



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 11:09 AM UTC

PDB ID : 6LIV / pdb_00006liv
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

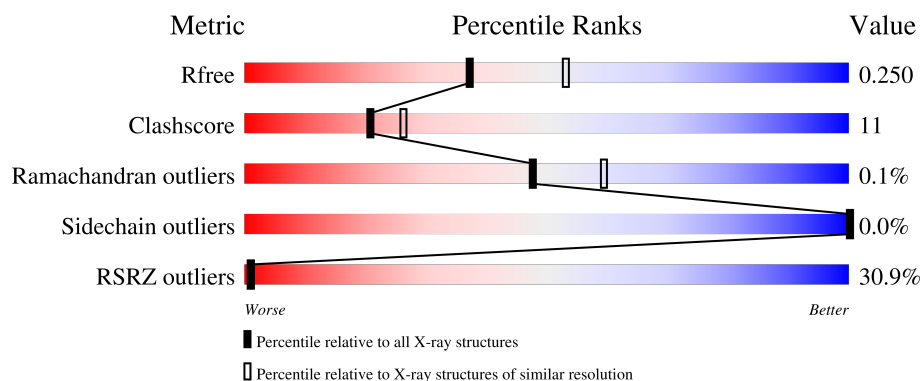
1 Overall quality at a glance

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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (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 ≥ 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	4% 80% 11% 9%
1	B	531	3% 81% 10% 9%
1	C	531	5% 79% 12% 9%
1	D	531	3% 81% 9% 9%
1	E	531	80% 56% 34% 10%

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Mol	Chain	Length	Quality of chain
1	F	531	72% 52% 37% 10%

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

2 Entry composition [i](#)

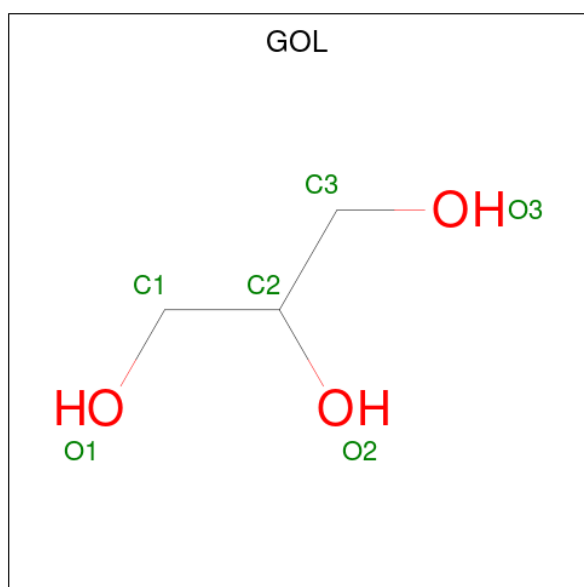
There are 3 unique types of molecules in this entry. The entry contains 23982 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

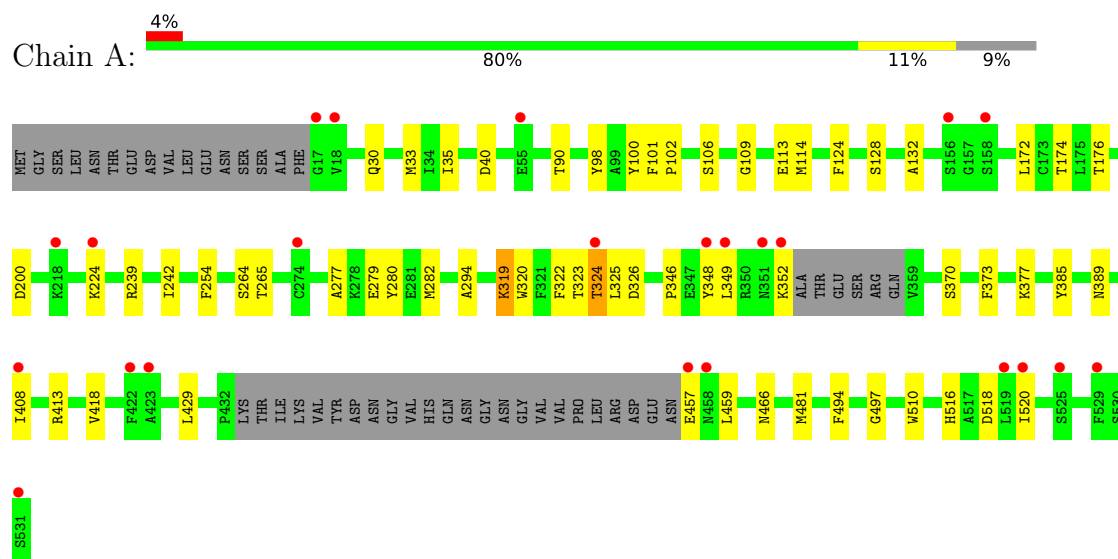
- Molecule 3 is water.

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

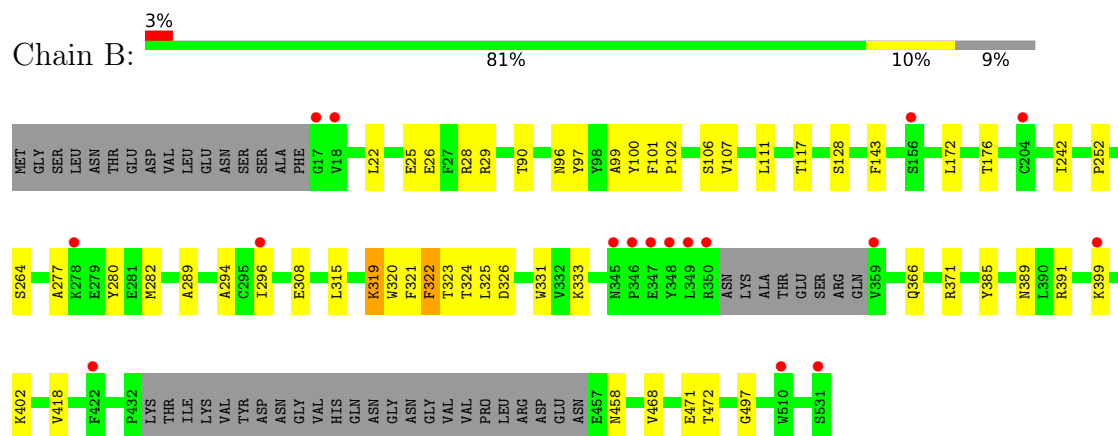
3 Residue-property plots [i](#)

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.

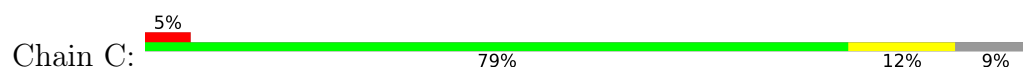
• Molecule 1: Tyrosine/DOPA decarboxylase 2

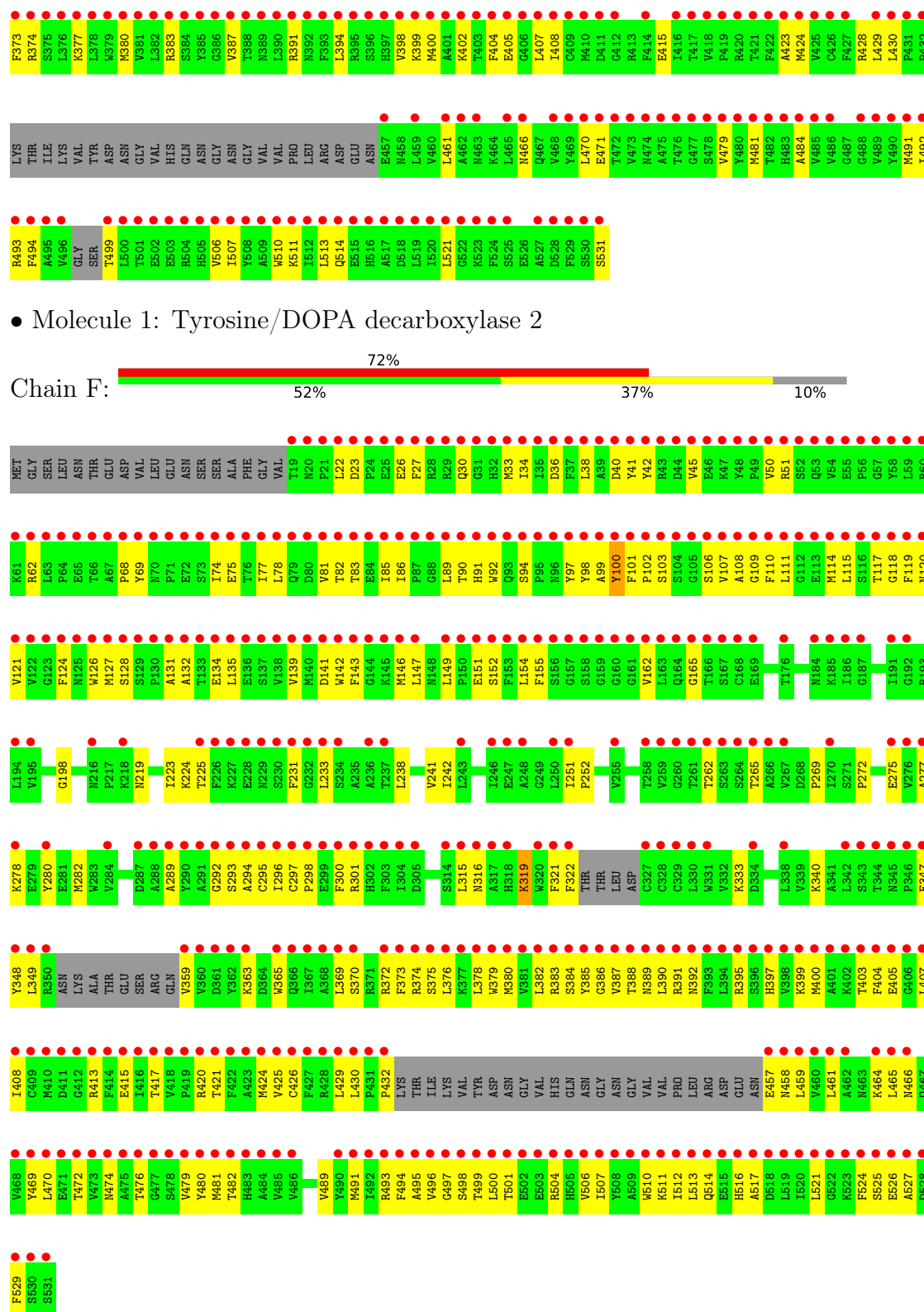


• Molecule 1: Tyrosine/DOPA decarboxylase 2



• Molecule 1: Tyrosine/DOPA decarboxylase 2





● Molecule 1: Tyrosine/DOPA decarboxylase 2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	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) 99.6 (49.84-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	10120 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23982	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, GOL

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	0.27	3/3909 (0.1%)	0.33	0/5307
1	B	0.36	4/3892 (0.1%)	0.40	4/5285 (0.1%)
1	C	0.34	4/3909 (0.1%)	0.36	1/5307 (0.0%)
1	D	0.20	0/3892	0.33	0/5285
1	E	0.25	1/3870 (0.0%)	0.40	0/5254
1	F	0.28	0/3850	0.50	2/5225 (0.0%)
All	All	0.29	12/23322 (0.1%)	0.39	7/31663 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	471	GLU	C-O	-8.10	1.14	1.24
1	C	100	TYR	C-O	-7.58	1.14	1.24
1	B	100	TYR	C-O	-6.95	1.15	1.24
1	A	100	TYR	C-O	-6.89	1.15	1.24
1	C	101	PHE	C-O	-6.32	1.17	1.24
1	B	101	PHE	C-O	-6.02	1.18	1.24
1	C	98	TYR	C-O	-5.91	1.16	1.24
1	C	97	TYR	C-O	-5.88	1.16	1.24
1	A	101	PHE	C-O	-5.65	1.18	1.24
1	E	100	TYR	C-O	-5.23	1.17	1.24
1	A	98	TYR	C-O	-5.23	1.16	1.24
1	B	96	ASN	C-O	-5.06	1.17	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	PHE	N-CA-C	8.54	123.38	113.38
1	B	321	PHE	N-CA-C	7.57	122.01	111.56
1	B	323	THR	N-CA-C	6.92	119.84	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	263	SER	N-CA-C	6.49	118.14	111.14
1	B	324	THR	N-CA-CB	5.42	119.64	110.49
1	F	100	TYR	CA-C-N	5.38	133.38	122.45
1	F	100	TYR	C-N-CA	5.38	133.38	122.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3840	0	3783	42	0
1	B	3823	0	3764	35	0
1	C	3840	0	3783	52	0
1	D	3823	0	3764	43	0
1	E	3802	0	3743	156	0
1	F	3782	0	3721	227	0
2	A	6	0	8	3	0
2	B	18	0	24	3	0
2	C	18	0	24	10	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	22630	506	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (506) 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:C:277:ALA:HA	1:C:282:MET:HE3	1.56	0.87
1:F:74:ILE:HA	1:F:77:ILE:HG22	1.59	0.85
1:D:277:ALA:HA	1:D:282:MET:HE3	1.62	0.82
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:B:277:ALA:HA	1:B:282:MET:HE3	1.64	0.79
1:C:280:TYR:HB2	1:C:282:MET:HE2	1.63	0.78
1:A:277:ALA:HA	1:A:282:MET:HE3	1.66	0.77
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:280:TYR:HB2	1:F:282:MET:HE2	1.69	0.75
1:F:277:ALA:HA	1:F:282:MET:HE3	1.70	0.73
1:A:280:TYR:HB2	1:A:282:MET:HE2	1.69	0.73
1:B:280:TYR:HB2	1:B:282:MET:HE2	1.69	0.73
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
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:C:30:GLN:HA	1:C:33:MET:HE3	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:D:280:TYR:HB2	1:D:282:MET:HE2	1.75	0.69
1:A:30:GLN:HA	1:A:33:MET:HE3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:131:ALA:C	1:F:135:LEU:HD12	2.21	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:A:35:ILE:HD11	1:A:114:MET:HE1	1.79	0.63
1:E:289:ALA:HA	1:E:316:ASN:H	1.63	0.62
1:F:385:TYR:C	1:F:389:ASN:HD21	2.06	0.62
1:C:25:GLU:OE2	1:C:28:ARG:NH1	2.32	0.62
1:E:481:MET:HE1	1:E:513:LEU:HD21	1.81	0.62
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:A:481:MET:HE3	1:A:494:PHE:HD1	1.65	0.62
1:B:319:LLP:H4'1	2:B:601:GOL:H2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:461:LEU:C	1:E:461:LEU:HD13	2.25	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: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:E:93:GLN:CD	1:E:93:GLN:H	2.10	0.58
1:E:206:LEU:HG	1:E:220:PHE:HE1	1.69	0.58
1:E:127:MET:HE2	1:F:51:ARG:HH21	1.67	0.57
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:242:ILE:HD13	1:F:282:MET:HE1	1.86	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:F:400:MET:HE3	1:F:506:VAL:HG21	1.87	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:F:510:TRP:CD1	1:F:511:LYS:HZ3	2.24	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:F:50:VAL:HG21	1:F:479:VAL:C	2.33	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:F:429:LEU:C	1:F:429:LEU:HD13	2.33	0.53
1:F:400:MET:HE2	1:F:496:VAL:HG11	1.91	0.53
1:E:140:MET:HE1	1:E:329:CYS:HB3	1.90	0.53
1:B:319:LLP:NZ	1:B:319:LLP:O3	2.38	0.53
1:C:242:ILE:HD13	1:C:282:MET:HE1	1.90	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:F:457:GLU:CD	1:F:458:ASN:H	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:292:GLY:O	1:F:295:CYS:HB2	2.10	0.51
1:E:29:ARG:HD2	1:E:33:MET:HE2	1.92	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:D:308:GLU:O	1:D:333:LYS:NZ	2.32	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:101:PHE:CE1	1:F:424:MET:HE3	2.47	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:E:126:TRP:C	1:E:128:SER:H	2.20	0.49
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:F:106:SER:HG	1:F:109:GLY:H	1.57	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:470:LEU:HD13	1:F:470:LEU:C	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:90:THR:OG1	1:F:127:MET:O	2.26	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:457:GLU:OE1	1:F:459:LEU:N	2.46	0.48
1:A:294:ALA:HB2	1:A:320:TRP:CZ3	2.48	0.48
1:E:278:LYS:HD2	1:E:278:LYS:C	2.37	0.48
1:F:143:PHE:HA	1:F:146:MET:HE3	1.94	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:E:326:ASP:CG	1:E:374:ARG:HH12	2.22	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:A:481:MET:HE3	1:A:494:PHE:CD1	2.48	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:B:308:GLU:O	1:B:333:LYS:NZ	2.35	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: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:F:525:SER:C	1:F:527:ALA:H	2.22	0.47
1:A:239:ARG:NH2	1:A:279:GLU:OE1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LEU:O	1:B:176:THR:HG23	2.15	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: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: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:A:242:ILE:HD13	1:A:282:MET:HE1	1.97	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
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:C:426:CYS:HB3	1:C:491:MET:HE3	1.98	0.46
1:F:375:SER:O	1:F:379:TRP:N	2.49	0.46
1:D:458:ASN:OD1	1:D:458:ASN:N	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: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:E:146:MET:HE3	1:E:146:MET:HB2	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:285:HIS:NE2	1:E:314:SER:OG	2.50	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:F:424:MET:HE1	1:F:493:ARG:HH21	1.81	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
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: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:E:283:TRP:HE1	1:E:312:SER:HG	1.64	0.44
1:F:127:MET:HE3	1:F:127:MET:HA	2.00	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:497:GLY:C	1:F:499:THR:H	2.26	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:F:101:PHE:HE1	1:F:424:MET:HE3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:114:MET:HE3	1:F:114:MET:HB3	1.70	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:140:MET:HE1	1:C:329:CYS:HB3	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:380:MET:HB2	1:E:380:MET:HE3	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:297:CYS:HB3	1:F:300:PHE:CD1	2.55	0.41
1:F:481:MET:HE3	1:F:494:PHE:HD2	1.85	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:E:461:LEU:C	1:E:461:LEU:CD1	2.93	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
1:F:457:GLU:CD	1:F:458:ASN:N	2.78	0.41
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:A:370:SER:OG	1:B:319:LLP:OP3	2.35	0.41
1:F:424:MET:HE2	1:F:495:ALA:HB2	2.01	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:B:242:ILE:HD13	1:B:282:MET:HE1	2.01	0.41
1:F:139:VAL:HG21	1:F:378:LEU:HD23	2.02	0.41
1:E:90:THR:HB	1:F:128:SER:C	2.45	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:278:LYS:NZ	3:D:704:HOH:O	2.34	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:F:275:GLU:HG3	1:F:278:LYS:HZ3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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%)	43	53
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%)	43	53
1	F	468/531 (88%)	443 (95%)	25 (5%)	0	100	100
All	All	2846/3186 (89%)	2758 (97%)	86 (3%)	2 (0%)	48	59

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%)	415 (100%)	0	100	100
1	B	413/455 (91%)	413 (100%)	0	100	100
1	C	415/455 (91%)	415 (100%)	0	100	100
1	D	413/455 (91%)	412 (100%)	1 (0%)	87	94
1	E	411/455 (90%)	411 (100%)	0	100	100
1	F	408/455 (90%)	408 (100%)	0	100	100
All	All	2475/2730 (91%)	2474 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	262	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	201	GLN
1	B	514	GLN
1	D	302	HIS
1	D	467	GLN
1	E	96	ASN
1	E	120	ASN
1	E	201	GLN
1	E	302	HIS
1	E	392	ASN
1	E	514	GLN
1	F	30	GLN

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Mol	Chain	Res	Type
1	F	120	ASN
1	F	514	GLN

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	D	319	1	23,24,25	2.50	6 (26%)	25,32,34	1.31	4 (16%)
1	LLP	E	319	1	23,24,25	2.48	6 (26%)	25,32,34	1.40	3 (12%)
1	LLP	A	319	1	23,24,25	2.48	6 (26%)	25,32,34	1.32	4 (16%)
1	LLP	C	319	1	23,24,25	2.49	6 (26%)	25,32,34	1.34	4 (16%)
1	LLP	F	319	1	23,24,25	2.48	6 (26%)	25,32,34	1.39	4 (16%)
1	LLP	B	319	1	23,24,25	2.49	6 (26%)	25,32,34	1.30	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	D	319	1	-	2/16/17/19	0/1/1/1
1	LLP	E	319	1	-	6/16/17/19	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	F	319	1	-	5/16/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	B	319	1	-	2/16/17/19	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	319	LLP	C4-C4'	7.23	1.62	1.46
1	D	319	LLP	C4-C4'	7.20	1.62	1.46
1	B	319	LLP	C4-C4'	7.16	1.61	1.46
1	F	319	LLP	C4-C4'	7.15	1.61	1.46
1	A	319	LLP	C4-C4'	7.14	1.61	1.46
1	C	319	LLP	C4-C4'	7.12	1.61	1.46
1	F	319	LLP	C4'-NZ	4.99	1.43	1.27
1	E	319	LLP	C4'-NZ	4.98	1.43	1.27
1	D	319	LLP	C4'-NZ	4.98	1.43	1.27
1	B	319	LLP	C4'-NZ	4.92	1.43	1.27
1	A	319	LLP	C4'-NZ	4.91	1.43	1.27
1	C	319	LLP	C4'-NZ	4.91	1.43	1.27
1	C	319	LLP	C2'-C2	3.76	1.56	1.50
1	F	319	LLP	C2'-C2	3.76	1.56	1.50
1	B	319	LLP	C2'-C2	3.76	1.56	1.50
1	D	319	LLP	C4-C5	-3.75	1.36	1.42
1	D	319	LLP	C2'-C2	3.75	1.56	1.50
1	C	319	LLP	C4-C5	-3.73	1.36	1.42
1	E	319	LLP	C2'-C2	3.73	1.56	1.50
1	A	319	LLP	C2'-C2	3.72	1.56	1.50
1	A	319	LLP	C4-C5	-3.71	1.36	1.42
1	B	319	LLP	C4-C5	-3.70	1.36	1.42
1	F	319	LLP	C4-C5	-3.51	1.37	1.42
1	E	319	LLP	C4-C5	-3.33	1.37	1.42
1	F	319	LLP	C6-N1	3.11	1.40	1.34
1	C	319	LLP	C6-N1	3.11	1.40	1.34
1	E	319	LLP	C6-N1	3.08	1.40	1.34
1	A	319	LLP	C6-N1	3.08	1.40	1.34
1	B	319	LLP	C6-N1	3.08	1.40	1.34
1	D	319	LLP	C6-N1	3.05	1.40	1.34
1	F	319	LLP	C5'-C5	2.27	1.56	1.50
1	E	319	LLP	C5'-C5	2.26	1.56	1.50
1	D	319	LLP	C5'-C5	2.12	1.56	1.50
1	C	319	LLP	C5'-C5	2.11	1.56	1.50
1	A	319	LLP	C5'-C5	2.08	1.56	1.50
1	B	319	LLP	C5'-C5	2.05	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	-3.69	107.01	124.04
1	F	319	LLP	C4-C4'-NZ	-3.45	108.11	124.04
1	B	319	LLP	C4-C4'-NZ	-3.44	108.15	124.04
1	C	319	LLP	C4-C4'-NZ	-3.44	108.15	124.04
1	A	319	LLP	C4-C4'-NZ	-3.41	108.29	124.04
1	D	319	LLP	C4-C4'-NZ	-3.39	108.40	124.04
1	C	319	LLP	CE-NZ-C4'	-2.74	109.94	118.72
1	A	319	LLP	CE-NZ-C4'	-2.73	109.97	118.72
1	D	319	LLP	CE-NZ-C4'	-2.70	110.07	118.72
1	B	319	LLP	CE-NZ-C4'	-2.69	110.11	118.72
1	F	319	LLP	CE-NZ-C4'	-2.69	110.11	118.72
1	C	319	LLP	C5-C6-N1	-2.54	119.70	123.83
1	B	319	LLP	C5-C6-N1	-2.52	119.73	123.83
1	A	319	LLP	C5-C6-N1	-2.51	119.75	123.83
1	D	319	LLP	C5-C6-N1	-2.47	119.81	123.83
1	E	319	LLP	CE-NZ-C4'	-2.31	111.33	118.72
1	C	319	LLP	C3-C4-C5	2.26	120.09	118.28
1	F	319	LLP	C5-C6-N1	-2.20	120.25	123.83
1	D	319	LLP	C3-C4-C5	2.19	120.03	118.28
1	A	319	LLP	C3-C4-C5	2.16	120.01	118.28
1	B	319	LLP	C3-C4-C5	2.13	119.99	118.28
1	F	319	LLP	C3-C4-C5	2.11	119.97	118.28
1	E	319	LLP	C5-C6-N1	-2.07	120.46	123.83

There are no chirality outliers.

All (19) 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	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	D	319	LLP	C4-C4'-NZ-CE
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

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Mol	Chain	Res	Type	Atoms
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	CE-CD-CG-CB
1	F	319	LLP	CD-CE-NZ-C4'
1	E	319	LLP	C-CA-CB-CG

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	319	LLP	4	0
1	E	319	LLP	1	0
1	A	319	LLP	3	0
1	C	319	LLP	2	0
1	F	319	LLP	1	0
1	B	319	LLP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	D	602	-	5,5,5	0.44	0	5,5,5	0.68	0
2	GOL	B	602	-	5,5,5	0.32	0	5,5,5	0.67	0
2	GOL	B	603	-	5,5,5	0.73	0	5,5,5	1.10	0
2	GOL	A	601	-	5,5,5	0.27	0	5,5,5	1.05	0
2	GOL	C	601	-	5,5,5	0.15	0	5,5,5	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	C	603	-	5,5,5	0.63	0	5,5,5	1.24	1 (20%)
2	GOL	B	601	-	5,5,5	0.44	0	5,5,5	0.73	0
2	GOL	D	601	-	5,5,5	0.61	0	5,5,5	0.46	0
2	GOL	C	602	-	5,5,5	0.25	0	5,5,5	0.59	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	D	602	-	-	2/4/4/4	-
2	GOL	B	602	-	-	0/4/4/4	-
2	GOL	B	603	-	-	2/4/4/4	-
2	GOL	A	601	-	-	4/4/4/4	-
2	GOL	C	601	-	-	4/4/4/4	-
2	GOL	C	603	-	-	2/4/4/4	-
2	GOL	B	601	-	-	2/4/4/4	-
2	GOL	D	601	-	-	4/4/4/4	-
2	GOL	C	602	-	-	2/4/4/4	-

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	2.23	120.42	110.38

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

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Mol	Chain	Res	Type	Atoms
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 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	602	GOL	4	0
2	A	601	GOL	3	0
2	C	601	GOL	6	0
2	C	603	GOL	2	0
2	B	601	GOL	3	0
2	D	601	GOL	4	0
2	C	602	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	484/531 (91%)	0.32	23 (4%) 35 38	21, 30, 47, 74	0
1	B	482/531 (90%)	0.18	17 (3%) 47 50	21, 28, 43, 86	0
1	C	484/531 (91%)	0.36	29 (5%) 27 30	20, 30, 51, 83	0
1	D	482/531 (90%)	0.21	16 (3%) 49 52	20, 28, 43, 77	0
1	E	478/531 (90%)	3.99	426 (89%) 0 0	52, 76, 91, 101	0
1	F	476/531 (89%)	3.99	382 (80%) 0 0	43, 74, 96, 104	0
All	All	2886/3186 (90%)	1.50	893 (30%) 1 1	20, 33, 89, 104	0

All (893) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	387	VAL	10.7
1	E	22	LEU	10.4
1	F	382	LEU	10.0
1	F	74	ILE	9.7
1	E	500	LEU	9.7
1	F	379	TRP	9.6
1	F	42	TYR	9.4
1	E	20	ASN	9.4
1	F	41	TYR	9.3
1	E	394	LEU	8.8
1	F	92	TRP	8.8
1	F	48	TYR	8.6
1	E	121	VAL	8.4
1	F	506	VAL	8.4
1	E	105	GLY	8.4
1	E	69	TYR	8.4
1	E	507	ILE	8.3
1	E	382	LEU	8.3
1	E	379	TRP	8.3

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Mol	Chain	Res	Type	RSRZ
1	E	59	LEU	8.2
1	E	21	PRO	8.1
1	F	59	LEU	8.1
1	F	384	SER	8.0
1	F	90	THR	8.0
1	F	45	VAL	7.9
1	F	77	ILE	7.9
1	B	348	TYR	7.9
1	E	24	PRO	7.9
1	E	479	VAL	7.8
1	F	393	PHE	7.7
1	E	68	PRO	7.7
1	F	480	TYR	7.6
1	F	423	ALA	7.6
1	E	42	TYR	7.6
1	F	35	ILE	7.5
1	F	89	LEU	7.5
1	F	394	LEU	7.5
1	F	318	HIS	7.5
1	F	513	LEU	7.5
1	F	327	CYS	7.4
1	F	119	PHE	7.4
1	F	67	ALA	7.4
1	E	506	VAL	7.3
1	F	404	PHE	7.3
1	F	403	THR	7.3
1	E	27	PHE	7.3
1	E	137	SER	7.3
1	F	296	ILE	7.2
1	F	71	PRO	7.2
1	E	142	TRP	7.2
1	F	406	GLY	7.1
1	F	510	TRP	7.1
1	E	45	VAL	7.1
1	E	88	GLY	7.0
1	F	381	VAL	7.0
1	E	35	ILE	7.0
1	E	496	VAL	6.9
1	F	33	MET	6.9
1	F	500	LEU	6.9
1	E	512	ILE	6.9
1	F	474	ASN	6.9

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Mol	Chain	Res	Type	RSRZ
1	F	21	PRO	6.9
1	F	407	LEU	6.9
1	F	425	VAL	6.9
1	F	24	PRO	6.8
1	F	82	THR	6.8
1	F	85	ILE	6.8
1	E	58	TYR	6.8
1	F	30	GLN	6.8
1	E	48	TYR	6.8
1	E	381	VAL	6.8
1	F	416	ILE	6.8
1	E	328	CYS	6.8
1	E	373	PHE	6.8
1	F	121	VAL	6.7
1	F	49	PRO	6.7
1	F	142	TRP	6.7
1	F	377	LYS	6.7
1	F	494	PHE	6.6
1	E	122	VAL	6.6
1	F	472	THR	6.6
1	E	383	ARG	6.6
1	F	99	ALA	6.6
1	F	373	PHE	6.6
1	E	82	THR	6.6
1	E	267	VAL	6.6
1	E	89	LEU	6.6
1	E	422	PHE	6.6
1	F	107	VAL	6.6
1	F	108	ALA	6.5
1	F	143	PHE	6.5
1	F	507	ILE	6.5
1	F	383	ARG	6.5
1	F	111	LEU	6.5
1	F	86	ILE	6.5
1	F	78	LEU	6.5
1	F	390	LEU	6.5
1	F	37	PHE	6.5
1	F	408	ILE	6.4
1	F	512	ILE	6.4
1	F	38	LEU	6.4
1	E	404	PHE	6.4
1	F	322	PHE	6.4

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Mol	Chain	Res	Type	RSRZ
1	F	128	SER	6.4
1	E	499	THR	6.4
1	F	50	VAL	6.4
1	F	63	LEU	6.4
1	F	66	THR	6.4
1	F	398	VAL	6.4
1	F	479	VAL	6.4
1	E	378	LEU	6.4
1	E	57	GLY	6.4
1	E	393	PHE	6.3
1	F	127	MET	6.3
1	E	109	GLY	6.3
1	F	96	ASN	6.3
1	F	97	TYR	6.3
1	E	372	ARG	6.3
1	F	498	SER	6.3
1	F	422	PHE	6.3
1	F	400	MET	6.3
1	E	81	VAL	6.2
1	F	39	ALA	6.2
1	F	105	GLY	6.2
1	F	317	ALA	6.2
1	E	390	LEU	6.2
1	E	54	VAL	6.2
1	E	115	LEU	6.2
1	E	123	GLY	6.2
1	F	429	LEU	6.2
1	E	41	TYR	6.2
1	F	94	SER	6.2
1	E	19	THR	6.2
1	F	95	PRO	6.2
1	E	423	ALA	6.1
1	F	401	ALA	6.1
1	F	497	GLY	6.1
1	F	104	SER	6.1
1	F	58	TYR	6.1
1	E	132	ALA	6.1
1	F	54	VAL	6.1
1	F	521	LEU	6.1
1	E	324	THR	6.0
1	F	83	THR	6.0
1	F	297	CYS	6.0

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Mol	Chain	Res	Type	RSRZ
1	F	76	THR	6.0
1	F	481	MET	6.0
1	F	386	GLY	6.0
1	F	385	TYR	6.0
1	F	427	PHE	6.0
1	F	396	SER	6.0
1	E	114	MET	6.0
1	E	74	ILE	6.0
1	F	378	LEU	5.9
1	F	294	ALA	5.9
1	E	92	TRP	5.9
1	E	52	SER	5.9
1	F	426	CYS	5.9
1	F	133	THR	5.9
1	F	88	GLY	5.9
1	F	520	ILE	5.8
1	F	321	PHE	5.8
1	E	131	ALA	5.8
1	F	81	VAL	5.8
1	E	330	LEU	5.8
1	F	91	HIS	5.8
1	E	106	SER	5.8
1	E	110	PHE	5.8
1	E	478	SER	5.8
1	E	107	VAL	5.8
1	E	509	ALA	5.8
1	B	349	LEU	5.7
1	F	432	PRO	5.7
1	E	365	TRP	5.7
1	A	348	TYR	5.7
1	E	380	MET	5.7
1	E	149	LEU	5.7
1	E	154	LEU	5.7
1	F	132	ALA	5.7
1	E	117	THR	5.7
1	E	87	PRO	5.7
1	E	86	ILE	5.6
1	F	122	VAL	5.6
1	E	403	THR	5.6
1	E	410	MET	5.6
1	F	457	GLU	5.6
1	F	412	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
1	E	163	LEU	5.6
1	F	93	GLN	5.6
1	F	473	VAL	5.5
1	F	375	SER	5.5
1	F	391	ARG	5.5
1	E	320	TRP	5.5
1	E	331	TRP	5.5
1	F	499	THR	5.5
1	E	292	GLY	5.5
1	E	387	VAL	5.5
1	E	519	LEU	5.5
1	E	162	VAL	5.5
1	F	110	PHE	5.5
1	F	410	MET	5.5
1	E	30	GLN	5.5
1	E	119	PHE	5.4
1	E	419	PRO	5.4
1	E	385	TYR	5.4
1	F	517	ALA	5.4
1	F	496	VAL	5.4
1	E	124	PHE	5.4
1	F	300	PHE	5.4
1	E	362	TYR	5.4
1	E	84	GLU	5.4
1	E	96	ASN	5.4
1	E	298	PRO	5.4
1	F	98	TYR	5.4
1	E	94	SER	5.3
1	F	501	THR	5.3
1	E	317	ALA	5.3
1	E	147	LEU	5.3
1	F	138	VAL	5.3
1	E	300	PHE	5.3
1	E	304	ILE	5.3
1	E	161	GLY	5.3
1	E	315	LEU	5.3
1	F	124	PHE	5.3
1	F	348	TYR	5.3
1	E	38	LEU	5.3
1	F	120	ASN	5.2
1	E	325	LEU	5.2
1	E	360	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	F	359	VAL	5.2
1	E	143	PHE	5.2
1	E	322	PHE	5.2
1	F	106	SER	5.2
1	F	370	SER	5.2
1	F	112	GLY	5.2
1	F	292	GLY	5.2
1	E	64	PRO	5.2
1	E	90	THR	5.2
1	E	395	ARG	5.2
1	F	421	THR	5.2
1	E	108	ALA	5.2
1	F	392	ASN	5.2
1	C	352	LYS	5.2
1	F	477	GLY	5.2
1	F	56	PRO	5.2
1	F	431	PRO	5.2
1	E	508	TYR	5.2
1	E	401	ALA	5.2
1	E	111	LEU	5.2
1	F	129	SER	5.2
1	E	323	THR	5.2
1	F	430	LEU	5.1
1	F	475	ALA	5.1
1	E	376	LEU	5.1
1	F	349	LEU	5.1
1	F	470	LEU	5.1
1	F	80	ASP	5.1
1	F	331	TRP	5.1
1	E	307	VAL	5.1
1	F	529	PHE	5.1
1	D	324	THR	5.1
1	F	117	THR	5.1
1	E	513	LEU	5.1
1	F	22	LEU	5.1
1	F	36	ASP	5.1
1	E	427	PHE	5.1
1	F	34	ILE	5.1
1	F	380	MET	5.1
1	E	91	HIS	5.1
1	E	97	TYR	5.0
1	F	478	SER	5.0

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Mol	Chain	Res	Type	RSRZ
1	F	165	GLY	5.0
1	E	418	VAL	5.0
1	F	156	SER	5.0
1	F	414	PHE	5.0
1	E	296	ILE	5.0
1	E	514	GLN	5.0
1	E	398	VAL	5.0
1	F	114	MET	5.0
1	F	25	GLU	5.0
1	F	135	LEU	5.0
1	E	384	SER	4.9
1	F	469	TYR	4.9
1	C	529	PHE	4.9
1	F	51	ARG	4.9
1	E	72	GLU	4.9
1	F	31	GLY	4.9
1	F	315	LEU	4.9
1	F	84	GLU	4.9
1	F	64	PRO	4.9
1	F	109	GLY	4.9
1	F	118	GLY	4.9
1	E	511	LYS	4.9
1	E	139	VAL	4.9
1	F	69	TYR	4.9
1	E	83	THR	4.9
1	F	482	THR	4.9
1	E	326	ASP	4.9
1	E	104	SER	4.9
1	E	293	SER	4.9
1	F	32	HIS	4.9
1	F	265	THR	4.9
1	F	417	THR	4.9
1	F	115	LEU	4.8
1	F	519	LEU	4.8
1	E	39	ALA	4.8
1	E	510	TRP	4.8
1	F	495	ALA	4.8
1	E	73	SER	4.8
1	E	103	SER	4.8
1	F	28	ARG	4.8
1	E	474	ASN	4.8
1	E	503	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	F	103	SER	4.8
1	E	43	ARG	4.8
1	E	408	ILE	4.8
1	F	20	ASN	4.8
1	F	374	ARG	4.8
1	F	413	ARG	4.8
1	F	418	VAL	4.8
1	E	133	THR	4.8
1	E	391	ARG	4.8
1	E	61	LYS	4.8
1	E	174	THR	4.7
1	E	270	ILE	4.7
1	E	316	ASN	4.7
1	F	468	VAL	4.7
1	F	27	PHE	4.7
1	E	294	ALA	4.7
1	E	477	GLY	4.7
1	E	128	SER	4.7
1	F	163	LEU	4.7
1	E	98	TYR	4.7
1	E	290	TYR	4.7
1	E	289	ALA	4.7
1	E	116	SER	4.7
1	E	44	ASP	4.7
1	F	295	CYS	4.7
1	E	135	LEU	4.7
1	F	511	LYS	4.7
1	E	127	MET	4.7
1	E	120	ASN	4.6
1	E	397	HIS	4.6
1	F	397	HIS	4.6
1	F	409	CYS	4.6
1	F	320	TRP	4.6
1	F	100	TYR	4.6
1	F	514	GLN	4.6
1	E	23	ASP	4.6
1	E	77	ILE	4.6
1	A	457	GLU	4.6
1	E	126	TRP	4.6
1	E	150	PRO	4.6
1	E	531	SER	4.6
1	F	389	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	388	THR	4.6
1	E	465	LEU	4.6
1	F	46	GLU	4.6
1	E	93	GLN	4.6
1	F	388	THR	4.6
1	E	138	VAL	4.6
1	F	424	MET	4.6
1	E	494	PHE	4.5
1	A	531	SER	4.5
1	F	52	SER	4.5
1	E	51	ARG	4.5
1	E	175	LEU	4.5
1	E	321	PHE	4.5
1	C	531	SER	4.5
1	E	155	PHE	4.5
1	E	471	GLU	4.5
1	F	369	LEU	4.5
1	E	457	GLU	4.5
1	E	274	CYS	4.5
1	F	298	PRO	4.4
1	F	303	PHE	4.4
1	F	141	ASP	4.4
1	E	63	LEU	4.4
1	E	71	PRO	4.4
1	E	284	VAL	4.4
1	F	57	GLY	4.4
1	E	402	LYS	4.4
1	F	411	ASP	4.4
1	E	335	PRO	4.4
1	F	19	THR	4.4
1	F	476	THR	4.4
1	E	85	ILE	4.4
1	E	359	VAL	4.4
1	E	140	MET	4.4
1	F	368	ALA	4.4
1	F	329	CYS	4.4
1	E	348	TYR	4.4
1	E	377	LYS	4.4
1	F	140	MET	4.4
1	C	457	GLU	4.3
1	E	46	GLU	4.3
1	E	283	TRP	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	146	MET	4.3
1	E	392	ASN	4.3
1	E	495	ALA	4.3
1	E	32	HIS	4.3
1	E	95	PRO	4.3
1	E	130	PRO	4.3
1	E	295	CYS	4.3
1	E	329	CYS	4.3
1	F	328	CYS	4.3
1	F	267	VAL	4.3
1	F	509	ALA	4.3
1	E	78	LEU	4.3
1	E	480	TYR	4.3
1	F	372	ARG	4.3
1	E	50	VAL	4.2
1	F	360	VAL	4.2
1	E	129	SER	4.2
1	F	73	SER	4.2
1	E	141	ASP	4.2
1	F	518	ASP	4.2
1	F	505	HIS	4.2
1	F	376	LEU	4.2
1	E	113	GLU	4.2
1	F	508	TYR	4.2
1	E	475	ALA	4.2
1	F	87	PRO	4.2
1	E	166	THR	4.2
1	E	265	THR	4.2
1	E	259	VAL	4.2
1	F	139	VAL	4.2
1	E	56	PRO	4.2
1	F	68	PRO	4.2
1	E	37	PHE	4.2
1	E	407	LEU	4.2
1	F	395	ARG	4.2
1	A	18	VAL	4.2
1	F	525	SER	4.2
1	E	146	MET	4.2
1	C	348	TYR	4.2
1	F	47	LYS	4.2
1	E	327	CYS	4.1
1	E	53	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	165	GLY	4.1
1	C	458	ASN	4.1
1	E	425	VAL	4.1
1	E	493	ARG	4.1
1	F	29	ARG	4.1
1	B	346	PRO	4.1
1	F	291	ALA	4.1
1	F	290	TYR	4.1
1	E	476	THR	4.1
1	F	419	PRO	4.1
1	E	170	ALA	4.1
1	E	232	GLY	4.1
1	E	482	THR	4.0
1	E	153	PHE	4.0
1	D	348	TYR	4.0
1	E	399	LYS	4.0
1	E	375	SER	4.0
1	F	299	GLU	4.0
1	E	470	LEU	4.0
1	B	347	GLU	4.0
1	E	65	GLU	4.0
1	E	136	GLU	4.0
1	F	304	ILE	4.0
1	D	349	LEU	4.0
1	F	149	LEU	4.0
1	E	112	GLY	4.0
1	E	469	TYR	4.0
1	F	70	ASN	4.0
1	E	60	ARG	4.0
1	E	238	LEU	4.0
1	F	72	GLU	4.0
1	F	402	LYS	3.9
1	E	516	HIS	3.9
1	F	126	TRP	3.9
1	E	481	MET	3.9
1	E	118	GLY	3.9
1	E	341	ALA	3.9
1	E	421	THR	3.9
1	F	262	THR	3.9
1	E	313	PHE	3.9
1	E	269	PRO	3.9
1	E	306	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	276	VAL	3.9
1	E	286	VAL	3.9
1	E	409	CYS	3.9
1	F	367	ILE	3.9
1	A	17	GLY	3.9
1	E	66	THR	3.9
1	E	99	ALA	3.9
1	E	337	ALA	3.9
1	F	266	ALA	3.9
1	E	371	ARG	3.9
1	E	426	CYS	3.8
1	E	303	PHE	3.8
1	F	130	PRO	3.8
1	F	134	GLU	3.8
1	C	351	ASN	3.8
1	F	365	TRP	3.8
1	F	524	PHE	3.8
1	E	102	PRO	3.8
1	E	62	ARG	3.8
1	E	429	LEU	3.8
1	F	147	LEU	3.8
1	E	76	THR	3.8
1	E	501	THR	3.8
1	E	49	PRO	3.8
1	E	47	LYS	3.8
1	F	43	ARG	3.8
1	E	195	VAL	3.8
1	E	197	TYR	3.8
1	E	261	THR	3.8
1	E	517	ALA	3.8
1	E	75	GLU	3.8
1	F	75	GLU	3.8
1	E	424	MET	3.8
1	E	529	PHE	3.8
1	E	472	THR	3.7
1	E	389	ASN	3.7
1	F	345	ASN	3.7
1	F	399	LYS	3.7
1	E	374	ARG	3.7
1	E	521	LEU	3.7
1	F	465	LEU	3.7
1	E	420	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	346	PRO	3.7
1	E	164	GLN	3.7
1	E	336	SER	3.7
1	F	516	HIS	3.7
1	C	523	LYS	3.7
1	F	231	PHE	3.6
1	F	157	GLY	3.6
1	E	29	ARG	3.6
1	E	260	GLY	3.6
1	E	504	ARG	3.6
1	E	67	ALA	3.6
1	E	310	ALA	3.6
1	F	293	SER	3.6
1	E	28	ARG	3.6
1	E	520	ILE	3.6
1	E	224	LYS	3.6
1	F	125	ASN	3.6
1	E	473	VAL	3.6
1	E	505	HIS	3.6
1	E	151	GLU	3.6
1	F	131	ALA	3.6
1	E	416	ILE	3.5
1	E	226	PHE	3.5
1	E	386	GLY	3.5
1	F	233	LEU	3.5
1	E	299	GLU	3.5
1	E	432	PRO	3.5
1	F	502	GLU	3.5
1	E	205	ALA	3.5
1	E	158	SER	3.5
1	E	26	GLU	3.5
1	E	288	ALA	3.5
1	D	158	SER	3.5
1	E	271	SER	3.5
1	E	100	TYR	3.5
1	E	198	GLY	3.5
1	E	101	PHE	3.5
1	F	113	GLU	3.5
1	F	62	ARG	3.5
1	F	102	PRO	3.5
1	E	334	ASP	3.5
1	C	422	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	262	THR	3.4
1	F	491	MET	3.4
1	F	462	ALA	3.4
1	E	314	SER	3.4
1	E	396	SER	3.4
1	E	157	GLY	3.4
1	F	428	ARG	3.4
1	A	324	THR	3.4
1	E	25	GLU	3.4
1	E	79	GLN	3.4
1	E	191	ILE	3.4
1	E	361	ASP	3.4
1	E	430	LEU	3.4
1	D	346	PRO	3.4
1	F	527	ALA	3.4
1	F	461	LEU	3.4
1	E	199	SER	3.4
1	F	289	ALA	3.4
1	F	101	PHE	3.3
1	F	137	SER	3.3
1	E	40	ASP	3.3
1	E	264	SER	3.3
1	F	61	LYS	3.3
1	F	53	GLN	3.3
1	E	159	GLY	3.3
1	F	123	GLY	3.3
1	F	251	ILE	3.3
1	F	493	ARG	3.3
1	E	414	PHE	3.3
1	E	523	LYS	3.3
1	F	366	GLN	3.3
1	E	332	VAL	3.3
1	F	144	GLY	3.3
1	F	232	GLY	3.3
1	E	36	ASP	3.3
1	E	80	ASP	3.3
1	E	349	LEU	3.3
1	E	256	CYS	3.3
1	E	492	ILE	3.3
1	C	527	ALA	3.2
1	E	33	MET	3.2
1	E	518	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	243	LEU	3.2
1	E	338	LEU	3.2
1	F	154	LEU	3.2
1	F	116	SER	3.2
1	B	278	LYS	3.2
1	F	136	GLU	3.2
1	A	520	ILE	3.2
1	E	273	ILE	3.2
1	E	145	LYS	3.2
1	F	44	ASP	3.2
1	F	361	ASP	3.2
1	E	233	LEU	3.2
1	F	166	THR	3.2
1	F	522	GLY	3.2
1	E	70	ASN	3.2
1	E	411	ASP	3.2
1	E	206	LEU	3.2
1	F	350	ARG	3.1
1	E	168	CYS	3.1
1	E	254	PHE	3.1
1	E	171	ILE	3.1
1	E	282	MET	3.1
1	E	134	GLU	3.1
1	E	515	GLU	3.1
1	F	314	SER	3.1
1	E	522	GLY	3.1
1	F	458	ASN	3.1
1	F	164	GLN	3.1
1	C	18	VAL	3.1
1	E	255	VAL	3.1
1	E	485	VAL	3.1
1	C	114	MET	3.1
1	F	275	GLU	3.1
1	F	503	GLU	3.1
1	E	258	THR	3.1
1	E	156	SER	3.1
1	E	160	GLY	3.1
1	E	213	ALA	3.1
1	F	60	ARG	3.1
1	F	301	ARG	3.1
1	E	369	LEU	3.1
1	F	186	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	261	THR	3.0
1	E	167	SER	3.0
1	E	231	PHE	3.0
1	E	235	ALA	3.0
1	F	79	GLN	3.0
1	F	263	SER	3.0
1	F	531	SER	3.0
1	F	278	LYS	3.0
1	E	220	PHE	3.0
1	F	155	PHE	3.0
1	E	177	ALA	3.0
1	E	266	ALA	3.0
1	E	183	LEU	3.0
1	F	526	GLU	3.0
1	F	227	LYS	3.0
1	F	363	LYS	3.0
1	F	504	ARG	3.0
1	F	152	SER	3.0
1	B	345	ASN	3.0
1	E	318	HIS	3.0
1	E	34	ILE	3.0
1	E	242	ILE	3.0
1	F	191	ILE	3.0
1	E	490	TYR	3.0
1	F	226	PHE	2.9
1	F	362	TYR	2.9
1	E	31	GLY	2.9
1	E	491	MET	2.9
1	F	161	GLY	2.9
1	A	529	PHE	2.9
1	F	276	VAL	2.9
1	E	297	CYS	2.9
1	F	168	CYS	2.9
1	C	525	SER	2.9
1	E	230	SER	2.9
1	F	530	SER	2.9
1	F	484	ALA	2.9
1	E	366	GLN	2.9
1	B	18	VAL	2.9
1	F	162	VAL	2.9
1	E	275	GLU	2.9
1	F	515	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	158	SER	2.9
1	E	406	GLY	2.9
1	D	185	LYS	2.9
1	E	181	ARG	2.9
1	C	349	LEU	2.9
1	F	316	ASN	2.9
1	E	278	LYS	2.8
1	F	195	VAL	2.8
1	D	323	THR	2.8
1	E	246	ILE	2.8
1	F	492	ILE	2.8
1	E	148	ASN	2.8
1	E	268	ASP	2.8
1	E	287	ASP	2.8
1	F	466	ASN	2.8
1	E	236	ALA	2.8
1	F	288	ALA	2.8
1	E	502	GLU	2.8
1	E	483	HIS	2.8
1	F	55	GLU	2.8
1	F	65	GLU	2.8
1	E	178	ALA	2.8
1	E	400	MET	2.8
1	F	523	LYS	2.8
1	E	285	HIS	2.8
1	F	229	ASN	2.8
1	F	490	TYR	2.8
1	B	359	VAL	2.8
1	E	125	ASN	2.7
1	E	466	ASN	2.7
1	F	40	ASP	2.7
1	D	510	TRP	2.7
1	E	152	SER	2.7
1	E	530	SER	2.7
1	E	291	ALA	2.7
1	E	524	PHE	2.7
1	E	202	THR	2.7
1	E	223	ILE	2.7
1	E	251	ILE	2.7
1	E	257	PRO	2.7
1	F	228	GLU	2.7
1	A	224	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	185	LYS	2.7
1	E	196	VAL	2.7
1	F	258	THR	2.7
1	C	530	SER	2.7
1	F	169	GLU	2.7
1	E	459	LEU	2.7
1	F	420	ARG	2.7
1	E	461	LEU	2.7
1	A	351	ASN	2.6
1	E	339	VAL	2.6
1	F	338	LEU	2.6
1	F	184	ASN	2.6
1	E	417	THR	2.6
1	F	259	VAL	2.6
1	E	302	HIS	2.6
1	E	333	LYS	2.6
1	E	204	CYS	2.6
1	D	347	GLU	2.6
1	E	368	ALA	2.6
1	A	458	ASN	2.6
1	E	463	ASN	2.6
1	F	284	VAL	2.6
1	A	352	LYS	2.6
1	E	172	LEU	2.6
1	E	250	LEU	2.6
1	E	347	GLU	2.6
1	F	471	GLU	2.6
1	F	236	ALA	2.6
1	B	422	PHE	2.6
1	E	412	GLY	2.6
1	C	519	LEU	2.5
1	F	528	ASP	2.5
1	F	486	VAL	2.5
1	C	520	ILE	2.5
1	C	409	CYS	2.5
1	E	229	ASN	2.5
1	E	462	ALA	2.5
1	F	287	ASP	2.5
1	C	278	LYS	2.5
1	E	218	LYS	2.5
1	E	272	PRO	2.5
1	F	187	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	489	VAL	2.5
1	F	264	SER	2.5
1	F	460	VAL	2.5
1	E	405	GLU	2.5
1	F	280	TYR	2.5
1	E	245	ASP	2.5
1	F	334	ASP	2.5
1	F	160	GLY	2.5
1	F	260	GLY	2.5
1	E	281	GLU	2.5
1	D	408	ILE	2.5
1	E	186	ILE	2.5
1	C	324	THR	2.4
1	F	230	SER	2.4
1	A	349	LEU	2.4
1	C	17	GLY	2.4
1	A	158	SER	2.4
1	B	531	SER	2.4
1	E	234	SER	2.4
1	E	370	SER	2.4
1	B	296	ILE	2.4
1	E	241	VAL	2.4
1	E	301	ARG	2.4
1	F	216	ASN	2.4
1	F	247	GLU	2.4
1	E	144	GLY	2.4
1	F	192	GLY	2.4
1	E	263	SER	2.4
1	E	484	ALA	2.4
1	E	340	LYS	2.4
1	F	246	ILE	2.4
1	F	270	ILE	2.4
1	C	432	PRO	2.3
1	F	150	PRO	2.3
1	E	192	GLY	2.3
1	F	248	ALA	2.3
1	F	167	SER	2.3
1	E	309	GLU	2.3
1	F	26	GLU	2.3
1	F	347	GLU	2.3
1	E	527	ALA	2.3
1	A	408	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	255	VAL	2.3
1	F	302	HIS	2.3
1	E	201	GLN	2.3
1	C	461	LEU	2.3
1	F	243	LEU	2.3
1	F	330	LEU	2.3
1	F	342	LEU	2.3
1	D	278	LYS	2.3
1	E	227	LYS	2.3
1	F	464	LYS	2.3
1	D	17	GLY	2.3
1	A	423	ALA	2.3
1	D	530	SER	2.3
1	C	497	GLY	2.3
1	C	410	MET	2.3
1	C	69	TYR	2.3
1	E	169	GLU	2.3
1	F	459	LEU	2.2
1	A	55	GLU	2.2
1	F	344	THR	2.2
1	F	415	GLU	2.2
1	A	156	SER	2.2
1	B	399	LYS	2.2
1	E	528	ASP	2.2
1	F	159	GLY	2.2
1	E	55	GLU	2.2
1	F	151	GLU	2.2
1	F	237	THR	2.2
1	F	194	LEU	2.2
1	F	485	VAL	2.2
1	E	219	ASN	2.2
1	E	350	ARG	2.2
1	E	173	CYS	2.2
1	F	483	HIS	2.2
1	D	156	SER	2.2
1	E	525	SER	2.2
1	F	225	THR	2.2
1	E	215	ILE	2.2
1	A	422	PHE	2.2
1	F	23	ASP	2.2
1	F	305	ASP	2.2
1	A	218	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	308	GLU	2.2
1	B	17	GLY	2.2
1	E	187	GLY	2.2
1	E	488	GLY	2.2
1	A	525	SER	2.2
1	F	277	ALA	2.2
1	B	350	ARG	2.1
1	F	250	LEU	2.1
1	F	145	LYS	2.1
1	F	218	LYS	2.1
1	F	343	SER	2.1
1	A	519	LEU	2.1
1	E	184	ASN	2.1
1	F	405	GLU	2.1
1	E	188	ARG	2.1
1	C	423	ALA	2.1
1	C	526	GLU	2.1
1	E	228	GLU	2.1
1	E	280	TYR	2.1
1	E	431	PRO	2.1
1	E	486	VAL	2.1
1	A	274	CYS	2.1
1	F	234	SER	2.1
1	E	367	ILE	2.1
1	F	153	PHE	2.1
1	E	193	ARG	2.1
1	B	156	SER	2.0
1	C	76	THR	2.0
1	F	176	THR	2.0
1	B	204	CYS	2.0
1	D	62	ARG	2.0
1	E	468	VAL	2.0
1	D	529	PHE	2.0
1	B	510	TRP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	LLP	E	319	24/25	0.80	0.20	60,68,78,81	0
1	LLP	F	319	24/25	0.85	0.20	44,56,72,76	0
1	LLP	C	319	24/25	0.95	0.08	21,28,31,34	0
1	LLP	D	319	24/25	0.95	0.08	19,23,28,29	0
1	LLP	A	319	24/25	0.96	0.07	19,24,30,31	0
1	LLP	B	319	24/25	0.96	0.08	19,25,29,30	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	C	601	6/6	0.76	0.18	26,35,37,38	6
2	GOL	C	602	6/6	0.76	0.20	29,38,40,43	6
2	GOL	B	603	6/6	0.80	0.18	18,26,28,31	6
2	GOL	B	601	6/6	0.82	0.17	24,30,32,35	6
2	GOL	C	603	6/6	0.84	0.17	28,35,38,39	6
2	GOL	B	602	6/6	0.85	0.15	29,31,32,33	6
2	GOL	D	601	6/6	0.86	0.15	23,28,34,34	6
2	GOL	A	601	6/6	0.88	0.14	27,31,32,35	6
2	GOL	D	602	6/6	0.88	0.14	30,32,32,36	6

6.5 Other polymers [i](#)

There are no such residues in this entry.