



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 10:53 PM EDT

PDB ID : 6LIV  
Title : Crystal structure of Tyrosine decarboxylase in complex with PLP  
Authors : Wang, H.; Yu, J.; Yao, M.  
Deposited on : 2019-12-13  
Resolution : 2.31 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

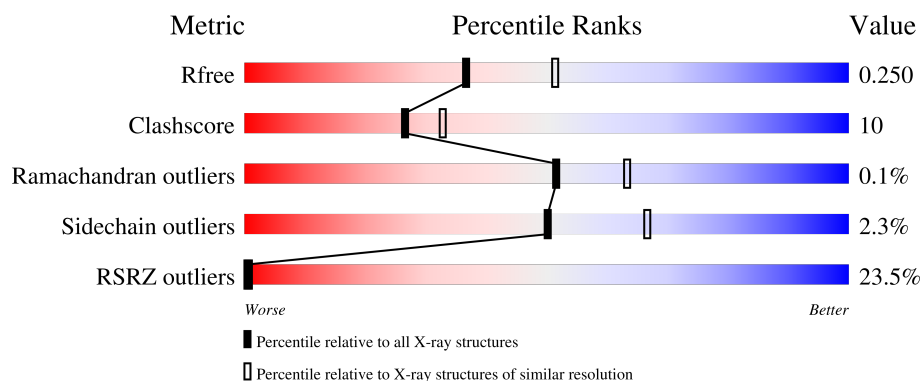
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	531	<div> <div>5%</div> <div> <div>81%</div> <div>9%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	531	<div> <div>4%</div> <div> <div>82%</div> <div>9%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	531	<div> <div>6%</div> <div> <div>80%</div> <div>11%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	531	<div> <div>2%</div> <div> <div>81%</div> <div>9%</div> <div>•</div> <div>9%</div> </div> </div>
1	E	531	<div> <div>57%</div> <div> <div>55%</div> <div>34%</div> <div>•</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	531	<p>52% 51% 36% 10%</p>

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	GOL	C	601	-	-	X	-
2	GOL	C	602	-	-	-	X
2	GOL	D	601	-	-	X	-
2	GOL	D	602	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 23982 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 Tyrosine/DOPA decarboxylase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	P	S	0	0	0
			3840	2464	643	708	1	24			
1	B	483	Total	C	N	O	P	S	0	0	0
			3823	2454	639	705	1	24			
1	C	485	Total	C	N	O	P	S	0	0	0
			3840	2464	643	708	1	24			
1	D	483	Total	C	N	O	P	S	0	0	0
			3823	2454	639	705	1	24			
1	E	479	Total	C	N	O	P	S	0	0	0
			3802	2442	635	700	1	24			
1	F	477	Total	C	N	O	P	S	0	0	0
			3782	2429	633	695	1	24			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0

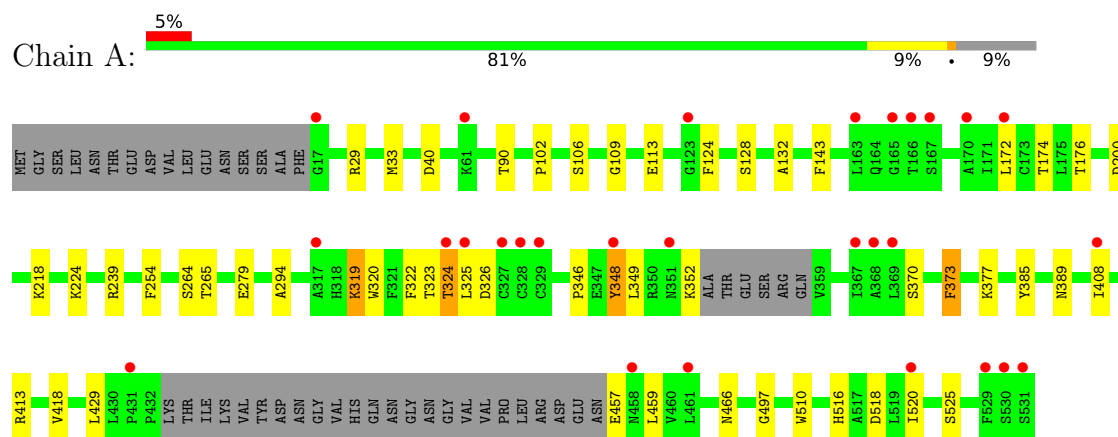
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	213	Total O 213 213	0	0
3	B	262	Total O 262 262	0	0
3	C	204	Total O 204 204	0	0
3	D	269	Total O 269 269	0	0
3	E	29	Total O 29 29	0	0
3	F	41	Total O 41 41	0	0

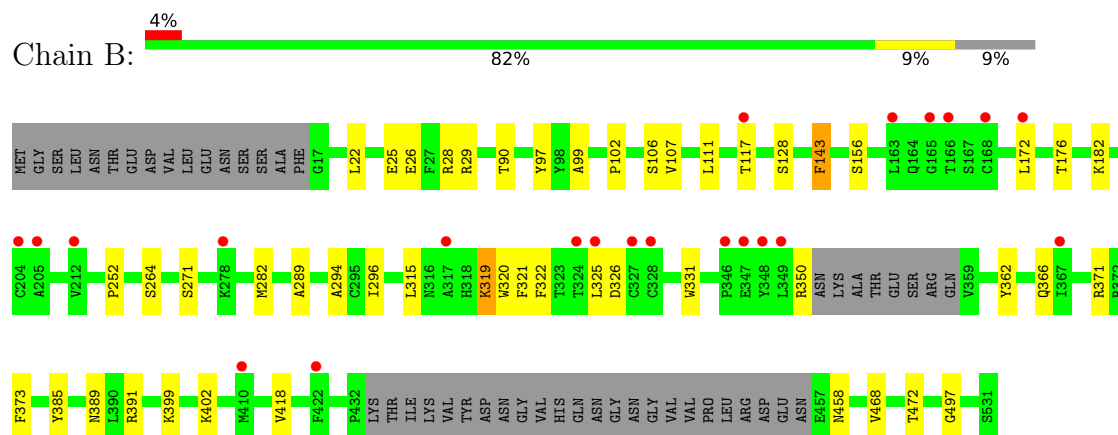
### 3 Residue-property plots [i](#)

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.

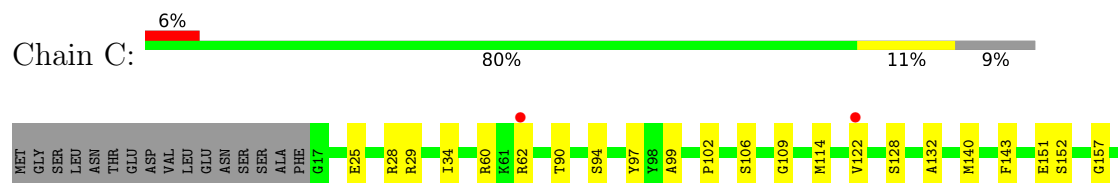
#### • Molecule 1: Tyrosine/DOPA decarboxylase 2

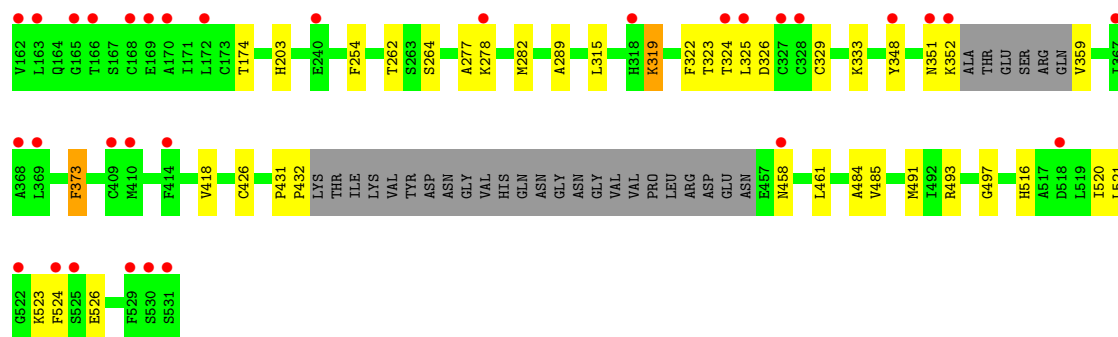


#### • Molecule 1: Tyrosine/DOPA decarboxylase 2

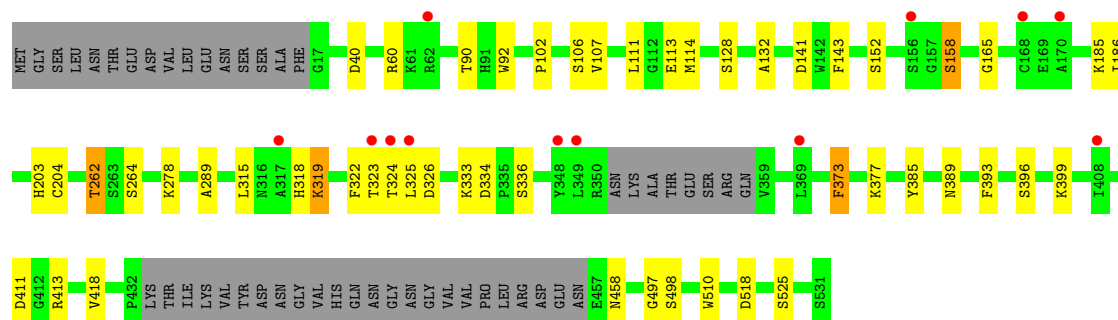
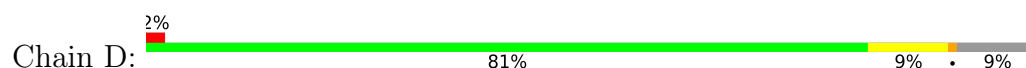


#### • Molecule 1: Tyrosine/DOPA decarboxylase 2

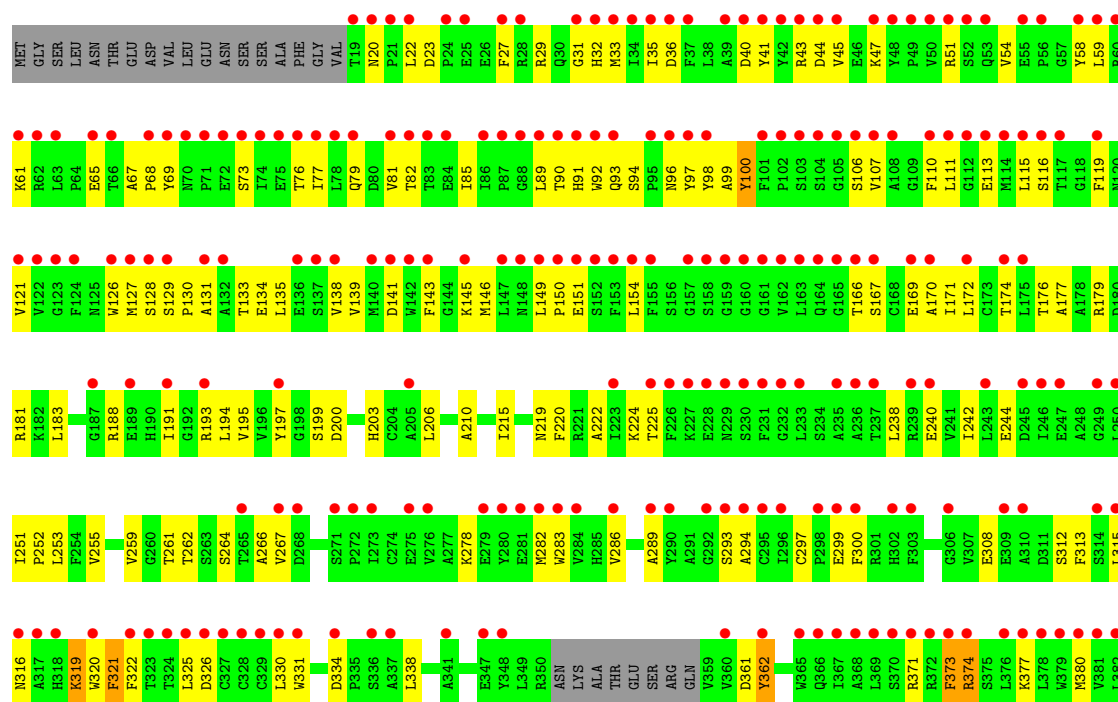


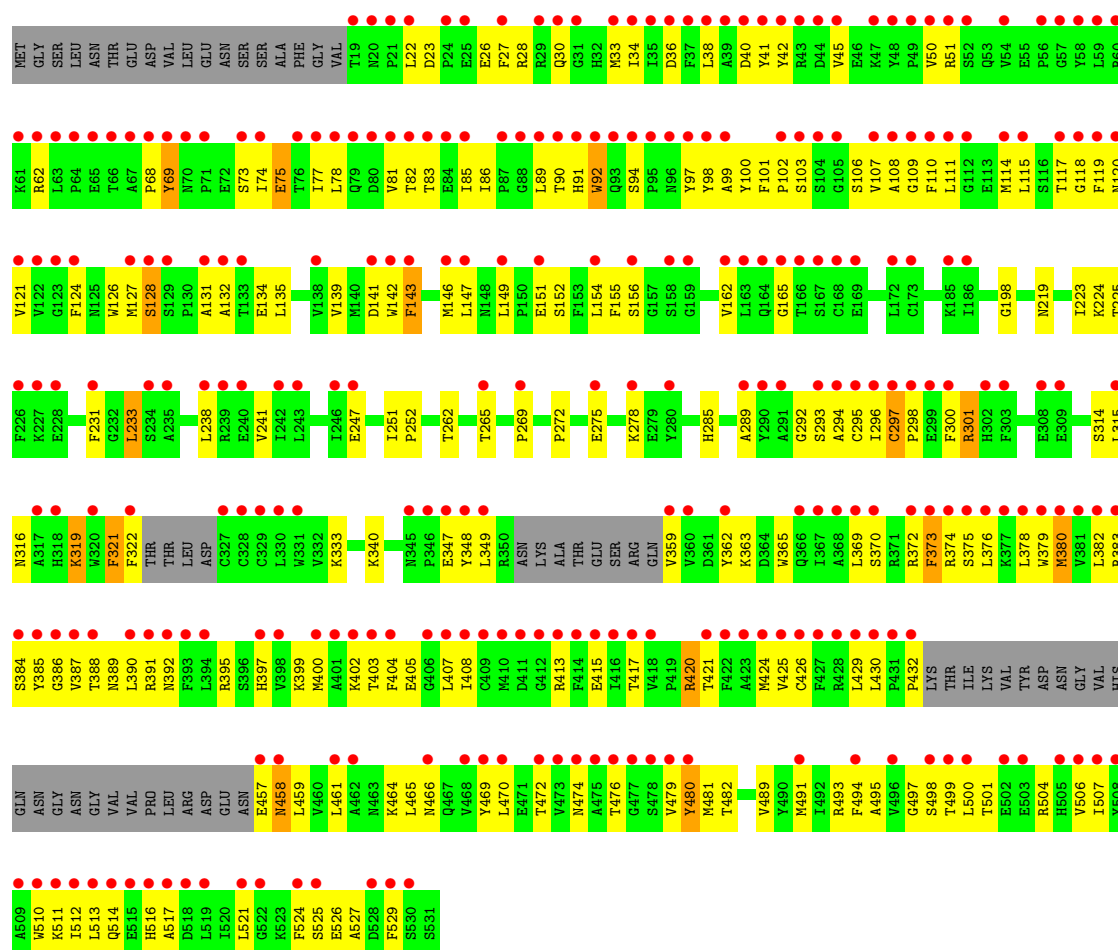


• Molecule 1: Tyrosine/DOPA decarboxylase 2



• Molecule 1: Tyrosine/DOPA decarboxylase 2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.91Å 180.41Å 218.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 2.31 49.84 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.84-2.31) 99.7 (49.84-2.31)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.227 , 0.250 0.227 , 0.250	Depositor DCC
$R_{free}$ test set	10115 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23982	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6058e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, LLP

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	0.36	0/3909	0.42	0/5307
1	B	0.38	0/3892	0.44	0/5285
1	C	0.39	0/3909	0.42	0/5307
1	D	0.28	0/3892	0.42	0/5285
1	E	0.33	0/3870	0.47	0/5254
1	F	0.37	0/3850	0.52	0/5225
All	All	0.36	0/23322	0.45	0/31663

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	3840	0	3782	36	0
1	B	3823	0	3763	30	0
1	C	3840	0	3782	50	0
1	D	3823	0	3763	40	0
1	E	3802	0	3742	150	0
1	F	3782	0	3721	210	0
2	A	6	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	18	0	24	3	0
2	C	18	0	24	11	0
2	D	12	0	16	7	0
3	A	213	0	0	2	0
3	B	262	0	0	1	0
3	C	204	0	0	3	0
3	D	269	0	0	3	0
3	E	29	0	0	1	0
3	F	41	0	0	3	0
All	All	23982	0	22625	470	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 10.

All (470) 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:C:319:LLP:H4'1	2:C:601:GOL:H11	1.23	1.14
1:C:203:HIS:NE2	2:C:601:GOL:H12	1.67	1.08
1:C:203:HIS:HE2	2:C:601:GOL:H12	1.00	1.07
1:F:385:TYR:HB3	1:F:390:LEU:HD21	1.44	0.99
1:F:131:ALA:O	1:F:135:LEU:HD12	1.61	0.98
1:C:319:LLP:C4'	2:C:601:GOL:H11	1.93	0.97
1:F:340:LYS:HE3	1:F:347:GLU:OE1	1.65	0.96
1:D:319:LLP:H4'1	2:D:601:GOL:H12	1.45	0.96
1:F:98:TYR:OH	1:F:506:VAL:HA	1.69	0.91
1:E:51:ARG:HA	1:E:90:THR:HG23	1.52	0.89
1:F:74:ILE:HA	1:F:77:ILE:HG22	1.59	0.85
1:F:415:GLU:HB2	1:F:430:LEU:HD11	1.62	0.82
1:C:203:HIS:HE2	2:C:601:GOL:C1	1.91	0.80
1:E:151:GLU:HA	1:E:154:LEU:HG	1.66	0.77
1:D:318:HIS:CD2	1:D:325:LEU:HD12	2.21	0.76
1:F:285:HIS:HE2	1:F:314:SER:HG	1.35	0.74
1:D:319:LLP:H4'1	2:D:601:GOL:C1	2.18	0.73
1:E:107:VAL:HA	1:E:110:PHE:HB3	1.69	0.72
1:F:135:LEU:HD13	1:F:373:PHE:HZ	1.53	0.72
1:E:128:SER:HB3	1:F:92:TRP:HH2	1.53	0.72
1:F:293:SER:HB3	1:F:321:PHE:CE1	2.24	0.71
1:F:413:ARG:HH21	1:F:517:ALA:HB3	1.55	0.71
1:E:96:ASN:HB3	1:E:479:VAL:HG22	1.73	0.71
1:D:264:SER:HB2	1:D:418:VAL:HG21	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:ALA:HB1	1:F:135:LEU:HD11	1.72	0.70
1:E:113:GLU:HG3	1:E:377:LYS:HE2	1.74	0.70
1:F:143:PHE:O	1:F:147:LEU:CD2	2.40	0.70
1:F:110:PHE:HD2	1:F:111:LEU:HG	1.55	0.69
1:F:139:VAL:HG12	1:F:382:LEU:HD11	1.73	0.69
1:E:67:ALA:HB2	1:F:142:TRP:HB3	1.74	0.69
1:B:264:SER:HB2	1:B:418:VAL:HG21	1.75	0.69
1:F:98:TYR:CE1	1:F:494:PHE:CZ	2.81	0.68
1:C:262:THR:HG21	2:C:602:GOL:O2	1.93	0.68
1:F:420:ARG:HG3	1:F:425:VAL:HB	1.76	0.68
1:F:110:PHE:CD2	1:F:111:LEU:HG	2.29	0.68
1:F:135:LEU:HD13	1:F:373:PHE:CZ	2.28	0.68
1:F:143:PHE:HE1	1:F:296:ILE:HD11	1.58	0.68
1:C:28:ARG:NH2	1:D:40:ASP:OD1	2.26	0.67
1:C:526:GLU:HB3	1:E:224:LYS:HE2	1.76	0.67
1:F:397:HIS:CE1	1:F:499:THR:HG22	2.29	0.67
1:E:481:MET:HE1	1:E:513:LEU:HD21	1.74	0.67
1:E:197:TYR:HB2	1:E:255:VAL:HG12	1.76	0.67
1:E:511:LYS:HA	1:E:514:GLN:HG2	1.76	0.67
1:F:521:LEU:HA	1:F:524:PHE:HB2	1.77	0.67
1:E:149:LEU:HD23	1:E:150:PRO:HD2	1.76	0.66
1:A:346:PRO:HG2	1:A:349:LEU:HD12	1.78	0.66
1:F:151:GLU:HA	1:F:154:LEU:HG	1.78	0.66
1:C:106:SER:HB3	1:C:322:PHE:HB3	1.78	0.65
1:C:60:ARG:NH2	1:D:141:ASP:OD2	2.29	0.65
1:F:417:THR:HG21	1:F:491:MET:HB2	1.78	0.65
1:A:113:GLU:HG2	1:A:377:LYS:HD3	1.77	0.65
1:E:166:THR:HG23	1:E:169:GLU:H	1.61	0.65
1:D:319:LLP:C4'	2:D:601:GOL:H12	2.24	0.65
1:F:297:CYS:HA	1:F:391:ARG:HH11	1.62	0.65
1:E:380:MET:HA	1:F:77:ILE:HD11	1.80	0.64
1:F:143:PHE:O	1:F:147:LEU:HD22	1.97	0.64
1:E:31:GLY:HA2	1:F:111:LEU:HD11	1.80	0.64
1:F:404:PHE:HA	1:F:407:LEU:HD12	1.80	0.64
1:E:111:LEU:HD22	1:F:34:ILE:HG13	1.79	0.63
1:E:107:VAL:HG21	1:F:27:PHE:HA	1.79	0.63
1:F:74:ILE:O	1:F:78:LEU:HG	1.98	0.63
1:F:432:PRO:HG3	1:F:521:LEU:HD23	1.81	0.63
1:F:51:ARG:HA	1:F:90:THR:HG23	1.80	0.63
1:E:289:ALA:HA	1:E:316:ASN:H	1.63	0.62
1:C:25:GLU:OE2	1:C:28:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:388:THR:HA	1:F:391:ARG:HG3	1.81	0.62
1:F:397:HIS:HE1	1:F:499:THR:HG22	1.64	0.62
1:B:319:LLP:H4'1	2:B:601:GOL:H2	1.81	0.62
1:C:359:VAL:N	3:C:709:HOH:O	2.33	0.61
1:E:183:LEU:HB3	1:E:188:ARG:HG2	1.82	0.61
1:E:261:THR:HG22	1:E:266:ALA:H	1.65	0.61
1:E:398:VAL:HG22	1:E:423:ALA:HB2	1.82	0.61
1:F:111:LEU:O	1:F:115:LEU:HD12	2.01	0.61
1:F:429:LEU:HD12	1:F:465:LEU:HD21	1.83	0.61
1:E:90:THR:HB	1:F:128:SER:O	2.01	0.61
1:A:90:THR:HB	1:B:128:SER:O	2.01	0.60
1:C:90:THR:HB	1:D:128:SER:O	2.01	0.60
1:E:22:LEU:HB2	1:F:500:LEU:HD11	1.83	0.60
1:A:413:ARG:NH1	1:A:518:ASP:OD1	2.33	0.60
1:B:102:PRO:HG3	1:B:497:GLY:HA3	1.82	0.60
1:F:131:ALA:C	1:F:135:LEU:HD12	2.21	0.60
1:E:44:ASP:HB2	1:E:47:LYS:HD3	1.83	0.60
1:A:516:HIS:O	1:A:520:ILE:HG12	2.02	0.59
1:C:128:SER:O	1:D:90:THR:HB	2.02	0.59
1:E:402:LYS:HA	1:E:405:GLU:HB3	1.85	0.59
1:F:417:THR:OG1	1:F:426:CYS:HB2	2.02	0.59
1:F:100:TYR:O	1:F:493:ARG:NH2	2.36	0.58
1:E:111:LEU:HD11	1:F:30:GLN:HB3	1.85	0.58
1:E:133:THR:HG22	1:E:362:TYR:HD2	1.68	0.58
1:E:371:ARG:NH1	3:E:602:HOH:O	2.29	0.58
1:F:298:PRO:HD3	1:F:391:ARG:HH12	1.69	0.58
1:F:461:LEU:HD21	1:F:526:GLU:HG2	1.84	0.58
1:D:106:SER:HB3	1:D:322:PHE:HB3	1.85	0.58
1:F:385:TYR:C	1:F:389:ASN:HD21	2.06	0.58
1:E:206:LEU:HG	1:E:220:PHE:HE1	1.69	0.58
1:A:102:PRO:HG3	1:A:497:GLY:HA3	1.87	0.57
1:E:40:ASP:OD1	1:E:43:ARG:NH1	2.34	0.57
1:E:461:LEU:C	1:E:461:LEU:HD13	2.25	0.57
1:E:131:ALA:HB1	1:F:85:ILE:HD13	1.86	0.57
1:F:385:TYR:O	1:F:389:ASN:ND2	2.35	0.57
1:E:299:GLU:HG2	1:E:300:PHE:HD1	1.69	0.57
1:A:457:GLU:OE1	1:A:459:LEU:N	2.37	0.57
1:F:293:SER:HB3	1:F:321:PHE:CD1	2.39	0.57
1:A:102:PRO:CG	1:A:497:GLY:HA3	2.35	0.57
1:D:204:CYS:SG	2:D:602:GOL:H11	2.45	0.57
1:E:41:TYR:OH	1:E:91:HIS:ND1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:PRO:HG3	1:F:497:GLY:HA3	1.85	0.57
1:F:289:ALA:HA	1:F:315:LEU:HA	1.87	0.57
1:A:128:SER:O	1:B:90:THR:HB	2.04	0.57
1:F:413:ARG:NH2	1:F:514:GLN:O	2.36	0.56
1:B:106:SER:HB3	1:B:322:PHE:HB3	1.86	0.56
1:E:424:MET:SD	1:E:493:ARG:NH1	2.79	0.56
1:F:404:PHE:HD1	1:F:407:LEU:HD12	1.71	0.56
1:E:85:ILE:HD11	1:F:135:LEU:HD21	1.86	0.56
1:E:193:ARG:HB2	1:E:251:ILE:HD12	1.87	0.56
1:F:319:LLP:NZ	1:F:319:LLP:O3	2.35	0.56
1:F:359:VAL:N	3:F:619:HOH:O	2.38	0.56
1:A:109:GLY:HA3	1:A:323:THR:O	2.06	0.56
1:C:352:LYS:NZ	3:C:712:HOH:O	2.39	0.56
1:E:293:SER:HB3	1:E:321:PHE:HD1	1.70	0.56
1:E:121:VAL:HA	1:F:92:TRP:HE1	1.71	0.56
1:E:128:SER:HB3	1:F:92:TRP:CH2	2.38	0.56
1:E:176:THR:HG22	1:E:179:ARG:HH21	1.71	0.56
1:E:387:VAL:HB	1:F:69:TYR:HA	1.88	0.56
1:B:25:GLU:OE2	1:B:28:ARG:NH1	2.39	0.56
1:A:352:LYS:NZ	3:A:704:HOH:O	2.31	0.55
1:D:262:THR:HG21	2:D:602:GOL:O2	2.06	0.55
1:C:348:TYR:O	1:C:351:ASN:ND2	2.38	0.55
1:E:499:THR:HG23	1:F:22:LEU:HD23	1.86	0.55
1:E:115:LEU:O	1:E:119:PHE:N	2.36	0.55
1:A:319:LLP:H4'1	2:A:601:GOL:H11	1.88	0.55
1:E:135:LEU:O	1:E:139:VAL:HG22	2.07	0.55
1:F:81:VAL:HG13	1:F:85:ILE:HB	1.88	0.55
1:E:113:GLU:HB2	1:E:377:LYS:HG2	1.88	0.55
1:D:152:SER:HA	1:D:158:SER:HB3	1.89	0.54
1:E:222:ALA:O	1:E:224:LYS:NZ	2.40	0.54
1:F:119:PHE:O	1:F:121:VAL:HG13	2.06	0.54
1:B:102:PRO:CG	1:B:497:GLY:HA3	2.37	0.54
1:C:521:LEU:HA	1:C:524:PHE:HB2	1.89	0.54
1:E:166:THR:OG1	1:E:319:LLP:OP2	2.26	0.54
1:F:108:ALA:HB1	1:F:380:MET:HB3	1.89	0.54
1:F:98:TYR:CD1	1:F:494:PHE:CE1	2.96	0.54
1:A:324:THR:HG21	1:B:117:THR:HG23	1.90	0.54
1:E:100:TYR:HA	1:E:493:ARG:HH22	1.72	0.54
1:C:523:LYS:HD2	1:F:348:TYR:HE2	1.73	0.54
1:E:470:LEU:HD22	1:E:492:ILE:HG12	1.89	0.54
1:D:323:THR:O	1:D:324:THR:HG22	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:ILE:HD12	1:E:194:LEU:HD12	1.90	0.54
1:F:233:LEU:HD21	1:F:238:LEU:HB2	1.89	0.54
1:C:516:HIS:O	1:C:520:ILE:HG12	2.08	0.54
1:E:195:VAL:HG12	1:E:219:ASN:HB3	1.90	0.53
1:F:98:TYR:CE1	1:F:494:PHE:CE1	2.96	0.53
1:F:126:TRP:NE1	1:F:134:GLU:OE2	2.41	0.53
1:F:420:ARG:HG2	1:F:424:MET:O	2.08	0.53
1:F:482:THR:OG1	1:F:493:ARG:NH1	2.41	0.53
1:E:151:GLU:HG3	1:E:154:LEU:HB2	1.90	0.53
1:F:322:PHE:HE1	1:F:499:THR:HG21	1.72	0.53
1:E:429:LEU:HD11	1:E:521:LEU:HD11	1.89	0.53
1:E:92:TRP:HA	1:E:97:TYR:CG	2.44	0.53
1:E:100:TYR:HA	1:E:493:ARG:NH2	2.24	0.53
1:F:30:GLN:NE2	1:F:74:ILE:HD12	2.24	0.53
1:E:92:TRP:H	1:F:121:VAL:HG12	1.73	0.53
1:E:93:GLN:CD	1:E:93:GLN:H	2.10	0.53
1:E:68:PRO:HG2	1:F:383:ARG:HG2	1.90	0.53
1:E:171:ILE:HA	1:E:174:THR:HG22	1.91	0.53
1:F:81:VAL:HG12	1:F:86:ILE:HG13	1.89	0.53
1:D:102:PRO:CG	1:D:497:GLY:HA3	2.38	0.52
1:F:275:GLU:HG3	1:F:278:LYS:NZ	2.24	0.52
1:F:457:GLU:CG	1:F:458:ASN:H	2.22	0.52
1:C:458:ASN:OD1	1:C:458:ASN:N	2.41	0.52
1:E:98:TYR:CD1	1:E:494:PHE:CE1	2.97	0.52
1:E:286:VAL:HB	1:E:313:PHE:HD1	1.75	0.52
1:F:92:TRP:CD1	1:F:103:SER:HB3	2.44	0.52
1:B:143:PHE:CE1	1:B:296:ILE:HD11	2.45	0.52
1:D:102:PRO:HG3	1:D:497:GLY:HA3	1.92	0.52
1:E:150:PRO:HG3	1:E:308:GLU:HG3	1.91	0.52
1:E:170:ALA:HB1	1:E:330:LEU:HD22	1.92	0.52
1:F:51:ARG:HD3	1:F:480:TYR:CZ	2.45	0.52
1:F:363:LYS:HE2	1:F:369:LEU:HD22	1.92	0.52
1:E:259:VAL:HG13	1:E:267:VAL:HG13	1.90	0.52
1:F:510:TRP:CD1	1:F:511:LYS:HG3	2.45	0.52
1:E:129:SER:HA	1:F:89:LEU:HA	1.91	0.51
1:E:404:PHE:CE1	1:E:408:ILE:HD11	2.46	0.51
1:F:297:CYS:HA	1:F:391:ARG:NH1	2.24	0.51
1:C:114:MET:HG2	1:D:114:MET:SD	2.50	0.51
1:E:106:SER:OG	1:E:322:PHE:HB3	2.10	0.51
1:E:54:VAL:HG13	1:E:58:TYR:CD2	2.46	0.51
1:E:127:MET:HE2	1:F:51:ARG:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:292:GLY:O	1:F:295:CYS:HB2	2.10	0.51
1:E:283:TRP:HE1	1:E:312:SER:HG	1.58	0.51
1:F:100:TYR:HA	1:F:493:ARG:HH22	1.75	0.51
1:F:289:ALA:HB1	1:F:316:ASN:HD21	1.75	0.51
1:A:319:LLP:H5'1	2:A:601:GOL:O3	2.11	0.50
1:B:143:PHE:HE1	1:B:296:ILE:HD11	1.76	0.50
1:C:34:ILE:HG13	1:D:111:LEU:HD22	1.93	0.50
1:E:77:ILE:HG23	1:F:383:ARG:HH12	1.76	0.50
1:E:325:LEU:HD11	1:F:370:SER:OG	2.11	0.50
2:D:601:GOL:O2	2:D:602:GOL:H32	2.11	0.50
1:E:107:VAL:O	1:E:111:LEU:HG	2.10	0.50
1:F:405:GLU:O	1:F:408:ILE:HG12	2.11	0.50
1:E:415:GLU:HB2	1:E:430:LEU:HD11	1.92	0.50
1:E:299:GLU:HG2	1:E:300:PHE:CD1	2.45	0.50
1:F:147:LEU:HB2	1:F:149:LEU:HG	1.92	0.50
1:C:203:HIS:CE1	2:C:601:GOL:H12	2.43	0.50
1:D:203:HIS:CD2	2:D:602:GOL:H12	2.47	0.50
1:F:481:MET:SD	1:F:513:LEU:HD21	2.52	0.50
1:F:62:ARG:NH2	1:F:83:THR:O	2.43	0.49
1:F:74:ILE:CA	1:F:77:ILE:HG22	2.39	0.49
1:F:132:ALA:HA	1:F:373:PHE:CE1	2.47	0.49
1:E:98:TYR:HB2	1:E:481:MET:HG2	1.94	0.49
1:E:294:ALA:HB2	1:E:320:TRP:CZ3	2.47	0.49
1:F:98:TYR:HA	1:F:495:ALA:O	2.12	0.49
1:F:295:CYS:O	1:F:301:ARG:HB3	2.12	0.49
1:E:383:ARG:HG2	1:F:68:PRO:HG3	1.95	0.49
1:A:370:SER:OG	2:B:601:GOL:H31	2.13	0.49
1:E:484:ALA:O	1:E:491:MET:HG2	2.12	0.49
1:F:50:VAL:HG21	1:F:479:VAL:C	2.33	0.49
1:B:458:ASN:ND2	3:B:718:HOH:O	2.44	0.49
1:F:38:LEU:O	1:F:41:TYR:HB3	2.13	0.49
1:F:162:VAL:HB	1:F:365:TRP:CE3	2.47	0.49
1:B:26:GLU:OE2	1:B:29:ARG:NH2	2.35	0.49
1:C:323:THR:O	1:C:324:THR:HG23	2.13	0.48
1:F:224:LYS:HE2	1:F:225:THR:O	2.13	0.48
1:F:386:GLY:O	1:F:390:LEU:HG	2.13	0.48
1:A:40:ASP:OD1	1:B:28:ARG:NH2	2.46	0.48
1:E:240:GLU:O	1:E:244:GLU:HG3	2.13	0.48
1:F:223:ILE:HG23	1:F:241:VAL:HG21	1.94	0.48
1:F:429:LEU:C	1:F:429:LEU:HD13	2.33	0.48
1:F:457:GLU:OE1	1:F:459:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ALA:HB2	1:A:320:TRP:CZ3	2.48	0.48
1:F:348:TYR:CD1	1:F:349:LEU:HG	2.48	0.48
1:E:252:PRO:HB2	1:E:282:MET:SD	2.54	0.48
1:F:100:TYR:CA	1:F:493:ARG:HH22	2.26	0.48
1:C:493:ARG:NE	2:C:603:GOL:H32	2.27	0.48
1:E:98:TYR:CD2	1:E:479:VAL:HG13	2.48	0.48
1:F:289:ALA:HB1	1:F:316:ASN:ND2	2.29	0.48
1:C:523:LYS:O	1:C:523:LYS:HD3	2.14	0.48
1:C:29:ARG:NH1	3:C:713:HOH:O	2.40	0.48
1:E:97:TYR:CZ	1:E:99:ALA:HB3	2.49	0.48
1:A:200:ASP:OD2	1:A:224:LYS:HD3	2.13	0.48
1:E:113:GLU:HA	1:E:116:SER:OG	2.14	0.48
1:F:98:TYR:CD1	1:F:494:PHE:CZ	3.02	0.48
1:F:111:LEU:O	1:F:114:MET:N	2.46	0.48
1:F:429:LEU:HD13	1:F:430:LEU:N	2.29	0.48
1:D:60:ARG:NH1	3:D:710:HOH:O	2.46	0.47
1:E:41:TYR:O	1:E:45:VAL:HG13	2.13	0.47
1:F:322:PHE:CE1	1:F:499:THR:HG21	2.49	0.47
1:A:323:THR:O	1:A:324:THR:HB	2.14	0.47
1:F:380:MET:O	1:F:384:SER:HB2	2.14	0.47
1:A:319:LLP:NZ	1:A:319:LLP:O3	2.39	0.47
1:E:111:LEU:HB3	1:F:34:ILE:HG13	1.95	0.47
1:F:143:PHE:O	1:F:147:LEU:HD23	2.12	0.47
1:C:152:SER:HB2	1:C:333:LYS:HD3	1.95	0.47
1:F:142:TRP:CE3	1:F:382:LEU:HD13	2.50	0.47
1:F:404:PHE:HE1	1:F:510:TRP:CZ3	2.32	0.47
1:A:239:ARG:NH2	1:A:279:GLU:OE1	2.32	0.47
1:B:172:LEU:O	1:B:176:THR:HG23	2.15	0.47
1:E:29:ARG:HD2	1:E:33:MET:HE2	1.95	0.47
1:E:177:ALA:HB2	1:E:338:LEU:HD23	1.96	0.47
1:F:251:ILE:HD12	1:F:252:PRO:HD2	1.97	0.47
1:A:174:THR:HG22	1:A:254:PHE:HE2	1.79	0.47
1:B:319:LLP:NZ	1:B:319:LLP:O3	2.38	0.47
1:B:458:ASN:N	1:B:458:ASN:OD1	2.48	0.47
1:C:102:PRO:CG	1:C:497:GLY:HA3	2.45	0.47
1:C:426:CYS:HB3	1:C:491:MET:HE3	1.97	0.47
1:E:31:GLY:O	1:E:35:ILE:HG12	2.14	0.47
1:E:224:LYS:HA	1:E:224:LYS:HD3	1.51	0.47
1:F:457:GLU:CD	1:F:458:ASN:H	2.17	0.47
1:F:42:TYR:HA	1:F:45:VAL:HG23	1.97	0.47
1:F:142:TRP:O	1:F:146:MET:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:399:LYS:O	1:F:403:THR:HG23	2.16	0.46
1:F:429:LEU:HD11	1:F:521:LEU:HD11	1.97	0.46
1:B:294:ALA:HB2	1:B:320:TRP:CZ3	2.50	0.46
1:E:69:TYR:O	1:F:388:THR:HG22	2.15	0.46
1:E:167:SER:O	1:E:171:ILE:HG13	2.15	0.46
1:F:293:SER:HB3	1:F:321:PHE:HE1	1.76	0.46
1:F:198:GLY:O	1:F:223:ILE:HG12	2.16	0.46
1:F:375:SER:O	1:F:379:TRP:N	2.49	0.46
1:D:278:LYS:NZ	3:D:704:HOH:O	2.34	0.46
1:D:458:ASN:N	1:D:458:ASN:OD1	2.48	0.46
1:E:89:LEU:HD23	1:E:91:HIS:ND1	2.31	0.46
1:E:126:TRP:CE2	1:E:130:PRO:HB3	2.51	0.46
1:E:264:SER:O	1:E:264:SER:OG	2.31	0.46
1:F:51:ARG:HE	1:F:474:ASN:HB2	1.81	0.46
1:F:420:ARG:HB3	1:F:420:ARG:CZ	2.46	0.46
1:F:464:LYS:HG3	1:F:529:PHE:HB3	1.98	0.46
1:E:20:ASN:HB3	1:E:23:ASP:HB2	1.97	0.46
1:A:319:LLP:H4'1	2:A:601:GOL:H2	1.98	0.46
1:C:151:GLU:HG2	1:C:157:GLY:HA3	1.98	0.46
1:F:106:SER:HG	1:F:109:GLY:H	1.58	0.46
1:C:264:SER:HB2	1:C:418:VAL:HG21	1.96	0.46
1:F:459:LEU:HD11	1:F:489:VAL:HA	1.98	0.46
1:A:124:PHE:CD1	2:B:601:GOL:H32	2.51	0.45
1:A:264:SER:HB2	1:A:418:VAL:HG21	1.97	0.45
1:D:185:LYS:HG3	1:D:186:ILE:HG23	1.97	0.45
1:C:109:GLY:HA3	1:C:323:THR:O	2.17	0.45
1:E:89:LEU:HD23	1:E:91:HIS:HD1	1.80	0.45
1:F:75:GLU:HA	1:F:78:LEU:HD12	1.98	0.45
1:F:392:ASN:HA	1:F:395:ARG:NH2	2.32	0.45
1:F:101:PHE:CE2	1:F:262:THR:HA	2.52	0.45
1:F:378:LEU:HG	1:F:382:LEU:HD21	1.98	0.45
1:F:400:MET:O	1:F:403:THR:OG1	2.29	0.45
1:C:484:ALA:HB2	1:C:493:ARG:HD2	1.98	0.45
1:D:319:LLP:NZ	1:D:319:LLP:O3	2.38	0.45
1:E:181:ARG:NH1	1:E:334:ASP:OD2	2.50	0.45
1:F:469:TYR:OH	1:F:513:LEU:HB3	2.17	0.45
1:C:122:VAL:HB	1:D:92:TRP:CZ2	2.52	0.45
1:C:493:ARG:CZ	2:C:603:GOL:H32	2.46	0.45
1:E:98:TYR:HD2	1:E:479:VAL:HG13	1.82	0.45
1:A:429:LEU:N	1:A:466:ASN:OD1	2.45	0.45
1:B:107:VAL:O	1:B:111:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ILE:HG22	1:B:391:ARG:HG2	1.98	0.45
1:E:106:SER:HB2	1:E:322:PHE:O	2.17	0.45
1:E:116:SER:HB3	1:E:373:PHE:HB3	1.98	0.45
1:A:29:ARG:NH1	1:A:33:MET:HE1	2.31	0.45
1:A:174:THR:HG22	1:A:254:PHE:CE2	2.52	0.45
1:D:262:THR:HG22	3:D:779:HOH:O	2.17	0.45
1:F:75:GLU:HG2	1:F:78:LEU:HD12	1.97	0.45
1:F:141:ASP:OD2	1:F:155:PHE:HB2	2.16	0.45
1:D:107:VAL:O	1:D:111:LEU:HG	2.17	0.44
1:E:407:LEU:HD11	1:E:507:ILE:HD13	1.98	0.44
1:F:376:LEU:HA	1:F:379:TRP:HB2	1.99	0.44
1:F:512:ILE:N	3:F:618:HOH:O	2.37	0.44
1:E:73:SER:OG	1:E:76:THR:HG22	2.18	0.44
1:F:294:ALA:O	1:F:300:PHE:HD1	2.00	0.44
1:C:62:ARG:HE	1:C:62:ARG:HB3	1.65	0.44
1:E:126:TRP:C	1:E:128:SER:H	2.20	0.44
1:E:325:LEU:HD23	1:F:372:ARG:HG2	1.99	0.44
1:A:408:ILE:HG12	1:A:510:TRP:CZ3	2.53	0.44
1:D:289:ALA:HA	1:D:315:LEU:HA	1.99	0.44
1:D:323:THR:O	1:D:377:LYS:HD2	2.17	0.44
1:F:224:LYS:HD2	1:F:224:LYS:HA	1.79	0.44
1:F:470:LEU:HD13	1:F:470:LEU:C	2.37	0.44
1:F:470:LEU:HD13	1:F:474:ASN:OD1	2.18	0.44
1:B:468:VAL:O	1:B:472:THR:HG23	2.18	0.44
1:E:96:ASN:HA	1:E:98:TYR:CE2	2.52	0.44
1:F:82:THR:HA	1:F:86:ILE:HD12	1.98	0.44
1:B:399:LYS:NZ	1:B:402:LYS:HB3	2.32	0.44
1:E:146:MET:SD	1:E:387:VAL:HG22	2.58	0.44
1:E:238:LEU:O	1:E:242:ILE:HG13	2.17	0.44
1:E:315:LEU:HG	1:E:331:TRP:CH2	2.53	0.44
1:F:124:PHE:CE1	1:F:363:LYS:HE3	2.53	0.44
1:F:135:LEU:CD1	1:F:373:PHE:HZ	2.28	0.44
1:D:165:GLY:O	1:D:326:ASP:HB2	2.18	0.44
1:E:98:TYR:HD2	1:E:479:VAL:CG1	2.31	0.44
1:E:166:THR:HG23	1:E:169:GLU:HB2	2.00	0.44
1:D:132:ALA:HA	1:D:373:PHE:CE1	2.52	0.44
1:D:411:ASP:HB2	1:D:510:TRP:HH2	1.82	0.44
1:E:278:LYS:HD2	1:E:278:LYS:C	2.37	0.44
1:E:27:PHE:HA	1:F:107:VAL:HG21	1.99	0.44
1:F:74:ILE:O	1:F:77:ILE:HG22	2.18	0.44
1:C:203:HIS:CD2	2:C:602:GOL:H12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:ARG:HD3	1:F:480:TYR:CE1	2.53	0.43
1:F:131:ALA:HB1	1:F:135:LEU:CD1	2.45	0.43
1:F:294:ALA:HB1	1:F:300:PHE:CD1	2.53	0.43
1:F:382:LEU:HB2	1:F:383:ARG:HG3	2.00	0.43
1:F:457:GLU:OE1	1:F:458:ASN:N	2.50	0.43
1:A:325:LEU:HA	1:A:326:ASP:HA	1.66	0.43
1:C:352:LYS:HD2	1:C:352:LYS:HA	1.72	0.43
1:D:113:GLU:HB2	1:D:377:LYS:HD3	1.98	0.43
1:E:326:ASP:CG	1:E:374:ARG:HH12	2.22	0.43
1:E:407:LEU:HD13	1:E:510:TRP:CD1	2.52	0.43
1:F:457:GLU:CG	1:F:458:ASN:N	2.82	0.43
1:B:289:ALA:HA	1:B:315:LEU:HA	2.01	0.43
1:E:172:LEU:O	1:E:176:THR:HG23	2.19	0.43
1:E:394:LEU:O	1:E:398:VAL:HG23	2.18	0.43
1:F:296:ILE:HD12	1:F:321:PHE:HZ	1.83	0.43
1:C:523:LYS:HD2	1:F:348:TYR:CE2	2.53	0.43
1:B:385:TYR:O	1:B:389:ASN:HB2	2.19	0.43
1:F:117:THR:O	1:F:120:ASN:HB2	2.18	0.43
1:F:127:MET:HE3	1:F:127:MET:HA	2.01	0.43
1:C:174:THR:HG22	1:C:254:PHE:CE1	2.54	0.43
1:E:59:LEU:HG	1:F:134:GLU:CB	2.49	0.43
1:F:23:ASP:HB3	1:F:26:GLU:HB3	2.00	0.43
1:F:62:ARG:HE	1:F:62:ARG:HB3	1.61	0.43
1:F:219:ASN:ND2	3:F:614:HOH:O	2.35	0.43
1:F:501:THR:HG22	1:F:506:VAL:HG23	2.01	0.43
1:E:59:LEU:HG	1:F:134:GLU:HB2	2.01	0.43
1:E:325:LEU:HA	1:E:326:ASP:HA	1.59	0.43
1:A:106:SER:HB3	1:A:322:PHE:HB3	2.00	0.43
1:B:252:PRO:HB2	1:B:282:MET:SD	2.59	0.43
1:E:194:LEU:HB3	1:E:253:LEU:HD22	2.01	0.43
1:F:97:TYR:CZ	1:F:99:ALA:HB3	2.53	0.43
1:E:69:TYR:HA	1:F:387:VAL:HB	2.01	0.43
1:F:86:ILE:HA	1:F:89:LEU:HG	2.01	0.43
1:E:113:GLU:HG2	1:E:116:SER:HB2	2.00	0.42
1:E:141:ASP:O	1:E:145:LYS:HG3	2.19	0.42
1:E:195:VAL:HG12	1:E:219:ASN:CB	2.49	0.42
1:F:525:SER:C	1:F:527:ALA:H	2.22	0.42
1:E:41:TYR:OH	1:E:93:GLN:NE2	2.45	0.42
1:E:61:LYS:NZ	1:E:65:GLU:OE2	2.46	0.42
1:E:315:LEU:HG	1:E:331:TRP:HH2	1.83	0.42
1:E:325:LEU:H	1:F:120:ASN:HD21	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:470:LEU:HG	1:E:471:GLU:OE2	2.18	0.42
1:F:36:ASP:O	1:F:40:ASP:N	2.37	0.42
1:F:143:PHE:CE1	1:F:296:ILE:HD11	2.45	0.42
1:E:289:ALA:HA	1:E:315:LEU:HA	2.01	0.42
1:D:334:ASP:OD1	1:D:336:SER:OG	2.38	0.42
1:F:265:THR:O	1:F:421:THR:OG1	2.31	0.42
1:F:269:PRO:HB2	1:F:272:PRO:HD2	2.00	0.42
1:E:399:LYS:HG3	1:E:400:MET:N	2.35	0.42
1:C:97:TYR:CZ	1:C:99:ALA:HB3	2.54	0.42
1:D:413:ARG:NH1	1:D:518:ASP:OD1	2.48	0.42
1:F:30:GLN:HA	1:F:33:MET:SD	2.59	0.42
1:F:91:HIS:O	1:F:94:SER:OG	2.30	0.42
1:F:99:ALA:HB1	1:F:482:THR:HG23	2.00	0.42
1:A:346:PRO:HB2	1:A:348:TYR:CZ	2.55	0.42
1:D:325:LEU:HG	1:D:326:ASP:HB3	2.01	0.42
1:E:32:HIS:NE2	1:F:36:ASP:OD1	2.48	0.42
1:E:79:GLN:HG2	1:E:82:THR:OG1	2.19	0.42
1:F:99:ALA:HB2	1:F:481:MET:HA	2.01	0.42
1:F:458:ASN:N	1:F:458:ASN:OD1	2.53	0.42
1:C:277:ALA:HA	1:C:282:MET:HE2	2.02	0.42
1:C:431:PRO:HA	1:C:432:PRO:HD3	1.90	0.42
1:D:318:HIS:CG	1:D:325:LEU:HD12	2.52	0.42
1:E:294:ALA:HB1	1:E:300:PHE:CD2	2.55	0.42
1:E:400:MET:HB3	1:E:506:VAL:HG21	2.00	0.42
1:F:225:THR:HB	1:F:231:PHE:HA	2.00	0.42
1:F:385:TYR:CB	1:F:390:LEU:HD21	2.31	0.42
1:F:390:LEU:N	1:F:390:LEU:HD23	2.34	0.42
1:A:265:THR:HG21	3:A:740:HOH:O	2.20	0.42
1:F:497:GLY:O	1:F:498:SER:HB3	2.20	0.42
1:A:385:TYR:O	1:A:389:ASN:HB2	2.20	0.41
1:B:325:LEU:HA	1:B:326:ASP:HA	1.60	0.41
1:E:200:ASP:OD1	1:E:225:THR:OG1	2.33	0.41
1:F:297:CYS:HB3	1:F:300:PHE:CD1	2.55	0.41
1:C:289:ALA:HA	1:C:315:LEU:HA	2.01	0.41
1:F:147:LEU:HD22	1:F:147:LEU:H	1.84	0.41
1:A:132:ALA:HA	1:A:373:PHE:CE1	2.55	0.41
1:C:325:LEU:HA	1:C:326:ASP:HA	1.66	0.41
1:D:152:SER:HB2	1:D:333:LYS:HG2	2.01	0.41
1:E:398:VAL:HA	1:E:423:ALA:HB2	2.01	0.41
1:F:34:ILE:HG22	1:F:38:LEU:HD12	2.01	0.41
1:F:162:VAL:HB	1:F:365:TRP:HE3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:472:THR:O	1:F:476:THR:HG23	2.20	0.41
1:F:504:ARG:HA	1:F:507:ILE:HD12	2.01	0.41
1:A:172:LEU:O	1:A:176:THR:HG23	2.19	0.41
1:E:179:ARG:HE	1:E:179:ARG:HB3	1.69	0.41
1:F:97:TYR:CE1	1:F:99:ALA:HB3	2.56	0.41
1:F:429:LEU:N	1:F:466:ASN:OD1	2.46	0.41
1:F:511:LYS:HA	1:F:514:GLN:HB3	2.02	0.41
1:B:22:LEU:HD12	1:B:22:LEU:HA	1.90	0.41
1:C:132:ALA:HA	1:C:373:PHE:CE1	2.56	0.41
1:F:152:SER:HB2	1:F:333:LYS:HD3	2.03	0.41
1:F:470:LEU:HA	1:F:470:LEU:HD22	1.76	0.41
1:F:139:VAL:HG21	1:F:378:LEU:HD23	2.02	0.41
1:E:210:ALA:HB1	1:E:215:ILE:HB	2.02	0.41
1:F:512:ILE:O	1:F:516:HIS:ND1	2.53	0.41
1:D:322:PHE:CZ	1:D:393:PHE:HB3	2.56	0.41
1:D:385:TYR:O	1:D:389:ASN:HB2	2.21	0.41
1:E:77:ILE:O	1:E:81:VAL:HG23	2.21	0.41
1:E:98:TYR:CD2	1:E:479:VAL:CG1	3.04	0.41
1:E:203:HIS:HD2	1:E:262:THR:HG21	1.85	0.41
1:B:366:GLN:OE1	1:B:371:ARG:HD2	2.20	0.41
1:E:133:THR:HG22	1:E:362:TYR:CD2	2.51	0.41
1:E:325:LEU:O	1:F:372:ARG:HD3	2.21	0.41
1:E:428:ARG:HB2	1:E:466:ASN:ND2	2.35	0.41
1:F:429:LEU:CD1	1:F:465:LEU:HD21	2.50	0.41
1:F:114:MET:O	1:F:118:GLY:N	2.53	0.40
1:F:139:VAL:HG12	1:F:382:LEU:CD1	2.47	0.40
1:F:165:GLY:N	1:F:374:ARG:HH21	2.19	0.40
1:B:97:TYR:CZ	1:B:99:ALA:HB3	2.56	0.40
1:B:143:PHE:HB3	1:B:331:TRP:HZ2	1.87	0.40
1:E:134:GLU:O	1:E:138:VAL:HG12	2.21	0.40
1:F:376:LEU:HA	1:F:376:LEU:HD23	1.84	0.40
1:F:388:THR:HA	1:F:391:ARG:CG	2.49	0.40
1:C:140:MET:HE1	1:C:329:CYS:HB3	2.04	0.40
1:C:262:THR:HG21	2:C:602:GOL:HO2	1.87	0.40
1:C:485:VAL:HB	1:E:531:SER:HA	2.02	0.40
1:E:297:CYS:SG	1:E:391:ARG:HG2	2.62	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	478/531 (90%)	466 (98%)	11 (2%)	1 (0%)	47	58
1	B	476/531 (90%)	465 (98%)	11 (2%)	0	100	100
1	C	478/531 (90%)	465 (97%)	13 (3%)	0	100	100
1	D	476/531 (90%)	465 (98%)	11 (2%)	0	100	100
1	E	470/531 (88%)	454 (97%)	15 (3%)	1 (0%)	47	58
1	F	468/531 (88%)	443 (95%)	25 (5%)	0	100	100
All	All	2846/3186 (89%)	2758 (97%)	86 (3%)	2 (0%)	51	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	100	TYR
1	A	324	THR

### 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	415/455 (91%)	410 (99%)	5 (1%)	71	83
1	B	413/455 (91%)	405 (98%)	8 (2%)	57	73
1	C	415/455 (91%)	410 (99%)	5 (1%)	71	83
1	D	413/455 (91%)	405 (98%)	8 (2%)	57	73
1	E	411/455 (90%)	401 (98%)	10 (2%)	49	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	408/455 (90%)	388 (95%)	20 (5%)	25	34
All	All	2475/2730 (91%)	2419 (98%)	56 (2%)	50	66

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	PHE
1	A	218	LYS
1	A	348	TYR
1	A	373	PHE
1	A	525	SER
1	B	143	PHE
1	B	156	SER
1	B	182	LYS
1	B	271	SER
1	B	321	PHE
1	B	350	ARG
1	B	362	TYR
1	B	373	PHE
1	C	94	SER
1	C	143	PHE
1	C	278	LYS
1	C	373	PHE
1	C	461	LEU
1	D	143	PHE
1	D	158	SER
1	D	262	THR
1	D	373	PHE
1	D	396	SER
1	D	399	LYS
1	D	498	SER
1	D	525	SER
1	E	36	ASP
1	E	94	SER
1	E	143	PHE
1	E	199	SER
1	E	321	PHE
1	E	361	ASP
1	E	362	TYR
1	E	373	PHE
1	E	374	ARG
1	E	420	ARG

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Mol	Chain	Res	Type
1	F	28	ARG
1	F	69	TYR
1	F	73	SER
1	F	75	GLU
1	F	92	TRP
1	F	128	SER
1	F	143	PHE
1	F	156	SER
1	F	233	LEU
1	F	247	GLU
1	F	297	CYS
1	F	301	ARG
1	F	321	PHE
1	F	362	TYR
1	F	373	PHE
1	F	380	MET
1	F	402	LYS
1	F	420	ARG
1	F	458	ASN
1	F	480	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	392	ASN
1	F	30	GLN
1	F	120	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	LLP	E	319	1	23,24,25	2.59	6 (26%)	25,32,34	1.40	3 (12%)
1	LLP	F	319	1	23,24,25	2.59	6 (26%)	25,32,34	1.39	4 (16%)
1	LLP	D	319	1	23,24,25	2.61	6 (26%)	25,32,34	1.33	4 (16%)
1	LLP	A	319	1	23,24,25	2.59	6 (26%)	25,32,34	1.34	4 (16%)
1	LLP	C	319	1	23,24,25	2.60	6 (26%)	25,32,34	1.36	4 (16%)
1	LLP	B	319	1	23,24,25	2.60	5 (21%)	25,32,34	1.32	4 (16%)

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
1	LLP	E	319	1	-	5/16/17/19	0/1/1/1
1	LLP	F	319	1	-	5/16/17/19	0/1/1/1
1	LLP	D	319	1	-	2/16/17/19	0/1/1/1
1	LLP	A	319	1	-	2/16/17/19	0/1/1/1
1	LLP	C	319	1	-	2/16/17/19	0/1/1/1
1	LLP	B	319	1	-	2/16/17/19	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	319	LLP	C4-C4'	8.10	1.62	1.46
1	D	319	LLP	C4-C4'	8.07	1.62	1.46
1	B	319	LLP	C4-C4'	8.02	1.61	1.46
1	F	319	LLP	C4-C4'	8.01	1.61	1.46
1	A	319	LLP	C4-C4'	8.00	1.61	1.46
1	C	319	LLP	C4-C4'	7.98	1.61	1.46
1	F	319	LLP	C4'-NZ	4.95	1.43	1.27
1	E	319	LLP	C4'-NZ	4.94	1.43	1.27
1	D	319	LLP	C4'-NZ	4.93	1.43	1.27
1	B	319	LLP	C4'-NZ	4.88	1.43	1.27
1	A	319	LLP	C4'-NZ	4.87	1.43	1.27
1	C	319	LLP	C4'-NZ	4.86	1.43	1.27
1	D	319	LLP	C4-C5	-4.15	1.36	1.42
1	C	319	LLP	C4-C5	-4.13	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	319	LLP	C4-C5	-4.10	1.36	1.42
1	B	319	LLP	C4-C5	-4.09	1.36	1.42
1	F	319	LLP	C4-C5	-3.88	1.37	1.42
1	E	319	LLP	C4-C5	-3.68	1.37	1.42
1	C	319	LLP	C2'-C2	3.52	1.56	1.50
1	F	319	LLP	C2'-C2	3.52	1.56	1.50
1	B	319	LLP	C2'-C2	3.51	1.56	1.50
1	D	319	LLP	C2'-C2	3.51	1.56	1.50
1	E	319	LLP	C2'-C2	3.49	1.56	1.50
1	A	319	LLP	C2'-C2	3.48	1.56	1.50
1	F	319	LLP	C6-N1	3.00	1.40	1.34
1	C	319	LLP	C6-N1	3.00	1.40	1.34
1	E	319	LLP	C6-N1	2.97	1.40	1.34
1	A	319	LLP	C6-N1	2.97	1.40	1.34
1	B	319	LLP	C6-N1	2.97	1.40	1.34
1	D	319	LLP	C6-N1	2.94	1.40	1.34
1	F	319	LLP	C5'-C5	2.18	1.56	1.50
1	E	319	LLP	C5'-C5	2.17	1.56	1.50
1	D	319	LLP	C5'-C5	2.03	1.56	1.50
1	C	319	LLP	C5'-C5	2.03	1.56	1.50
1	A	319	LLP	C5'-C5	2.00	1.56	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	319	LLP	C4-C4'-NZ	-3.77	107.01	124.31
1	F	319	LLP	C4-C4'-NZ	-3.53	108.11	124.31
1	B	319	LLP	C4-C4'-NZ	-3.52	108.15	124.31
1	C	319	LLP	C4-C4'-NZ	-3.52	108.15	124.31
1	A	319	LLP	C4-C4'-NZ	-3.49	108.29	124.31
1	D	319	LLP	C4-C4'-NZ	-3.46	108.40	124.31
1	C	319	LLP	CE-NZ-C4'	-2.92	109.94	118.90
1	A	319	LLP	CE-NZ-C4'	-2.91	109.97	118.90
1	D	319	LLP	CE-NZ-C4'	-2.88	110.07	118.90
1	B	319	LLP	CE-NZ-C4'	-2.86	110.11	118.90
1	F	319	LLP	CE-NZ-C4'	-2.86	110.11	118.90
1	C	319	LLP	C5-C6-N1	-2.47	119.70	123.82
1	E	319	LLP	CE-NZ-C4'	-2.46	111.33	118.90
1	B	319	LLP	C5-C6-N1	-2.45	119.73	123.82
1	A	319	LLP	C5-C6-N1	-2.44	119.75	123.82
1	D	319	LLP	C5-C6-N1	-2.41	119.81	123.82
1	C	319	LLP	C3-C4-C5	2.39	120.09	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	319	LLP	C3-C4-C5	2.31	120.03	118.26
1	A	319	LLP	C3-C4-C5	2.29	120.01	118.26
1	B	319	LLP	C3-C4-C5	2.25	119.99	118.26
1	F	319	LLP	C3-C4-C5	2.22	119.97	118.26
1	F	319	LLP	C5-C6-N1	-2.14	120.25	123.82
1	E	319	LLP	C5-C6-N1	-2.02	120.46	123.82

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	319	LLP	C-CA-CB-CG
1	B	319	LLP	C-CA-CB-CG
1	C	319	LLP	C-CA-CB-CG
1	D	319	LLP	C4-C4'-NZ-CE
1	D	319	LLP	C-CA-CB-CG
1	E	319	LLP	O-C-CA-CB
1	E	319	LLP	CG-CD-CE-NZ
1	F	319	LLP	N-CA-CB-CG
1	F	319	LLP	C-CA-CB-CG
1	A	319	LLP	C4-C4'-NZ-CE
1	B	319	LLP	C4-C4'-NZ-CE
1	C	319	LLP	C4-C4'-NZ-CE
1	F	319	LLP	C4-C4'-NZ-CE
1	E	319	LLP	CA-CB-CG-CD
1	E	319	LLP	CD-CE-NZ-C4'
1	E	319	LLP	C3-C4-C4'-NZ
1	F	319	LLP	CD-CE-NZ-C4'
1	F	319	LLP	CE-CD-CG-CB

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	319	LLP	1	0
1	F	319	LLP	1	0
1	D	319	LLP	4	0
1	A	319	LLP	4	0
1	C	319	LLP	2	0
1	B	319	LLP	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

9 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	GOL	B	603	-	5,5,5	0.71	0	5,5,5	1.05	0
2	GOL	C	601	-	5,5,5	0.14	0	5,5,5	0.72	0
2	GOL	C	603	-	5,5,5	0.61	0	5,5,5	1.19	1 (20%)
2	GOL	D	601	-	5,5,5	0.60	0	5,5,5	0.45	0
2	GOL	D	602	-	5,5,5	0.43	0	5,5,5	0.64	0
2	GOL	C	602	-	5,5,5	0.24	0	5,5,5	0.56	0
2	GOL	A	601	-	5,5,5	0.27	0	5,5,5	0.99	0
2	GOL	B	601	-	5,5,5	0.42	0	5,5,5	0.67	0
2	GOL	B	602	-	5,5,5	0.31	0	5,5,5	0.61	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
2	GOL	B	603	-	-	2/4/4/4	-
2	GOL	C	601	-	-	4/4/4/4	-
2	GOL	C	603	-	-	2/4/4/4	-
2	GOL	D	601	-	-	4/4/4/4	-
2	GOL	D	602	-	-	2/4/4/4	-
2	GOL	C	602	-	-	2/4/4/4	-
2	GOL	A	601	-	-	4/4/4/4	-
2	GOL	B	601	-	-	2/4/4/4	-
2	GOL	B	602	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	603	GOL	O3-C3-C2	2.13	120.42	110.20

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	O1-C1-C2-C3
2	B	601	GOL	O1-C1-C2-C3
2	C	601	GOL	C1-C2-C3-O3
2	C	602	GOL	C1-C2-C3-O3
2	C	603	GOL	O1-C1-C2-C3
2	D	601	GOL	O1-C1-C2-O2
2	D	601	GOL	O1-C1-C2-C3
2	D	602	GOL	C1-C2-C3-O3
2	C	603	GOL	O1-C1-C2-O2
2	A	601	GOL	C1-C2-C3-O3
2	B	603	GOL	O1-C1-C2-C3
2	C	601	GOL	O1-C1-C2-C3
2	D	601	GOL	C1-C2-C3-O3
2	A	601	GOL	O2-C2-C3-O3
2	B	603	GOL	O1-C1-C2-O2
2	C	601	GOL	O2-C2-C3-O3
2	C	602	GOL	O2-C2-C3-O3
2	A	601	GOL	O1-C1-C2-O2
2	D	602	GOL	O2-C2-C3-O3
2	B	601	GOL	O1-C1-C2-O2
2	D	601	GOL	O2-C2-C3-O3
2	C	601	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	GOL	6	0
2	C	603	GOL	2	0
2	D	601	GOL	4	0
2	D	602	GOL	4	0
2	C	602	GOL	3	0
2	A	601	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	GOL	3	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	484/531 (91%)	0.47	28 (5%)	23 29	21, 30, 47, 74	0
1	B	482/531 (90%)	0.31	22 (4%)	32 40	21, 28, 43, 86	0
1	C	484/531 (91%)	0.47	34 (7%)	16 22	20, 30, 51, 83	0
1	D	482/531 (90%)	0.27	12 (2%)	57 64	20, 28, 43, 77	0
1	E	478/531 (90%)	2.87	303 (63%)	0 0	52, 76, 91, 101	0
1	F	476/531 (89%)	2.86	278 (58%)	0 0	43, 74, 96, 104	0
All	All	2886/3186 (90%)	1.20	677 (23%)	0 1	20, 33, 89, 104	0

All (677) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	22	LEU	18.8
1	F	379	TRP	13.4
1	F	48	TYR	12.0
1	F	33	MET	11.9
1	F	387	VAL	11.7
1	F	45	VAL	10.6
1	F	384	SER	10.0
1	E	42	TYR	10.0
1	E	509	ALA	9.7
1	F	66	THR	9.6
1	F	74	ILE	9.6
1	F	83	THR	9.5
1	F	383	ARG	9.4
1	F	42	TYR	9.2
1	F	37	PHE	9.1
1	F	76	THR	8.9
1	E	20	ASN	8.9
1	E	27	PHE	8.7
1	F	77	ILE	8.5

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Mol	Chain	Res	Type	RSRZ
1	F	404	PHE	8.4
1	E	382	LEU	8.4
1	F	89	LEU	8.3
1	F	297	CYS	8.1
1	F	85	ILE	8.0
1	E	66	THR	7.9
1	E	404	PHE	7.8
1	F	518	ASP	7.7
1	F	513	LEU	7.6
1	F	41	TYR	7.5
1	E	96	ASN	7.5
1	F	348	TYR	7.4
1	F	67	ALA	7.4
1	F	327	CYS	7.4
1	F	78	LEU	7.3
1	F	474	ASN	7.3
1	E	35	ILE	7.3
1	B	348	TYR	7.2
1	F	411	ASP	7.2
1	E	41	TYR	7.2
1	F	90	THR	7.2
1	E	394	LEU	7.1
1	E	479	VAL	7.1
1	F	409	CYS	7.0
1	E	513	LEU	7.0
1	E	82	THR	6.9
1	F	507	ILE	6.9
1	F	522	GLY	6.9
1	F	529	PHE	6.9
1	F	410	MET	6.8
1	F	382	LEU	6.8
1	F	92	TRP	6.8
1	E	121	VAL	6.8
1	E	507	ILE	6.7
1	E	148	ASN	6.7
1	E	403	THR	6.7
1	E	478	SER	6.7
1	E	83	THR	6.6
1	C	529	PHE	6.6
1	F	84	GLU	6.6
1	E	68	PRO	6.5
1	E	298	PRO	6.5

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Mol	Chain	Res	Type	RSRZ
1	F	521	LEU	6.5
1	F	59	LEU	6.5
1	E	522	GLY	6.5
1	F	24	PRO	6.5
1	F	61	LYS	6.4
1	F	472	THR	6.4
1	E	110	PHE	6.4
1	F	406	GLY	6.3
1	E	51	ARG	6.2
1	E	409	CYS	6.2
1	E	381	VAL	6.1
1	F	373	PHE	6.1
1	E	65	GLU	6.0
1	E	410	MET	6.0
1	F	430	LEU	6.0
1	E	24	PRO	5.9
1	F	88	GLY	5.9
1	F	38	LEU	5.9
1	E	520	ILE	5.9
1	E	418	VAL	5.8
1	E	147	LEU	5.8
1	F	79	GLN	5.8
1	E	430	LEU	5.7
1	F	403	THR	5.7
1	E	165	GLY	5.7
1	F	121	VAL	5.7
1	E	81	VAL	5.6
1	E	19	THR	5.6
1	F	65	GLU	5.6
1	F	35	ILE	5.6
1	E	69	TYR	5.6
1	E	149	LEU	5.6
1	F	431	PRO	5.5
1	F	432	PRO	5.5
1	E	44	ASP	5.5
1	F	480	TYR	5.4
1	E	383	ARG	5.4
1	F	457	GLU	5.4
1	F	39	ALA	5.4
1	E	117	THR	5.4
1	E	58	TYR	5.4
1	E	372	ARG	5.3

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Mol	Chain	Res	Type	RSRZ
1	F	322	PHE	5.3
1	E	36	ASP	5.3
1	E	518	ASP	5.3
1	E	76	THR	5.2
1	F	119	PHE	5.2
1	E	348	TYR	5.2
1	F	128	SER	5.2
1	E	500	LEU	5.2
1	E	48	TYR	5.2
1	F	499	THR	5.1
1	E	21	PRO	5.1
1	F	412	GLY	5.0
1	F	298	PRO	5.0
1	F	517	ALA	5.0
1	F	25	GLU	5.0
1	E	79	GLN	5.0
1	E	510	TRP	5.0
1	F	427	PHE	5.0
1	E	511	LYS	4.9
1	F	429	LEU	4.9
1	E	336	SER	4.9
1	E	292	GLY	4.8
1	F	408	ILE	4.8
1	F	49	PRO	4.8
1	E	175	LEU	4.8
1	E	328	CYS	4.8
1	E	72	GLU	4.8
1	F	107	VAL	4.8
1	F	458	ASN	4.8
1	E	88	GLY	4.8
1	E	43	ARG	4.8
1	F	63	LEU	4.8
1	F	494	PHE	4.8
1	E	379	TRP	4.8
1	F	105	GLY	4.8
1	F	390	LEU	4.7
1	F	506	VAL	4.7
1	E	150	PRO	4.7
1	F	99	ALA	4.7
1	E	506	VAL	4.7
1	E	87	PRO	4.7
1	E	107	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	62	ARG	4.6
1	D	348	TYR	4.6
1	E	337	ALA	4.6
1	F	470	LEU	4.6
1	F	36	ASP	4.6
1	F	423	ALA	4.5
1	F	30	GLN	4.5
1	E	276	VAL	4.5
1	E	191	ILE	4.5
1	E	373	PHE	4.5
1	F	149	LEU	4.5
1	E	246	ILE	4.5
1	F	413	ARG	4.5
1	E	71	PRO	4.5
1	E	300	PHE	4.5
1	E	166	THR	4.5
1	F	349	LEU	4.5
1	F	511	LYS	4.5
1	F	91	HIS	4.5
1	E	378	LEU	4.5
1	A	348	TYR	4.5
1	E	530	SER	4.4
1	F	278	LYS	4.4
1	E	387	VAL	4.4
1	F	69	TYR	4.4
1	F	426	CYS	4.4
1	F	73	SER	4.4
1	F	226	PHE	4.3
1	E	142	TRP	4.3
1	F	19	THR	4.3
1	E	151	GLU	4.3
1	E	78	LEU	4.3
1	E	45	VAL	4.3
1	E	395	ARG	4.3
1	E	137	SER	4.3
1	F	299	GLU	4.3
1	E	516	HIS	4.3
1	C	522	GLY	4.3
1	F	142	TRP	4.3
1	F	132	ALA	4.2
1	F	422	PHE	4.2
1	E	325	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	458	ASN	4.2
1	F	80	ASP	4.2
1	C	530	SER	4.2
1	F	104	SER	4.2
1	F	300	PHE	4.2
1	D	324	THR	4.2
1	F	64	PRO	4.1
1	E	330	LEU	4.1
1	F	508	TYR	4.1
1	E	104	SER	4.1
1	F	156	SER	4.1
1	F	372	ARG	4.1
1	F	22	LEU	4.1
1	F	70	ASN	4.1
1	E	326	ASP	4.1
1	E	514	GLN	4.1
1	D	325	LEU	4.1
1	E	124	PHE	4.1
1	E	39	ALA	4.1
1	F	81	VAL	4.1
1	E	37	PHE	4.1
1	F	71	PRO	4.0
1	E	273	ILE	4.0
1	E	411	ASP	4.0
1	E	52	SER	4.0
1	F	40	ASP	4.0
1	F	167	SER	4.0
1	F	318	HIS	4.0
1	F	510	TRP	4.0
1	F	93	GLN	4.0
1	E	235	ALA	3.9
1	E	422	PHE	3.9
1	F	479	VAL	3.9
1	E	160	GLY	3.9
1	E	315	LEU	3.9
1	F	418	VAL	3.9
1	F	425	VAL	3.9
1	E	77	ILE	3.9
1	F	400	MET	3.9
1	E	424	MET	3.9
1	E	63	LEU	3.9
1	E	228	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	405	GLU	3.9
1	E	75	GLU	3.9
1	F	296	ILE	3.9
1	E	47	LYS	3.9
1	F	475	ALA	3.9
1	F	367	ILE	3.9
1	F	496	VAL	3.9
1	F	165	GLY	3.8
1	F	103	SER	3.8
1	E	205	ALA	3.8
1	F	151	GLU	3.8
1	F	96	ASN	3.8
1	E	115	LEU	3.8
1	F	234	SER	3.8
1	F	369	LEU	3.8
1	F	469	TYR	3.8
1	E	86	ILE	3.8
1	F	509	ALA	3.8
1	F	500	LEU	3.8
1	E	157	GLY	3.8
1	F	380	MET	3.8
1	F	124	PHE	3.7
1	E	164	GLN	3.7
1	E	427	PHE	3.7
1	E	499	THR	3.7
1	E	92	TRP	3.7
1	E	114	MET	3.7
1	E	89	LEU	3.7
1	E	275	GLU	3.7
1	F	428	ARG	3.7
1	F	414	PHE	3.7
1	E	152	SER	3.7
1	E	163	LEU	3.7
1	F	394	LEU	3.7
1	E	393	PHE	3.7
1	E	529	PHE	3.7
1	E	412	GLY	3.7
1	F	246	ILE	3.7
1	F	519	LEU	3.7
1	E	327	CYS	3.6
1	F	502	GLU	3.6
1	F	94	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	525	SER	3.6
1	E	398	VAL	3.6
1	B	327	CYS	3.6
1	E	170	ALA	3.6
1	E	303	PHE	3.6
1	C	351	ASN	3.6
1	F	163	LEU	3.6
1	F	359	VAL	3.6
1	E	377	LYS	3.6
1	F	87	PRO	3.6
1	E	362	TYR	3.6
1	E	385	TYR	3.6
1	E	413	ARG	3.6
1	E	236	ALA	3.6
1	E	317	ALA	3.6
1	F	47	LYS	3.6
1	F	416	ILE	3.6
1	F	461	LEU	3.6
1	E	59	LEU	3.5
1	E	272	PRO	3.5
1	E	419	PRO	3.5
1	E	229	ASN	3.5
1	E	390	LEU	3.5
1	F	95	PRO	3.5
1	F	477	GLY	3.5
1	E	226	PHE	3.5
1	F	186	ILE	3.5
1	F	421	THR	3.5
1	E	429	LEU	3.5
1	E	519	LEU	3.5
1	E	161	GLY	3.5
1	E	280	TYR	3.5
1	F	51	ARG	3.5
1	F	515	GLU	3.4
1	F	120	ASN	3.4
1	F	275	GLU	3.4
1	E	331	TRP	3.4
1	E	122	VAL	3.4
1	E	432	PRO	3.4
1	C	328	CYS	3.4
1	E	40	ASP	3.4
1	F	127	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	377	LYS	3.4
1	E	423	ALA	3.4
1	E	283	TRP	3.4
1	F	280	TYR	3.4
1	F	385	TYR	3.4
1	F	243	LEU	3.4
1	F	328	CYS	3.4
1	E	320	TRP	3.4
1	F	269	PRO	3.4
1	E	281	GLU	3.4
1	F	82	THR	3.4
1	E	162	VAL	3.3
1	E	284	VAL	3.3
1	F	265	THR	3.3
1	C	458	ASN	3.3
1	F	345	ASN	3.3
1	F	393	PHE	3.3
1	F	415	GLU	3.3
1	F	303	PHE	3.3
1	F	122	VAL	3.3
1	E	103	SER	3.3
1	A	461	LEU	3.3
1	F	512	ILE	3.3
1	F	68	PRO	3.3
1	E	128	SER	3.3
1	E	240	GLU	3.3
1	E	299	GLU	3.3
1	E	496	VAL	3.3
1	F	473	VAL	3.3
1	C	409	CYS	3.3
1	A	529	PHE	3.3
1	E	143	PHE	3.3
1	E	245	ASP	3.3
1	E	504	ARG	3.3
1	E	105	GLY	3.3
1	E	131	ALA	3.3
1	E	295	CYS	3.3
1	E	316	ASN	3.2
1	E	106	SER	3.2
1	F	21	PRO	3.2
1	F	34	ILE	3.2
1	E	90	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	324	THR	3.2
1	F	368	ALA	3.2
1	E	239	ARG	3.2
1	F	374	ARG	3.2
1	E	322	PHE	3.2
1	E	31	GLY	3.2
1	E	323	THR	3.2
1	E	431	PRO	3.2
1	E	461	LEU	3.2
1	F	97	TYR	3.2
1	E	457	GLU	3.2
1	B	166	THR	3.2
1	F	54	VAL	3.2
1	A	369	LEU	3.2
1	F	44	ASP	3.2
1	E	401	ALA	3.2
1	E	374	ARG	3.2
1	F	31	GLY	3.2
1	F	392	ASN	3.2
1	F	111	LEU	3.2
1	E	265	THR	3.1
1	C	348	TYR	3.1
1	F	346	PRO	3.1
1	E	521	LEU	3.1
1	E	485	VAL	3.1
1	F	476	THR	3.1
1	E	368	ALA	3.1
1	F	498	SER	3.1
1	E	296	ILE	3.1
1	F	247	GLU	3.1
1	B	349	LEU	3.1
1	E	250	LEU	3.1
1	F	242	ILE	3.1
1	E	108	ALA	3.1
1	F	462	ALA	3.1
1	E	397	HIS	3.1
1	A	327	CYS	3.1
1	E	310	ALA	3.1
1	F	528	ASP	3.0
1	F	424	MET	3.0
1	E	408	ILE	3.0
1	E	366	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	478	SER	3.0
1	A	170	ALA	3.0
1	F	131	ALA	3.0
1	F	235	ALA	3.0
1	C	168	CYS	3.0
1	E	129	SER	3.0
1	E	98	TYR	3.0
1	C	324	THR	3.0
1	F	378	LEU	3.0
1	E	84	GLU	3.0
1	E	472	THR	3.0
1	E	392	ASN	3.0
1	F	397	HIS	3.0
1	F	108	ALA	3.0
1	C	524	PHE	3.0
1	E	34	ILE	3.0
1	E	155	PHE	3.0
1	F	468	VAL	3.0
1	E	73	SER	2.9
1	E	28	ARG	2.9
1	E	91	HIS	2.9
1	E	93	GLN	2.9
1	E	481	MET	2.9
1	F	123	GLY	2.9
1	E	56	PRO	2.9
1	C	122	VAL	2.9
1	E	290	TYR	2.9
1	E	279	GLU	2.9
1	F	109	GLY	2.9
1	E	138	VAL	2.9
1	F	398	VAL	2.9
1	E	116	SER	2.9
1	E	169	GLU	2.9
1	F	503	GLU	2.9
1	B	165	GLY	2.9
1	E	243	LEU	2.9
1	C	327	CYS	2.9
1	E	293	SER	2.9
1	E	488	GLY	2.9
1	F	290	TYR	2.9
1	F	27	PHE	2.9
1	F	530	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	306	GLY	2.9
1	F	386	GLY	2.9
1	E	70	ASN	2.8
1	F	162	VAL	2.8
1	E	367	ILE	2.8
1	F	185	LYS	2.8
1	A	351	ASN	2.8
1	F	347	GLU	2.8
1	E	286	VAL	2.8
1	B	163	LEU	2.8
1	E	32	HIS	2.8
1	F	168	CYS	2.8
1	F	417	THR	2.8
1	E	153	PHE	2.8
1	F	50	VAL	2.8
1	B	410	MET	2.8
1	E	380	MET	2.8
1	F	330	LEU	2.8
1	F	62	ARG	2.8
1	E	61	LYS	2.8
1	F	295	CYS	2.8
1	C	367	ILE	2.8
1	E	119	PHE	2.8
1	E	360	VAL	2.8
1	E	460	VAL	2.8
1	F	289	ALA	2.8
1	B	347	GLU	2.8
1	F	114	MET	2.8
1	F	402	LYS	2.8
1	E	463	ASN	2.8
1	D	317	ALA	2.7
1	E	50	VAL	2.7
1	E	289	ALA	2.7
1	E	334	ASP	2.7
1	E	132	ALA	2.7
1	E	495	ALA	2.7
1	C	162	VAL	2.7
1	E	60	ARG	2.7
1	E	112	GLY	2.7
1	B	328	CYS	2.7
1	E	515	GLU	2.7
1	A	325	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	407	LEU	2.7
1	E	371	ARG	2.7
1	F	133	THR	2.7
1	F	388	THR	2.7
1	E	302	HIS	2.7
1	E	55	GLU	2.7
1	E	123	GLY	2.7
1	A	530	SER	2.7
1	F	370	SER	2.7
1	E	517	ALA	2.7
1	E	508	TYR	2.7
1	E	231	PHE	2.7
1	F	20	ASN	2.7
1	F	524	PHE	2.7
1	B	325	LEU	2.7
1	E	33	MET	2.7
1	E	309	GLU	2.7
1	F	401	ALA	2.7
1	E	318	HIS	2.7
1	E	365	TRP	2.6
1	A	317	ALA	2.6
1	F	466	ASN	2.6
1	E	526	GLU	2.6
1	E	267	VAL	2.6
1	F	376	LEU	2.6
1	D	156	SER	2.6
1	E	126	TRP	2.6
1	F	320	TRP	2.6
1	A	520	ILE	2.6
1	E	459	LEU	2.6
1	F	58	TYR	2.6
1	F	239	ARG	2.6
1	E	249	GLY	2.6
1	D	62	ARG	2.6
1	C	410	MET	2.6
1	A	165	GLY	2.6
1	F	514	GLN	2.6
1	F	166	THR	2.5
1	B	172	LEU	2.5
1	E	172	LEU	2.5
1	E	414	PHE	2.5
1	F	240	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	317	ALA	2.5
1	F	29	ARG	2.5
1	A	408	ILE	2.5
1	D	323	THR	2.5
1	C	166	THR	2.5
1	F	228	GLU	2.5
1	E	187	GLY	2.5
1	E	376	LEU	2.5
1	F	138	VAL	2.5
1	C	525	SER	2.5
1	C	531	SER	2.5
1	D	170	ALA	2.5
1	E	97	TYR	2.5
1	F	98	TYR	2.5
1	E	113	GLU	2.5
1	E	154	LEU	2.5
1	F	147	LEU	2.5
1	B	422	PHE	2.5
1	C	518	ASP	2.5
1	F	143	PHE	2.5
1	F	231	PHE	2.5
1	E	247	GLU	2.5
1	F	102	PRO	2.5
1	F	118	GLY	2.5
1	F	164	GLN	2.5
1	C	278	LYS	2.4
1	E	233	LEU	2.4
1	E	271	SER	2.4
1	F	60	ARG	2.4
1	F	315	LEU	2.4
1	E	294	ALA	2.4
1	E	49	PRO	2.4
1	F	505	HIS	2.4
1	F	331	TRP	2.4
1	F	309	GLU	2.4
1	E	407	LEU	2.4
1	F	360	VAL	2.4
1	C	240	GLU	2.4
1	C	352	LYS	2.4
1	E	416	ILE	2.4
1	E	158	SER	2.4
1	A	328	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	329	CYS	2.4
1	E	406	GLY	2.4
1	E	237	THR	2.4
1	E	391	ARG	2.4
1	F	43	ARG	2.4
1	E	314	SER	2.4
1	E	417	THR	2.4
1	E	223	ILE	2.4
1	F	391	ARG	2.4
1	E	282	MET	2.4
1	F	291	ALA	2.4
1	B	168	CYS	2.4
1	F	52	SER	2.4
1	C	165	GLY	2.3
1	E	111	LEU	2.3
1	A	166	THR	2.3
1	E	53	GLN	2.3
1	B	212	VAL	2.3
1	E	141	ASP	2.3
1	E	347	GLU	2.3
1	F	308	GLU	2.3
1	A	368	ALA	2.3
1	A	324	THR	2.3
1	E	225	THR	2.3
1	B	204	CYS	2.3
1	D	349	LEU	2.3
1	F	110	PHE	2.3
1	F	516	HIS	2.3
1	E	268	ASP	2.3
1	E	370	SER	2.3
1	F	294	ALA	2.3
1	E	421	THR	2.3
1	F	117	THR	2.3
1	F	238	LEU	2.3
1	E	232	GLY	2.3
1	A	367	ILE	2.3
1	D	369	LEU	2.2
1	E	420	ARG	2.2
1	E	503	GLU	2.2
1	F	141	ASP	2.2
1	E	341	ALA	2.2
1	B	324	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	174	THR	2.2
1	C	325	LEU	2.2
1	D	168	CYS	2.2
1	C	170	ALA	2.2
1	A	163	LEU	2.2
1	E	95	PRO	2.2
1	F	381	VAL	2.2
1	E	74	ILE	2.2
1	E	470	LEU	2.2
1	E	197	TYR	2.2
1	F	366	GLN	2.2
1	A	431	PRO	2.2
1	A	123	GLY	2.2
1	E	524	PHE	2.2
1	F	227	LYS	2.2
1	E	329	CYS	2.2
1	E	189	GLU	2.2
1	E	389	ASN	2.1
1	F	112	GLY	2.2
1	C	62	ARG	2.1
1	C	414	PHE	2.1
1	F	302	HIS	2.1
1	C	163	LEU	2.1
1	E	369	LEU	2.1
1	A	61	LYS	2.1
1	A	167	SER	2.1
1	F	293	SER	2.1
1	B	205	ALA	2.1
1	C	368	ALA	2.1
1	A	17	GLY	2.1
1	E	193	ARG	2.1
1	E	480	TYR	2.1
1	E	101	PHE	2.1
1	E	230	SER	2.1
1	F	154	LEU	2.1
1	F	169	GLU	2.1
1	E	140	MET	2.1
1	C	318	HIS	2.1
1	E	145	LYS	2.1
1	F	173	CYS	2.1
1	B	117	THR	2.1
1	B	278	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	369	LEU	2.1
1	E	127	MET	2.1
1	F	375	SER	2.1
1	F	56	PRO	2.1
1	D	408	ILE	2.1
1	E	25	GLU	2.1
1	F	491	MET	2.1
1	B	317	ALA	2.1
1	A	329	CYS	2.1
1	E	102	PRO	2.1
1	C	169	GLU	2.0
1	E	136	GLU	2.0
1	B	367	ILE	2.0
1	F	172	LEU	2.0
1	E	227	LYS	2.0
1	F	146	MET	2.0
1	E	159	GLY	2.0
1	F	158	SER	2.0
1	F	159	GLY	2.0
1	F	362	TYR	2.0
1	A	172	LEU	2.0
1	F	57	GLY	2.0
1	E	167	SER	2.0
1	F	129	SER	2.0
1	B	346	PRO	2.0
1	C	172	LEU	2.0
1	F	115	LEU	2.0
1	A	531	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	E	319	24/25	0.79	0.25	60,68,78,81	0
1	LLP	F	319	24/25	0.90	0.28	44,56,72,76	0
1	LLP	C	319	24/25	0.93	0.23	21,28,31,34	0
1	LLP	D	319	24/25	0.93	0.23	19,23,28,29	0
1	LLP	A	319	24/25	0.94	0.22	19,24,30,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	LLP	B	319	24/25	0.94	0.22	19,25,29,30	0

### 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, 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( $\text{\AA}^2$ )	Q<0.9
2	GOL	C	602	6/6	0.76	0.42	29,38,40,43	6
2	GOL	B	603	6/6	0.79	0.36	18,26,28,31	6
2	GOL	C	601	6/6	0.84	0.49	26,35,37,38	6
2	GOL	B	602	6/6	0.85	0.47	29,31,32,33	6
2	GOL	C	603	6/6	0.86	0.23	28,35,38,39	6
2	GOL	D	601	6/6	0.86	0.49	23,28,34,34	6
2	GOL	D	602	6/6	0.87	0.50	30,32,32,36	6
2	GOL	B	601	6/6	0.90	0.48	24,30,32,35	6
2	GOL	A	601	6/6	0.90	0.45	27,31,32,35	6

### 6.5 Other polymers [i](#)

There are no such residues in this entry.