



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:44 PM GMT

PDB ID : 1LS3  
Title : Crystal Structure of the Complex between Rabbit Cytosolic Serine Hydroxymethyltransferase and TriGlu-5-formyl-tetrahydrofolate  
Authors : Fu, T.F.; Scarsdale, J.N.; Kazanina, G.; Schirch, V.; Wright, H.T.  
Deposited on : 2002-05-16  
Resolution : 2.70 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

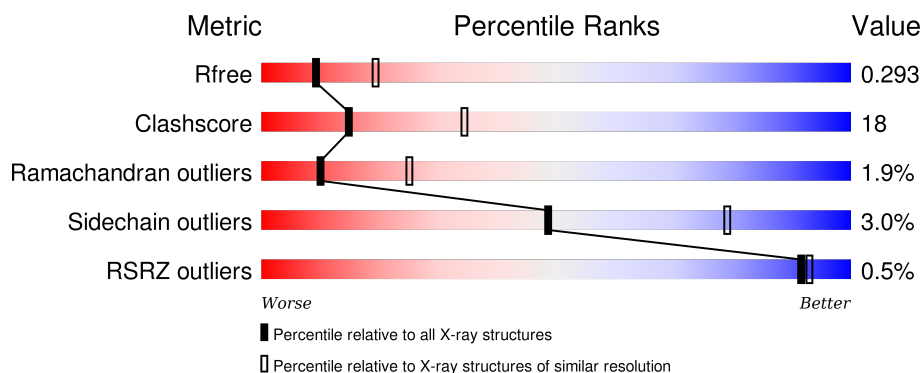
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*





The reported resolution of this entry is 2.70 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	483	 65% 28% • •
1	B	483	 61% 31% • 6%
1	C	483	 66% 28% • •
1	D	483	 62% 29% • 6%

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	PLP	B	419(A)	-	-	-	X
4	TGF	D	420(F)[A]	-	-	-	X
4	TGF	D	420(F)[B]	-	-	-	X
5	GOL	B	422	-	-	-	X
5	GOL	C	421	-	-	-	X

## 2 Entry composition [i](#)

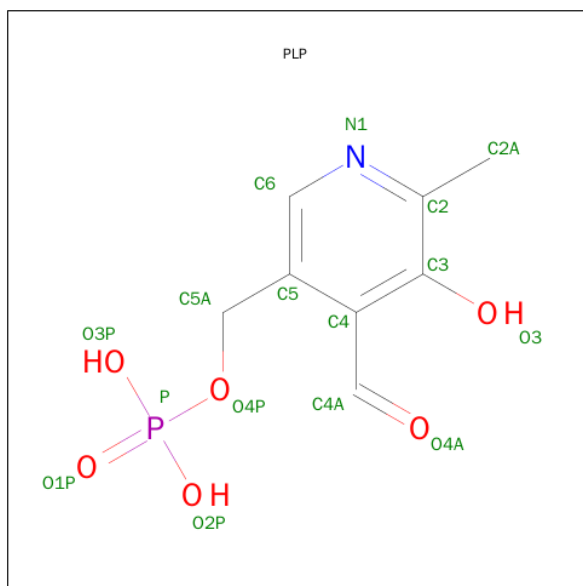
There are 6 unique types of molecules in this entry. The entry contains 14342 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serine Hydroxymethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	1	0
			3489	2187	620	664	18			
1	B	455	Total	C	N	O	S	0	3	0
			3404	2132	611	643	18			
1	C	465	Total	C	N	O	S	0	0	0
			3470	2178	616	658	18			
1	D	456	Total	C	N	O	S	0	0	0
			3374	2115	601	640	18			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



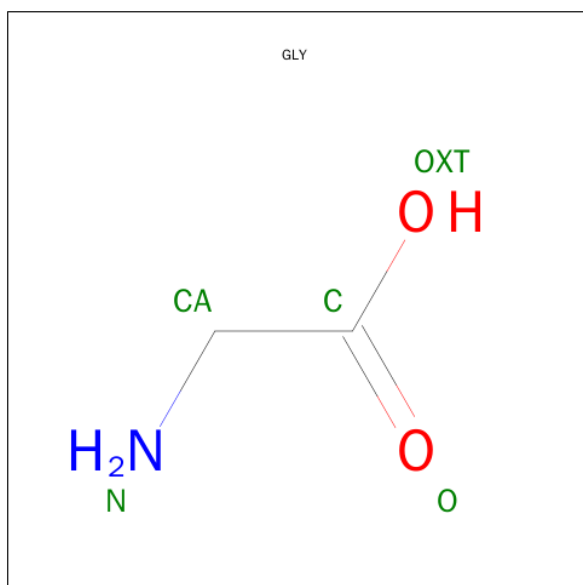
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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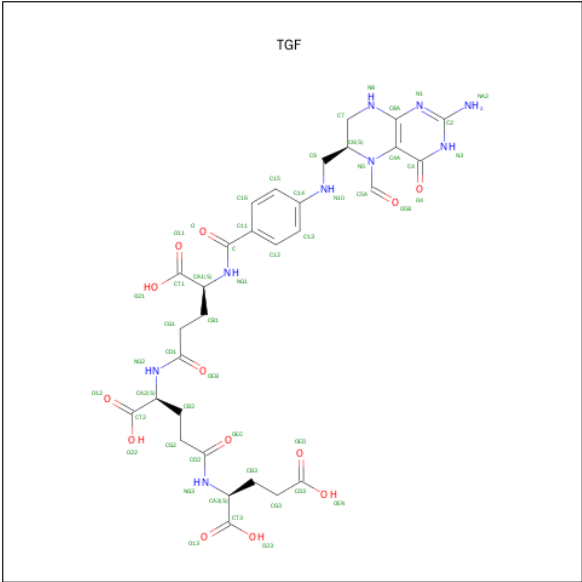
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula:  $C_2H_5NO_2$ ).



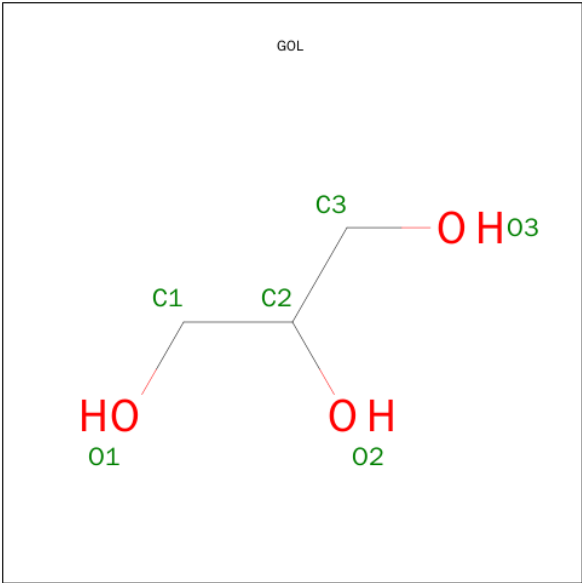
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	2	1	2		
3	C	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 4 is 2-[4-(4-{4-[(2-AMINO-5-FORMYL-4-OXO-3,4,5,6,7,8-HEXAHYDRO-PTERIDIN-6-YLMETHYL)-AMINO]-BENZOYLAMINO}-4-CARBOXY-BUTYRYLAMINO)-4-CARBOXY-BUTYRYLAMINO]-PENTANEDIOIC ACID (three-letter code: TGF) (formula:  $C_{30}H_{37}N_9O_{13}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	1
			60	34	9	17		
4	D	1	Total	C	N	O	0	1
			73	41	11	21		

- Molecule 5 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
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

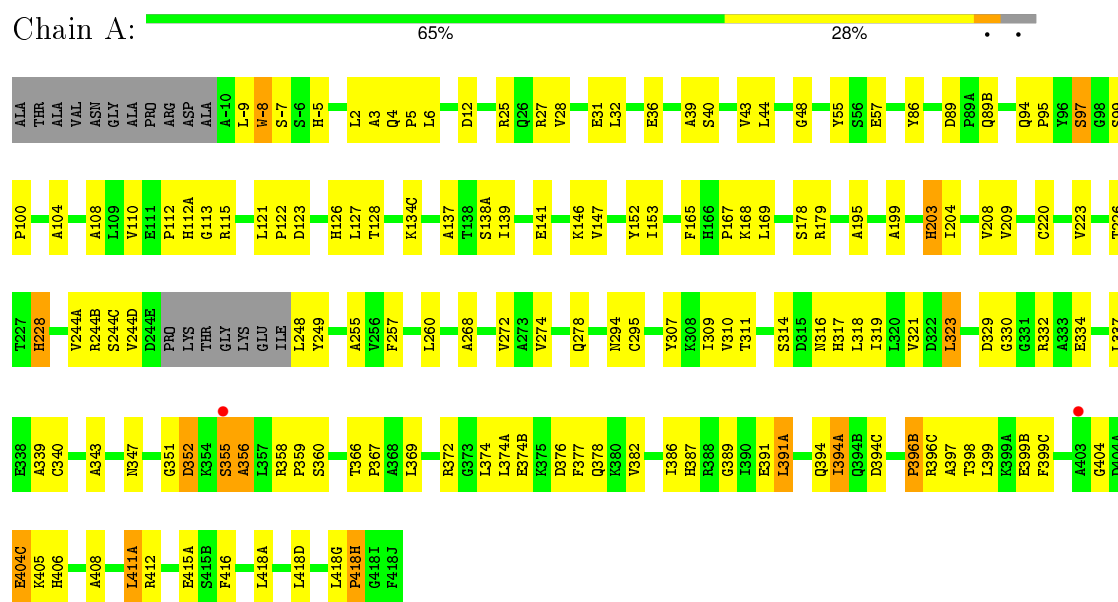
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	99	Total	O	0	0
			99	99		
6	B	107	Total	O	0	0
			107	107		
6	C	99	Total	O	0	0
			99	99		
6	D	73	Total	O	0	0
			73	73		

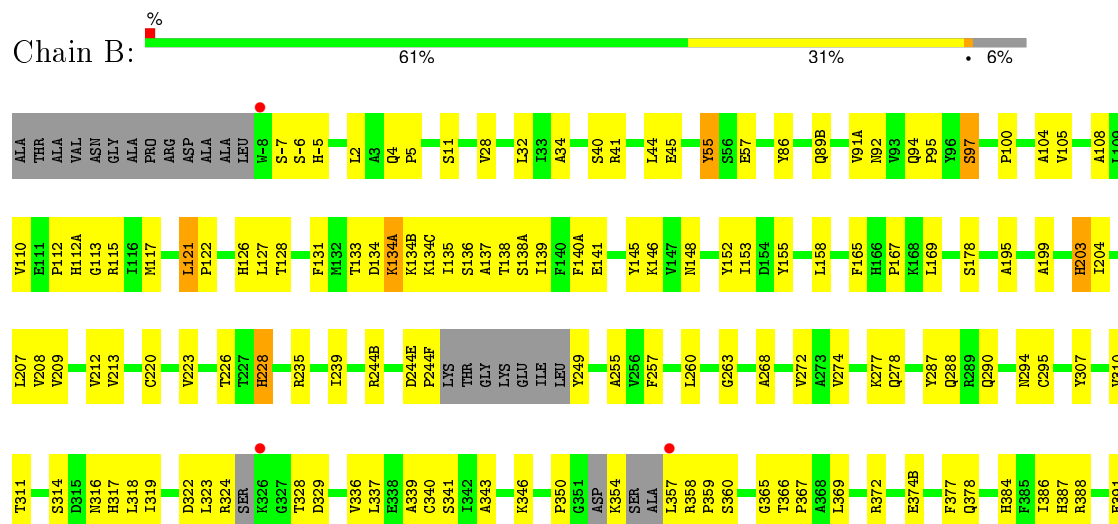
### 3 Residue-property plots

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

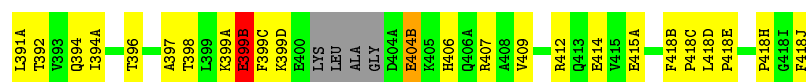
#### • Molecule 1: Serine Hydroxymethyltransferase



#### • Molecule 1: Serine Hydroxymethyltransferase

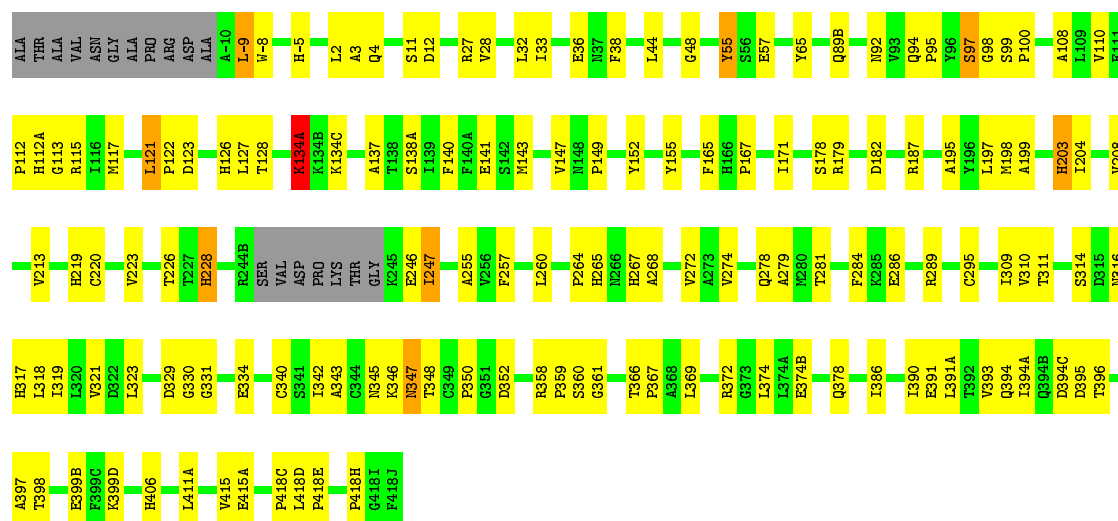






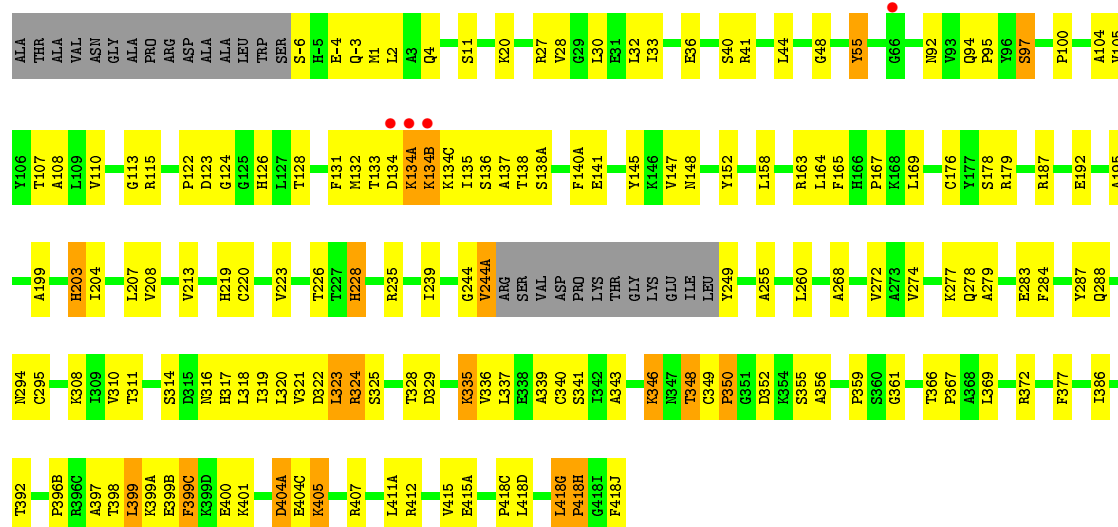
• Molecule 1: Serine Hydroxymethyltransferase

Chain C: 66% 28%



• Molecule 1: Serine Hydroxymethyltransferase

Chain D: 62% 29% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.08Å 114.08Å 156.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.79 – 2.70 35.16 – 2.70	Depositor EDS
% Data completeness (in resolution range)	86.7 (19.79-2.70) 86.7 (35.16-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.68Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.220 , 0.294 0.221 , 0.293	Depositor DCC
$R_{free}$ test set	4794 reflections (10.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 25.7	EDS
Estimated twinning fraction	0.470 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	0 of 47665 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14342	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, TGF, PLP

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	0.38	0/3560	0.62	1/4828 (0.0%)
1	B	0.39	0/3471	0.62	1/4706 (0.0%)
1	C	0.38	0/3541	0.62	0/4804
1	D	0.38	0/3442	0.63	0/4671
All	All	0.38	0/14014	0.62	2/19009 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244(F)	PRO	N-CA-CB	5.76	110.21	103.30
1	A	418(H)	PRO	N-CA-CB	5.61	110.03	103.30

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	3489	0	3326	116	0
1	B	3404	0	3204	134	0
1	C	3470	0	3301	115	0
1	D	3374	0	3201	143	0
2	A	15	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	6	0	0
2	C	15	0	6	0	0
2	D	15	0	6	0	0
3	A	5	0	2	0	0
3	C	5	0	2	2	0
4	B	60	0	10	2	0
4	D	73	0	28	4	0
5	B	12	0	16	1	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	99	0	0	5	0
6	B	107	0	0	4	0
6	C	99	0	0	5	0
6	D	73	0	0	3	0
All	All	14342	0	13130	481	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 18.

All (481) 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:398:THR:HG22	1:C:399(B):GLU:HG3	1.17	1.07
1:C:398:THR:HG22	1:C:399(B):GLU:CG	1.89	1.01
1:C:398:THR:CG2	1:C:399(B):GLU:HG3	1.88	1.01
1:D:418(G):LEU:HD12	1:D:418(J):PHE:HD2	1.36	0.90
1:B:346:LYS:HD2	1:B:359:PRO:HG2	1.55	0.85
1:B:374(B):GLU:O	1:B:378:GLN:HG3	1.76	0.85
1:B:134(A):LYS:HD2	1:B:134(B):LYS:N	1.94	0.82
1:B:354:LYS:HD3	1:B:358:ARG:CD	2.11	0.81
1:A:391(A):LEU:O	1:A:394(A):ILE:HG23	1.80	0.81
1:B:407:ARG:NH1	1:B:407:ARG:HB3	1.96	0.81
1:A:134(C):LYS:HD3	1:A:138(A):SER:O	1.82	0.79
1:C:374(B):GLU:O	1:C:378:GLN:HG3	1.81	0.79
1:B:134(C):LYS:HD3	1:B:138(A):SER:O	1.84	0.77
1:B:357:LEU:HG	4:B:420(C)[A]:TGF:HG32	1.68	0.76
1:B:407:ARG:HH11	1:B:407:ARG:HB3	1.51	0.75
1:C:398:THR:HG23	1:C:399(B):GLU:H	1.50	0.75
1:B:133:THR:OG1	1:B:134(A):LYS:HG3	1.87	0.74
1:A:396(C):ARG:O	1:A:398:THR:HG22	1.88	0.73
1:D:33:ILE:HB	1:D:36:GLU:HG3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:GLU:O	1:C:394:GLN:HG3	1.89	0.73
1:C:203:HIS:HE1	3:C:420(B):GLY:HA3	1.54	0.72
1:D:134(C):LYS:HD3	1:D:138(A):SER:O	1.88	0.72
1:A:398:THR:OG1	1:A:399:LEU:HD22	1.90	0.72
1:B:336:VAL:HG21	1:B:392:THR:OG1	1.89	0.72
1:A:6:LEU:N	1:B:45:GLU:OE1	2.21	0.72
1:C:310:VAL:HG12	1:C:311:THR:HG23	1.71	0.71
1:A:391:GLU:O	1:A:394:GLN:HG3	1.90	0.71
1:B:203:HIS:HD2	1:B:317:HIS:HE2	1.38	0.70
1:D:134(A):LYS:HD2	1:D:134(B):LYS:N	2.07	0.70
1:D:133:THR:OG1	1:D:134(A):LYS:HE2	1.92	0.70
1:D:199:ALA:HB3	1:D:223:VAL:HG22	1.73	0.70
1:C:330:GLY:O	1:C:334:GLU:HB2	1.91	0.69
1:C:213:VAL:HB	6:C:537:HOH:O	1.93	0.69
1:D:418(G):LEU:HD12	1:D:418(J):PHE:CD2	2.25	0.68
1:D:336:VAL:HG21	1:D:392:THR:OG1	1.94	0.67
1:A:268:ALA:O	1:A:272:VAL:HG23	1.94	0.67
1:D:323:LEU:C	1:D:325:SER:H	1.95	0.67
1:D:369:LEU:O	1:D:372:ARG:HB2	1.95	0.67
1:C:4:GLN:HG3	1:C:11:SER:HB2	1.76	0.67
1:B:86:TYR:CZ	1:B:209:VAL:HG23	2.30	0.67
1:D:203:HIS:HD2	1:D:317:HIS:HE2	1.43	0.67
1:A:310:VAL:HG12	1:A:311:THR:HG23	1.76	0.67
1:D:244(A):VAL:HA	1:D:249:TYR:HD2	1.60	0.66
1:C:390:ILE:O	1:C:393:VAL:HG23	1.96	0.66
1:A:330:GLY:O	1:A:334:GLU:HB2	1.94	0.66
1:B:134(B):LYS:HG2	1:B:134(C):LYS:N	2.09	0.66
1:D:244:GLY:O	1:D:249:TYR:HB2	1.95	0.66
1:C:281:THR:HG21	1:D:1:MET:HE1	1.78	0.66
1:D:310:VAL:HG12	1:D:311:THR:HG23	1.78	0.65
1:B:134(B):LYS:HG2	1:B:134(C):LYS:H	1.61	0.65
1:B:369:LEU:O	1:B:372:ARG:HB2	1.97	0.65
1:A:317:HIS:H	1:A:317:HIS:HD1	1.45	0.64
1:C:398:THR:CG2	1:C:399(B):GLU:H	2.09	0.64
1:B:310:VAL:HG12	1:B:311:THR:HG23	1.81	0.63
1:C:317:HIS:HD1	1:C:317:HIS:H	1.44	0.63
1:C:268:ALA:O	1:C:272:VAL:HG23	1.99	0.63
1:A:374(B):GLU:O	1:A:378:GLN:HG3	1.98	0.63
1:C:27:ARG:NH2	6:C:795:HOH:O	2.30	0.63
1:A:332:ARG:NH2	1:A:398:THR:OG1	2.31	0.63
1:B:199:ALA:HB3	1:B:223:VAL:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ARG:HD2	6:B:783:HOH:O	1.99	0.62
1:A:394(A):ILE:HD11	1:A:399(C):PHE:CZ	2.33	0.62
1:C:203:HIS:CE1	3:C:420(B):GLY:HA3	2.34	0.62
1:C:55:TYR:HB2	1:D:36:GLU:OE2	1.99	0.61
1:C:134(C):LYS:HD3	1:C:138(A):SER:O	2.00	0.61
1:C:-9:LEU:HD13	1:C:-8:TRP:H	1.65	0.61
1:A:86:TYR:CZ	1:A:209:VAL:HG23	2.35	0.61
1:C:366:THR:H	1:C:367:PRO:HD3	1.67	0.60
1:D:123:ASP:HB3	1:D:147:VAL:HG13	1.83	0.60
1:A:398:THR:OG1	1:A:399:LEU:N	2.34	0.60
1:A:36:GLU:OE2	1:B:55:TYR:HB2	2.01	0.60
1:D:115:ARG:HB3	1:D:165:PHE:CE2	2.37	0.60
1:B:110:VAL:CG1	1:B:113:GLY:HA3	2.31	0.60
1:B:274:VAL:O	1:B:278:GLN:HG3	2.02	0.60
1:A:352:ASP:OD1	1:A:360:SER:OG	2.18	0.60
1:B:354:LYS:HD3	1:B:358:ARG:HD2	1.83	0.59
1:D:349:CYS:SG	1:D:350:PRO:HD2	2.42	0.59
1:A:366:THR:N	1:A:367:PRO:CD	2.66	0.59
1:A:394:GLN:O	1:A:394(C):ASP:HB2	2.03	0.59
1:C:366:THR:N	1:C:367:PRO:CD	2.66	0.59
1:D:135:ILE:HG13	1:D:136:SER:N	2.18	0.59
1:B:366:THR:N	1:B:367:PRO:CD	2.65	0.59
1:B:354:LYS:CB	1:B:358:ARG:HB3	2.33	0.59
1:D:324:ARG:N	1:D:328:THR:O	2.36	0.59
1:C:199:ALA:HB3	1:C:223:VAL:HG22	1.85	0.58
1:A:332:ARG:HH22	1:A:398:THR:CB	2.15	0.58
1:A:228:HIS:CD2	1:A:228:HIS:H	2.20	0.58
1:C:36:GLU:OE2	1:D:55:TYR:HB2	2.04	0.58
1:D:55:TYR:HA	6:D:635:HOH:O	2.03	0.58
1:B:138:THR:O	1:B:140(A):PHE:HB2	2.03	0.58
1:D:108:ALA:HB2	1:D:255:ALA:HB2	1.86	0.58
1:C:3:ALA:O	1:D:41:ARG:HD3	2.03	0.58
1:D:133:THR:OG1	1:D:134(A):LYS:HG3	2.04	0.58
1:C:112:PRO:O	1:C:112(A):HIS:HB2	2.04	0.57
1:A:115:ARG:HB3	1:A:165:PHE:CE2	2.39	0.57
1:C:352:ASP:OD1	1:C:360:SER:OG	2.20	0.57
1:B:346:LYS:HD2	1:B:359:PRO:CG	2.31	0.57
1:D:204:ILE:O	1:D:208:VAL:HG23	2.05	0.57
1:C:246:GLU:HG3	1:C:246:GLU:O	2.05	0.57
1:C:228:HIS:CD2	1:C:228:HIS:H	2.21	0.57
1:A:366:THR:H	1:A:367:PRO:HD3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:HD21	1:B:127:LEU:HD23	1.86	0.57
1:B:-6:SER:O	1:B:-5:HIS:HB3	2.05	0.57
1:D:203:HIS:CD2	1:D:317:HIS:HE2	2.23	0.56
1:B:244(B):ARG:HB2	1:B:249:TYR:CE1	2.40	0.56
1:D:32:LEU:HD13	1:D:386:ILE:HD11	1.87	0.56
1:C:203:HIS:HD2	1:C:317:HIS:NE2	2.04	0.56
1:D:412:ARG:O	1:D:415(A):GLU:HG3	2.06	0.56
1:B:392:THR:C	1:B:394:GLN:H	2.08	0.56
1:C:331:GLY:HA2	1:C:346:LYS:HD3	1.88	0.56
1:B:366:THR:H	1:B:367:PRO:HD3	1.70	0.56
1:B:418(H):PRO:O	5:B:422:GOL:H32	2.05	0.56
1:D:110:VAL:CG1	1:D:113:GLY:HA3	2.35	0.56
1:A:358:ARG:O	1:A:358:ARG:HG2	2.06	0.56
1:C:369:LEU:O	1:C:372:ARG:HB2	2.06	0.56
1:A:32:LEU:HB2	1:A:343:ALA:O	2.06	0.56
1:A:2:LEU:HA	1:B:40:SER:HB2	1.87	0.55
1:C:199:ALA:HB2	1:C:220:CYS:SG	2.46	0.55
1:D:404(C):GLU:O	1:D:405:LYS:HB2	2.06	0.55
1:B:360:SER:CB	6:B:861:HOH:O	2.54	0.55
1:B:392:THR:C	1:B:394:GLN:N	2.60	0.55
1:A:340:CYS:SG	1:A:411(A):LEU:HD13	2.47	0.55
1:D:323:LEU:O	1:D:325:SER:N	2.40	0.55
1:C:48:GLY:O	1:D:44:LEU:HD23	2.07	0.55
1:A:-9:LEU:HD22	1:A:-7:SER:HB3	1.88	0.55
1:D:418(G):LEU:HB3	1:D:418(H):PRO:CD	2.36	0.54
1:B:203:HIS:CD2	1:B:317:HIS:HE2	2.20	0.54
1:A:309:ILE:CD1	1:A:321:VAL:HG22	2.37	0.54
1:C:32:LEU:HB2	1:C:343:ALA:O	2.08	0.54
1:B:115:ARG:HA	1:B:141:GLU:O	2.07	0.54
1:D:323:LEU:C	1:D:325:SER:N	2.61	0.54
1:B:391(A):LEU:O	1:B:394(A):ILE:HG13	2.07	0.54
1:D:399(C):PHE:C	1:D:399(C):PHE:CD2	2.80	0.54
1:D:92:ASN:OD1	1:D:95:PRO:HD3	2.07	0.54
1:A:397:ALA:HB1	1:A:399(B):GLU:OE1	2.07	0.54
1:D:321:VAL:O	1:D:361:GLY:HA2	2.07	0.54
1:C:366:THR:N	1:C:367:PRO:HD3	2.23	0.54
1:B:178:SER:HB2	1:B:314:SER:HB2	1.89	0.54
1:C:204:ILE:O	1:C:208:VAL:HG23	2.07	0.54
1:D:418(C):PRO:HA	6:D:558:HOH:O	2.08	0.54
1:C:121:LEU:HD21	1:C:127:LEU:HD23	1.88	0.54
1:A:203:HIS:HD2	1:A:317:HIS:NE2	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ARG:HB3	1:B:165:PHE:CE2	2.42	0.54
1:A:394(A):ILE:HG22	1:A:406:HIS:CE1	2.42	0.54
1:A:178:SER:HB2	1:A:314:SER:HB2	1.89	0.54
1:B:391:GLU:O	1:B:394:GLN:HB2	2.08	0.53
1:D:346:LYS:HE2	4:D:420(F)[A]:TGF:O13	2.08	0.53
1:C:123:ASP:HB3	1:C:147:VAL:HG13	1.89	0.53
1:B:126:HIS:CE1	1:B:128:THR:HG23	2.42	0.53
1:A:416:PHE:O	1:A:418(A):LEU:HB2	2.08	0.53
1:D:126:HIS:CE1	1:D:128:THR:HG23	2.44	0.53
1:C:182:ASP:HA	6:C:585:HOH:O	2.07	0.53
1:C:347:ASN:HD22	1:C:348:THR:N	2.07	0.53
1:D:366:THR:N	1:D:367:PRO:CD	2.72	0.53
1:A:309:ILE:HD13	1:A:321:VAL:HG22	1.91	0.53
1:C:108:ALA:HB2	1:C:255:ALA:HB2	1.90	0.53
1:D:407:ARG:HG3	1:D:407:ARG:HH11	1.73	0.53
1:A:112:PRO:O	1:A:112(A):HIS:HB2	2.09	0.52
1:B:354:LYS:HD3	1:B:358:ARG:HD3	1.91	0.52
1:A:244(B):ARG:HA	1:A:249:TYR:CE2	2.44	0.52
1:D:28:VAL:HB	1:D:415(A):GLU:HB3	1.90	0.52
1:B:294:ASN:HB3	1:B:377:PHE:CD2	2.45	0.52
1:B:134(A):LYS:HD2	1:B:134(B):LYS:H	1.70	0.52
1:C:418(E):PRO:HA	6:C:804:HOH:O	2.10	0.52
1:A:110:VAL:CG1	1:A:113:GLY:HA3	2.40	0.52
1:D:308:LYS:HB3	1:D:322:ASP:HB3	1.92	0.52
1:B:228:HIS:CD2	1:B:228:HIS:H	2.28	0.52
1:B:346:LYS:CD	1:B:359:PRO:HG2	2.34	0.52
1:D:340:CYS:SG	1:D:411(A):LEU:HD23	2.50	0.52
1:C:134(A):LYS:HB3	1:C:134(A):LYS:NZ	2.25	0.52
1:C:286:GLU:CB	1:C:289:ARG:NH2	2.73	0.52
1:D:178:SER:HB2	1:D:314:SER:HB2	1.92	0.52
1:C:115:ARG:HB3	1:C:165:PHE:CE2	2.45	0.52
1:B:374(B):GLU:HB2	6:B:640:HOH:O	2.09	0.51
1:B:354:LYS:HB3	1:B:358:ARG:HB3	1.92	0.51
1:D:4:GLN:NE2	1:D:11:SER:HA	2.25	0.51
1:C:12:ASP:HA	1:D:277:LYS:NZ	2.26	0.51
1:A:351:GLY:O	1:A:352:ASP:C	2.49	0.51
1:C:33:ILE:HB	1:C:36:GLU:HG3	1.92	0.51
1:B:108:ALA:HB2	1:B:255:ALA:HB2	1.92	0.51
1:A:199:ALA:HB2	1:A:220:CYS:SG	2.49	0.51
1:B:354:LYS:HB2	1:B:358:ARG:HB3	1.92	0.51
1:B:105:VAL:HG23	1:B:239:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-5:HIS:CD2	1:B:287:TYR:HB2	2.45	0.51
1:D:4:GLN:HG3	1:D:11:SER:HB2	1.93	0.51
1:D:27:ARG:HB2	1:D:418(D):LEU:HD22	1.92	0.51
1:B:366:THR:N	1:B:367:PRO:HD3	2.26	0.51
1:A:141:GLU:HG3	1:C:141:GLU:HG3	1.93	0.51
1:B:134(A):LYS:HD2	1:B:134(B):LYS:CB	2.41	0.51
1:B:110:VAL:HG12	1:B:113:GLY:HA3	1.93	0.51
1:A:355:SER:O	1:A:356:ALA:O	2.28	0.51
1:D:366:THR:N	1:D:367:PRO:HD3	2.26	0.50
1:B:4:GLN:HG3	1:B:11:SER:HB2	1.93	0.50
1:D:228:HIS:CD2	1:D:228:HIS:H	2.28	0.50
1:A:316:ASN:HB2	1:A:317:HIS:HD1	1.76	0.50
1:A:-9:LEU:HD22	1:A:-7:SER:CB	2.42	0.50
1:D:105:VAL:HG23	1:D:239:ILE:HD13	1.93	0.50
1:D:310:VAL:HG21	1:D:320:LEU:HD23	1.92	0.50
1:D:207:LEU:HB3	1:D:213:VAL:HG22	1.94	0.50
1:D:418(H):PRO:C	1:D:418(J):PHE:H	2.15	0.50
1:A:12:ASP:HA	1:B:277:LYS:NZ	2.27	0.50
1:B:112:PRO:O	1:B:112(A):HIS:HB2	2.12	0.50
1:C:321:VAL:O	1:C:361:GLY:HA2	2.12	0.50
1:D:97:SER:C	1:D:100:PRO:HD2	2.32	0.50
1:B:384[B]:HIS:HD2	6:B:836:HOH:O	1.94	0.50
1:A:404(C):GLU:CD	1:A:405:LYS:H	2.15	0.50
1:B:94:GLN:N	1:B:95:PRO:CD	2.75	0.50
1:D:322:ASP:C	1:D:323:LEU:O	2.50	0.49
1:A:-9:LEU:C	1:A:-7:SER:H	2.16	0.49
1:C:94:GLN:N	1:C:95:PRO:CD	2.75	0.49
1:D:-3:GLN:HE21	1:D:2:LEU:HD12	1.77	0.49
1:B:135:ILE:HG13	1:B:136:SER:N	2.27	0.49
1:C:187:ARG:NH1	1:C:219:HIS:O	2.43	0.49
1:D:324:ARG:HG2	1:D:324:ARG:O	2.12	0.49
1:D:4:GLN:HE21	1:D:11:SER:HA	1.78	0.49
1:A:369:LEU:O	1:A:372:ARG:HB2	2.13	0.49
1:C:110:VAL:CG1	1:C:113:GLY:HA3	2.41	0.49
1:B:167:PRO:O	1:B:195:ALA:HB2	2.12	0.49
1:A:274:VAL:O	1:A:278:GLN:HG3	2.12	0.49
1:B:336:VAL:HG23	1:B:337:LEU:N	2.27	0.49
1:C:316:ASN:HB2	1:C:317:HIS:HD1	1.77	0.49
1:D:122:PRO:HA	1:D:348:THR:HB	1.95	0.48
1:B:412:ARG:O	1:B:415(A):GLU:HG3	2.13	0.48
1:B:268:ALA:O	1:B:272:VAL:HG23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ALA:HB2	1:A:255:ALA:HB2	1.94	0.48
1:B:329:ASP:HB2	1:B:359:PRO:O	2.12	0.48
1:B:178:SER:HB2	1:B:314:SER:CB	2.44	0.48
1:B:97:SER:C	1:B:100:PRO:HD2	2.34	0.48
1:D:398:THR:C	1:D:399(A):LYS:H	2.16	0.48
1:A:115:ARG:HA	1:A:141:GLU:O	2.14	0.48
1:A:356:ALA:C	1:A:358:ARG:H	2.15	0.48
1:B:121:LEU:CB	1:B:122:PRO:HD3	2.44	0.48
1:D:366:THR:H	1:D:367:PRO:HD3	1.78	0.48
1:C:137:ALA:CB	1:D:260:LEU:HD23	2.44	0.48
1:C:340:CYS:SG	1:C:411(A):LEU:HD23	2.52	0.48
1:D:399(B):GLU:O	1:D:400:GLU:N	2.45	0.48
1:D:356:ALA:HB1	4:D:420(F)[B]:TGF:O12	2.14	0.48
1:B:126:HIS:HE1	1:B:128:THR:HG23	1.78	0.48
1:A:94:GLN:N	1:A:95:PRO:CD	2.76	0.48
1:B:207:LEU:HB3	1:B:213:VAL:HG22	1.94	0.48
1:C:187:ARG:HA	1:C:197:LEU:HD22	1.95	0.48
1:D:30:LEU:HG	1:D:415:VAL:HG13	1.96	0.48
1:C:2:LEU:HA	1:D:40:SER:HB2	1.96	0.48
1:D:94:GLN:N	1:D:95:PRO:CD	2.77	0.48
1:C:398:THR:HG22	1:C:399(B):GLU:CB	2.44	0.47
1:D:346:LYS:H	1:D:346:LYS:HD3	1.79	0.47
1:A:366:THR:N	1:A:367:PRO:HD3	2.28	0.47
1:A:-9:LEU:O	1:A:-7:SER:N	2.47	0.47
1:C:178:SER:HB2	1:C:314:SER:HB2	1.96	0.47
1:B:34:ALA:HA	1:B:365:GLY:HA3	1.95	0.47
1:B:322:ASP:C	1:B:324:ARG:H	2.16	0.47
1:D:199:ALA:HB2	1:D:220:CYS:SG	2.54	0.47
1:D:340:CYS:O	1:D:341:SER:HB2	2.14	0.47
1:A:126:HIS:CE1	1:A:128:THR:HG23	2.50	0.47
1:C:149:PRO:HA	1:C:350:PRO:HB3	1.96	0.47
1:D:167:PRO:O	1:D:195:ALA:HB2	2.14	0.47
1:D:4:GLN:HE21	1:D:11:SER:CA	2.28	0.47
1:D:318:LEU:HD12	1:D:318:LEU:C	2.34	0.47
1:A:3:ALA:O	1:B:41:ARG:HD3	2.15	0.47
1:C:115:ARG:HA	1:C:141:GLU:O	2.15	0.47
1:D:295:CYS:SG	1:D:319:ILE:HG23	2.55	0.47
1:A:244(A):VAL:HG23	1:A:244(A):VAL:O	2.15	0.47
1:C:98:GLY:HA3	1:C:226:THR:HG22	1.97	0.47
1:B:32:LEU:HB2	1:B:343:ALA:O	2.14	0.47
1:D:115:ARG:HA	1:D:141:GLU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:TYR:CE2	1:A:209:VAL:HG23	2.50	0.47
1:A:374(A):LEU:HB3	6:A:826:HOH:O	2.14	0.47
1:C:121:LEU:CB	1:C:122:PRO:HD3	2.45	0.46
1:D:274:VAL:O	1:D:278:GLN:HG3	2.15	0.46
1:D:336:VAL:HG23	1:D:337:LEU:N	2.29	0.46
1:C:28:VAL:O	1:C:415(A):GLU:HA	2.16	0.46
1:B:104:ALA:HA	1:B:260:LEU:CD1	2.44	0.46
1:B:145:TYR:CD2	1:B:158:LEU:HD13	2.50	0.46
1:D:-6:SER:C	1:D:-4:GLU:H	2.18	0.46
1:B:357:LEU:O	1:B:357:LEU:HD23	2.15	0.46
1:A:332:ARG:NH2	1:A:398:THR:CB	2.78	0.46
1:D:135:ILE:HG13	1:D:136:SER:H	1.78	0.46
1:B:-5:HIS:HE1	1:B:2:LEU:HD11	1.79	0.46
1:D:122:PRO:HA	1:D:348:THR:CB	2.45	0.46
1:D:126:HIS:HE1	1:D:128:THR:HG23	1.80	0.46
1:C:309:ILE:CD1	1:C:321:VAL:HG22	2.45	0.46
1:C:152:TYR:CE1	1:C:179:ARG:HG3	2.50	0.46
1:A:28:VAL:O	1:A:415(A):GLU:HA	2.16	0.46
1:A:27:ARG:HA	1:A:418(D):LEU:HD13	1.98	0.46
1:A:339:ALA:O	1:A:412:ARG:HD2	2.16	0.46
1:D:228:HIS:CD2	1:D:235:ARG:HA	2.50	0.46
1:C:345:ASN:HB2	6:C:555:HOH:O	2.16	0.46
1:C:32:LEU:HD13	1:C:386:ILE:HD11	1.98	0.46
1:D:399(C):PHE:C	1:D:399(C):PHE:HD2	2.19	0.46
1:C:279:ALA:HA	1:C:284:PHE:CG	2.51	0.46
1:D:323:LEU:O	1:D:324:ARG:HB3	2.15	0.46
1:C:-9:LEU:HD11	1:D:283:GLU:HG3	1.97	0.46
1:A:343:ALA:HB3	6:A:776:HOH:O	2.15	0.46
1:A:152:TYR:CE1	1:A:179:ARG:HG3	2.51	0.46
1:D:207:LEU:HD23	1:D:288:GLN:OE1	2.16	0.45
1:A:204:ILE:O	1:A:208:VAL:HG23	2.16	0.45
1:C:-9:LEU:HD13	1:C:-8:TRP:N	2.29	0.45
1:C:92:ASN:OD1	1:C:95:PRO:HD3	2.17	0.45
1:B:207:LEU:HD22	1:B:212:VAL:HG21	1.97	0.45
1:B:146:LYS:HD2	1:D:164:LEU:HD21	1.98	0.45
1:C:55:TYR:N	1:D:36:GLU:OE2	2.44	0.45
1:B:117:MET:HG3	1:B:167:PRO:HB3	1.97	0.45
1:A:294:ASN:HB3	1:A:377:PHE:CD2	2.51	0.45
1:C:318:LEU:C	1:C:318:LEU:HD12	2.36	0.45
1:A:25:ARG:NH2	6:A:656:HOH:O	2.49	0.45
1:A:40:SER:OG	1:A:43:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLY:O	1:B:44:LEU:HD23	2.15	0.45
1:C:246:GLU:O	1:C:247:ILE:CB	2.64	0.45
1:B:228:HIS:CD2	1:B:235:ARG:HA	2.52	0.45
1:C:126:HIS:CE1	1:C:128:THR:HG23	2.51	0.45
1:B:137:ALA:HA	1:B:139:ILE:HD12	1.98	0.45
1:D:322:ASP:O	1:D:323:LEU:O	2.34	0.45
1:A:99:SER:HA	1:A:128:THR:HG21	1.98	0.45
1:D:148:ASN:N	1:D:152:TYR:O	2.47	0.45
1:C:358:ARG:O	1:C:358:ARG:HG2	2.17	0.44
1:C:330:GLY:O	1:C:346:LYS:HB3	2.16	0.44
1:D:336:VAL:HG23	1:D:337:LEU:H	1.83	0.44
1:C:97:SER:C	1:C:100:PRO:HD2	2.37	0.44
1:D:418(G):LEU:O	1:D:418(H):PRO:O	2.35	0.44
1:B:55:TYR:CE1	1:B:263:GLY:HA3	2.53	0.44
1:D:28:VAL:HG11	6:D:514:HOH:O	2.16	0.44
1:B:92:ASN:OD1	1:B:95:PRO:HD3	2.18	0.44
1:B:148:ASN:N	1:B:152:TYR:O	2.49	0.44
1:A:147:VAL:HA	1:A:153:ILE:HA	1.99	0.44
1:B:399(B):GLU:C	1:B:399(D):LYS:H	2.20	0.44
1:D:268:ALA:O	1:D:272:VAL:HG23	2.17	0.44
1:B:134(A):LYS:CD	1:B:134(B):LYS:N	2.75	0.44
1:A:323:LEU:HB2	1:A:360:SER:O	2.17	0.44
1:C:99:SER:HA	1:C:128:THR:HG21	1.99	0.44
1:B:340:CYS:O	1:B:341:SER:HB2	2.16	0.44
1:D:187:ARG:NH1	1:D:219:HIS:O	2.49	0.44
1:C:329:ASP:HB2	1:C:359:PRO:O	2.17	0.44
1:C:394(A):ILE:HA	1:C:406:HIS:NE2	2.33	0.44
1:A:310:VAL:C	1:A:311:THR:HG23	2.38	0.44
1:A:199:ALA:HB3	1:A:223:VAL:HG22	1.98	0.44
1:B:91(A):VAL:HG22	1:B:92:ASN:N	2.33	0.44
1:B:91(A):VAL:CG2	1:B:92:ASN:N	2.81	0.44
1:D:404(A):ASP:OD1	1:D:405:LYS:HB3	2.17	0.44
1:C:309:ILE:HD13	1:C:321:VAL:HG22	1.99	0.44
1:B:28:VAL:HB	1:B:415(A):GLU:HB3	1.99	0.44
1:A:126:HIS:HE1	1:A:128:THR:HG23	1.83	0.44
1:A:244(A):VAL:HA	1:A:248:LEU:HA	2.00	0.44
1:A:137:ALA:CB	1:B:260:LEU:HD23	2.47	0.44
1:B:316:ASN:HB2	1:B:317:HIS:H	1.65	0.44
1:D:396(B):PRO:C	1:D:397:ALA:N	2.69	0.44
1:A:-8:TRP:CZ2	1:B:290:GLN:HG2	2.53	0.44
1:B:169:LEU:HD23	1:B:169:LEU:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:THR:O	1:C:397:ALA:HB2	2.18	0.44
1:A:94:GLN:N	1:A:95:PRO:HD3	2.32	0.44
1:B:207:LEU:HD23	1:B:288:GLN:OE1	2.18	0.44
1:C:99:SER:HB2	1:C:100:PRO:HD3	2.00	0.44
1:A:123:ASP:HB3	1:A:147:VAL:HG13	2.00	0.44
1:D:294:ASN:HB3	1:D:377:PHE:CD2	2.52	0.44
1:B:203:HIS:HD2	1:B:317:HIS:NE2	2.11	0.43
1:D:203:HIS:HD2	1:D:317:HIS:NE2	2.13	0.43
1:D:399:LEU:HA	1:D:399(C):PHE:CB	2.48	0.43
1:B:131:PHE:O	1:B:135:ILE:HG12	2.18	0.43
1:B:336:VAL:HG23	1:B:337:LEU:H	1.83	0.43
1:A:376:ASP:O	1:A:382:VAL:HG23	2.18	0.43
1:A:169:LEU:C	1:A:169:LEU:HD23	2.38	0.43
1:A:406:HIS:O	1:A:408:ALA:HB3	2.18	0.43
1:A:329:ASP:HB2	1:A:359:PRO:O	2.18	0.43
1:D:178:SER:HB2	1:D:314:SER:CB	2.49	0.43
1:A:40:SER:HB2	6:A:712:HOH:O	2.19	0.43
1:A:167:PRO:O	1:A:195:ALA:HB2	2.17	0.43
1:C:140:PHE:HZ	1:D:107:THR:HG1	1.66	0.43
1:A:260:LEU:HD23	1:B:137:ALA:CB	2.49	0.43
1:D:138:THR:O	1:D:140(A):PHE:HB2	2.18	0.43
1:D:134(A):LYS:C	1:D:134(A):LYS:HD2	2.39	0.43
1:D:316:ASN:HB2	1:D:317:HIS:H	1.60	0.43
1:C:110:VAL:HG13	1:C:113:GLY:HA3	2.01	0.43
1:A:27:ARG:HB2	1:A:418(D):LEU:HD22	1.99	0.43
1:A:121:LEU:CB	1:A:122:PRO:HD3	2.48	0.43
1:B:307:TYR:HE1	1:B:387:HIS:HD1	1.67	0.43
1:C:57:GLU:HB3	1:C:257:PHE:CZ	2.53	0.43
4:D:420(F)[A]:TGF:HB21	4:D:420(F)[A]:TGF:HG3	1.44	0.43
1:D:108:ALA:HB2	1:D:255:ALA:CB	2.47	0.43
1:D:104:ALA:HA	1:D:260:LEU:CD1	2.48	0.43
1:A:123:ASP:OD1	1:A:146:LYS:HB3	2.18	0.43
1:B:57:GLU:HB3	1:B:257:PHE:CZ	2.53	0.43
1:D:397:ALA:C	1:D:399:LEU:H	2.22	0.43
1:A:318:LEU:C	1:A:318:LEU:HD12	2.39	0.43
1:B:318:LEU:HD12	1:B:318:LEU:C	2.39	0.43
1:B:354:LYS:HD3	1:B:358:ARG:CG	2.49	0.43
1:B:358:ARG:CG	1:B:358:ARG:O	2.67	0.43
1:C:274:VAL:O	1:C:278:GLN:HG3	2.19	0.43
1:D:244(A):VAL:CA	1:D:249:TYR:HD2	2.30	0.42
1:A:369:LEU:HB3	1:A:374:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:HD13	1:B:386:ILE:HD11	2.01	0.42
1:C:167:PRO:O	1:C:195:ALA:HB2	2.19	0.42
1:D:279:ALA:HA	1:D:284:PHE:CG	2.53	0.42
1:A:89:ASP:OD2	1:A:89(B):GLN:HB2	2.20	0.42
1:C:94:GLN:HG2	1:C:264:PRO:HB3	2.00	0.42
1:C:126:HIS:HE1	1:C:128:THR:HG23	1.84	0.42
1:D:335:LYS:HA	1:D:335:LYS:HD2	1.86	0.42
1:B:86:TYR:CE2	1:B:209:VAL:HG23	2.54	0.42
1:B:418(H):PRO:C	1:B:418(J):PHE:H	2.22	0.42
1:A:31:GLU:HA	6:A:776:HOH:O	2.18	0.42
1:D:226:THR:HB	1:D:228:HIS:CD2	2.55	0.42
1:D:145:TYR:CD2	1:D:158:LEU:HD13	2.54	0.42
1:C:108:ALA:HB2	1:C:255:ALA:CB	2.49	0.42
1:B:418(D):LEU:HD12	1:B:418(D):LEU:HA	1.90	0.42
1:B:204:ILE:O	1:B:208:VAL:HG23	2.19	0.42
1:B:354:LYS:NZ	1:B:358:ARG:HH11	2.18	0.42
1:C:394:GLN:O	1:C:394(C):ASP:HB2	2.20	0.42
1:D:320:LEU:HD21	1:D:349:CYS:HA	2.02	0.42
1:A:108:ALA:HB2	1:A:255:ALA:CB	2.50	0.42
1:D:399(B):GLU:O	1:D:401:LYS:N	2.52	0.42
1:A:57:GLU:HB3	1:A:257:PHE:CZ	2.55	0.42
1:D:169:LEU:HD23	1:D:169:LEU:C	2.40	0.42
1:D:131:PHE:H	1:D:138(A):SER:HB2	1.85	0.42
4:D:420(F)[B]:TGF:HB21	4:D:420(F)[B]:TGF:HG3	1.73	0.42
1:B:399(A):LYS:O	1:B:399(C):PHE:N	2.52	0.42
1:C:44:LEU:HD23	1:D:48:GLY:O	2.19	0.42
1:D:336:VAL:O	1:D:339:ALA:N	2.52	0.42
1:B:226:THR:HB	1:B:228:HIS:CD2	2.55	0.42
1:A:121:LEU:HD21	1:A:127:LEU:HD23	2.01	0.42
1:C:260:LEU:HD23	1:D:137:ALA:CB	2.50	0.42
1:A:97:SER:C	1:A:100:PRO:HD2	2.39	0.42
1:A:115:ARG:HH21	1:C:141:GLU:HB3	1.84	0.42
1:B:339:ALA:HB1	1:B:409:VAL:HG11	2.01	0.42
1:A:168:LYS:HB3	1:A:168:LYS:HE2	1.88	0.42
1:B:328:THR:OG1	1:B:329:ASP:N	2.52	0.41
1:D:346:LYS:H	1:D:346:LYS:CD	2.32	0.41
1:B:108:ALA:HB2	1:B:255:ALA:CB	2.49	0.41
1:B:121:LEU:HB3	1:B:122:PRO:HD3	2.02	0.41
1:A:358:ARG:N	1:A:359:PRO:HD3	2.34	0.41
1:C:369:LEU:HB3	1:C:374:LEU:HD22	2.02	0.41
1:C:155:TYR:CE2	1:C:182:ASP:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:ASN:HB2	1:C:317:HIS:H	1.60	0.41
1:D:314:SER:HB2	1:D:319:ILE:HG22	2.03	0.41
1:A:39:ALA:HB3	1:A:44:LEU:HD11	2.02	0.41
1:A:337:LEU:CD2	1:A:389:GLY:HA3	2.51	0.41
1:A:226:THR:HB	1:A:228:HIS:CD2	2.56	0.41
1:B:121:LEU:HD11	1:B:127:LEU:HA	2.02	0.41
1:C:38:PHE:CE2	1:C:418(D):LEU:HD11	2.55	0.41
1:C:265:HIS:HB3	1:C:267:HIS:CE1	2.55	0.41
1:B:295:CYS:SG	1:B:319:ILE:HG23	2.59	0.41
1:B:134(A):LYS:HD2	1:B:134(B):LYS:HB3	2.01	0.41
1:C:65:TYR:CD1	1:D:33:ILE:HD13	2.55	0.41
1:D:133:THR:OG1	1:D:134:ASP:N	2.51	0.41
1:D:328:THR:OG1	1:D:329:ASP:N	2.53	0.41
1:B:228:HIS:CD2	1:B:228:HIS:N	2.88	0.41
1:A:137:ALA:HA	1:A:139:ILE:HD12	2.02	0.41
1:B:404(B):GLU:C	1:B:406:HIS:N	2.74	0.41
1:B:357:LEU:HG	4:B:420(C)[A]:TGF:CG3	2.44	0.41
1:B:4:GLN:HA	1:B:5:PRO:HD3	1.89	0.41
1:D:152:TYR:CE1	1:D:179:ARG:HG3	2.56	0.41
1:A:295:CYS:SG	1:A:319:ILE:HG23	2.61	0.41
1:C:171:ILE:HA	1:C:198:MET:O	2.21	0.41
1:C:-5:HIS:CD2	1:D:287:TYR:HB2	2.56	0.41
1:B:153:ILE:HB	1:B:155:TYR:CE1	2.56	0.41
1:C:295:CYS:SG	1:C:319:ILE:HG23	2.60	0.41
1:D:163:ARG:NE	1:D:192:GLU:OE2	2.42	0.41
1:B:388:ARG:HH22	1:B:414:GLU:CD	2.25	0.41
1:D:110:VAL:HG12	1:D:113:GLY:HA3	2.03	0.41
1:A:178:SER:HB2	1:A:314:SER:CB	2.50	0.41
1:C:372:ARG:HD2	1:C:418(C):PRO:O	2.21	0.40
1:A:32:LEU:HD13	1:A:386:ILE:HD11	2.03	0.40
1:C:395:ASP:O	1:C:396:THR:C	2.60	0.40
1:C:391(A):LEU:HD13	1:C:391(A):LEU:O	2.21	0.40
1:D:132:MET:HB3	1:D:138(A):SER:OG	2.22	0.40
1:D:32:LEU:HB2	1:D:343:ALA:O	2.21	0.40
1:A:4:GLN:HA	1:A:5:PRO:HD3	1.97	0.40
1:D:418(G):LEU:HB3	1:D:418(H):PRO:HD2	2.03	0.40
1:B:134(A):LYS:CD	1:B:134(B):LYS:H	2.33	0.40
1:A:398:THR:HG23	1:A:399:LEU:CD2	2.52	0.40
1:C:281:THR:OG1	1:D:1:MET:HE3	2.20	0.40
1:B:418(B):PHE:HA	1:B:418(C):PRO:HD3	1.80	0.40
1:B:199:ALA:HB2	1:B:220:CYS:SG	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:LEU:N	1:C:360:SER:O	2.55	0.40
1:A:-9:LEU:C	1:A:-7:SER:N	2.75	0.40
1:D:398:THR:C	1:D:399(A):LYS:N	2.75	0.40
1:A:104:ALA:HA	1:A:260:LEU:CD1	2.50	0.40
1:C:342:ILE:HD11	1:C:415:VAL:HG21	2.04	0.40
1:A:307:TYR:HE1	1:A:387:HIS:HD1	1.68	0.40
1:C:117:MET:HA	1:C:143:MET:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	462/483 (96%)	412 (89%)	39 (8%)	11 (2%)	7	19
1	B	447/483 (92%)	404 (90%)	34 (8%)	9 (2%)	9	24
1	C	461/483 (95%)	427 (93%)	31 (7%)	3 (1%)	26	55
1	D	452/483 (94%)	404 (89%)	36 (8%)	12 (3%)	6	16
All	All	1822/1932 (94%)	1647 (90%)	140 (8%)	35 (2%)	10	25

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244(C)	SER
1	A	244(D)	VAL
1	A	355	SER
1	A	356	ALA
1	A	396(B)	PRO
1	A	418(G)	LEU
1	A	418(H)	PRO
1	B	244(E)	ASP

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Mol	Chain	Res	Type
1	B	396	THR
1	B	397	ALA
1	D	355	SER
1	D	404(A)	ASP
1	D	405	LYS
1	D	418(H)	PRO
1	A	-8	TRP
1	B	398	THR
1	B	399(B)	GLU
1	B	418(E)	PRO
1	D	323	LEU
1	D	418(G)	LEU
1	A	404	GLY
1	A	404(C)	GLU
1	B	350	PRO
1	C	134(A)	LYS
1	D	348	THR
1	D	352	ASP
1	D	399	LEU
1	A	323	LEU
1	C	418(H)	PRO
1	B	323	LEU
1	C	247	ILE
1	D	134(B)	LYS
1	B	-7	SER
1	D	350	PRO
1	D	359	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	350/391 (90%)	340 (97%)	10 (3%)	50	80
1	B	335/391 (86%)	324 (97%)	11 (3%)	45	76
1	C	345/391 (88%)	335 (97%)	10 (3%)	50	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	333/391 (85%)	322 (97%)	11 (3%)	45	76
All	All	1363/1564 (87%)	1321 (97%)	42 (3%)	48	78

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	TYR
1	A	97	SER
1	A	203	HIS
1	A	228	HIS
1	A	347	ASN
1	A	352	ASP
1	A	391(A)	LEU
1	A	394(A)	ILE
1	A	396(B)	PRO
1	A	411(A)	LEU
1	B	55	TYR
1	B	89(B)[A]	GLN
1	B	89(B)[B]	GLN
1	B	97	SER
1	B	121	LEU
1	B	134	ASP
1	B	134(A)	LYS
1	B	203	HIS
1	B	228	HIS
1	B	399(B)	GLU
1	B	404(B)	GLU
1	C	-9	LEU
1	C	55	TYR
1	C	89(B)	GLN
1	C	97	SER
1	C	121	LEU
1	C	134(A)	LYS
1	C	203	HIS
1	C	228	HIS
1	C	347	ASN
1	C	399(D)	LYS
1	D	20	LYS
1	D	55	TYR
1	D	97	SER
1	D	134(A)	LYS
1	D	203	HIS

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Mol	Chain	Res	Type
1	D	228	HIS
1	D	244(A)	VAL
1	D	324	ARG
1	D	335	LYS
1	D	346	LYS
1	D	399(C)	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	203	HIS
1	A	228	HIS
1	A	250	ASN
1	A	347	ASN
1	A	394(B)	GLN
1	B	203	HIS
1	B	228	HIS
1	C	4	GLN
1	C	166	HIS
1	C	203	HIS
1	C	228	HIS
1	C	347	ASN
1	D	-3	GLN
1	D	4	GLN
1	D	203	HIS
1	D	228	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

14 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	PLP	A	419(A)	1,3	15,15,16	1.81	3 (20%)	21,22,23	2.94	9 (42%)
3	GLY	A	420(B)	2	1,4,4	0.57	0	0,4,4	0.00	-
2	PLP	B	419(A)	1	15,15,16	1.74	4 (26%)	21,22,23	3.10	10 (47%)
4	TGF	B	420(C)[A]	-	39,54,54	2.49	10 (25%)	40,74,74	3.22	16 (40%)
4	TGF	B	420(C)[B]	-	39,54,54	2.49	10 (25%)	40,74,74	3.22	16 (40%)
5	GOL	B	421	-	5,5,5	0.54	0	5,5,5	0.28	0
5	GOL	B	422	-	5,5,5	0.77	0	5,5,5	0.27	0
2	PLP	C	419(A)	1,3	15,15,16	1.61	3 (20%)	21,22,23	3.02	8 (38%)
3	GLY	C	420(B)	2	1,4,4	0.58	0	0,4,4	0.00	-
5	GOL	C	421	-	5,5,5	0.89	0	5,5,5	0.23	0
2	PLP	D	419(A)	1	15,15,16	1.46	2 (13%)	21,22,23	3.09	10 (47%)
4	TGF	D	420(F)[A]	-	39,54,54	2.40	12 (30%)	40,74,74	3.24	15 (37%)
4	TGF	D	420(F)[B]	-	39,54,54	2.39	12 (30%)	40,74,74	3.22	14 (35%)
5	GOL	D	421	-	5,5,5	0.62	0	5,5,5	0.27	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	PLP	A	419(A)	1,3	-	0/6/6/8	0/1/1/1
3	GLY	A	420(B)	2	-	0/0/2/2	0/0/0/0
2	PLP	B	419(A)	1	-	0/6/6/8	0/1/1/1
4	TGF	B	420(C)[A]	-	-	2/36/63/63	0/2/3/3
4	TGF	B	420(C)[B]	-	-	2/36/63/63	0/2/3/3
5	GOL	B	421	-	-	0/4/4/4	0/0/0/0
5	GOL	B	422	-	-	0/4/4/4	0/0/0/0
2	PLP	C	419(A)	1,3	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLY	C	420(B)	2	-	0/0/2/2	0/0/0/0
5	GOL	C	421	-	-	0/4/4/4	0/0/0/0
2	PLP	D	419(A)	1	-	0/6/6/8	0/1/1/1
4	TGF	D	420(F)[A]	-	-	2/36/63/63	0/2/3/3
4	TGF	D	420(F)[B]	-	-	2/36/63/63	0/2/3/3
5	GOL	D	421	-	-	0/4/4/4	0/0/0/0

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	420(F)[B]	TGF	C7-N8	-4.27	1.40	1.46
4	D	420(F)[A]	TGF	C7-N8	-4.27	1.40	1.46
4	B	420(C)[B]	TGF	C7-N8	-4.14	1.40	1.46
4	B	420(C)[A]	TGF	C7-N8	-4.14	1.40	1.46
2	B	419(A)	PLP	C4A-C4	-3.03	1.45	1.51
2	D	419(A)	PLP	C4A-C4	-2.85	1.45	1.51
2	C	419(A)	PLP	O3-C3	-2.29	1.31	1.37
2	D	419(A)	PLP	O3-C3	-2.17	1.31	1.37
2	B	419(A)	PLP	O3-C3	-2.04	1.32	1.37
2	A	419(A)	PLP	O3-C3	-2.02	1.32	1.37
4	D	420(F)[B]	TGF	CA1-NG1	2.19	1.49	1.46
4	D	420(F)[A]	TGF	CA1-NG1	2.19	1.49	1.46
4	D	420(F)[B]	TGF	CB1-CA1	2.23	1.56	1.53
4	D	420(F)[A]	TGF	CB1-CA1	2.23	1.56	1.53
2	B	419(A)	PLP	C6-C5	2.27	1.42	1.37
2	A	419(A)	PLP	C6-C5	2.33	1.42	1.37
2	C	419(A)	PLP	C6-C5	2.34	1.42	1.37
4	B	420(C)[B]	TGF	CA1-NG1	2.37	1.50	1.46
4	B	420(C)[A]	TGF	CA1-NG1	2.37	1.50	1.46
4	D	420(F)[B]	TGF	CB2-CA2	2.41	1.56	1.53
4	D	420(F)[A]	TGF	CA2-NG2	2.64	1.50	1.46
4	D	420(F)[B]	TGF	C9-N10	3.15	1.51	1.45
4	D	420(F)[A]	TGF	C9-N10	3.15	1.51	1.45
4	B	420(C)[B]	TGF	C2-N3	3.51	1.41	1.35
4	B	420(C)[A]	TGF	C2-N3	3.51	1.41	1.35
4	B	420(C)[B]	TGF	C16-C15	3.52	1.45	1.38
4	B	420(C)[A]	TGF	C16-C15	3.52	1.45	1.38
4	D	420(F)[B]	TGF	C16-C15	3.63	1.45	1.38
4	D	420(F)[A]	TGF	C16-C15	3.63	1.45	1.38
4	D	420(F)[B]	TGF	C2-N3	3.83	1.42	1.35
4	D	420(F)[A]	TGF	C2-N3	3.83	1.42	1.35
4	B	420(C)[B]	TGF	C9-N10	4.00	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	420(C)[A]	TGF	C9-N10	4.00	1.53	1.45
4	D	420(F)[B]	TGF	C8A-N1	4.02	1.41	1.34
4	D	420(F)[A]	TGF	C8A-N1	4.02	1.41	1.34
2	B	419(A)	PLP	C3-C2	4.02	1.43	1.40
4	B	420(C)[B]	TGF	C8A-N1	4.08	1.42	1.34
4	B	420(C)[A]	TGF	C8A-N1	4.08	1.42	1.34
2	C	419(A)	PLP	C3-C2	4.19	1.43	1.40
4	D	420(F)[B]	TGF	C4-N3	4.27	1.41	1.33
4	D	420(F)[A]	TGF	C4-N3	4.27	1.41	1.33
4	B	420(C)[B]	TGF	C4-N3	4.32	1.41	1.33
4	B	420(C)[A]	TGF	C4-N3	4.32	1.41	1.33
4	D	420(F)[B]	TGF	C12-C11	4.67	1.47	1.39
4	D	420(F)[A]	TGF	C12-C11	4.67	1.47	1.39
2	A	419(A)	PLP	C3-C2	5.00	1.44	1.40
4	B	420(C)[B]	TGF	C12-C11	5.48	1.48	1.39
4	B	420(C)[A]	TGF	C12-C11	5.48	1.48	1.39
4	D	420(F)[B]	TGF	C13-C14	5.53	1.48	1.39
4	D	420(F)[A]	TGF	C13-C14	5.53	1.48	1.39
4	B	420(C)[B]	TGF	C13-C14	6.35	1.49	1.39
4	B	420(C)[A]	TGF	C13-C14	6.35	1.49	1.39
4	D	420(F)[B]	TGF	C4A-N5	6.55	1.51	1.42
4	D	420(F)[A]	TGF	C4A-N5	6.55	1.51	1.42
4	B	420(C)[B]	TGF	C4A-N5	6.91	1.52	1.42
4	B	420(C)[A]	TGF	C4A-N5	6.91	1.52	1.42

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	420(C)[B]	TGF	N3-C2-N1	-7.13	113.85	125.53
4	B	420(C)[A]	TGF	N3-C2-N1	-7.13	113.85	125.53
4	D	420(F)[B]	TGF	N3-C2-N1	-7.05	113.97	125.53
4	D	420(F)[A]	TGF	N3-C2-N1	-7.05	113.97	125.53
4	D	420(F)[B]	TGF	C4A-C4-N3	-5.05	115.70	123.46
4	D	420(F)[A]	TGF	C4A-C4-N3	-5.05	115.70	123.46
4	B	420(C)[B]	TGF	C4A-C4-N3	-4.97	115.82	123.46
4	B	420(C)[A]	TGF	C4A-C4-N3	-4.97	115.82	123.46
4	D	420(F)[B]	TGF	C16-C15-C14	-4.82	114.87	120.28
4	D	420(F)[A]	TGF	C16-C15-C14	-4.82	114.87	120.28
4	D	420(F)[B]	TGF	C4A-N5-C6	-4.43	112.09	119.81
4	D	420(F)[A]	TGF	C4A-N5-C6	-4.43	112.09	119.81
4	B	420(C)[B]	TGF	C16-C15-C14	-4.28	115.48	120.28
4	B	420(C)[A]	TGF	C16-C15-C14	-4.28	115.48	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	420(C)[B]	TGF	O5B-C5A-N5	-4.27	117.79	124.21
4	B	420(C)[A]	TGF	O5B-C5A-N5	-4.27	117.79	124.21
4	B	420(C)[B]	TGF	C4A-N5-C6	-4.10	112.67	119.81
4	B	420(C)[A]	TGF	C4A-N5-C6	-4.10	112.67	119.81
4	D	420(F)[B]	TGF	O5B-C5A-N5	-4.07	118.10	124.21
4	D	420(F)[A]	TGF	O5B-C5A-N5	-4.07	118.10	124.21
4	B	420(C)[B]	TGF	C12-C13-C14	-3.76	116.06	120.28
4	B	420(C)[A]	TGF	C12-C13-C14	-3.76	116.06	120.28
2	C	419(A)	PLP	C5A-C5-C6	-3.75	112.19	119.28
2	A	419(A)	PLP	C5A-C5-C6	-3.67	112.35	119.28
4	D	420(F)[B]	TGF	C12-C13-C14	-3.60	116.23	120.28
4	D	420(F)[A]	TGF	C12-C13-C14	-3.60	116.23	120.28
2	D	419(A)	PLP	C5A-C5-C6	-3.57	112.54	119.28
2	B	419(A)	PLP	C5A-C5-C6	-3.51	112.65	119.28
4	D	420(F)[B]	TGF	C13-C14-N10	-3.43	114.48	121.06
4	D	420(F)[A]	TGF	C13-C14-N10	-3.43	114.48	121.06
2	B	419(A)	PLP	C3-C2-N1	-2.96	116.52	120.61
2	D	419(A)	PLP	C3-C2-N1	-2.93	116.56	120.61
2	C	419(A)	PLP	C3-C2-N1	-2.78	116.77	120.61
2	A	419(A)	PLP	C3-C2-N1	-2.61	117.01	120.61
4	D	420(F)[A]	TGF	OEB-CD1-CG1	-2.44	117.77	121.98
2	B	419(A)	PLP	C6-C5-C4	-2.40	116.11	118.15
4	B	420(C)[B]	TGF	O-C-C11	-2.39	116.89	120.97
4	B	420(C)[A]	TGF	O-C-C11	-2.39	116.89	120.97
2	D	419(A)	PLP	C6-C5-C4	-2.33	116.17	118.15
2	D	419(A)	PLP	C5-C6-N1	-2.19	120.05	123.86
2	B	419(A)	PLP	C5-C6-N1	-2.10	120.22	123.86
2	A	419(A)	PLP	C5-C6-N1	-2.07	120.27	123.86
4	B	420(C)[B]	TGF	C15-C14-N10	-2.07	117.10	121.06
4	B	420(C)[A]	TGF	C15-C14-N10	-2.07	117.10	121.06
4	B	420(C)[B]	TGF	C13-C14-N10	-2.02	117.20	121.06
4	B	420(C)[A]	TGF	C13-C14-N10	-2.02	117.20	121.06
2	C	419(A)	PLP	C3-C4-C5	2.01	120.98	118.78
2	A	419(A)	PLP	C3-C4-C5	2.04	121.00	118.78
4	D	420(F)[B]	TGF	C9-N10-C14	2.06	126.64	121.46
4	D	420(F)[A]	TGF	C9-N10-C14	2.06	126.64	121.46
4	D	420(F)[B]	TGF	C9-C6-N5	2.12	115.28	110.94
4	D	420(F)[A]	TGF	C9-C6-N5	2.12	115.28	110.94
4	B	420(C)[B]	TGF	C15-C16-C11	2.18	123.28	120.76
4	B	420(C)[A]	TGF	C15-C16-C11	2.18	123.28	120.76
2	C	419(A)	PLP	O3P-P-O4P	2.31	113.21	106.56
2	B	419(A)	PLP	O3P-P-O4P	2.34	113.29	106.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	420(C)[B]	TGF	C9-C6-N5	2.47	115.99	110.94
4	B	420(C)[A]	TGF	C9-C6-N5	2.47	115.99	110.94
2	A	419(A)	PLP	O3P-P-O4P	2.67	114.24	106.56
2	D	419(A)	PLP	C3-C4-C5	2.78	121.81	118.78
2	B	419(A)	PLP	C3-C4-C5	2.97	122.02	118.78
2	C	419(A)	PLP	C6-N1-C2	3.00	125.39	119.28
2	D	419(A)	PLP	O3P-P-O4P	3.01	115.23	106.56
2	A	419(A)	PLP	C6-N1-C2	3.12	125.64	119.28
2	B	419(A)	PLP	C6-N1-C2	3.21	125.84	119.28
2	D	419(A)	PLP	C6-N1-C2	3.36	126.14	119.28
4	B	420(C)[B]	TGF	C11-C-NG1	3.71	123.54	116.93
4	B	420(C)[A]	TGF	C11-C-NG1	3.71	123.54	116.93
4	D	420(F)[B]	TGF	CG1-CB1-CA1	3.82	120.74	112.98
4	D	420(F)[A]	TGF	CG1-CB1-CA1	3.82	120.74	112.98
4	B	420(C)[B]	TGF	C2-N1-C8A	4.43	124.49	114.54
4	B	420(C)[A]	TGF	C2-N1-C8A	4.43	124.49	114.54
4	D	420(F)[B]	TGF	C2-N1-C8A	4.43	124.50	114.54
4	D	420(F)[A]	TGF	C2-N1-C8A	4.43	124.50	114.54
2	C	419(A)	PLP	C2A-C2-C3	4.48	126.44	121.04
2	D	419(A)	PLP	C2A-C2-C3	4.51	126.48	121.04
2	B	419(A)	PLP	C2A-C2-C3	4.69	126.69	121.04
4	B	420(C)[B]	TGF	C15-C14-C13	4.77	125.70	119.06
4	B	420(C)[A]	TGF	C15-C14-C13	4.77	125.70	119.06
2	A	419(A)	PLP	C2A-C2-C3	4.82	126.85	121.04
4	D	420(F)[B]	TGF	C15-C14-C13	5.10	126.15	119.06
4	D	420(F)[A]	TGF	C15-C14-C13	5.10	126.15	119.06
2	A	419(A)	PLP	C5A-C5-C4	6.87	130.76	121.65
2	C	419(A)	PLP	C5A-C5-C4	6.89	130.78	121.65
2	B	419(A)	PLP	C5A-C5-C4	7.09	131.04	121.65
2	D	419(A)	PLP	C5A-C5-C4	7.16	131.14	121.65
2	A	419(A)	PLP	O4P-C5A-C5	7.19	120.87	108.99
2	D	419(A)	PLP	O4P-C5A-C5	7.57	121.51	108.99
2	B	419(A)	PLP	O4P-C5A-C5	7.98	122.18	108.99
2	C	419(A)	PLP	O4P-C5A-C5	8.21	122.56	108.99
4	D	420(F)[B]	TGF	C4-N3-C2	8.76	128.09	115.94
4	D	420(F)[A]	TGF	C4-N3-C2	8.76	128.09	115.94
4	D	420(F)[B]	TGF	NA2-C2-N1	8.83	131.82	117.20
4	D	420(F)[A]	TGF	NA2-C2-N1	8.83	131.82	117.20
4	B	420(C)[B]	TGF	C4-N3-C2	8.85	128.23	115.94
4	B	420(C)[A]	TGF	C4-N3-C2	8.85	128.23	115.94
4	B	420(C)[B]	TGF	NA2-C2-N1	9.07	132.21	117.20
4	B	420(C)[A]	TGF	NA2-C2-N1	9.07	132.21	117.20



There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	420(C)[B]	TGF	O5B-C5A-N5-C6
4	B	420(C)[A]	TGF	O5B-C5A-N5-C6
4	D	420(F)[B]	TGF	O5B-C5A-N5-C4A
4	D	420(F)[A]	TGF	O5B-C5A-N5-C4A
4	B	420(C)[B]	TGF	O5B-C5A-N5-C4A
4	B	420(C)[A]	TGF	O5B-C5A-N5-C4A
4	D	420(F)[B]	TGF	CB1-CA1-NG1-C
4	D	420(F)[A]	TGF	CB1-CA1-NG1-C

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	420(C)[A]	TGF	2	0
5	B	422	GOL	1	0
3	C	420(B)	GLY	2	0
4	D	420(F)[A]	TGF	2	0
4	D	420(F)[B]	TGF	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	465/483 (96%)	-0.48	2 (0%) 93 94	24, 44, 78, 153	0
1	B	455/483 (94%)	-0.43	3 (0%) 89 90	21, 45, 92, 155	1 (0%)
1	C	465/483 (96%)	-0.51	0 100 100	22, 43, 73, 125	0
1	D	456/483 (94%)	-0.42	4 (0%) 85 86	20, 46, 94, 156	0
All	All	1841/1932 (95%)	-0.46	9 (0%) 91 93	20, 44, 83, 156	1 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	134(B)	LYS	3.9
1	A	355	SER	3.1
1	B	357	LEU	2.8
1	D	66	GLY	2.8
1	D	134(A)	LYS	2.5
1	B	326	LYS	2.4
1	B	-8	TRP	2.2
1	A	403	ALA	2.1
1	D	134	ASP	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	C	421	6/6	0.76	0.40	4.71	75,75,75,75	0
4	TGF	D	420(F)[A]	52/52	0.79	0.36	3.31	8,54,92,99	52
5	GOL	B	422	6/6	0.83	0.25	2.20	77,77,77,77	0
2	PLP	B	419(A)	15/16	0.96	0.17	2.13	45,45,45,45	0
4	TGF	B	420(C)[B]	52/52	0.83	0.28	1.53	24,61,107,122	52
4	TGF	B	420(C)[A]	52/52	0.83	0.28	1.53	20,58,107,122	52
3	GLY	A	420(B)	5/5	0.90	0.20	1.49	67,67,67,67	0
2	PLP	D	419(A)	15/16	0.97	0.15	0.89	37,37,37,37	0
4	TGF	D	420(F)[B]	52/52	0.79	0.36	0.53	20,59,94,99	52
3	GLY	C	420(B)	5/5	0.96	0.13	-0.17	51,51,51,51	0
2	PLP	C	419(A)	15/16	0.97	0.12	-0.19	36,36,36,36	0
2	PLP	A	419(A)	15/16	0.98	0.12	-0.22	37,37,37,37	0
5	GOL	D	421	6/6	0.95	0.12	-	56,56,56,56	0
5	GOL	B	421	6/6	0.95	0.17	-	58,58,58,58	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.