,4,4	0.21	0	6,6,6	0.10	0
2	SO4	E	1302	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	F	1304	-	4,4,4	0.19	0	6,6,6	0.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	THM	C	1405	-	-	2/6/18/18	0/2/2/2
3	THM	H	1407	-	-	2/6/18/18	0/2/2/2
3	THM	E	1402	-	-	2/6/18/18	0/2/2/2
3	THM	D	1401	-	-	2/6/18/18	0/2/2/2
3	THM	F	1404	-	-	2/6/18/18	0/2/2/2
3	THM	A	1400	-	-	2/6/18/18	0/2/2/2
3	THM	G	1403	-	-	1/6/18/18	0/2/2/2
3	THM	B	1406	-	-	2/6/18/18	0/2/2/2

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1406	THM	C6-C5	5.15	1.43	1.34
3	D	1401	THM	O4-C4	4.65	1.32	1.23
3	H	1407	THM	O2-C2	4.62	1.31	1.23
3	E	1402	THM	O4-C4	4.51	1.32	1.23
3	H	1407	THM	C6-C5	4.50	1.42	1.34
3	E	1402	THM	C6-C5	4.42	1.41	1.34
3	B	1406	THM	O4-C4	4.38	1.31	1.23
3	F	1404	THM	O4-C4	4.36	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1400	THM	C6-C5	4.35	1.41	1.34
3	C	1405	THM	O4-C4	4.35	1.31	1.23
3	D	1401	THM	C6-C5	4.20	1.41	1.34
3	C	1405	THM	C6-C5	4.18	1.41	1.34
3	G	1403	THM	O4-C4	4.14	1.31	1.23
3	G	1403	THM	C6-C5	4.14	1.41	1.34
3	G	1403	THM	O3'-C3'	4.09	1.52	1.43
3	H	1407	THM	O4-C4	4.00	1.31	1.23
3	A	1400	THM	O4-C4	3.96	1.31	1.23
3	F	1404	THM	C6-C5	3.94	1.41	1.34
3	A	1400	THM	O3'-C3'	3.84	1.51	1.43
3	E	1402	THM	O3'-C3'	3.81	1.51	1.43
3	F	1404	THM	O3'-C3'	3.67	1.51	1.43
3	C	1405	THM	O3'-C3'	3.60	1.51	1.43
3	H	1407	THM	C3'-C4'	3.56	1.62	1.53
3	D	1401	THM	O3'-C3'	3.42	1.50	1.43
3	B	1406	THM	O3'-C3'	3.39	1.50	1.43
3	B	1406	THM	C4-N3	-3.13	1.33	1.38
3	A	1400	THM	C4-N3	-3.13	1.33	1.38
3	F	1404	THM	C4-N3	-2.92	1.33	1.38
3	F	1404	THM	O2-C2	2.90	1.28	1.23
3	G	1403	THM	C4-N3	-2.87	1.33	1.38
3	C	1405	THM	C4-N3	-2.74	1.33	1.38
3	D	1401	THM	C4-N3	-2.72	1.33	1.38
3	A	1400	THM	O2-C2	2.70	1.28	1.23
3	B	1406	THM	O2-C2	2.67	1.27	1.23
3	E	1402	THM	C4-N3	-2.63	1.33	1.38
3	E	1402	THM	O2-C2	2.60	1.27	1.23
3	H	1407	THM	C5'-C4'	2.43	1.60	1.51
3	D	1401	THM	O2-C2	2.42	1.27	1.23
3	F	1404	THM	C6-N1	-2.37	1.34	1.38
3	H	1407	THM	C2-N3	-2.37	1.33	1.38
3	A	1400	THM	C2-N3	-2.33	1.33	1.38
3	H	1407	THM	O3'-C3'	2.30	1.48	1.43
3	H	1407	THM	C4-C5	-2.27	1.41	1.44
3	G	1403	THM	O2-C2	2.25	1.27	1.23
3	E	1402	THM	C5'-C4'	2.20	1.59	1.51
3	C	1405	THM	O2-C2	2.15	1.27	1.23
3	H	1407	THM	C6-N1	-2.12	1.34	1.38
3	F	1404	THM	C5'-C4'	2.12	1.59	1.51
3	D	1401	THM	C4-C5	-2.12	1.41	1.44
3	B	1406	THM	C4-C5	-2.08	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1400	THM	C4-C5	-2.04	1.41	1.44

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1407	THM	C4-N3-C2	-6.19	119.34	127.35
3	B	1406	THM	N3-C2-N1	6.03	122.89	114.89
3	F	1404	THM	C4-N3-C2	-5.98	119.61	127.35
3	G	1403	THM	C4-N3-C2	-5.83	119.80	127.35
3	G	1403	THM	N3-C2-N1	5.80	122.58	114.89
3	H	1407	THM	C5-C4-N3	5.78	120.24	115.31
3	E	1402	THM	N3-C2-N1	5.76	122.54	114.89
3	E	1402	THM	C4-N3-C2	-5.75	119.90	127.35
3	C	1405	THM	N3-C2-N1	5.75	122.52	114.89
3	A	1400	THM	N3-C2-N1	5.74	122.51	114.89
3	D	1401	THM	C4-N3-C2	-5.74	119.92	127.35
3	B	1406	THM	C4-N3-C2	-5.73	119.94	127.35
3	C	1405	THM	C4-N3-C2	-5.69	119.99	127.35
3	F	1404	THM	N3-C2-N1	5.66	122.41	114.89
3	D	1401	THM	N3-C2-N1	5.61	122.33	114.89
3	A	1400	THM	C4-N3-C2	-5.57	120.14	127.35
3	H	1407	THM	N3-C2-N1	5.50	122.19	114.89
3	A	1400	THM	C5-C6-N1	-5.47	117.71	123.34
3	B	1406	THM	C5-C6-N1	-5.45	117.73	123.34
3	A	1400	THM	C5-C4-N3	5.43	119.95	115.31
3	H	1407	THM	C5-C6-N1	-5.38	117.80	123.34
3	B	1406	THM	C5-C4-N3	5.38	119.91	115.31
3	H	1407	THM	O4'-C4'-C5'	5.37	120.82	109.21
3	D	1401	THM	C5-C4-N3	5.35	119.88	115.31
3	F	1404	THM	C5-C4-N3	5.33	119.86	115.31
3	C	1405	THM	C5-C4-N3	5.30	119.83	115.31
3	G	1403	THM	C5-C4-N3	5.25	119.79	115.31
3	E	1402	THM	C5-C4-N3	5.17	119.72	115.31
3	C	1405	THM	C5-C6-N1	-4.95	118.25	123.34
3	F	1404	THM	C5-C6-N1	-4.90	118.30	123.34
3	G	1403	THM	C5-C6-N1	-4.84	118.36	123.34
3	D	1401	THM	C5-C6-N1	-4.83	118.37	123.34
3	E	1402	THM	C5-C6-N1	-4.78	118.42	123.34
3	E	1402	THM	O4'-C4'-C5'	4.78	119.54	109.21
3	D	1401	THM	O4'-C4'-C5'	4.72	119.41	109.21
3	G	1403	THM	O4'-C4'-C5'	4.67	119.31	109.21
3	F	1404	THM	O4'-C4'-C5'	4.63	119.22	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1405	THM	O4'-C4'-C5'	4.40	118.72	109.21
3	A	1400	THM	O4'-C4'-C5'	4.31	118.53	109.21
3	B	1406	THM	O4'-C4'-C5'	4.11	118.10	109.21
3	G	1403	THM	O4'-C4'-C3'	-4.02	96.29	105.67
3	H	1407	THM	C2'-C3'-C4'	-3.92	94.59	102.76
3	H	1407	THM	O4'-C4'-C3'	-3.79	96.82	105.67
3	D	1401	THM	O4'-C4'-C3'	-3.79	96.82	105.67
3	B	1406	THM	O2-C2-N1	-3.77	117.78	122.79
3	E	1402	THM	O4'-C4'-C3'	-3.73	96.96	105.67
3	A	1400	THM	O4'-C4'-C3'	-3.73	96.97	105.67
3	F	1404	THM	O4'-C4'-C3'	-3.73	96.98	105.67
3	C	1405	THM	O2-C2-N1	-3.68	117.90	122.79
3	G	1403	THM	C5'-C4'-C3'	3.67	124.08	114.81
3	A	1400	THM	O2-C2-N1	-3.61	117.99	122.79
3	D	1401	THM	C2'-C3'-C4'	-3.60	95.26	102.76
3	G	1403	THM	C2'-C3'-C4'	-3.59	95.27	102.76
3	A	1400	THM	C2'-C3'-C4'	-3.56	95.35	102.76
3	F	1404	THM	C2'-C3'-C4'	-3.54	95.38	102.76
3	B	1406	THM	O4'-C4'-C3'	-3.53	97.44	105.67
3	H	1407	THM	O4-C4-C5	-3.53	120.81	124.90
3	E	1402	THM	C5'-C4'-C3'	3.53	123.72	114.81
3	B	1406	THM	C2'-C3'-C4'	-3.50	95.46	102.76
3	G	1403	THM	O2-C2-N1	-3.48	118.16	122.79
3	A	1400	THM	C5'-C4'-C3'	3.47	123.57	114.81
3	E	1402	THM	C2'-C3'-C4'	-3.46	95.56	102.76
3	F	1404	THM	C5'-C4'-C3'	3.45	123.53	114.81
3	H	1407	THM	O2-C2-N1	-3.43	118.22	122.79
3	F	1404	THM	O2-C2-N1	-3.43	118.22	122.79
3	D	1401	THM	O4-C4-C5	-3.43	120.93	124.90
3	C	1405	THM	C5'-C4'-C3'	3.43	123.47	114.81
3	C	1405	THM	O4'-C4'-C3'	-3.42	97.68	105.67
3	D	1401	THM	C5'-C4'-C3'	3.39	123.38	114.81
3	C	1405	THM	C2'-C3'-C4'	-3.38	95.73	102.76
3	D	1401	THM	O2-C2-N1	-3.35	118.33	122.79
3	E	1402	THM	O2-C2-N1	-3.33	118.36	122.79
3	B	1406	THM	C5'-C4'-C3'	3.28	123.09	114.81
3	A	1400	THM	O4-C4-C5	-3.27	121.11	124.90
3	F	1404	THM	O4-C4-C5	-3.22	121.16	124.90
3	B	1406	THM	O4-C4-C5	-3.07	121.34	124.90
3	C	1405	THM	O4-C4-C5	-3.05	121.37	124.90
3	H	1407	THM	O3'-C3'-C2'	3.05	121.80	110.90
3	G	1403	THM	O4-C4-C5	-3.04	121.38	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1403	THM	O3'-C3'-C2'	3.03	121.74	110.90
3	D	1401	THM	O3'-C3'-C2'	2.96	121.50	110.90
3	E	1402	THM	O4-C4-C5	-2.93	121.51	124.90
3	A	1400	THM	O3'-C3'-C2'	2.91	121.30	110.90
3	B	1406	THM	O3'-C3'-C2'	2.89	121.25	110.90
3	E	1402	THM	O3'-C3'-C2'	2.87	121.17	110.90
3	F	1404	THM	O3'-C3'-C2'	2.85	121.11	110.90
3	C	1405	THM	O3'-C3'-C2'	2.85	121.08	110.90
3	E	1402	THM	O4'-C1'-C2'	-2.70	101.14	106.25
3	G	1403	THM	O4'-C1'-C2'	-2.67	101.21	106.25
3	F	1404	THM	C5M-C5-C6	-2.67	119.29	122.85
3	H	1407	THM	O4'-C1'-C2'	-2.59	101.35	106.25
3	G	1403	THM	C2'-C1'-N1	2.59	119.74	113.77
3	D	1401	THM	O4'-C1'-C2'	-2.57	101.39	106.25
3	G	1403	THM	C5M-C5-C6	-2.56	119.43	122.85
3	D	1401	THM	C2'-C1'-N1	2.55	119.64	113.77
3	H	1407	THM	C5M-C5-C4	2.53	121.55	118.77
3	H	1407	THM	C5'-C4'-C3'	2.52	121.18	114.81
3	B	1406	THM	O4'-C1'-C2'	-2.47	101.59	106.25
3	F	1404	THM	C5M-C5-C4	2.46	121.47	118.77
3	H	1407	THM	C5M-C5-C6	-2.42	119.61	122.85
3	F	1404	THM	C2'-C1'-N1	2.40	119.30	113.77
3	G	1403	THM	C5M-C5-C4	2.40	121.40	118.77
3	E	1402	THM	C5M-C5-C6	-2.39	119.65	122.85
3	F	1404	THM	O4'-C1'-C2'	-2.37	101.77	106.25
3	E	1402	THM	C2'-C1'-N1	2.36	119.21	113.77
3	D	1401	THM	C5M-C5-C6	-2.32	119.74	122.85
3	C	1405	THM	C5M-C5-C6	-2.32	119.75	122.85
3	C	1405	THM	C5M-C5-C4	2.26	121.26	118.77
3	C	1405	THM	O4'-C1'-C2'	-2.23	102.04	106.25
3	A	1400	THM	O3'-C3'-C4'	2.21	118.57	110.10
3	A	1400	THM	C5M-C5-C6	-2.18	119.94	122.85
3	E	1402	THM	C5M-C5-C4	2.18	121.16	118.77
3	A	1400	THM	O4'-C1'-C2'	-2.13	102.23	106.25
3	C	1405	THM	C2'-C1'-N1	2.06	118.51	113.77
3	E	1402	THM	C4'-O4'-C1'	2.04	114.38	109.45
3	H	1407	THM	O3'-C3'-C4'	2.03	117.86	110.10
3	D	1401	THM	C5M-C5-C4	2.01	120.98	118.77
3	C	1405	THM	O3'-C3'-C4'	2.01	117.79	110.10
3	B	1406	THM	O3'-C3'-C4'	2.00	117.76	110.10

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1400	THM	O4'-C4'-C5'-O5'
3	A	1400	THM	C3'-C4'-C5'-O5'
3	B	1406	THM	C3'-C4'-C5'-O5'
3	D	1401	THM	C3'-C4'-C5'-O5'
3	E	1402	THM	C3'-C4'-C5'-O5'
3	F	1404	THM	C3'-C4'-C5'-O5'
3	H	1407	THM	O4'-C4'-C5'-O5'
3	H	1407	THM	C3'-C4'-C5'-O5'
3	B	1406	THM	O4'-C4'-C5'-O5'
3	D	1401	THM	O4'-C4'-C5'-O5'
3	E	1402	THM	O4'-C4'-C5'-O5'
3	F	1404	THM	O4'-C4'-C5'-O5'
3	C	1405	THM	O4'-C4'-C5'-O5'
3	C	1405	THM	C3'-C4'-C5'-O5'
3	G	1403	THM	O4'-C4'-C5'-O5'

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	197/250 (78%)	-0.02	5 (2%) 57 61	20, 37, 59, 97	0
1	B	192/250 (76%)	0.47	22 (11%) 4 4	28, 57, 98, 110	0
1	C	197/250 (78%)	0.43	14 (7%) 16 16	36, 65, 106, 115	0
1	D	191/250 (76%)	0.60	20 (10%) 6 6	41, 72, 103, 114	0
1	E	192/250 (76%)	0.33	9 (4%) 31 33	36, 61, 95, 110	0
1	F	192/250 (76%)	0.92	33 (17%) 1 1	42, 79, 107, 116	0
1	G	192/250 (76%)	0.61	17 (8%) 9 9	32, 69, 108, 123	0
1	H	192/250 (76%)	-0.18	2 (1%) 82 84	21, 35, 55, 71	0
All	All	1545/2000 (77%)	0.39	122 (7%) 12 12	20, 60, 103, 123	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	12	THR	7.7
1	F	168	ALA	5.4
1	F	95	PRO	5.0
1	F	170	SER	5.0
1	G	206	ASP	4.8
1	D	192	ILE	4.8
1	G	207	ALA	4.7
1	F	173	SER	4.6
1	F	18	THR	4.5
1	G	166	GLN	4.4
1	C	169	ARG	4.4
1	G	173	SER	4.3
1	B	170	SER	4.2
1	E	169	ARG	4.0
1	G	169	ARG	4.0
1	C	207	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	169	ARG	4.0
1	C	208	ASP	3.7
1	C	172	GLU	3.7
1	D	12	THR	3.7
1	C	18	THR	3.6
1	B	168	ALA	3.5
1	A	97	ASN	3.5
1	C	199	SER	3.4
1	F	17	GLY	3.4
1	E	12	THR	3.4
1	D	193	HIS	3.3
1	F	145	VAL	3.3
1	G	170	SER	3.3
1	A	199	SER	3.3
1	G	168	ALA	3.3
1	F	105	ARG	3.2
1	D	169	ARG	3.2
1	E	166	GLN	3.2
1	G	42	LYS	3.1
1	G	203	LEU	3.1
1	A	208	ASP	3.0
1	D	95	PRO	3.0
1	A	12	THR	3.0
1	E	168	ALA	3.0
1	F	25	ILE	2.9
1	E	17	GLY	2.9
1	E	18	THR	2.9
1	D	200	CYS	2.9
1	B	110	ALA	2.9
1	D	97	ASN	2.8
1	B	45	ASN	2.8
1	D	114	PHE	2.8
1	F	94	ALA	2.7
1	B	44	LYS	2.7
1	B	201	LYS	2.7
1	F	27	GLY	2.7
1	B	85	THR	2.7
1	F	208	ASP	2.7
1	F	82	SER	2.7
1	F	144	HIS	2.7
1	C	95	PRO	2.7
1	D	15	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	106	SER	2.7
1	F	193	HIS	2.7
1	G	48	CYS	2.6
1	F	201	LYS	2.6
1	F	200	CYS	2.6
1	D	165	ARG	2.6
1	G	205	LEU	2.6
1	F	97	ASN	2.5
1	B	173	SER	2.5
1	F	166	GLN	2.5
1	F	165	ARG	2.5
1	A	207	ALA	2.5
1	E	97	ASN	2.5
1	D	27	GLY	2.5
1	H	85	THR	2.5
1	D	173	SER	2.5
1	D	144	HIS	2.4
1	D	168	ALA	2.4
1	F	207	ALA	2.4
1	F	203	LEU	2.4
1	D	78	MET	2.4
1	C	17	GLY	2.4
1	G	208	ASP	2.4
1	F	104	GLU	2.4
1	G	85	THR	2.4
1	B	18	THR	2.4
1	F	99	LYS	2.3
1	D	106	SER	2.3
1	B	200	CYS	2.3
1	H	208	ASP	2.3
1	B	192	ILE	2.3
1	F	12	THR	2.3
1	F	194	GLN	2.3
1	B	17	GLY	2.3
1	B	194	GLN	2.3
1	B	174	CYS	2.3
1	D	18	THR	2.2
1	F	108	PHE	2.2
1	B	41	GLU	2.2
1	B	208	ASP	2.2
1	G	82	SER	2.2
1	B	97	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	173	SER	2.2
1	F	84	VAL	2.2
1	B	16	GLU	2.2
1	G	185	GLU	2.2
1	C	44	LYS	2.2
1	G	47	ILE	2.2
1	C	170	SER	2.2
1	D	44	LYS	2.1
1	G	84	VAL	2.1
1	B	169	ARG	2.1
1	B	42	LYS	2.1
1	D	201	LYS	2.1
1	B	206	ASP	2.1
1	B	95	PRO	2.1
1	E	25	ILE	2.1
1	C	165	ARG	2.1
1	C	173	SER	2.1
1	F	103	MET	2.1
1	F	202	VAL	2.0
1	F	42	LYS	2.0
1	C	82	SER	2.0
1	D	99	LYS	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 monosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
3	THM	C	1405	17/17	0.92	0.27	55,58,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	THM	G	1403	17/17	0.94	0.28	66,70,72,73	0
2	SO4	D	1301	5/5	0.95	0.15	55,56,60,61	0
2	SO4	F	1304	5/5	0.96	0.16	65,67,68,70	0
3	THM	D	1401	17/17	0.96	0.26	48,51,58,60	0
3	THM	E	1402	17/17	0.96	0.19	39,44,52,52	0
3	THM	F	1404	17/17	0.96	0.20	45,49,56,58	0
3	THM	B	1406	17/17	0.96	0.23	29,37,45,45	0
2	SO4	G	1303	5/5	0.97	0.12	69,69,69,72	0
3	THM	A	1400	17/17	0.97	0.20	27,31,36,38	0
2	SO4	C	1305	5/5	0.98	0.11	66,67,68,69	0
3	THM	H	1407	17/17	0.98	0.18	16,26,30,31	0
2	SO4	A	1300	5/5	0.99	0.09	29,29,33,35	0
2	SO4	H	1307	5/5	0.99	0.14	30,31,33,34	0
2	SO4	A	1308	5/5	0.99	0.19	43,46,49,50	0
2	SO4	E	1302	5/5	0.99	0.12	49,49,51,52	0
2	SO4	B	1306	5/5	0.99	0.12	43,44,47,50	0

6.5 Other polymers (i)

There are no such residues in this entry.