



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:18 PM UTC

PDB ID : 1OT3 / pdb_00001ot3
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

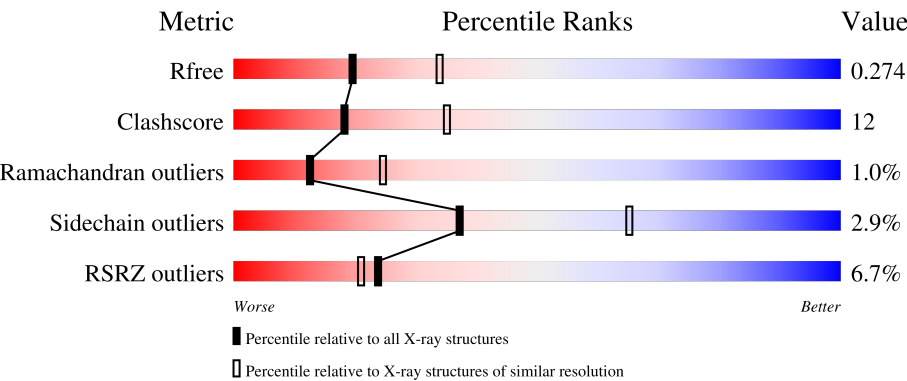
1 Overall quality at a glance i

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	2% 54% 22% • 21%
1	B	250	7% 58% 16% • 23%
1	C	250	5% 57% 20% • 21%
1	D	250	7% 54% 21% • 24%
1	E	250	2% 54% 21% • 23%

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

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

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.

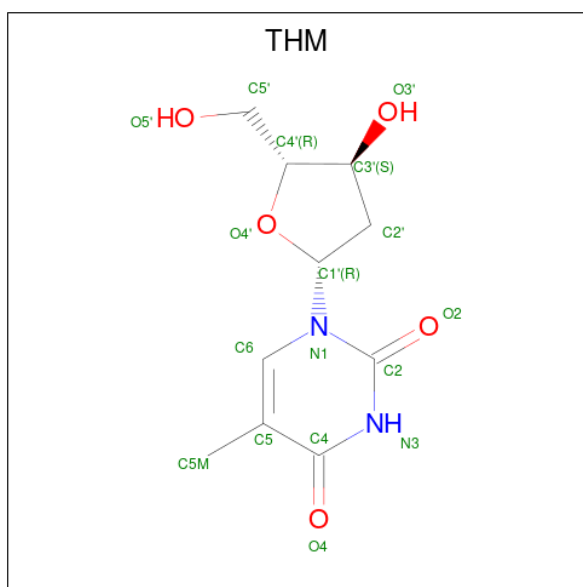
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1640	1046	282	302	10			
1	B	192	Total	C	N	O	S	0	0	0
			1596	1021	270	295	10			
1	C	197	Total	C	N	O	S	0	0	0
			1640	1046	282	302	10			
1	D	191	Total	C	N	O	S	0	0	0
			1587	1016	268	293	10			
1	E	192	Total	C	N	O	S	0	0	0
			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 (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is THYMIDINE (CCD ID: THM) (formula: C₁₀H₁₄N₂O₅).



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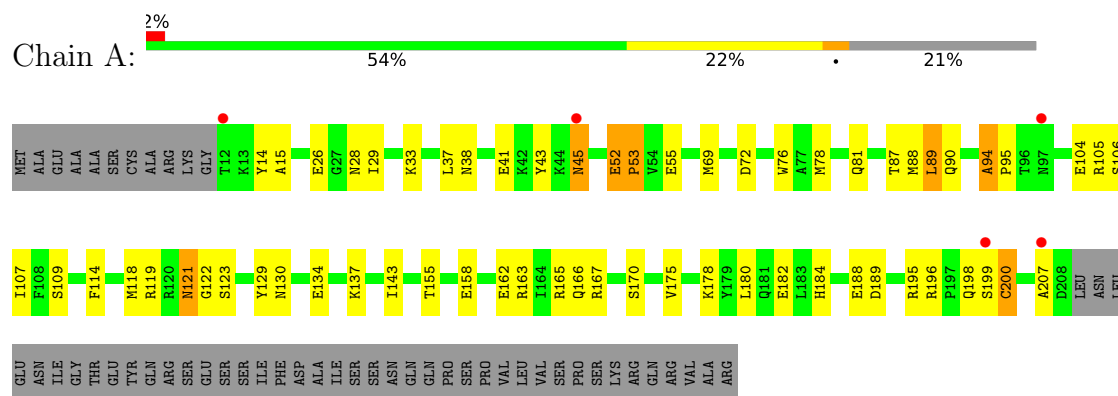
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	27	Total 27	O 27	0	0
4	F	16	Total 16	O 16	0	0
4	G	18	Total 18	O 18	0	0
4	H	65	Total 65	O 65	0	0

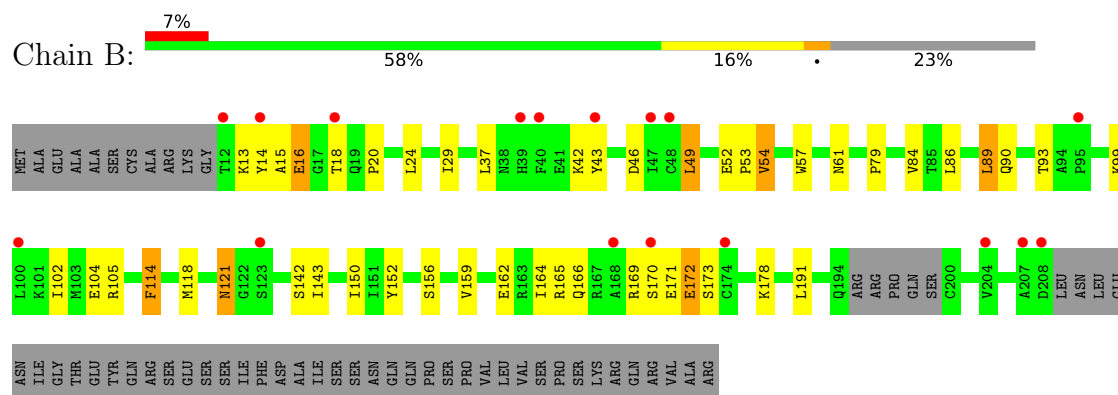
3 Residue-property plots

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.

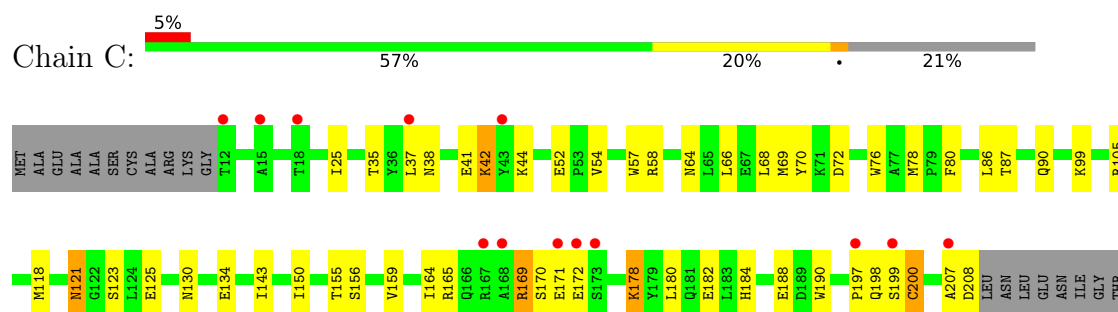
• Molecule 1: Deoxyribonucleoside Kinase



• Molecule 1: Deoxyribonucleoside Kinase



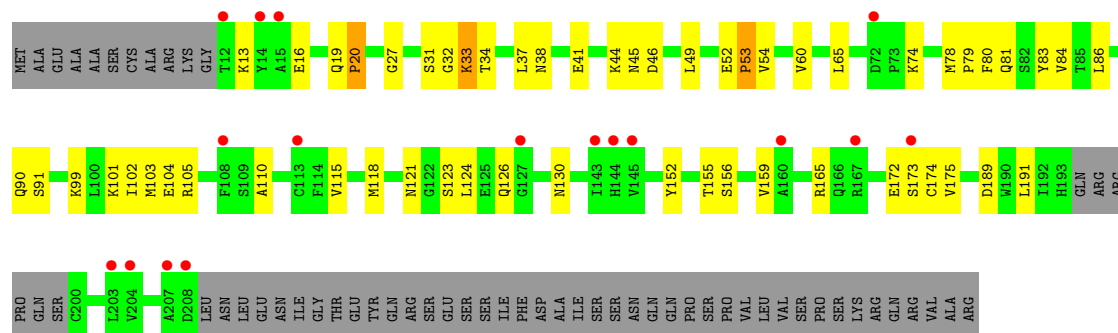
• Molecule 1: Deoxyribonucleoside Kinase



GLU TYR ARG ARG SER GLU SER SER ILE PHE ASP ALA ILE SER SER ASN GLN PRO PRO VAL VAL SER PRO SER LYS GLN ARG VAL ALA ARG

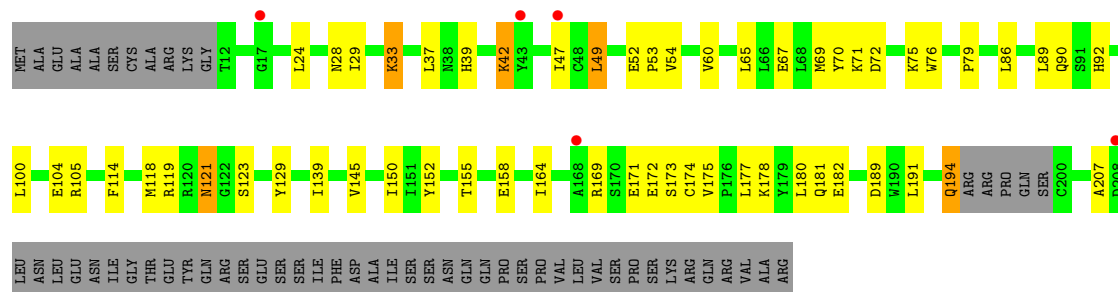
• Molecule 1: Deoxyribonucleoside Kinase

Chain D: 7% 54% 21% 24%



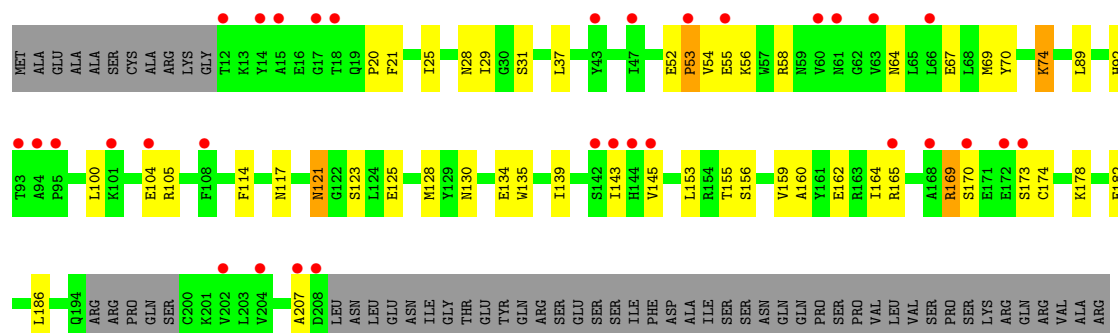
• Molecule 1: Deoxyribonucleoside Kinase

Chain E: 2% 54% 21% 23%



• Molecule 1: Deoxyribonucleoside Kinase

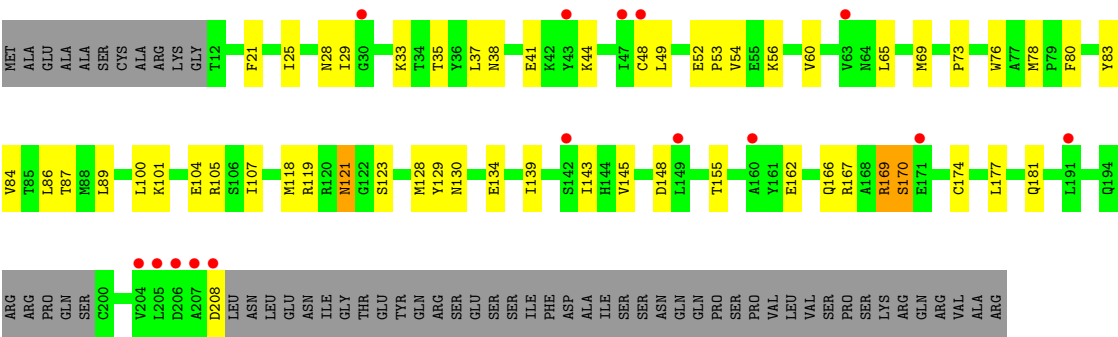
Chain F: 13% 56% 19% 23%



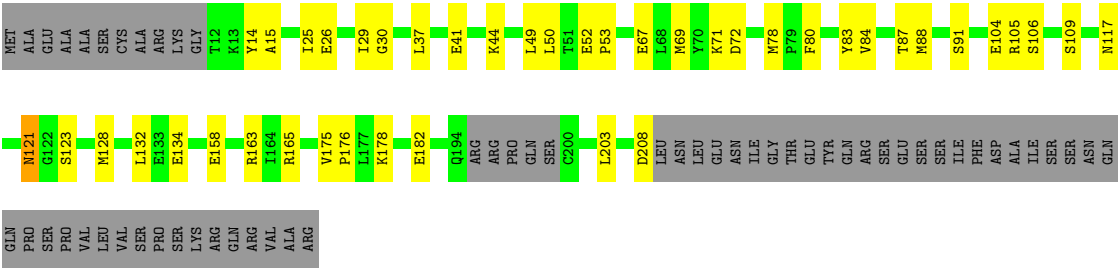
• Molecule 1: Deoxyribonucleoside Kinase

Chain G: 6% 55% 21% 23%





● Molecule 1: Deoxyribonucleoside Kinase



4 Data and refinement statistics

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 25.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.8 (25.00-2.50) 89.8 (25.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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%)	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)	0.31 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.56	0/1678	0.96	6/2268 (0.3%)
1	B	0.40	0/1632	0.80	1/2205 (0.0%)
1	C	0.38	0/1678	0.77	2/2268 (0.1%)
1	D	0.36	0/1623	0.77	0/2193
1	E	0.38	0/1632	0.76	1/2205 (0.0%)
1	F	0.35	0/1632	0.76	1/2205 (0.0%)
1	G	0.36	0/1632	0.77	0/2205
1	H	0.55	0/1632	0.86	3/2205 (0.1%)
All	All	0.43	0/13139	0.81	14/17754 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	PHE	N-CA-C	6.02	117.84	111.28
1	A	52	GLU	CA-C-N	6.00	127.34	119.84
1	A	52	GLU	C-N-CA	6.00	127.34	119.84
1	F	114	PHE	N-CA-C	5.94	117.44	110.97
1	H	29	ILE	N-CA-C	-5.93	101.93	109.58
1	A	114	PHE	N-CA-C	5.72	117.20	111.07
1	C	72	ASP	CA-C-N	5.32	124.51	118.97
1	C	72	ASP	C-N-CA	5.32	124.51	118.97
1	E	114	PHE	N-CA-C	5.29	116.73	111.07
1	H	72	ASP	CA-C-N	5.17	124.62	119.24
1	H	72	ASP	C-N-CA	5.17	124.62	119.24
1	A	94	ALA	CA-C-N	5.04	124.80	119.76
1	A	94	ALA	C-N-CA	5.04	124.80	119.76
1	A	200	CYS	N-CA-C	5.00	115.78	107.73

There are no chirality outliers.

There are no planarity outliers.

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	1640	0	1629	48	0
1	B	1596	0	1582	37	0
1	C	1640	0	1629	43	0
1	D	1587	0	1574	42	0
1	E	1596	0	1582	43	0
1	F	1596	0	1582	38	0
1	G	1596	0	1582	39	0
1	H	1596	0	1582	28	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	6	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	312	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 12.

All (312) 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:D:19:GLN:HE22	1:D:101:LYS:HZ1	1.25	0.84
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	0.77
1:G:21:PHE:HB3	1:G:100:LEU:HD12	1.67	0.76
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:H:121:ASN:C	1:H:121:ASN:HD22	1.96	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:F:125:GLU:H	1:F:128:MET:HE3	1.54	0.71
1:A:155:THR:HG22	1:A:207:ALA:HB2	1.73	0.70
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:A:121:ASN:C	1:A:121:ASN:HD22	2.02	0.68
1:D:156:SER:HB3	1:D:159:VAL:HG23	1.76	0.67
1:A:198:GLN:CD	1:A:199:SER:H	2.01	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:H:41:GLU:O	1:H:44:LYS:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:121:ASN:C	1:F:121:ASN:HD22	2.07	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: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:D:91:SER:HB3	1:D:103:MET:HE3	1.88	0.55
1:A:121:ASN:C	1:A:121:ASN:ND2	2.65	0.55
1:F:89:LEU:HD22	1:F:143:ILE:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:156:SER:HB3	1:C:159:VAL:CG2	2.37	0.54
1:B:121:ASN:C	1:B:121:ASN:ND2	2.66	0.53
1:A:143:ILE:H	1:A:143:ILE:CD1	2.22	0.53
1:F:52:GLU:C	1:F:54:VAL:H	2.17	0.53
1:F:121:ASN:ND2	1:F:123:SER:H	2.07	0.53
1:D:19:GLN:NE2	1:D:101:LYS:NZ	2.54	0.52
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:52:GLU:C	1:G:54:VAL:H	2.17	0.52
1:G:53:PRO:HB3	1:G:56:LYS:HD2	1.92	0.52
1:F:69:MET:SD	1:F:69:MET:C	2.92	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
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:121:ASN:C	1:E:121:ASN:HD22	2.18	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:B:29:ILE:HG22	1:B:164:ILE:HD11	1.93	0.51
1:C:171:GLU:CD	1:C:171:GLU:H	2.19	0.51
1:D:81:GLN:OE1	1:D:118:MET:HE1	2.11	0.51
1:G:44:LYS:NZ	1:G:49:LEU:HB3	2.26	0.51
1:G:44:LYS:HZ3	1:G:49:LEU:HB3	1.76	0.51
1:E:104:GLU:O	1:E:105:ARG:HB2	2.11	0.50
1:F:104:GLU:O	1:F:105:ARG:HB2	2.11	0.50
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:G:121:ASN:C	1:G:121:ASN:HD22	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:78:MET:HE2	1:B:79:PRO:HA	1.95	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: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:E:158:GLU:CD	1:E:158:GLU:H	2.21	0.49
1:F:169:ARG:HB2	1:F:173:SER:HB3	1.95	0.49
1:H:158:GLU:H	1:H:158:GLU:CD	2.20	0.49
1:C:121:ASN:ND2	1:C:121:ASN:C	2.70	0.49
1:D:44:LYS:C	1:D:46:ASP:H	2.20	0.49
1:F:105:ARG:HD3	4:F:1411:HOH:O	2.12	0.49
1:C:78:MET:HE2	1:D:79:PRO:HA	1.95	0.48
1:A:143:ILE:HD12	1:A:143:ILE:N	2.28	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: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:D:172:GLU:C	1:D:174:CYS:H	2.22	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: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:C:121:ASN:C	1:C:121:ASN:HD22	2.21	0.47
1:C:178:LYS:O	1:C:182:GLU:HG3	2.13	0.47

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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	0.47
1:D:172:GLU:HB3	3:D:1401:THM:HO3'	1.79	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:B:121:ASN:C	1:B:121:ASN:HD22	2.22	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:69:MET:HE1	1:F:70:TYR:CZ	2.51	0.46
1:F:153:LEU:HD22	1:F:207:ALA:HB2	1.98	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:F:121:ASN:C	1:F:121:ASN:ND2	2.74	0.46
1:C:35:THR:O	1:C:38:ASN:HB2	2.16	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
1:A:118:MET:HE3	4:A:1491:HOH:O	2.15	0.46
1:B:52:GLU:C	1:B:54:VAL:H	2.24	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:C:41:GLU:O	1:C:44:LYS:HG2	2.16	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:76:TRP:CZ3	1:H:128:MET:HE2	2.51	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: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:D:52:GLU:C	1:D:54:VAL:H	2.24	0.44
1:H:88:MET:HG2	1:H:106:SER:C	2.42	0.44
1:B:20:PRO:HB2	1:B:99:LYS:C	2.42	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: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: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
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:G:28:ASN:OD1	1:G:29:ILE:N	2.51	0.43
1:G:121:ASN:ND2	1:G:121:ASN:C	2.75	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:E:52:GLU:HA	1:E:53:PRO:HD3	1.90	0.43
1:E:76:TRP:C	1:E:79:PRO:HD2	2.43	0.43
1:G:177:LEU:O	1:G:181:GLN:HG3	2.19	0.43
1:H:78:MET:HE2	1:H:132:LEU:CD2	2.49	0.43
1:E:69:MET:SD	1:E:69:MET:C	3.02	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:C:105:ARG:HG3	1:C:105:ARG:HH11	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:SER:O	1:A:200:CYS:HB3	2.18	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:F:69:MET:HE1	1:F:70:TYR:CE2	2.55	0.42
1:G:78:MET:CB	1:G:128:MET:HE2	2.50	0.42
1:A:88:MET:HG2	1:A:106:SER:C	2.44	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:B:52:GLU:CD	1:B:105:ARG:HG3	2.44	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:52:GLU:OE2	1:A:105:ARG:HG3	2.20	0.42
1:G:49:LEU:HD13	1:G:49:LEU:C	2.44	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
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:A:43:TYR:C	1:A:45:ASN:N	2.78	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:A:158:GLU:H	1:A:158:GLU:CD	2.28	0.41
1:C:52:GLU:C	1:C:54:VAL:H	2.28	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:A:33:LYS:HZ1	1:A:105:ARG:NH2	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:52:GLU:C	1:E:54:VAL:H	2.28	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:E:39:HIS:C	1:E:42:LYS:HE3	2.46	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:H:121:ASN:C	1:H:121:ASN:ND2	2.67	0.40
1:A:94:ALA:HA	1:A:95:PRO:HD3	1.80	0.40
1:E:28:ASN:CG	1:E:29:ILE:N	2.80	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%)	24	43
1	B	188/250 (75%)	158 (84%)	29 (15%)	1 (0%)	24	43
1	C	195/250 (78%)	177 (91%)	17 (9%)	1 (0%)	24	43
1	D	187/250 (75%)	168 (90%)	15 (8%)	4 (2%)	5	9
1	E	188/250 (75%)	171 (91%)	16 (8%)	1 (0%)	24	43
1	F	188/250 (75%)	170 (90%)	14 (7%)	4 (2%)	5	9
1	G	188/250 (75%)	157 (84%)	28 (15%)	3 (2%)	7	14
1	H	188/250 (75%)	173 (92%)	15 (8%)	0	100	100
All	All	1517/2000 (76%)	1358 (90%)	144 (10%)	15 (1%)	12	24

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%)	33	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	177/227 (78%)	168 (95%)	9 (5%)	21	43
1	C	182/227 (80%)	175 (96%)	7 (4%)	29	56
1	D	176/227 (78%)	174 (99%)	2 (1%)	65	84
1	E	177/227 (78%)	172 (97%)	5 (3%)	38	66
1	F	177/227 (78%)	172 (97%)	5 (3%)	38	66
1	G	177/227 (78%)	174 (98%)	3 (2%)	53	78
1	H	177/227 (78%)	172 (97%)	5 (3%)	38	66
All	All	1425/1816 (78%)	1383 (97%)	42 (3%)	37	65

All (42) 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	54	VAL
1	B	61	ASN
1	B	89	LEU
1	B	121	ASN
1	B	165	ARG
1	B	172	GLU
1	C	42	LYS
1	C	121	ASN
1	C	125	GLU
1	C	165	ARG
1	C	169	ARG
1	C	178	LYS
1	C	200	CYS
1	D	33	LYS
1	D	189	ASP
1	E	33	LYS
1	E	42	LYS
1	E	49	LEU
1	E	121	ASN

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Mol	Chain	Res	Type
1	E	194	GLN
1	F	74	LYS
1	F	121	ASN
1	F	162	GLU
1	F	165	ARG
1	F	169	ARG
1	G	121	ASN
1	G	145	VAL
1	G	169	ARG
1	H	49	LEU
1	H	121	ASN
1	H	165	ARG
1	H	203	LEU
1	H	208	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	121	ASN
1	A	193	HIS
1	A	198	GLN
1	B	121	ASN
1	B	130	ASN
1	B	193	HIS
1	B	194	GLN
1	C	38	ASN
1	C	59	ASN
1	C	61	ASN
1	C	117	ASN
1	C	121	ASN
1	C	144	HIS
1	C	198	GLN
1	D	19	GLN
1	D	38	ASN
1	D	45	ASN
1	D	61	ASN
1	D	126	GLN
1	E	28	ASN
1	E	121	ASN
1	E	130	ASN
1	E	144	HIS

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Mol	Chain	Res	Type
1	F	121	ASN
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	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 oligosaccharides 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	0.42	0	6,6,6	0.19	0
2	SO4	C	1305	-	4,4,4	0.36	0	6,6,6	0.08	0
2	SO4	D	1301	-	4,4,4	0.39	0	6,6,6	0.11	0
3	THM	F	1404	-	18,18,18	2.23	7 (38%)	26,26,26	3.10	15 (57%)
2	SO4	B	1306	-	4,4,4	0.32	0	6,6,6	0.08	0
2	SO4	A	1308	-	4,4,4	0.28	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	F	1304	-	4,4,4	0.31	0	6,6,6	0.07	0
2	SO4	H	1307	-	4,4,4	0.30	0	6,6,6	0.26	0
3	THM	E	1402	-	18,18,18	2.24	6 (33%)	26,26,26	3.06	16 (61%)
2	SO4	E	1302	-	4,4,4	0.43	0	6,6,6	0.11	0
3	THM	C	1405	-	18,18,18	2.12	5 (27%)	26,26,26	3.01	15 (57%)
3	THM	H	1407	-	18,18,18	2.51	9 (50%)	26,26,26	3.21	15 (57%)
3	THM	G	1403	-	18,18,18	2.18	5 (27%)	26,26,26	3.14	15 (57%)
3	THM	D	1401	-	18,18,18	2.19	7 (38%)	26,26,26	3.08	15 (57%)
3	THM	B	1406	-	18,18,18	2.32	6 (33%)	26,26,26	3.04	13 (50%)
3	THM	A	1400	-	18,18,18	2.29	7 (38%)	26,26,26	3.06	14 (53%)
2	SO4	G	1303	-	4,4,4	0.37	0	6,6,6	0.08	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	F	1404	-	-	2/6/18/18	0/2/2/2
3	THM	E	1402	-	-	2/6/18/18	0/2/2/2
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	G	1403	-	-	1/6/18/18	0/2/2/2
3	THM	D	1401	-	-	2/6/18/18	0/2/2/2
3	THM	B	1406	-	-	2/6/18/18	0/2/2/2
3	THM	A	1400	-	-	2/6/18/18	0/2/2/2

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1406	THM	C6-C5	5.18	1.43	1.34
3	H	1407	THM	O2-C2	4.76	1.31	1.23
3	D	1401	THM	O4-C4	4.67	1.32	1.23
3	H	1407	THM	C6-C5	4.53	1.42	1.34
3	E	1402	THM	O4-C4	4.53	1.32	1.23
3	E	1402	THM	C6-C5	4.44	1.41	1.34
3	B	1406	THM	O4-C4	4.40	1.31	1.23
3	F	1404	THM	O4-C4	4.39	1.31	1.23
3	A	1400	THM	C6-C5	4.38	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1405	THM	O4-C4	4.37	1.31	1.23
3	D	1401	THM	C6-C5	4.23	1.41	1.34
3	C	1405	THM	C6-C5	4.20	1.41	1.34
3	G	1403	THM	O4-C4	4.16	1.31	1.23
3	G	1403	THM	C6-C5	4.16	1.41	1.34
3	G	1403	THM	O3'-C3'	4.14	1.52	1.43
3	H	1407	THM	O4-C4	4.02	1.31	1.23
3	A	1400	THM	O4-C4	3.99	1.31	1.23
3	F	1404	THM	C6-C5	3.96	1.41	1.34
3	A	1400	THM	O3'-C3'	3.89	1.51	1.43
3	E	1402	THM	O3'-C3'	3.85	1.51	1.43
3	H	1407	THM	C3'-C4'	3.72	1.62	1.53
3	F	1404	THM	O3'-C3'	3.72	1.51	1.43
3	C	1405	THM	O3'-C3'	3.65	1.51	1.43
3	D	1401	THM	O3'-C3'	3.46	1.50	1.43
3	B	1406	THM	O3'-C3'	3.43	1.50	1.43
3	B	1406	THM	C4-N3	-3.11	1.33	1.38
3	A	1400	THM	C4-N3	-3.11	1.33	1.38
3	F	1404	THM	O2-C2	2.98	1.28	1.23
3	F	1404	THM	C4-N3	-2.91	1.33	1.38
3	G	1403	THM	C4-N3	-2.85	1.33	1.38
3	A	1400	THM	O2-C2	2.78	1.28	1.23
3	B	1406	THM	O2-C2	2.74	1.27	1.23
3	C	1405	THM	C4-N3	-2.73	1.33	1.38
3	D	1401	THM	C4-N3	-2.70	1.33	1.38
3	E	1402	THM	O2-C2	2.67	1.27	1.23
3	E	1402	THM	C4-N3	-2.62	1.33	1.38
3	D	1401	THM	O2-C2	2.48	1.27	1.23
3	H	1407	THM	C5'-C4'	2.44	1.60	1.51
3	H	1407	THM	C2-N3	-2.42	1.33	1.38
3	A	1400	THM	C2-N3	-2.38	1.33	1.38
3	F	1404	THM	C6-N1	-2.36	1.34	1.38
3	H	1407	THM	C4-C5	-2.34	1.41	1.44
3	H	1407	THM	O3'-C3'	2.33	1.48	1.43
3	G	1403	THM	O2-C2	2.32	1.27	1.23
3	E	1402	THM	C5'-C4'	2.21	1.59	1.51
3	C	1405	THM	O2-C2	2.21	1.27	1.23
3	D	1401	THM	C4-C5	-2.19	1.41	1.44
3	B	1406	THM	C4-C5	-2.15	1.41	1.44
3	F	1404	THM	C5'-C4'	2.13	1.59	1.51
3	A	1400	THM	C4-C5	-2.11	1.41	1.44
3	H	1407	THM	C6-N1	-2.11	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1401	THM	C2-N3	-2.02	1.34	1.38

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1406	THM	N3-C2-N1	6.15	122.89	114.89
3	H	1407	THM	C4-N3-C2	-6.10	119.34	127.34
3	G	1403	THM	N3-C2-N1	5.91	122.58	114.89
3	F	1404	THM	C4-N3-C2	-5.90	119.61	127.34
3	E	1402	THM	N3-C2-N1	5.88	122.54	114.89
3	C	1405	THM	N3-C2-N1	5.86	122.52	114.89
3	A	1400	THM	N3-C2-N1	5.86	122.51	114.89
3	F	1404	THM	N3-C2-N1	5.77	122.41	114.89
3	G	1403	THM	C4-N3-C2	-5.75	119.80	127.34
3	D	1401	THM	N3-C2-N1	5.72	122.33	114.89
3	E	1402	THM	C4-N3-C2	-5.67	119.90	127.34
3	H	1407	THM	C5-C4-N3	5.66	120.24	115.32
3	D	1401	THM	C4-N3-C2	-5.66	119.92	127.34
3	B	1406	THM	C4-N3-C2	-5.65	119.94	127.34
3	C	1405	THM	C4-N3-C2	-5.61	119.99	127.34
3	H	1407	THM	N3-C2-N1	5.60	122.19	114.89
3	A	1400	THM	C4-N3-C2	-5.49	120.14	127.34
3	H	1407	THM	O4'-C4'-C5'	5.49	120.82	109.22
3	A	1400	THM	C5-C4-N3	5.32	119.95	115.32
3	B	1406	THM	C5-C4-N3	5.27	119.91	115.32
3	D	1401	THM	C5-C4-N3	5.24	119.88	115.32
3	F	1404	THM	C5-C4-N3	5.22	119.86	115.32
3	C	1405	THM	C5-C4-N3	5.19	119.83	115.32
3	A	1400	THM	C5-C6-N1	-5.16	117.71	123.31
3	G	1403	THM	C5-C4-N3	5.14	119.79	115.32
3	B	1406	THM	C5-C6-N1	-5.14	117.73	123.31
3	H	1407	THM	C5-C6-N1	-5.08	117.80	123.31
3	E	1402	THM	C5-C4-N3	5.06	119.72	115.32
3	E	1402	THM	O4'-C4'-C5'	4.88	119.54	109.22
3	D	1401	THM	O4'-C4'-C5'	4.82	119.41	109.22
3	G	1403	THM	O4'-C4'-C5'	4.77	119.31	109.22
3	F	1404	THM	O4'-C4'-C5'	4.73	119.22	109.22
3	C	1405	THM	C5-C6-N1	-4.66	118.25	123.31
3	F	1404	THM	C5-C6-N1	-4.62	118.30	123.31
3	G	1403	THM	C5-C6-N1	-4.56	118.36	123.31
3	D	1401	THM	C5-C6-N1	-4.55	118.37	123.31
3	E	1402	THM	C5-C6-N1	-4.50	118.42	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1405	THM	O4'-C4'-C5'	4.49	118.72	109.22
3	A	1400	THM	O4'-C4'-C5'	4.41	118.53	109.22
3	B	1406	THM	O4'-C4'-C5'	4.20	118.10	109.22
3	G	1403	THM	O4'-C4'-C3'	-4.10	96.29	105.65
3	H	1407	THM	C2'-C3'-C4'	-4.05	94.59	102.80
3	H	1407	THM	O4'-C4'-C3'	-3.87	96.82	105.65
3	D	1401	THM	O4'-C4'-C3'	-3.87	96.82	105.65
3	B	1406	THM	O2-C2-N1	-3.86	117.78	122.80
3	E	1402	THM	O4'-C4'-C3'	-3.81	96.96	105.65
3	A	1400	THM	O4'-C4'-C3'	-3.81	96.97	105.65
3	F	1404	THM	O4'-C4'-C3'	-3.80	96.98	105.65
3	C	1405	THM	O2-C2-N1	-3.76	117.90	122.80
3	D	1401	THM	C2'-C3'-C4'	-3.72	95.26	102.80
3	G	1403	THM	C5'-C4'-C3'	3.72	124.08	114.82
3	G	1403	THM	C2'-C3'-C4'	-3.71	95.27	102.80
3	A	1400	THM	O2-C2-N1	-3.69	117.99	122.80
3	A	1400	THM	C2'-C3'-C4'	-3.67	95.35	102.80
3	F	1404	THM	C2'-C3'-C4'	-3.66	95.38	102.80
3	B	1406	THM	C2'-C3'-C4'	-3.62	95.46	102.80
3	B	1406	THM	O4'-C4'-C3'	-3.60	97.44	105.65
3	H	1407	THM	O4-C4-C5	-3.59	120.81	124.92
3	E	1402	THM	C2'-C3'-C4'	-3.57	95.56	102.80
3	E	1402	THM	C5'-C4'-C3'	3.57	123.72	114.82
3	G	1403	THM	O2-C2-N1	-3.56	118.16	122.80
3	H	1407	THM	O2-C2-N1	-3.51	118.22	122.80
3	F	1404	THM	O2-C2-N1	-3.51	118.22	122.80
3	A	1400	THM	C5'-C4'-C3'	3.51	123.57	114.82
3	C	1405	THM	O4'-C4'-C3'	-3.49	97.68	105.65
3	F	1404	THM	C5'-C4'-C3'	3.49	123.53	114.82
3	D	1401	THM	O4-C4-C5	-3.49	120.93	124.92
3	C	1405	THM	C2'-C3'-C4'	-3.49	95.73	102.80
3	C	1405	THM	C5'-C4'-C3'	3.47	123.47	114.82
3	D	1401	THM	C5'-C4'-C3'	3.43	123.38	114.82
3	D	1401	THM	O2-C2-N1	-3.43	118.33	122.80
3	E	1402	THM	O2-C2-N1	-3.41	118.36	122.80
3	A	1400	THM	O4-C4-C5	-3.33	121.11	124.92
3	B	1406	THM	C5'-C4'-C3'	3.32	123.09	114.82
3	F	1404	THM	O4-C4-C5	-3.28	121.16	124.92
3	H	1407	THM	O3'-C3'-C2'	3.14	121.80	110.88
3	B	1406	THM	O4-C4-C5	-3.13	121.34	124.92
3	G	1403	THM	O3'-C3'-C2'	3.13	121.74	110.88
3	C	1405	THM	O4-C4-C5	-3.10	121.37	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1403	THM	O4-C4-C5	-3.09	121.38	124.92
3	D	1401	THM	O3'-C3'-C2'	3.06	121.50	110.88
3	A	1400	THM	O3'-C3'-C2'	3.00	121.30	110.88
3	B	1406	THM	O3'-C3'-C2'	2.98	121.25	110.88
3	E	1402	THM	O4-C4-C5	-2.98	121.51	124.92
3	E	1402	THM	O3'-C3'-C2'	2.96	121.17	110.88
3	F	1404	THM	O3'-C3'-C2'	2.94	121.11	110.88
3	C	1405	THM	O3'-C3'-C2'	2.94	121.08	110.88
3	E	1402	THM	O4'-C1'-C2'	-2.73	101.14	106.25
3	G	1403	THM	O4'-C1'-C2'	-2.69	101.21	106.25
3	F	1404	THM	C5M-C5-C6	-2.63	119.29	122.85
3	H	1407	THM	O4'-C1'-C2'	-2.62	101.35	106.25
3	D	1401	THM	O4'-C1'-C2'	-2.60	101.39	106.25
3	H	1407	THM	C5M-C5-C4	2.59	121.55	118.78
3	H	1407	THM	C5'-C4'-C3'	2.55	121.18	114.82
3	G	1403	THM	C5M-C5-C6	-2.53	119.43	122.85
3	F	1404	THM	C5M-C5-C4	2.52	121.47	118.78
3	B	1406	THM	O4'-C1'-C2'	-2.49	101.59	106.25
3	G	1403	THM	C5M-C5-C4	2.46	121.40	118.78
3	F	1404	THM	O4'-C1'-C2'	-2.39	101.77	106.25
3	H	1407	THM	C5M-C5-C6	-2.39	119.61	122.85
3	G	1403	THM	C2'-C1'-N1	2.37	119.74	113.81
3	E	1402	THM	C5M-C5-C6	-2.36	119.65	122.85
3	D	1401	THM	C2'-C1'-N1	2.33	119.64	113.81
3	C	1405	THM	C5M-C5-C4	2.32	121.26	118.78
3	D	1401	THM	C5M-C5-C6	-2.30	119.74	122.85
3	C	1405	THM	C5M-C5-C6	-2.29	119.75	122.85
3	C	1405	THM	O4'-C1'-C2'	-2.25	102.04	106.25
3	A	1400	THM	O3'-C3'-C4'	2.24	118.57	110.07
3	E	1402	THM	C5M-C5-C4	2.23	121.16	118.78
3	F	1404	THM	C2'-C1'-N1	2.20	119.30	113.81
3	E	1402	THM	C2'-C1'-N1	2.16	119.21	113.81
3	A	1400	THM	C5M-C5-C6	-2.15	119.94	122.85
3	A	1400	THM	O4'-C1'-C2'	-2.15	102.23	106.25
3	D	1401	THM	C5M-C5-C4	2.06	120.98	118.78
3	H	1407	THM	O3'-C3'-C4'	2.05	117.86	110.07
3	E	1402	THM	C4'-O4'-C1'	2.05	114.38	109.51
3	C	1405	THM	O3'-C3'-C4'	2.04	117.79	110.07
3	B	1406	THM	O3'-C3'-C4'	2.03	117.76	110.07

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

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, 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%)	-0.11	5 (2%) 58 54	20, 37, 59, 97	0
1	B	192/250 (76%)	0.58	17 (8%) 15 13	28, 57, 98, 110	0
1	C	197/250 (78%)	0.50	13 (6%) 24 21	36, 65, 106, 115	0
1	D	191/250 (76%)	0.76	17 (8%) 15 13	41, 72, 103, 114	0
1	E	192/250 (76%)	0.43	5 (2%) 57 52	36, 61, 95, 110	0
1	F	192/250 (76%)	0.98	32 (16%) 4 3	42, 79, 107, 116	0
1	G	192/250 (76%)	0.71	15 (7%) 19 17	32, 69, 108, 123	0
1	H	192/250 (76%)	-0.23	0 100 100	21, 35, 55, 71	0
All	All	1545/2000 (77%)	0.45	104 (6%) 24 21	20, 60, 103, 123	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	207	ALA	4.4
1	F	173	SER	4.2
1	B	168	ALA	4.0
1	D	143	ILE	4.0
1	B	174	CYS	3.7
1	B	208	ASP	3.3
1	G	142	SER	3.3
1	F	18	THR	3.3
1	F	208	ASP	3.2
1	C	207	ALA	3.2
1	C	168	ALA	3.1
1	E	168	ALA	3.1
1	D	207	ALA	3.1
1	F	207	ALA	3.1
1	F	145	VAL	3.1
1	F	170	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	208	ASP	3.0
1	C	199	SER	3.0
1	B	12	THR	3.0
1	F	15	ALA	3.0
1	F	12	THR	3.0
1	F	108	PHE	3.0
1	D	144	HIS	2.9
1	G	205	LEU	2.9
1	G	43	TYR	2.9
1	F	17	GLY	2.9
1	F	95	PRO	2.9
1	F	53	PRO	2.8
1	G	191	LEU	2.7
1	A	199	SER	2.7
1	D	203	LEU	2.7
1	A	12	THR	2.7
1	G	206	ASP	2.6
1	C	171	GLU	2.6
1	F	55	GLU	2.6
1	F	168	ALA	2.6
1	C	12	THR	2.6
1	B	207	ALA	2.6
1	D	12	THR	2.6
1	B	14	TYR	2.6
1	C	197	PRO	2.5
1	C	172	GLU	2.5
1	F	43	TYR	2.5
1	E	208	ASP	2.5
1	A	45	ASN	2.5
1	F	63	VAL	2.5
1	G	160	ALA	2.5
1	F	142	SER	2.5
1	A	97	ASN	2.5
1	G	204	VAL	2.5
1	F	172	GLU	2.4
1	F	144	HIS	2.4
1	A	207	ALA	2.4
1	F	94	ALA	2.4
1	F	14	TYR	2.4
1	B	95	PRO	2.4
1	D	15	ALA	2.4
1	E	47	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	208	ASP	2.3
1	B	40	PHE	2.3
1	F	61	ASN	2.3
1	D	173	SER	2.3
1	F	47	ILE	2.3
1	G	149	LEU	2.3
1	D	160	ALA	2.3
1	D	127	GLY	2.3
1	B	204	VAL	2.3
1	F	202	VAL	2.3
1	B	43	TYR	2.3
1	C	15	ALA	2.2
1	C	43	TYR	2.3
1	G	30	GLY	2.2
1	C	37	LEU	2.2
1	D	72	ASP	2.2
1	D	14	TYR	2.2
1	C	173	SER	2.2
1	F	104	GLU	2.2
1	D	167	ARG	2.2
1	F	60	VAL	2.2
1	F	93	THR	2.2
1	D	113	CYS	2.2
1	G	48	CYS	2.2
1	D	108	PHE	2.2
1	F	204	VAL	2.1
1	B	100	LEU	2.1
1	E	17	GLY	2.1
1	E	43	TYR	2.1
1	B	123	SER	2.1
1	D	145	VAL	2.1
1	D	204	VAL	2.1
1	B	48	CYS	2.1
1	B	170	SER	2.1
1	G	63	VAL	2.1
1	B	18	THR	2.1
1	C	18	THR	2.1
1	F	101	LYS	2.1
1	F	66	LEU	2.0
1	G	171	GLU	2.0
1	B	39	HIS	2.0
1	C	167	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	165	ARG	2.0
1	B	47	ILE	2.0
1	F	143	ILE	2.0
1	G	47	ILE	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 oligosaccharides 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	0.91	0.10	55,58,64,65	0
3	THM	G	1403	17/17	0.92	0.11	66,70,72,73	0
3	THM	D	1401	17/17	0.93	0.09	48,51,58,60	0
2	SO4	D	1301	5/5	0.93	0.09	55,56,60,61	0
3	THM	B	1406	17/17	0.94	0.07	29,37,45,45	0
2	SO4	F	1304	5/5	0.94	0.08	65,67,68,70	0
2	SO4	C	1305	5/5	0.95	0.09	66,67,68,69	0
3	THM	E	1402	17/17	0.95	0.06	39,44,52,52	0
2	SO4	G	1303	5/5	0.95	0.06	69,69,69,72	0
3	THM	A	1400	17/17	0.96	0.06	27,31,36,38	0
3	THM	F	1404	17/17	0.96	0.07	45,49,56,58	0
2	SO4	E	1302	5/5	0.96	0.06	49,49,51,52	0
2	SO4	A	1308	5/5	0.97	0.10	43,46,49,50	0
3	THM	H	1407	17/17	0.97	0.05	16,26,30,31	0
2	SO4	B	1306	5/5	0.98	0.06	43,44,47,50	0
2	SO4	A	1300	5/5	0.98	0.07	29,29,33,35	0
2	SO4	H	1307	5/5	0.99	0.04	30,31,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.