



# Full wwPDB X-ray Structure Validation Report

Mar 8, 2026 – 08:41 AM UTC


PDB ID : 4E1V / pdb\_00004e1v  
Title : X-RAY Structure of the Uridine Phosphorylase from Salmonella Typhimurium  
in Complex with 5-Fluorouracil at 2.15 Å Resolution  
Authors : Lashkov, A.A.; Sotnichenko, S.E.; Prokofev, I.I.; Gabdoulkhakov, A.G.;  
Mikhailov, A.M.  
Deposited on : 2012-03-07  
Resolution : 2.15 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

<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>.

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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

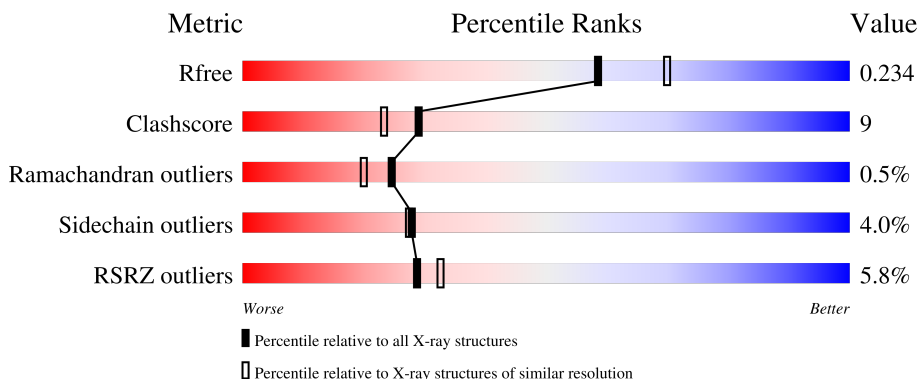
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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  $\geq 3$ , 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	253	 76% 20% ..
1	B	253	 85% 11% ..
1	C	253	 82% 13% ..
1	D	253	 83% 13% ..
1	E	253	 84% 11% ..

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Mol	Chain	Length	Quality of chain
1	F	253	
1	G	253	
1	H	253	
1	I	253	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	URF	A	1301	-	X	-	-
2	URF	B	1301	-	X	-	-
2	URF	C	1301	-	X	-	-
2	URF	D	1301	-	X	-	-
2	URF	E	1301	-	X	-	-
2	URF	F	1301	-	X	-	-
2	URF	G	1301	-	X	-	-
2	URF	H	1301	-	X	-	-
5	EDO	C	1302	-	-	X	-

## 2 Entry composition [i](#)

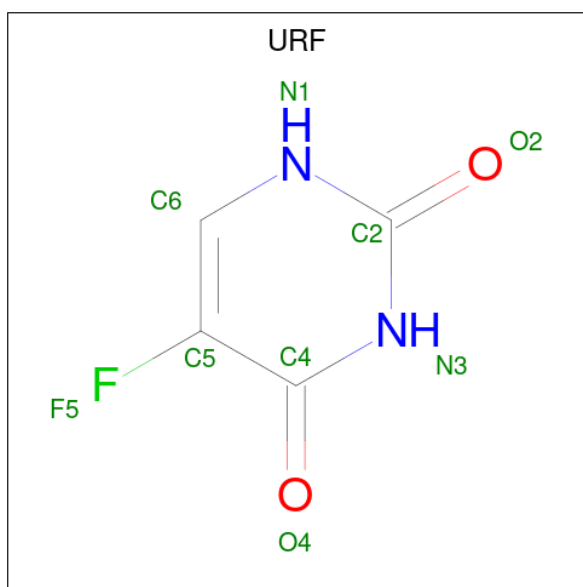
There are 6 unique types of molecules in this entry. The entry contains 17042 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	248	1868	1171	330	356	11	0	1	0
1	E	245	1835	1149	323	352	11	0	0	0
1	F	242	1814	1137	320	346	11	0	0	0
1	D	245	1843	1156	325	351	11	0	1	0
1	C	246	1846	1156	325	354	11	0	0	0
1	B	244	1838	1153	324	350	11	0	1	0
1	H	243	1824	1143	321	349	11	0	0	0
1	I	243	1823	1143	322	347	11	0	0	0
1	G	242	1814	1137	320	346	11	0	0	0

- Molecule 2 is 5-FLUOROURACIL (CCD ID: URF) (formula: C<sub>4</sub>H<sub>3</sub>FN<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	F	N			O	
2	A	1	Total	9	4	1	2	2	0	0
2	E	1	Total	9	4	1	2	2	0	0
2	F	1	Total	9	4	1	2	2	0	0
2	D	1	Total	9	4	1	2	2	0	0
2	C	1	Total	9	4	1	2	2	0	0
2	B	1	Total	9	4	1	2	2	0	0
2	H	1	Total	9	4	1	2	2	0	0
2	G	1	Total	9	4	1	2	2	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0
4	E	1	Total K 1 1	0	0
4	D	1	Total K 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	C O	0	0
			4	2 2		

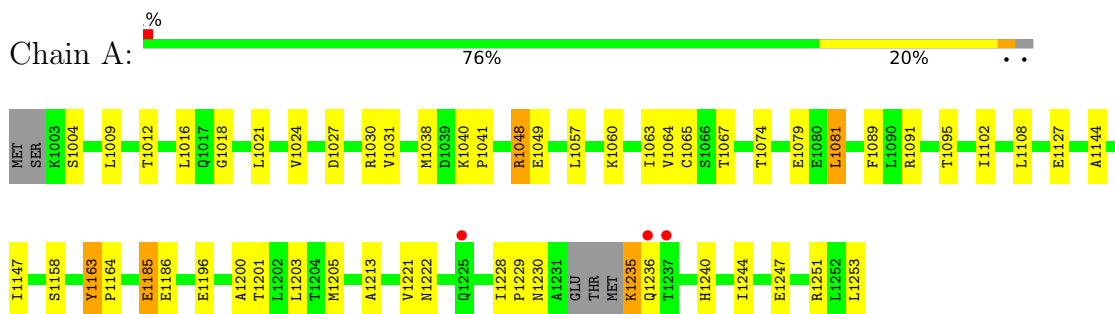
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	61	Total	O	0	1
			62	62		
6	E	62	Total	O	0	0
			62	62		
6	F	67	Total	O	0	0
			67	67		
6	D	69	Total	O	0	1
			70	70		
6	C	58	Total	O	0	0
			58	58		
6	B	66	Total	O	0	0
			66	66		
6	H	16	Total	O	0	0
			16	16		
6	I	12	Total	O	0	0
			12	12		
6	G	15	Total	O	0	0
			15	15		

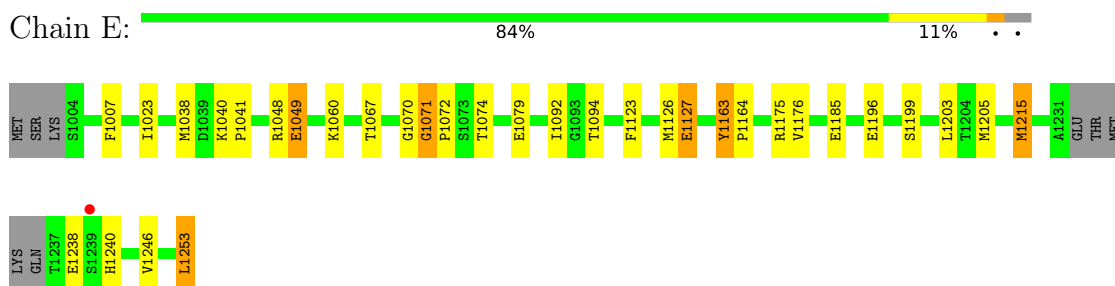
### 3 Residue-property plots [i](#)

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.

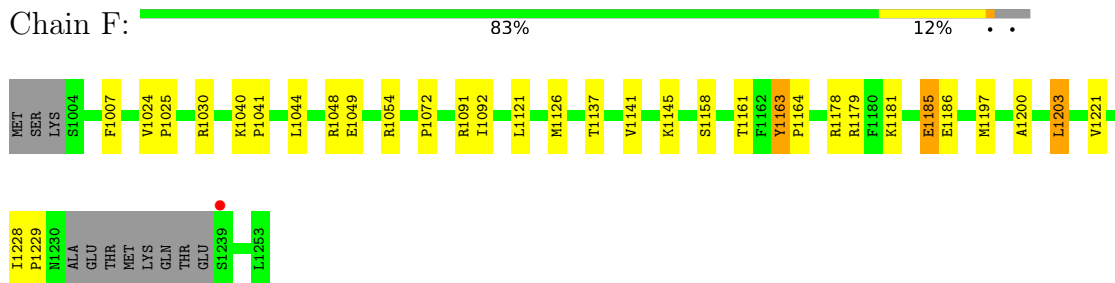
- Molecule 1: Uridine phosphorylase



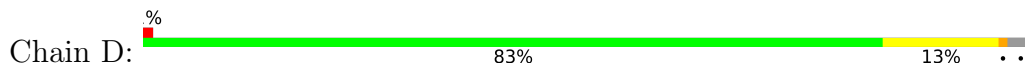
- Molecule 1: Uridine phosphorylase

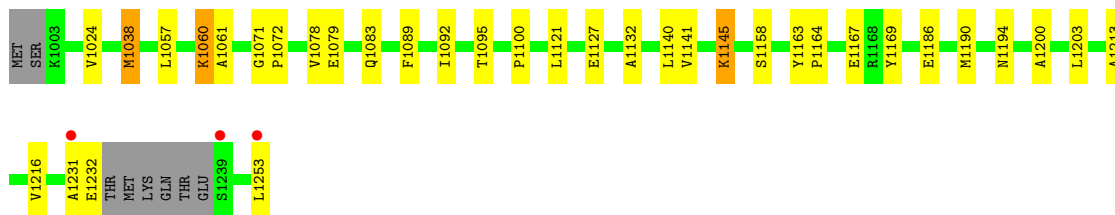


- Molecule 1: Uridine phosphorylase

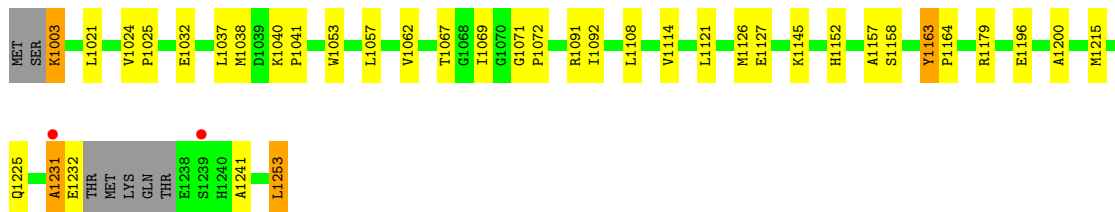
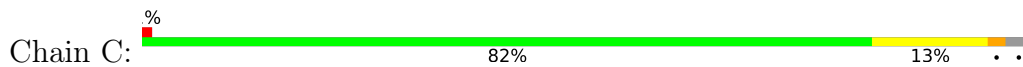


- Molecule 1: Uridine phosphorylase

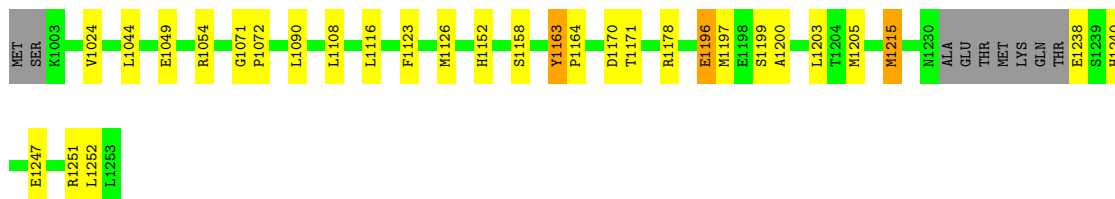
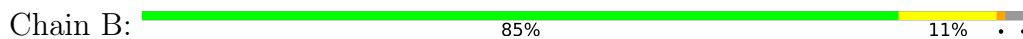




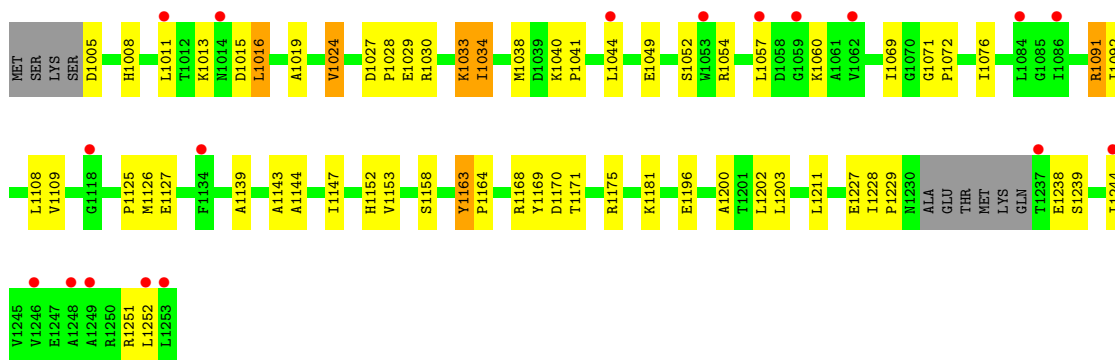
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase

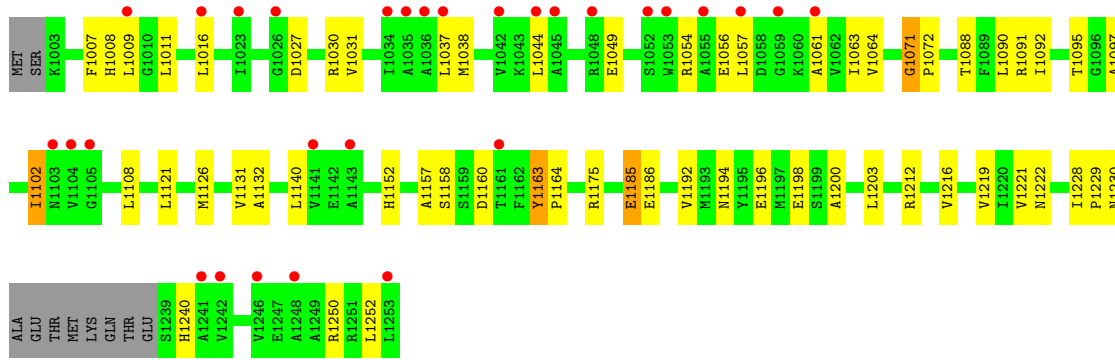


- Molecule 1: Uridine phosphorylase

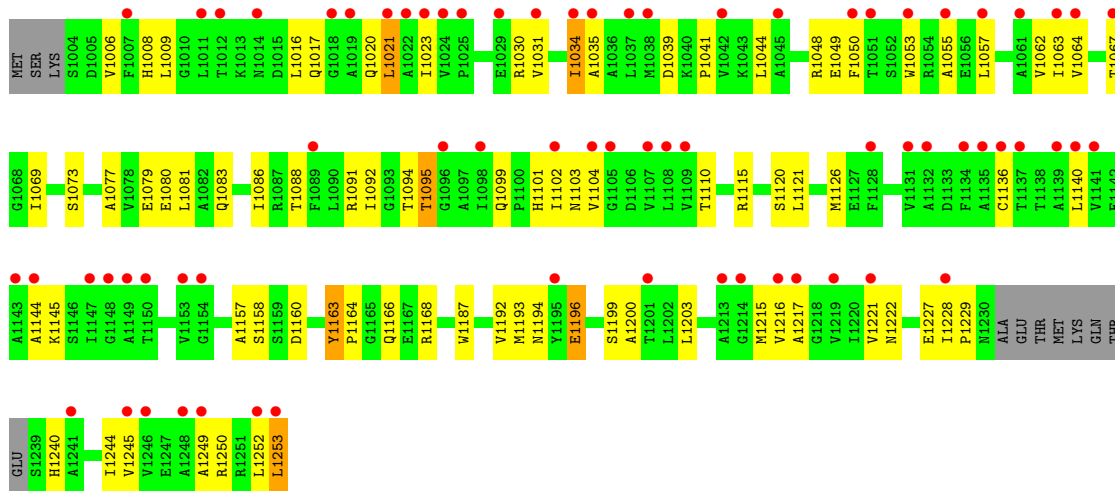


- Molecule 1: Uridine phosphorylase





- Molecule 1: Uridine phosphorylase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.49Å 93.21Å 149.97Å 90.00° 90.82° 90.00°	Depositor
Resolution (Å)	28.88 – 2.15 28.88 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.9 (28.88-2.15) 96.8 (28.88-2.15)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, $R_{free}$	0.194 , 0.238 0.192 , 0.234	Depositor DCC
$R_{free}$ test set	5750 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.027 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.026 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.077 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.057 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.028 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17042	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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, 0.333 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: GOL, URF, EDO, K

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	0/1900	0.79	1/2571 (0.0%)
1	B	0.49	0/1870	0.80	0/2531
1	C	0.49	0/1875	0.80	1/2539 (0.0%)
1	D	0.54	1/1875 (0.1%)	0.79	1/2538 (0.0%)
1	E	0.48	0/1864	0.84	4/2526 (0.2%)
1	F	0.48	0/1843	0.82	2/2497 (0.1%)
1	G	0.38	0/1843	0.80	2/2497 (0.1%)
1	H	0.42	0/1853	0.77	0/2511
1	I	0.34	0/1852	0.78	1/2508 (0.0%)
All	All	0.46	1/16775 (0.0%)	0.80	12/22718 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1164	PRO	C-O	-5.81	1.17	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1194	ASN	N-CA-C	6.06	117.44	108.60
1	E	1071	GLY	CA-C-N	5.92	125.12	118.97
1	E	1071	GLY	C-N-CA	5.92	125.12	118.97
1	D	1024	VAL	N-CA-C	5.87	113.96	108.15
1	E	1070	GLY	N-CA-C	5.79	118.77	112.29
1	F	1007	PHE	N-CA-C	5.58	117.16	111.14
1	C	1069	ILE	CB-CA-C	-5.38	104.78	111.08
1	E	1048	ARG	CB-CA-C	-5.30	110.44	116.54
1	F	1048	ARG	CB-CA-C	-5.12	110.65	116.54
1	G	1021	LEU	N-CA-C	5.11	117.15	109.23
1	I	1071	GLY	O-C-N	5.08	122.90	121.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1048	ARG	CB-CA-C	-5.06	110.72	116.54

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	1868	0	1890	38	0
1	B	1838	0	1857	20	0
1	C	1846	0	1855	26	0
1	D	1843	0	1862	21	0
1	E	1835	0	1843	24	0
1	F	1814	0	1825	27	0
1	G	1814	0	1825	72	0
1	H	1824	0	1833	39	0
1	I	1823	0	1838	35	0
2	A	9	0	3	1	0
2	B	9	0	3	2	0
2	C	9	0	3	2	0
2	D	9	0	3	0	0
2	E	9	0	3	1	0
2	F	9	0	3	1	0
2	G	9	0	3	0	0
2	H	9	0	3	0	0
3	A	6	0	8	1	0
3	B	6	0	8	3	0
3	C	6	0	8	2	0
3	E	6	0	8	2	0
3	F	6	0	8	1	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	C	4	0	6	4	0
6	A	62	0	0	0	0
6	B	66	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	58	0	0	0	0
6	D	70	0	0	1	0
6	E	62	0	0	0	0
6	F	67	0	0	1	0
6	G	15	0	0	0	0
6	H	16	0	0	0	0
6	I	12	0	0	1	0
All	All	17042	0	16698	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 9.

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:1095:THR:CG2	1:G:1217:ALA:HB1	1.97	0.94
2:E:1301:URF:HN1	3:E:1302:GOL:H2	1.36	0.91
1:H:1069:ILE:HD11	1:G:1048:ARG:HD3	1.55	0.88
1:G:1021:LEU:HD21	1:G:1088:THR:HB	1.59	0.84
1:I:1163:TYR:HB2	1:I:1164:PRO:HD3	1.61	0.83
1:G:1095:THR:HG22	1:G:1217:ALA:HB1	1.60	0.82
1:G:1095:THR:HG21	1:G:1217:ALA:CB	2.10	0.82
1:G:1020:GLN:C	1:G:1021:LEU:HD12	2.09	0.77
2:A:1301:URF:HN1	3:A:1302:GOL:H2	1.51	0.75
1:G:1055:ALA:O	1:G:1062:VAL:N	2.20	0.75
1:C:1179:ARG:HD2	5:C:1302:EDO:H21	1.68	0.74
1:H:1016:LEU:HG	1:H:1019:ALA:HB3	1.70	0.74
1:G:1166:GLN:OE1	1:G:1168:ARG:NH1	2.22	0.72
1:G:1020:GLN:O	1:G:1021:LEU:HD12	1.88	0.71
1:F:1158:SER:HB3	1:F:1200:ALA:HB2	1.71	0.71
1:H:1144:ALA:HA	1:H:1244:ILE:HD12	1.72	0.71
1:C:1067:THR:OG1	1:C:1091:ARG:NH1	2.24	0.70
1:I:1228:ILE:HB	1:I:1229:PRO:HD2	1.73	0.69
1:G:1006:VAL:HG11	1:G:1080:GLU:O	1.94	0.68
1:A:1144:ALA:HA	1:A:1244:ILE:HD12	1.76	0.68
1:G:1021:LEU:HD21	1:G:1088:THR:CB	2.25	0.67
1:G:1081:LEU:HB3	1:G:1086:ILE:HD12	1.75	0.67
1:G:1031:VAL:HG13	1:G:1064:VAL:HG12	1.75	0.67
1:E:1049:GLU:HB3	1:F:1049:GLU:HG2	1.78	0.66
1:D:1167:GLU:HG2	1:D:1169:TYR:CE1	2.32	0.65
1:A:1024:VAL:O	1:A:1091:ARG:HD2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1221:VAL:HB	1:F:1229:PRO:HB3	1.78	0.65
1:I:1044:LEU:HD11	1:I:1054:ARG:HB2	1.79	0.65
1:G:1021:LEU:CD2	1:G:1088:THR:HB	2.26	0.65
1:G:1095:THR:HG21	1:G:1217:ALA:HB1	1.67	0.65
1:H:1033:LYS:HA	1:H:1033:LYS:HE3	1.78	0.65
1:I:1228:ILE:HB	1:I:1229:PRO:CD	2.28	0.64
1:G:1101:HIS:O	1:G:1102:ILE:HD12	1.98	0.64
1:D:1231:ALA:O	1:D:1232:GLU:HB3	1.97	0.64
1:C:1038:MET:HE3	1:C:1057:LEU:HB2	1.79	0.63
1:G:1095:THR:HG21	1:G:1217:ALA:HB3	1.79	0.63
1:G:1034:ILE:HG22	1:G:1064:VAL:HG21	1.80	0.63
1:A:1018:GLY:O	1:A:1060[A]:LYS:NZ	2.33	0.62
1:G:1102:ILE:O	1:G:1222:ASN:ND2	2.33	0.62
1:C:1092:ILE:HD11	1:C:1241:ALA:HB1	1.81	0.61
1:G:1101:HIS:ND1	1:G:1102:ILE:HD12	2.14	0.61
2:C:1301:URF:HN1	3:C:1303:GOL:H2	1.65	0.61
1:G:1158:SER:HB3	1:G:1200:ALA:HB2	1.83	0.61
1:G:1031:VAL:HG13	1:G:1064:VAL:CG1	2.31	0.61
1:A:1240:HIS:O	1:A:1244:ILE:HG12	2.00	0.60
1:C:1179:ARG:NH1	5:C:1302:EDO:O1	2.34	0.60
1:G:1101:HIS:C	1:G:1102:ILE:HD12	2.27	0.60
1:D:1121:LEU:HD22	5:C:1302:EDO:H12	1.82	0.60
1:A:1144:ALA:HA	1:A:1244:ILE:CD1	2.31	0.60
1:G:1034:ILE:HG22	1:G:1035:ALA:N	2.17	0.59
1:G:1020:GLN:O	1:G:1086:ILE:HG23	2.03	0.59
1:G:1021:LEU:HD21	1:G:1088:THR:CG2	2.32	0.59
1:I:1158:SER:HB3	1:I:1200:ALA:HB2	1.84	0.59
2:F:1301:URF:HN1	3:F:1302:GOL:H11	1.67	0.57
1:I:1090:LEU:HD11	1:I:1252:LEU:HD12	1.86	0.57
1:E:1094:THR:HG1	3:E:1302:GOL:HO2	1.49	0.57
1:F:1044:LEU:HD11	1:F:1054:ARG:HB2	1.86	0.57
1:D:1100:PRO:HG2	6:D:1465:HOH:O	2.05	0.57
1:G:1101:HIS:ND1	1:G:1102:ILE:CD1	2.67	0.57
1:G:1121:LEU:HD21	1:G:1126:MET:HE2	1.87	0.56
1:D:1038:MET:HB3	1:D:1057:LEU:HD13	1.87	0.56
1:H:1028:PRO:HD2	1:G:1048:ARG:HA	1.87	0.56
1:G:1094:THR:C	1:G:1095:THR:HG22	2.29	0.56
1:A:1004:SER:HA	1:A:1012:THR:HG22	1.87	0.55
1:F:1054:ARG:NH2	6:F:1434:HOH:O	2.38	0.55
1:D:1140:LEU:HD22	1:D:1216:VAL:HB	1.88	0.55
1:H:1109:VAL:HB	1:H:1153:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1049:GLU:CD	1:G:1069:ILE:H	2.15	0.55
1:E:1049:GLU:HG2	1:F:1049:GLU:HG2	1.88	0.55
1:F:1121:LEU:HD21	1:F:1126:MET:HE2	1.89	0.55
1:C:1158:SER:HB3	1:C:1200:ALA:HB2	1.89	0.55
1:C:1179:ARG:CD	5:C:1302:EDO:H21	2.34	0.55
1:G:1044:LEU:HD11	1:G:1063:ILE:CD1	2.37	0.55
1:E:1060:LYS:HD2	1:E:1253:LEU:HB3	1.87	0.55
1:G:1163:TYR:HB2	1:G:1164:PRO:HD3	1.88	0.55
1:F:1163:TYR:HB2	1:F:1164:PRO:CD	2.36	0.55
1:D:1167:GLU:HG2	1:D:1169:TYR:HE1	1.70	0.55
1:G:1016:LEU:O	1:G:1017:GLN:HB2	2.06	0.55
1:G:1021:LEU:HG	1:G:1088:THR:O	2.07	0.55
1:E:1040:LYS:N	1:E:1041:PRO:HD3	2.22	0.54
1:H:1005:ASP:N	1:H:1005:ASP:OD2	2.40	0.54
1:C:1108:LEU:HD22	1:C:1152:HIS:HB2	1.89	0.54
1:H:1005:ASP:N	1:H:1011:LEU:O	2.41	0.54
1:H:1163:TYR:HB2	1:H:1164:PRO:CD	2.38	0.54
1:G:1021:LEU:CG	1:G:1088:THR:HB	2.38	0.54
1:H:1076:ILE:HD12	1:G:1069:ILE:HD13	1.89	0.53
1:H:1168:ARG:HG2	1:H:1227:GLU:HG3	1.91	0.53
1:E:1163:TYR:HB2	1:E:1164:PRO:CD	2.37	0.53
1:F:1161:THR:C	1:F:1197:MET:HE3	2.34	0.53
1:A:1040:LYS:N	1:A:1041:PRO:HD3	2.23	0.53
1:F:1040:LYS:N	1:F:1041:PRO:HD3	2.24	0.53
1:B:1123:PHE:CZ	1:B:1205:MET:HE3	2.44	0.53
1:E:1127:GLU:CD	1:E:1127:GLU:H	2.17	0.53
1:C:1121:LEU:HD21	1:C:1126:MET:HE2	1.91	0.53
1:H:1040:LYS:N	1:H:1041:PRO:HD3	2.23	0.53
1:H:1252:LEU:O	1:H:1252:LEU:HD12	2.09	0.53
1:E:1175:ARG:HG2	1:E:1176:VAL:N	2.24	0.52
1:C:1071:GLY:N	1:C:1072:PRO:CD	2.72	0.52
1:G:1030:ARG:O	1:G:1034:ILE:HD12	2.09	0.52
1:G:1008:HIS:H	1:G:1080:GLU:CD	2.17	0.52
1:A:1158:SER:HB3	1:A:1200:ALA:HB2	1.91	0.52
1:D:1060[B]:LYS:HD2	1:D:1061:ALA:N	2.25	0.52
1:I:1102:ILE:HD12	1:I:1108:LEU:HD21	1.91	0.52
1:E:1023:ILE:HD12	1:E:1038:MET:HE1	1.91	0.52
1:C:1091:ARG:HG2	1:C:1215:MET:SD	2.50	0.52
1:H:1163:TYR:CB	1:H:1164:PRO:CD	2.88	0.52
1:D:1060[A]:LYS:HD3	1:D:1061:ALA:N	2.24	0.52
1:B:1116:LEU:HB2	1:B:1158:SER:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:ASP:HB3	1:A:1030:ARG:HG3	1.91	0.51
1:B:1163:TYR:HB2	1:B:1164:PRO:CD	2.40	0.51
1:B:1163:TYR:CB	1:B:1164:PRO:CD	2.88	0.51
1:I:1071:GLY:N	1:I:1072:PRO:CD	2.74	0.51
1:F:1137:THR:O	1:F:1141:VAL:HG23	2.10	0.51
1:G:1110:THR:HB	1:G:1215:MET:HB3	1.92	0.51
1:A:1038:MET:HG2	1:A:1057:LEU:HD13	1.93	0.51
1:E:1007:PHE:CE1	1:F:1229:PRO:HG2	2.46	0.51
1:I:1016:LEU:HG	1:I:1063:ILE:HD12	1.93	0.50
1:B:1054:ARG:HG2	6:B:1406:HOH:O	2.11	0.50
1:I:1229:PRO:O	1:I:1230:ASN:CB	2.59	0.50
1:I:1088:THR:HA	1:I:1212:ARG:HB2	1.94	0.50
1:I:1196:GLU:CD	1:I:1198:GLU:H	2.19	0.50
1:H:1125:PRO:HB2	1:H:1127:GLU:OE2	2.12	0.50
1:G:1250:ARG:HA	1:G:1253:LEU:HD22	1.92	0.50
1:A:1163:TYR:HB2	1:A:1164:PRO:CD	2.42	0.49
1:I:1038:MET:HG2	1:I:1057:LEU:HD12	1.94	0.49
1:D:1079:GLU:O	1:D:1083:GLN:HG3	2.13	0.49
1:A:1095:THR:HG21	1:A:1108:LEU:HD12	1.94	0.49
1:E:1038:MET:HE2	1:E:1246:VAL:HG22	1.94	0.49
1:B:1158:SER:HB3	1:B:1200:ALA:HB2	1.95	0.49
1:E:1199:SER:HB3	1:E:1215:MET:HE2	1.93	0.49
1:A:1127:GLU:CD	1:A:1127:GLU:H	2.21	0.49
1:H:1071:GLY:N	1:H:1072:PRO:CD	2.76	0.48
1:G:1163:TYR:HB2	1:G:1164:PRO:CD	2.43	0.48
1:H:1091:ARG:HG3	1:H:1202:LEU:HD22	1.95	0.48
1:G:1067:THR:O	1:G:1073:SER:HB3	2.13	0.48
1:A:1009:LEU:CD1	1:A:1081:LEU:HD13	2.44	0.48
1:F:1163:TYR:CB	1:F:1164:PRO:CD	2.91	0.48
1:I:1071:GLY:N	1:I:1072:PRO:HD2	2.28	0.48
1:A:1230:ASN:HB2	1:A:1235:LYS:CE	2.44	0.48
1:F:1092:ILE:HG23	1:F:1092:ILE:O	2.12	0.48
1:H:1027:ASP:OD2	1:H:1029:GLU:HB2	2.13	0.48
1:I:1121:LEU:HD21	1:I:1126:MET:HE2	1.96	0.48
1:F:1024:VAL:O	1:F:1091:ARG:HD2	2.13	0.48
1:B:1044:LEU:HD11	1:B:1054:ARG:HB2	1.96	0.48
1:G:1030:ARG:O	1:G:1034:ILE:CD1	2.62	0.48
1:G:1030:ARG:HB3	1:G:1034:ILE:CD1	2.44	0.48
1:A:1102:ILE:O	1:A:1222:ASN:ND2	2.47	0.47
1:G:1240:HIS:O	1:G:1244:ILE:HG12	2.14	0.47
1:D:1089:PHE:O	1:D:1213:ALA:HA	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1090:LEU:HD11	1:B:1252:LEU:HD12	1.95	0.47
1:G:1221:VAL:HB	1:G:1229:PRO:HB3	1.97	0.47
1:I:1095:THR:OG1	1:I:1194:ASN:HB2	2.14	0.47
1:G:1168:ARG:HE	1:G:1227:GLU:HB2	1.80	0.47
1:A:1016:LEU:HG	1:A:1063:ILE:HG13	1.96	0.47
1:A:1021:LEU:C	1:A:1021:LEU:HD23	2.39	0.47
1:I:1057:LEU:HD21	1:I:1250:ARG:HB3	1.96	0.47
1:A:1009:LEU:HD12	1:A:1081:LEU:HD13	1.97	0.47
1:D:1158:SER:HB3	1:D:1200:ALA:HB2	1.97	0.47
1:E:1049:GLU:CB	1:F:1049:GLU:HG2	2.45	0.47
1:E:1071:GLY:N	1:E:1072:PRO:CD	2.78	0.47
1:F:1178:ARG:HH21	1:D:1186:GLU:CD	2.22	0.46
1:A:1163:TYR:HB2	1:A:1164:PRO:HD3	1.96	0.46
1:B:1247:GLU:HG3	1:B:1251:ARG:HH22	1.80	0.46
1:H:1015:ASP:O	1:H:1054:ARG:NE	2.47	0.46
1:H:1147:ILE:HG13	1:H:1244:ILE:HD13	1.98	0.46
1:E:1067:THR:HB	1:E:1074:THR:HA	1.98	0.46
1:C:1038:MET:HE1	1:C:1062:VAL:HG11	1.98	0.46
1:H:1008:HIS:CE1	1:H:1076:ILE:HD13	2.51	0.46
1:I:1027:ASP:HB3	1:I:1030:ARG:HB2	1.98	0.46
1:D:1132:ALA:HA	1:D:1203:LEU:HD22	1.97	0.46
1:F:1163:TYR:HB2	1:F:1164:PRO:HD3	1.98	0.46
1:C:1231:ALA:O	1:C:1232:GLU:HB3	2.15	0.46
1:H:1169:TYR:O	1:H:1171:THR:N	2.49	0.46
1:A:1163:TYR:CB	1:A:1164:PRO:CD	2.93	0.46
1:I:1221:VAL:HG22	1:I:1222:ASN:N	2.31	0.46
1:I:1031:VAL:HG13	1:I:1064:VAL:HG12	1.98	0.46
1:A:1067:THR:OG1	1:A:1091:ARG:NH1	2.46	0.45
1:I:1092:ILE:HA	1:I:1216:VAL:O	2.16	0.45
1:C:1057:LEU:HB3	1:C:1253:LEU:HD21	1.98	0.45
1:G:1193:MET:HE2	1:G:1193:MET:HB3	1.88	0.45
1:E:1238:GLU:O	1:E:1238:GLU:HG3	2.15	0.45
1:A:1147:ILE:HG22	1:A:1147:ILE:O	2.15	0.45
1:A:1185:GLU:HG3	1:A:1186:GLU:N	2.31	0.45
1:A:1247:GLU:HG3	1:A:1251:ARG:HH12	1.82	0.45
1:H:1024:VAL:HG23	1:H:1091:ARG:HA	1.99	0.45
1:G:1023:ILE:HD12	1:G:1245:VAL:HG22	1.99	0.45
1:D:1186:GLU:O	1:D:1190:MET:HG3	2.16	0.45
1:B:1196:GLU:OE2	1:B:1199:SER:OG	2.34	0.45
1:I:1011:LEU:HD11	1:I:1044:LEU:HD13	1.98	0.45
1:G:1041:PRO:HB2	1:G:1053:TRP:CZ3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1181:LYS:O	1:B:1178:ARG:NH2	2.50	0.45
1:C:1040:LYS:N	1:C:1041:PRO:CD	2.80	0.45
1:H:1163:TYR:HB2	1:H:1164:PRO:HD3	1.98	0.45
1:G:1157:ALA:HB2	1:G:1192:VAL:HG11	1.99	0.45
1:I:1009:LEU:HB3	1:I:1011:LEU:HD23	1.99	0.44
1:C:1163:TYR:HB2	1:C:1164:PRO:CD	2.47	0.44
1:H:1108:LEU:HD22	1:H:1152:HIS:HB2	1.99	0.44
1:H:1049:GLU:HG2	1:G:1049:GLU:HB3	1.99	0.44
1:G:1095:THR:CG2	1:G:1217:ALA:CB	2.71	0.44
1:E:1163:TYR:CB	1:E:1164:PRO:CD	2.95	0.44
1:B:1108:LEU:HD22	1:B:1152:HIS:HB2	2.00	0.44
1:H:1251:ARG:HA	1:H:1251:ARG:HD3	1.76	0.44
1:B:1197:MET:HB2	3:B:1302:GOL:O3	2.18	0.44
1:D:1141:VAL:O	1:D:1145:LYS:HG2	2.18	0.44
1:B:1071:GLY:N	1:B:1072:PRO:CD	2.81	0.44
1:G:1023:ILE:HD11	1:G:1249:ALA:HB2	2.00	0.44
1:C:1024:VAL:HA	1:C:1025:PRO:HD2	1.91	0.44
1:I:1131:VAL:HG22	1:I:1132:ALA:O	2.18	0.44
1:D:1071:GLY:N	1:D:1072:PRO:CD	2.81	0.43
1:B:1170:ASP:HA	1:H:1013:LYS:HD3	1.99	0.43
1:A:1067:THR:HB	1:A:1074:THR:HA	2.00	0.43
1:A:1201:THR:O	1:A:1205:MET:HG2	2.19	0.43
1:D:1078:VAL:HG13	1:D:1089:PHE:CZ	2.54	0.43
1:G:1145:LYS:HE3	1:G:1145:LYS:HB3	1.87	0.43
1:A:1048:ARG:HB3	1:A:1049:GLU:OE1	2.18	0.43
1:E:1049:GLU:HB3	1:F:1049:GLU:CG	2.47	0.43
1:H:1126:MET:HG3	1:I:1126:MET:HG3	2.01	0.43
1:I:1097:ALA:HB2	1:I:1102:ILE:HD11	2.00	0.43
1:G:1091:ARG:HG2	1:G:1215:MET:SD	2.58	0.43
1:G:1136:CYS:HA	1:G:1252:LEU:HD11	2.00	0.43
1:C:1127:GLU:CD	1:C:1127:GLU:H	2.27	0.43
1:G:1044:LEU:CD1	1:G:1063:ILE:HD12	2.49	0.43
1:G:1057:LEU:HB3	1:G:1253:LEU:HD21	2.00	0.43
1:E:1079:GLU:HG2	1:F:1163:TYR:CD2	2.54	0.43
1:H:1038:MET:SD	1:H:1057:LEU:HD11	2.58	0.43
1:C:1021:LEU:HD13	1:C:1253:LEU:CD1	2.49	0.43
2:B:1301:URF:HN1	3:B:1302:GOL:H31	1.84	0.43
1:A:1221:VAL:HB	1:A:1229:PRO:HG3	2.01	0.43
2:B:1301:URF:HN1	3:B:1302:GOL:C3	2.32	0.43
1:E:1253:LEU:HD12	1:E:1253:LEU:HA	1.83	0.42
1:H:1211:LEU:HD12	1:H:1211:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1228:ILE:HA	1:G:1229:PRO:HD3	1.81	0.42
1:E:1072:PRO:HG2	1:F:1072:PRO:HD2	2.01	0.42
1:C:1114:VAL:HB	1:C:1157:ALA:HA	2.00	0.42
1:C:1163:TYR:CB	1:C:1164:PRO:CD	2.97	0.42
1:B:1090:LEU:HD23	1:B:1090:LEU:HA	1.81	0.42
1:G:1163:TYR:HA	1:G:1168:ARG:HB2	2.00	0.42
1:C:1032:GLU:HG3	1:C:1053:TRP:CH2	2.55	0.42
1:C:1091:ARG:HG3	1:C:1092:ILE:N	2.34	0.42
1:H:1158:SER:HB2	1:H:1200:ALA:HB2	2.01	0.42
1:I:1140:LEU:HD12	1:I:1140:LEU:HA	1.82	0.42
1:A:1024:VAL:HA	1:A:1065:CYS:O	2.19	0.42
1:A:1089:PHE:O	1:A:1213:ALA:HA	2.19	0.42
1:E:1126:MET:SD	1:D:1127:GLU:HG3	2.60	0.42
1:F:1185:GLU:HG3	1:F:1186:GLU:N	2.29	0.42
1:F:1203:LEU:HA	1:F:1203:LEU:HD12	1.70	0.42
1:E:1123:PHE:CZ	1:E:1205:MET:HE3	2.54	0.42
1:I:1175:ARG:HD2	6:I:1309:HOH:O	2.19	0.42
1:G:1196:GLU:CD	1:G:1199:SER:H	2.27	0.42
1:A:1024:VAL:O	1:A:1024:VAL:HG23	2.20	0.42
1:D:1060[A]:LYS:HD3	1:D:1061:ALA:H	1.83	0.42
1:G:1136:CYS:O	1:G:1140:LEU:HD13	2.20	0.42
1:H:1030:ARG:O	1:H:1034:ILE:HG22	2.20	0.42
1:I:1007:PHE:HD2	1:I:1008:HIS:CE1	2.37	0.42
1:G:1115:ARG:NE	1:G:1120:SER:OG	2.51	0.42
1:A:1235:LYS:HD3	1:A:1236:GLN:H	1.85	0.42
1:H:1108:LEU:CD2	1:H:1152:HIS:HB2	2.50	0.42
1:H:1238:GLU:HG3	1:H:1239:SER:N	2.34	0.42
1:I:1185:GLU:HG2	1:I:1186:GLU:N	2.32	0.42
1:E:1049:GLU:CG	1:F:1049:GLU:HG2	2.49	0.42
1:C:1126:MET:HG3	1:B:1126:MET:HG3	2.01	0.41
1:I:1102:ILE:HD11	1:I:1219:VAL:HG21	2.01	0.41
1:G:1009:LEU:HD11	1:G:1081:LEU:HG	2.02	0.41
1:C:1003:LYS:HE2	1:C:1003:LYS:HB3	1.83	0.41
1:I:1108:LEU:HD22	1:I:1152:HIS:HB2	2.01	0.41
1:G:1079:GLU:O	1:G:1083:GLN:HG3	2.19	0.41
1:H:1139:ALA:O	1:H:1143:ALA:N	2.46	0.41
1:A:1081:LEU:HD12	1:A:1081:LEU:HA	1.91	0.41
1:A:1144:ALA:CA	1:A:1244:ILE:HD12	2.48	0.41
1:F:1158:SER:CB	1:F:1200:ALA:HB2	2.46	0.41
1:G:1103:ASN:O	1:G:1104:VAL:C	2.64	0.41
1:F:1024:VAL:HA	1:F:1025:PRO:HD2	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1215:MET:HE1	6:B:1443:HOH:O	2.21	0.41
1:C:1092:ILE:HG23	1:C:1092:ILE:O	2.21	0.41
1:I:1157:ALA:HB2	1:I:1192:VAL:HG11	2.03	0.41
1:I:1163:TYR:CB	1:I:1164:PRO:HD3	2.37	0.41
1:G:1050:PHE:HE2	1:G:1077:ALA:HB2	1.86	0.41
1:H:1228:ILE:HA	1:H:1229:PRO:HD3	1.92	0.40
1:A:1031:VAL:HG13	1:A:1064:VAL:HG12	2.02	0.40
1:A:1228:ILE:HA	1:A:1229:PRO:HD3	1.95	0.40
1:B:1024:VAL:HG23	1:B:1024:VAL:O	2.21	0.40
1:G:1144:ALA:HA	1:G:1244:ILE:HD12	2.03	0.40
1:G:1187:TRP:HB3	1:G:1192:VAL:HB	2.03	0.40
1:D:1095:THR:OG1	1:D:1194:ASN:HB2	2.21	0.40
2:C:1301:URF:N1	3:C:1303:GOL:H2	2.35	0.40
1:H:1163:TYR:CB	1:H:1164:PRO:HD3	2.51	0.40
1:G:1009:LEU:CD1	1:G:1081:LEU:HG	2.52	0.40
1:A:1079:GLU:OE1	1:B:1171:THR:HB	2.21	0.40
1:I:1056:GLU:HG2	1:I:1061:ALA:HA	2.02	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	245/253 (97%)	239 (98%)	5 (2%)	1 (0%)	30	26
1	B	241/253 (95%)	234 (97%)	6 (2%)	1 (0%)	30	26
1	C	242/253 (96%)	235 (97%)	5 (2%)	2 (1%)	16	10
1	D	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	30	26
1	E	241/253 (95%)	236 (98%)	4 (2%)	1 (0%)	30	26
1	F	238/253 (94%)	232 (98%)	5 (2%)	1 (0%)	30	26
1	G	238/253 (94%)	223 (94%)	14 (6%)	1 (0%)	30	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	239/253 (94%)	228 (95%)	9 (4%)	2 (1%)	16	10
1	I	239/253 (94%)	229 (96%)	9 (4%)	1 (0%)	30	26
All	All	2165/2277 (95%)	2093 (97%)	61 (3%)	11 (0%)	24	20

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	1163	TYR
1	F	1163	TYR
1	D	1163	TYR
1	C	1163	TYR
1	A	1163	TYR
1	E	1163	TYR
1	B	1163	TYR
1	C	1231	ALA
1	H	1170	ASP
1	G	1163	TYR
1	I	1163	TYR

### 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	198/202 (98%)	192 (97%)	6 (3%)	36	38
1	B	195/202 (96%)	189 (97%)	6 (3%)	35	37
1	C	195/202 (96%)	189 (97%)	6 (3%)	35	37
1	D	195/202 (96%)	189 (97%)	6 (3%)	35	37
1	E	194/202 (96%)	185 (95%)	9 (5%)	24	22
1	F	192/202 (95%)	186 (97%)	6 (3%)	35	37
1	G	192/202 (95%)	182 (95%)	10 (5%)	21	17
1	H	193/202 (96%)	180 (93%)	13 (7%)	15	10
1	I	193/202 (96%)	185 (96%)	8 (4%)	27	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1747/1818 (96%)	1677 (96%)	70 (4%)	28	27

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1081	LEU
1	A	1185	GLU
1	A	1196	GLU
1	A	1203	LEU
1	A	1235	LYS
1	A	1253	LEU
1	E	1049	GLU
1	E	1092	ILE
1	E	1127	GLU
1	E	1185	GLU
1	E	1196	GLU
1	E	1203	LEU
1	E	1215	MET
1	E	1240	HIS
1	E	1253	LEU
1	F	1030	ARG
1	F	1145	LYS
1	F	1179	ARG
1	F	1185	GLU
1	F	1203	LEU
1	F	1228	ILE
1	D	1038	MET
1	D	1060[A]	LYS
1	D	1060[B]	LYS
1	D	1092	ILE
1	D	1145	LYS
1	D	1253	LEU
1	C	1003	LYS
1	C	1037	LEU
1	C	1145	LYS
1	C	1196	GLU
1	C	1225	GLN
1	C	1253	LEU
1	B	1049	GLU
1	B	1196	GLU
1	B	1203	LEU
1	B	1215	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	1238	GLU
1	B	1240	HIS
1	H	1016	LEU
1	H	1024	VAL
1	H	1033	LYS
1	H	1034	ILE
1	H	1044	LEU
1	H	1052	SER
1	H	1060	LYS
1	H	1091	ARG
1	H	1092	ILE
1	H	1175	ARG
1	H	1181	LYS
1	H	1196	GLU
1	H	1203	LEU
1	I	1037	LEU
1	I	1049	GLU
1	I	1091	ARG
1	I	1102	ILE
1	I	1160	ASP
1	I	1185	GLU
1	I	1203	LEU
1	I	1240	HIS
1	G	1034	ILE
1	G	1039	ASP
1	G	1092	ILE
1	G	1095	THR
1	G	1099	GLN
1	G	1160	ASP
1	G	1196	GLU
1	G	1203	LEU
1	G	1216	VAL
1	G	1253	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1226	GLN
1	A	1236	GLN
1	E	1209	GLN
1	D	1020	GLN
1	C	1226	GLN

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Mol	Chain	Res	Type
1	C	1230	ASN
1	B	1240	HIS
1	I	1008	HIS
1	I	1226	GLN
1	G	1188	GLN

### 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](#)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 for Mogul analysis.

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	$\# Z  > 2$
3	GOL	A	1302	-	5,5,5	0.32	0	5,5,5	0.74	0
3	GOL	C	1303	-	5,5,5	0.37	0	5,5,5	0.20	0
2	URF	F	1301	-	9,9,9	3.31	5 (55%)	12,12,12	3.97	9 (75%)
2	URF	A	1301	-	9,9,9	3.43	5 (55%)	12,12,12	3.63	8 (66%)
3	GOL	F	1302	-	5,5,5	0.38	0	5,5,5	0.43	0
3	GOL	B	1302	-	5,5,5	0.39	0	5,5,5	0.13	0
5	EDO	C	1302	-	3,3,3	0.38	0	2,2,2	0.39	0
2	URF	G	1301	-	9,9,9	3.54	5 (55%)	12,12,12	3.84	9 (75%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	URF	D	1301	-	9,9,9	3.47	5 (55%)	12,12,12	3.63	6 (50%)
2	URF	C	1301	-	9,9,9	3.43	5 (55%)	12,12,12	3.62	7 (58%)
2	URF	B	1301	-	9,9,9	3.03	5 (55%)	12,12,12	4.02	7 (58%)
2	URF	E	1301	-	9,9,9	3.24	5 (55%)	12,12,12	4.11	7 (58%)
2	URF	H	1301	-	9,9,9	3.46	5 (55%)	12,12,12	3.96	9 (75%)
3	GOL	E	1302	-	5,5,5	0.39	0	5,5,5	0.37	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	GOL	A	1302	-	-	0/4/4/4	-
3	GOL	C	1303	-	-	2/4/4/4	-
2	URF	F	1301	-	-	-	0/1/1/1
2	URF	A	1301	-	-	-	0/1/1/1
3	GOL	F	1302	-	-	2/4/4/4	-
5	EDO	C	1302	-	-	0/1/1/1	-
2	URF	G	1301	-	-	-	0/1/1/1
2	URF	E	1301	-	-	-	0/1/1/1
2	URF	D	1301	-	-	-	0/1/1/1
2	URF	C	1301	-	-	-	0/1/1/1
2	URF	B	1301	-	-	-	0/1/1/1
3	GOL	B	1302	-	-	0/4/4/4	-
2	URF	H	1301	-	-	-	0/1/1/1
3	GOL	E	1302	-	-	2/4/4/4	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1301	URF	C2-N1	6.22	1.44	1.36
2	A	1301	URF	C2-N1	5.83	1.44	1.36
2	C	1301	URF	C2-N1	5.72	1.44	1.36
2	G	1301	URF	C2-N1	5.71	1.44	1.36
2	G	1301	URF	C6-N1	5.54	1.45	1.36
2	H	1301	URF	C2-N1	5.52	1.43	1.36
2	H	1301	URF	C6-N1	5.49	1.45	1.36
2	E	1301	URF	C6-N1	5.45	1.45	1.36
2	F	1301	URF	C6-N1	5.45	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	URF	C6-N1	5.42	1.45	1.36
2	C	1301	URF	C6-N1	5.41	1.45	1.36
2	B	1301	URF	C2-N1	5.36	1.43	1.36
2	F	1301	URF	C2-N1	5.33	1.43	1.36
2	D	1301	URF	C6-N1	5.26	1.44	1.36
2	G	1301	URF	C6-C5	5.25	1.38	1.33
2	E	1301	URF	C2-N1	5.13	1.43	1.36
2	H	1301	URF	C6-C5	4.83	1.37	1.33
2	B	1301	URF	C6-N1	4.79	1.44	1.36
2	A	1301	URF	C6-C5	4.74	1.37	1.33
2	E	1301	URF	C6-C5	4.74	1.37	1.33
2	D	1301	URF	C6-C5	4.69	1.37	1.33
2	C	1301	URF	C6-C5	4.69	1.37	1.33
2	F	1301	URF	C6-C5	4.27	1.37	1.33
2	B	1301	URF	C6-C5	3.78	1.37	1.33
2	C	1301	URF	C4-C5	3.69	1.49	1.44
2	F	1301	URF	C4-C5	3.47	1.48	1.44
2	H	1301	URF	C4-C5	3.40	1.48	1.44
2	G	1301	URF	C4-C5	3.29	1.48	1.44
2	A	1301	URF	C4-C5	3.27	1.48	1.44
2	D	1301	URF	C4-C5	3.19	1.48	1.44
2	H	1301	URF	C2-N3	2.95	1.42	1.37
2	G	1301	URF	C2-N3	2.85	1.42	1.37
2	B	1301	URF	C4-C5	2.84	1.47	1.44
2	E	1301	URF	C2-N3	2.70	1.41	1.37
2	A	1301	URF	C2-N3	2.68	1.41	1.37
2	F	1301	URF	C2-N3	2.65	1.41	1.37
2	D	1301	URF	C2-N3	2.52	1.41	1.37
2	C	1301	URF	C2-N3	2.50	1.41	1.37
2	B	1301	URF	C2-N3	2.49	1.41	1.37
2	E	1301	URF	C4-C5	2.40	1.47	1.44

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1301	URF	C5-C4-N3	8.89	120.77	112.64
2	B	1301	URF	C5-C4-N3	8.02	119.98	112.64
2	G	1301	URF	C5-C4-N3	7.63	119.62	112.64
2	F	1301	URF	C5-C4-N3	7.57	119.56	112.64
2	H	1301	URF	C5-C4-N3	7.52	119.52	112.64
2	C	1301	URF	C5-C4-N3	7.38	119.39	112.64
2	D	1301	URF	C5-C4-N3	7.33	119.34	112.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	URF	C5-C4-N3	7.19	119.22	112.64
2	E	1301	URF	O4-C4-C5	-7.06	119.68	125.69
2	B	1301	URF	O4-C4-C5	-6.88	119.84	125.69
2	G	1301	URF	O4-C4-C5	-6.22	120.39	125.69
2	H	1301	URF	O4-C4-C5	-6.08	120.52	125.69
2	F	1301	URF	O4-C4-C5	-6.07	120.53	125.69
2	C	1301	URF	O4-C4-C5	-6.02	120.57	125.69
2	A	1301	URF	O4-C4-C5	-5.92	120.65	125.69
2	D	1301	URF	O4-C4-C5	-5.82	120.73	125.69
2	E	1301	URF	C4-N3-C2	-5.16	119.27	126.37
2	D	1301	URF	N1-C2-N3	4.80	120.23	115.17
2	B	1301	URF	C4-N3-C2	-4.78	119.78	126.37
2	E	1301	URF	N1-C2-N3	4.73	120.16	115.17
2	F	1301	URF	F5-C5-C4	4.69	120.58	116.47
2	H	1301	URF	N1-C2-N3	4.66	120.08	115.17
2	F	1301	URF	N1-C2-N3	4.51	119.92	115.17
2	H	1301	URF	F5-C5-C4	4.50	120.41	116.47
2	H	1301	URF	C4-N3-C2	-4.48	120.20	126.37
2	F	1301	URF	C4-N3-C2	-4.47	120.22	126.37
2	D	1301	URF	C4-N3-C2	-4.47	120.22	126.37
2	G	1301	URF	N1-C2-N3	4.40	119.81	115.17
2	C	1301	URF	N1-C2-N3	4.37	119.78	115.17
2	G	1301	URF	C4-N3-C2	-4.30	120.44	126.37
2	B	1301	URF	F5-C5-C4	4.24	120.19	116.47
2	C	1301	URF	C4-N3-C2	-4.23	120.55	126.37
2	B	1301	URF	N1-C2-N3	4.19	119.58	115.17
2	A	1301	URF	N1-C2-N3	4.07	119.46	115.17
2	A	1301	URF	C4-N3-C2	-4.02	120.83	126.37
2	G	1301	URF	F5-C5-C4	3.94	119.92	116.47
2	A	1301	URF	F5-C5-C4	3.84	119.83	116.47
2	F	1301	URF	F5-C5-C6	-3.46	119.04	121.58
2	C	1301	URF	F5-C5-C4	3.23	119.30	116.47
2	D	1301	URF	C6-N1-C2	-3.14	119.78	122.69
2	F	1301	URF	O2-C2-N1	-3.07	119.62	122.79
2	B	1301	URF	F5-C5-C6	-3.02	119.36	121.58
2	H	1301	URF	C6-N1-C2	-3.01	119.90	122.69
2	H	1301	URF	O2-C2-N1	-2.98	119.72	122.79
2	H	1301	URF	F5-C5-C6	-2.93	119.43	121.58
2	G	1301	URF	C6-N1-C2	-2.84	120.05	122.69
2	A	1301	URF	F5-C5-C6	-2.80	119.53	121.58
2	D	1301	URF	F5-C5-C4	2.65	118.79	116.47
2	B	1301	URF	O2-C2-N1	-2.64	120.07	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1301	URF	F5-C5-C4	2.59	118.74	116.47
2	G	1301	URF	O2-C2-N1	-2.57	120.14	122.79
2	A	1301	URF	O2-C2-N1	-2.54	120.17	122.79
2	F	1301	URF	C6-N1-C2	-2.54	120.34	122.69
2	E	1301	URF	O2-C2-N1	-2.54	120.17	122.79
2	A	1301	URF	C6-N1-C2	-2.50	120.37	122.69
2	C	1301	URF	C6-N1-C2	-2.46	120.40	122.69
2	G	1301	URF	C6-C5-C4	-2.39	120.06	122.11
2	H	1301	URF	C6-C5-C4	-2.26	120.16	122.11
2	E	1301	URF	C6-N1-C2	-2.20	120.65	122.69
2	C	1301	URF	O2-C2-N1	-2.12	120.60	122.79
2	G	1301	URF	F5-C5-C6	-2.11	120.03	121.58
2	F	1301	URF	C6-C5-C4	-2.01	120.38	122.11

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1302	GOL	O1-C1-C2-C3
3	C	1303	GOL	O1-C1-C2-C3
3	E	1302	GOL	O1-C1-C2-O2
3	F	1302	GOL	O1-C1-C2-C3
3	F	1302	GOL	O1-C1-C2-O2
3	C	1303	GOL	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1302	GOL	1	0
3	C	1303	GOL	2	0
2	F	1301	URF	1	0
2	A	1301	URF	1	0
3	F	1302	GOL	1	0
3	B	1302	GOL	3	0
5	C	1302	EDO	4	0
2	C	1301	URF	2	0
2	B	1301	URF	2	0
2	E	1301	URF	1	0
3	E	1302	GOL	2	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	248/253 (98%)	-0.24	3 (1%) 76 79	26, 39, 62, 113	1 (0%)
1	B	244/253 (96%)	-0.15	0 100 100	27, 40, 64, 102	1 (0%)
1	C	246/253 (97%)	-0.19	2 (0%) 82 84	25, 39, 61, 107	0
1	D	245/253 (96%)	-0.24	3 (1%) 76 79	23, 38, 62, 96	1 (0%)
1	E	245/253 (96%)	-0.20	1 (0%) 88 90	26, 39, 60, 114	0
1	F	242/253 (95%)	-0.26	1 (0%) 88 90	26, 39, 57, 78	0
1	G	242/253 (95%)	1.49	71 (29%) 1 1	57, 89, 119, 135	0
1	H	243/253 (96%)	0.77	18 (7%) 20 23	45, 72, 104, 128	0
1	I	243/253 (96%)	0.97	29 (11%) 9 9	39, 77, 121, 130	0
All	All	2198/2277 (96%)	0.21	128 (5%) 29 32	23, 47, 108, 135	3 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1057	LEU	5.5
1	C	1231	ALA	4.5
1	G	1147	ILE	4.1
1	G	1245	VAL	4.1
1	G	1143	ALA	4.0
1	G	1252	LEU	3.9
1	G	1021	LEU	3.9
1	I	1045	ALA	3.7
1	G	1241	ALA	3.7
1	I	1246	VAL	3.6
1	G	1109	VAL	3.6
1	G	1034	ILE	3.6
1	H	1237	THR	3.6
1	I	1253	LEU	3.5
1	I	1103	ASN	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	1037	LEU	3.4
1	G	1139	ALA	3.4
1	H	1053	TRP	3.3
1	I	1036	ALA	3.3
1	G	1107	VAL	3.2
1	I	1016	LEU	3.2
1	G	1132	ALA	3.1
1	G	1014	ASN	3.1
1	G	1019	ALA	3.1
1	G	1104	VAL	3.1
1	A	1236	GLN	3.1
1	I	1052	SER	3.0
1	H	1134	PHE	3.0
1	G	1022	ALA	3.0
1	G	1042	VAL	3.0
1	G	1011	LEU	2.9
1	G	1031	VAL	2.9
1	G	1195	TYR	2.8
1	G	1105	GLY	2.8
1	G	1050	PHE	2.8
1	G	1253	LEU	2.8
1	I	1034	ILE	2.8
1	D	1231	ALA	2.8
1	G	1035	ALA	2.8
1	H	1044	LEU	2.8
1	G	1249	ALA	2.7
1	G	1153	VAL	2.7
1	G	1053	TRP	2.7
1	G	1045	ALA	2.7
1	E	1239	SER	2.7
1	G	1136	CYS	2.7
1	G	1018	GLY	2.7
1	G	1061	ALA	2.7
1	G	1134	PHE	2.7
1	I	1044	LEU	2.7
1	G	1012	THR	2.7
1	G	1108	LEU	2.7
1	G	1246	VAL	2.7
1	H	1118	GLY	2.7
1	I	1105	GLY	2.7
1	G	1135	ALA	2.6
1	H	1057	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	1253	LEU	2.6
1	I	1009	LEU	2.6
1	I	1057	LEU	2.6
1	I	1141	VAL	2.6
1	G	1064	VAL	2.6
1	H	1249	ALA	2.6
1	G	1055	ALA	2.6
1	H	1011	LEU	2.6
1	G	1023	ILE	2.6
1	G	1029	GLU	2.5
1	G	1102	ILE	2.5
1	G	1025	PRO	2.5
1	G	1144	ALA	2.5
1	H	1244	ILE	2.5
1	G	1140	LEU	2.5
1	H	1248	ALA	2.4
1	G	1089	PHE	2.4
1	G	1148	GLY	2.4
1	G	1216	VAL	2.4
1	F	1239	SER	2.4
1	G	1051	THR	2.4
1	G	1096	GLY	2.4
1	G	1063	ILE	2.4
1	I	1035	ALA	2.4
1	I	1061	ALA	2.3
1	I	1048	ARG	2.3
1	G	1149	ALA	2.3
1	I	1104	VAL	2.3
1	G	1214	GLY	2.3
1	G	1221	VAL	2.3
1	G	1067	THR	2.3
1	G	1217	ALA	2.3
1	G	1248	ALA	2.3
1	I	1053	TRP	2.3
1	G	1228	ILE	2.2
1	I	1055	ALA	2.2
1	D	1253	LEU	2.2
1	H	1084	LEU	2.2
1	H	1086	ILE	2.2
1	G	1150	THR	2.2
1	I	1042	VAL	2.2
1	G	1131	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	1248	ALA	2.2
1	H	1014	ASN	2.2
1	G	1137	THR	2.2
1	G	1154	GLY	2.2
1	I	1241	ALA	2.2
1	H	1246	VAL	2.1
1	G	1024	VAL	2.1
1	H	1059	GLY	2.1
1	G	1213	ALA	2.1
1	C	1239	SER	2.1
1	H	1252	LEU	2.1
1	G	1038	MET	2.1
1	A	1237	THR	2.1
1	G	1098	ILE	2.1
1	G	1007	PHE	2.1
1	G	1128	PHE	2.1
1	I	1242	VAL	2.1
1	I	1143	ALA	2.1
1	G	1201	THR	2.1
1	I	1059	GLY	2.1
1	G	1219	VAL	2.1
1	I	1037	LEU	2.0
1	A	1225	GLN	2.0
1	I	1026	GLY	2.0
1	I	1023	ILE	2.0
1	H	1062	VAL	2.0
1	G	1141	VAL	2.0
1	D	1239	SER	2.0
1	I	1161	THR	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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	K	D	1302	1/1	0.64	0.29	104,104,104,104	0
3	GOL	A	1302	6/6	0.80	0.16	66,68,68,69	0
5	EDO	C	1302	4/4	0.82	0.14	43,43,45,48	0
3	GOL	F	1302	6/6	0.83	0.16	61,65,66,66	0
4	K	A	1303	1/1	0.83	0.15	61,61,61,61	0
3	GOL	B	1302	6/6	0.86	0.13	55,56,58,58	0
2	URF	G	1301	9/9	0.86	0.10	72,73,73,73	0
4	K	E	1303	1/1	0.87	0.16	50,50,50,50	0
2	URF	H	1301	9/9	0.89	0.10	71,72,73,73	0
3	GOL	E	1302	6/6	0.89	0.12	60,63,64,64	0
3	GOL	C	1303	6/6	0.90	0.14	66,70,70,71	0
2	URF	D	1301	9/9	0.92	0.07	32,33,35,38	0
2	URF	A	1301	9/9	0.92	0.08	38,40,42,43	0
2	URF	B	1301	9/9	0.93	0.08	30,31,36,37	0
2	URF	C	1301	9/9	0.93	0.07	33,37,39,41	0
2	URF	E	1301	9/9	0.94	0.08	25,26,31,32	0
2	URF	F	1301	9/9	0.94	0.09	43,44,46,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.