



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:37 PM UTC

PDB ID : 1LS3 / pdb_00001ls3
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

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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

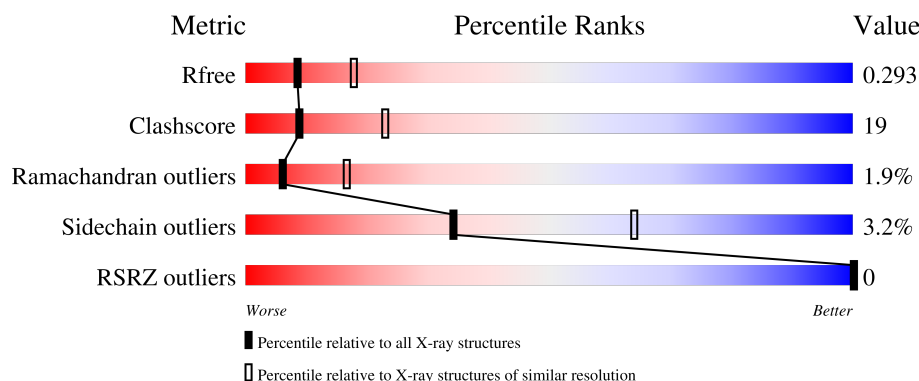
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	483	 62% 31% . .
1	B	483	 59% 31% . 6%
1	C	483	 63% 30% . .
1	D	483	 59% 30% 5% 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	-	-

2 Entry composition [i](#)

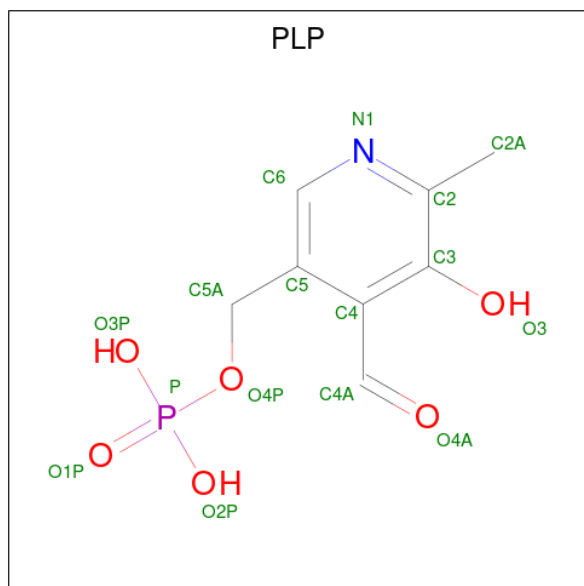
There are 6 unique types of molecules in this entry. The entry contains 14342 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



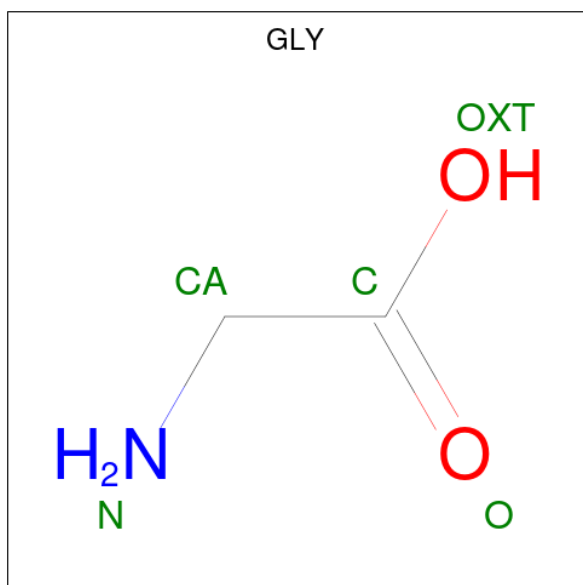
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

Continued on next page...

Continued from previous page...

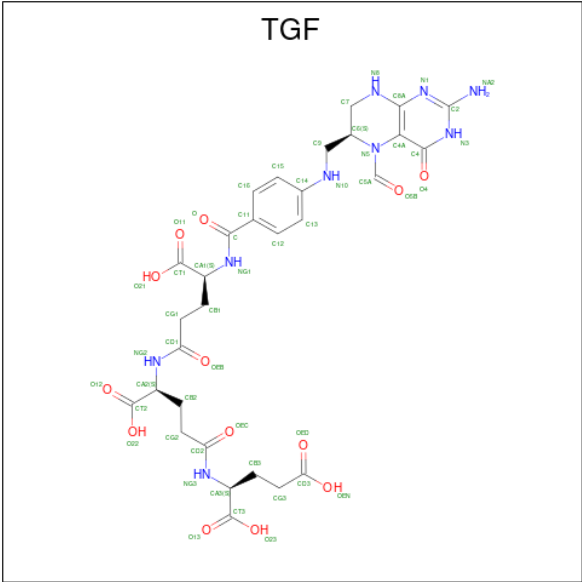
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂).



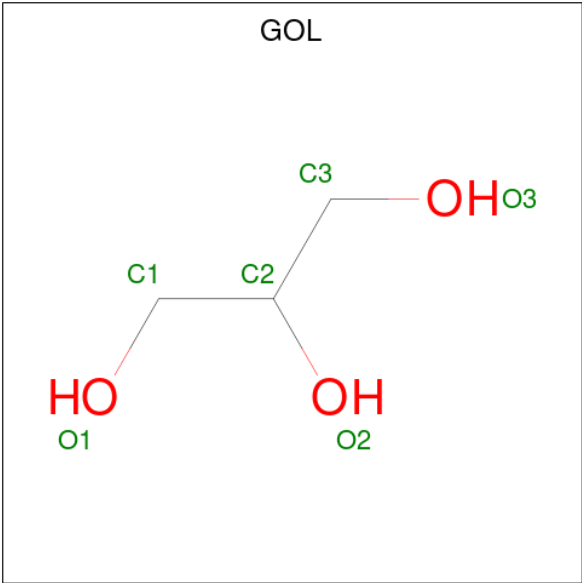
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	2	1	2		
3	C	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 4 is 2-[4-(4-{4-[(2-AMINO-5-FORMYL-4-OXO-3,4,5,6,7,8-HEXAHYDRO-PTE RIDIN-6-YLMETHYL)-AMINO]-BENZOYLAMINO}-4-CARBOXY-BUTYRYLAM INO)-4-CARBOXY-BUTYRYLAMINO]-PENTANEDIOIC ACID (CCD ID: TGF) (formula: C₃₀H₃₇N₉O₁₃).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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		

Continued on next page...

Continued from previous page...

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		

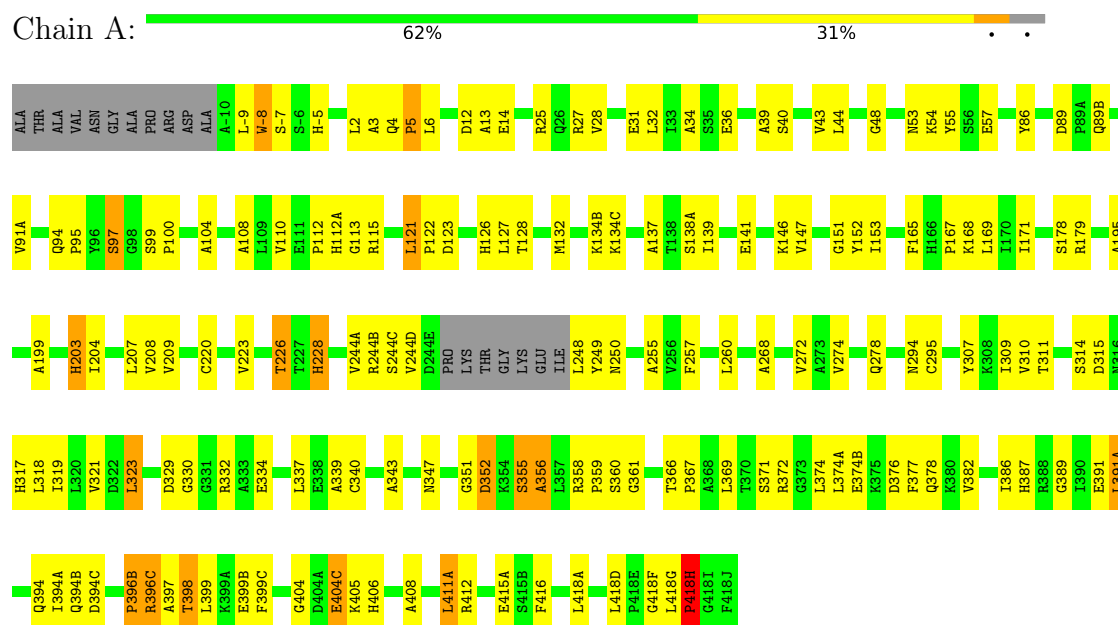
- Molecule 6 is water.

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		

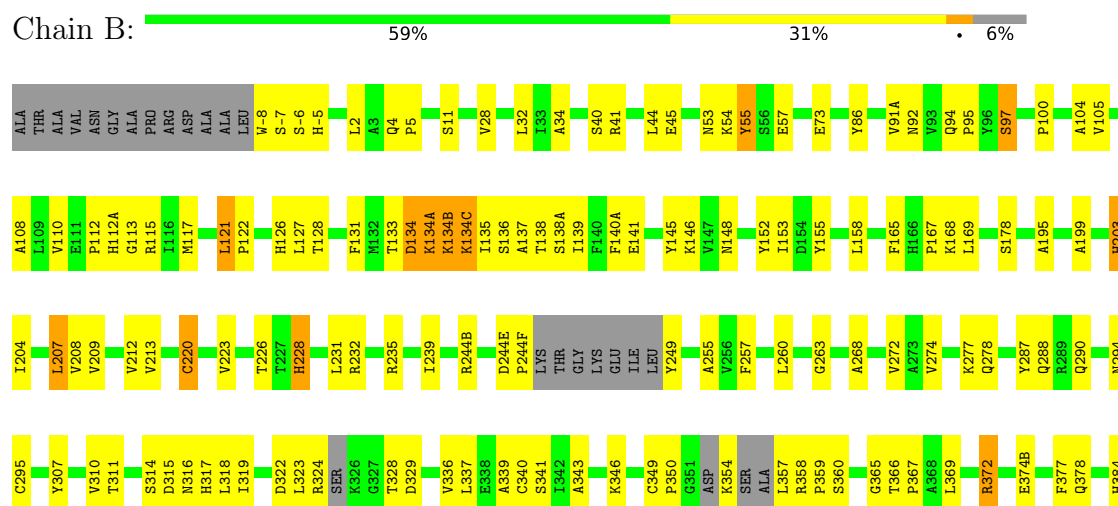
3 Residue-property plots

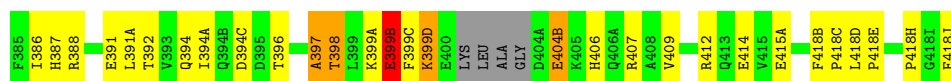
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Serine Hydroxymethyltransferase



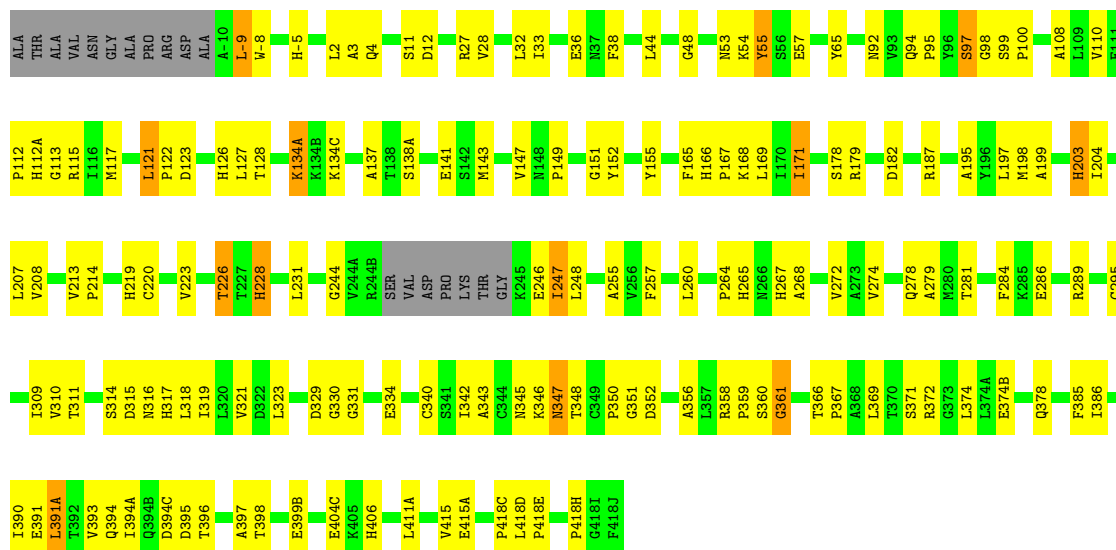
• Molecule 1: Serine Hydroxymethyltransferase





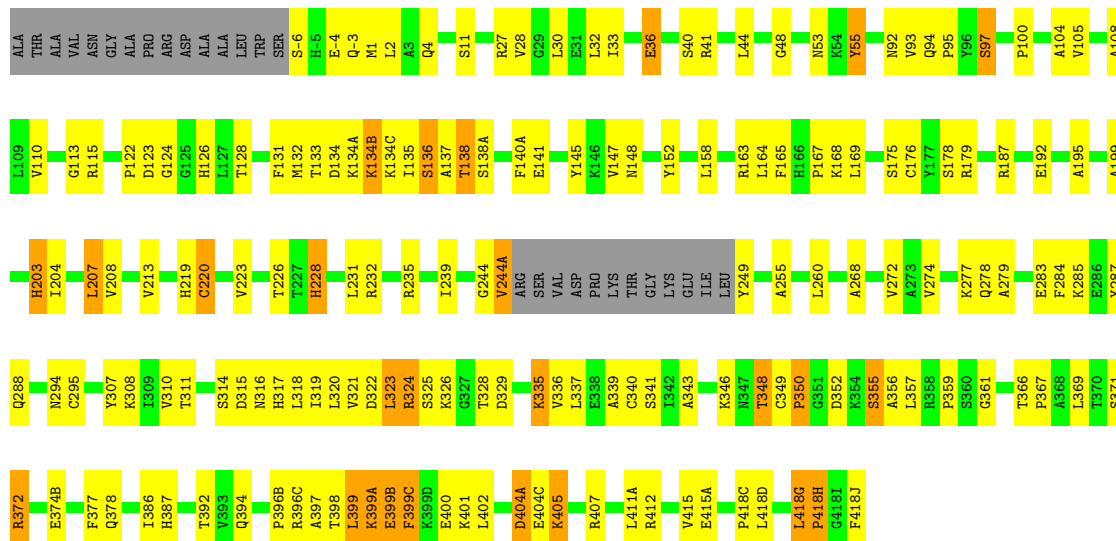
• Molecule 1: Serine Hydroxymethyltransferase

Chain C: 63% 30%



• Molecule 1: Serine Hydroxymethyltransferase

Chain D: 59% 30% 5% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	114.08Å 114.08Å 156.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.79 – 2.70 19.79 – 2.70	Depositor EDS
% Data completeness (in resolution range)	86.7 (19.79-2.70) 86.7 (19.79-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.68Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.294 0.221 , 0.293	Depositor DCC
R_{free} test set	4801 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 25.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.470 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14342	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: PLP, TGF, 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	0.48	0/3560	0.96	16/4828 (0.3%)
1	B	0.48	0/3471	0.95	13/4706 (0.3%)
1	C	0.48	0/3541	0.96	15/4804 (0.3%)
1	D	0.46	0/3442	1.00	19/4671 (0.4%)
All	All	0.47	0/14014	0.97	63/19009 (0.3%)

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	396(C)	ARG	N-CA-C	-9.70	100.71	112.54
1	D	399(C)	PHE	N-CA-C	-8.08	101.56	111.33
1	C	356	ALA	N-CA-C	-7.70	103.86	113.18
1	A	398	THR	N-CA-C	7.57	118.59	108.38
1	A	53	ASN	N-CA-C	7.30	120.28	111.82
1	C	53	ASN	N-CA-C	7.17	120.14	111.82
1	D	399(B)	GLU	N-CA-C	-7.13	105.76	114.75
1	D	402	LEU	N-CA-C	-7.07	103.32	112.23
1	B	244(F)	PRO	N-CA-CB	6.56	110.21	103.00
1	D	168	LYS	N-CA-C	-6.56	105.10	113.23
1	A	418(H)	PRO	N-CA-CB	6.46	110.03	103.25
1	A	361	GLY	N-CA-C	6.39	123.76	112.64
1	C	371	SER	N-CA-C	-6.14	105.64	113.01
1	B	53	ASN	N-CA-C	6.05	120.39	112.89
1	C	315	ASP	N-CA-C	-5.93	106.01	113.72
1	C	54	LYS	N-CA-C	5.91	119.15	109.76
1	D	53	ASN	N-CA-C	5.89	120.20	112.89
1	A	171	ILE	N-CA-C	5.87	116.56	107.99
1	A	54	LYS	N-CA-C	5.87	119.20	109.46
1	C	226	THR	N-CA-C	-5.83	102.14	110.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	ILE	N-CA-C	5.81	116.47	107.99
1	A	394(B)	GLN	N-CA-C	-5.76	105.51	112.54
1	B	73	GLU	N-CA-C	-5.75	105.09	111.36
1	C	231	LEU	N-CA-C	-5.71	106.31	113.28
1	B	394(C)	ASP	N-CA-C	-5.67	105.48	112.90
1	D	399(A)	LYS	N-CA-C	-5.62	106.01	112.92
1	D	326	LYS	N-CA-C	-5.55	105.48	114.09
1	D	232	ARG	N-CA-C	5.55	119.23	111.74
1	D	371	SER	N-CA-C	-5.51	105.65	112.38
1	D	136	SER	N-CA-C	5.50	118.90	110.20
1	B	168	LYS	N-CA-C	-5.48	106.43	113.23
1	D	138	THR	N-CA-C	-5.48	105.85	112.54
1	D	378	GLN	N-CA-C	-5.47	105.39	111.36
1	B	134	ASP	N-CA-C	-5.46	105.43	111.71
1	A	134(B)	LYS	N-CA-C	5.43	117.36	108.55
1	A	226	THR	N-CA-C	-5.40	102.76	110.59
1	D	231	LEU	N-CA-C	-5.40	106.69	113.28
1	A	91(A)	VAL	N-CA-C	5.38	115.46	108.35
1	B	232	ARG	N-CA-C	5.38	118.85	111.54
1	A	391(A)	LEU	N-CA-C	-5.37	105.33	111.07
1	C	244	GLY	N-CA-C	5.36	118.05	111.45
1	B	315	ASP	N-CA-C	-5.31	106.82	113.72
1	B	349	CYS	CA-C-N	5.28	126.44	119.84
1	B	349	CYS	C-N-CA	5.28	126.44	119.84
1	C	248	LEU	N-CA-C	5.27	117.89	110.14
1	D	175	SER	N-CA-C	-5.25	107.42	113.88
1	D	315	ASP	N-CA-C	-5.25	106.27	113.30
1	A	5	PRO	N-CA-C	-5.21	103.09	111.38
1	A	34	ALA	N-CA-C	5.19	118.39	111.75
1	C	151	GLY	N-CA-C	-5.17	108.49	115.36
1	A	371	SER	N-CA-C	-5.15	106.25	112.54
1	D	93	VAL	N-CA-C	5.15	117.06	112.17
1	B	220	CYS	N-CA-C	5.13	118.48	110.32
1	C	361	GLY	N-CA-C	5.13	120.50	111.57
1	A	315	ASP	N-CA-C	-5.08	107.11	113.72
1	C	168	LYS	N-CA-C	-5.06	106.95	113.23
1	D	220	CYS	N-CA-C	5.05	117.95	110.48
1	B	54	LYS	N-CA-C	5.04	118.02	109.76
1	A	151	GLY	N-CA-C	-5.03	108.67	115.36
1	C	385	PHE	N-CA-C	-5.03	105.71	111.14
1	C	391(A)	LEU	N-CA-C	-5.03	105.69	111.07
1	B	231	LEU	N-CA-C	-5.02	107.15	113.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	374(B)	GLU	N-CA-C	5.01	117.14	111.02

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	3489	0	3326	125	0
1	B	3404	0	3204	139	0
1	C	3470	0	3301	122	0
1	D	3374	0	3201	148	0
2	A	15	0	6	0	0
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	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 19.

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: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:C:203:HIS:HD2	1:C:317:HIS:HE2	1.23	0.86
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:C:281:THR:HG21	1:D:1:MET:HE1	1.58	0.85
1:A:203:HIS:HD2	1:A:317:HIS:HE2	1.25	0.84
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:HB3	1:B:407:ARG:NH1	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:HB3	1:B:407:ARG:HH11	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:D:323:LEU:C	1:D:325:SER:H	1.95	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
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:A:6:LEU:N	1:B:45:GLU:OE1	2.21	0.72
1:B:336:VAL:HG21	1:B:392:THR:OG1	1.89	0.72
1:A:391:GLU:O	1:A:394:GLN:HG3	1.90	0.71
1:C:310:VAL:HG12	1:C:311:THR:HG23	1.71	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:C:4:GLN:HG3	1:C:11:SER:HB2	1.76	0.67
1:D:369:LEU:O	1:D:372:ARG:HB2	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:330:GLY:O	1:A:334:GLU:HB2	1.94	0.66
1:C:390:ILE:O	1:C:393:VAL:HG23	1.96	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: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:C:398:THR:CG2	1:C:399(B):GLU:H	2.09	0.64
1:A:203:HIS:CD2	1:A:317:HIS:HE2	2.14	0.64
1:B:310:VAL:HG12	1:B:311:THR:HG23	1.81	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
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:A:86:TYR:CZ	1:A:209:VAL:HG23	2.35	0.61
1:C:-9:LEU:HD13	1:C:-8:TRP:H	1.65	0.61
1:B:392:THR:C	1:B:394:GLN:H	2.08	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:36:GLU:OE2	1:B:55:TYR:HB2	2.01	0.60
1:B:110:VAL:CG1	1:B:113:GLY:HA3	2.31	0.60
1:D:115:ARG:HB3	1:D:165:PHE:CE2	2.37	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:A:398:THR:OG1	1:A:399:LEU:N	2.34	0.60
1:C:352:ASP:OD1	1:C:360:SER:OG	2.20	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:B:366:THR:N	1:B:367:PRO:CD	2.65	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:399(C):PHE:CD2	1:D:399(C):PHE:C	2.80	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:B:138:THR:O	1:B:140(A):PHE:HB2	2.03	0.58
1:D:55:TYR:HA	6:D:635:HOH:O	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:B:392:THR:C	1:B:394:GLN:N	2.60	0.57
1:B:346:LYS:HD2	1:B:359:PRO:CG	2.31	0.57
1:C:203:HIS:CD2	1:C:317:HIS:HE2	2.12	0.57
1:D:204:ILE:O	1:D:208:VAL:HG23	2.05	0.57
1:C:228:HIS:H	1:C:228:HIS:CD2	2.21	0.57
1:C:246:GLU:HG3	1:C:246:GLU:O	2.05	0.57
1:A:366:THR:H	1:A:367:PRO:HD3	1.69	0.57
1:B:121:LEU:HD21	1:B:127:LEU:HD23	1.86	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:D:412:ARG:O	1:D:415(A):GLU:HG3	2.06	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:C:331:GLY:HA2	1:C:346:LYS:HD3	1.88	0.56
1:D:110:VAL:CG1	1:D:113:GLY:HA3	2.35	0.56
1:A:351:GLY:O	1:A:352:ASP:C	2.49	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:B:-6:SER:O	1:B:-5:HIS:HB3	2.05	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:CYS:SG	1:A:411(A):LEU:HD13	2.47	0.55
1:B:397:ALA:O	1:B:398:THR:OG1	2.23	0.55
1:C:48:GLY:O	1:D:44:LEU:HD23	2.07	0.55
1:D:323:LEU:O	1:D:325:SER:N	2.40	0.55
1:A:-9:LEU:HD22	1:A:-7:SER:HB3	1.88	0.55
1:D:97:SER:C	1:D:100:PRO:HD2	2.32	0.55
1:D:418(G):LEU:HB3	1:D:418(H):PRO:CD	2.36	0.54
1:A:309:ILE:CD1	1:A:321:VAL:HG22	2.37	0.54
1:A:404(C):GLU:CD	1:A:405:LYS:H	2.15	0.54
1:B:115:ARG:HA	1:B:141:GLU:O	2.07	0.54
1:B:203:HIS:CD2	1:B:317:HIS:HE2	2.20	0.54
1:C:32:LEU:HB2	1:C:343:ALA:O	2.08	0.54
1:B:391(A):LEU:O	1:B:394(A):ILE:HG13	2.07	0.54
1:A:397:ALA:HB1	1:A:399(B):GLU:OE1	2.07	0.54
1:D:92:ASN:OD1	1:D:95:PRO:HD3	2.07	0.54
1:D:321:VAL:O	1:D:361:GLY:HA2	2.07	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:C:366:THR:N	1:C:367:PRO:HD3	2.23	0.54
1:A:-9:LEU:C	1:A:-7:SER:H	2.16	0.54
1:C:121:LEU:HD21	1:C:127:LEU:HD23	1.88	0.54
1:D:418(C):PRO:HA	6:D:558:HOH:O	2.08	0.54
1:D:418(H):PRO:C	1:D:418(J):PHE:H	2.15	0.54
1:B:115:ARG:HB3	1:B:165:PHE:CE2	2.42	0.54
1:A:178:SER:HB2	1:A:314:SER:HB2	1.89	0.54
1:A:394(A):ILE:HG22	1:A:406:HIS:CE1	2.42	0.54
1:C:281:THR:CG2	1:D:1:MET:HE1	2.34	0.54
1:B:391:GLU:O	1:B:394:GLN:HB2	2.08	0.53
1:C:123:ASP:HB3	1:C:147:VAL:HG13	1.89	0.53
1:D:346:LYS:HE2	4:D:420(F)[A]:TGF:O13	2.08	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:322:ASP:C	1:D:323:LEU:O	2.50	0.53
1:D:126:HIS:CE1	1:D:128:THR:HG23	2.44	0.53
1:B:97:SER:C	1:B:100:PRO:HD2	2.34	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:398:THR:C	1:D:399(A):LYS:H	2.16	0.53
1:A:356:ALA:C	1:A:358:ARG:H	2.15	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ASP:C	1:B:324:ARG:H	2.16	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:D:323:LEU:C	1:D:325:SER:N	2.61	0.52
1:A:244(B):ARG:HA	1:A:249:TYR:CE2	2.44	0.52
1:B:354:LYS:HD3	1:B:358:ARG:HD3	1.91	0.52
1:B:294:ASN:HB3	1:B:377:PHE:CD2	2.45	0.52
1:D:28:VAL:HB	1:D:415(A):GLU:HB3	1.90	0.52
1:A:110:VAL:CG1	1:A:113:GLY:HA3	2.40	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:D:318:LEU:C	1:D:318:LEU:HD12	2.34	0.52
1:B:228:HIS:H	1:B:228:HIS:CD2	2.28	0.52
1:D:308:LYS:HB3	1:D:322:ASP:HB3	1.92	0.52
1:B:346:LYS:CD	1:B:359:PRO:HG2	2.34	0.52
1:C:134(A):LYS:NZ	1:C:134(A):LYS:HB3	2.25	0.52
1:C:286:GLU:CB	1:C:289:ARG:NH2	2.73	0.52
1:D:340:CYS:SG	1:D:411(A):LEU:HD23	2.50	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:354:LYS:HB3	1:B:358:ARG:HB3	1.92	0.51
1:B:374(B):GLU:HB2	6:B:640:HOH:O	2.09	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:B:108:ALA:HB2	1:B:255:ALA:HB2	1.92	0.51
1:C:33:ILE:HB	1:C:36:GLU:HG3	1.92	0.51
1:A:199:ALA:HB2	1:A:220:CYS:SG	2.49	0.51
1:A:-5:HIS:CD2	1:B:287:TYR:HB2	2.45	0.51
1:B:105:VAL:HG23	1:B:239:ILE:HD13	1.92	0.51
1:B:354:LYS:HB2	1:B:358:ARG:HB3	1.92	0.51
1:D:-6:SER:C	1:D:-4:GLU:H	2.18	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:A:141:GLU:HG3	1:C:141:GLU:HG3	1.93	0.51
1:B:366:THR:N	1:B:367:PRO:HD3	2.26	0.51
1:B:134(A):LYS:HD2	1:B:134(B):LYS:CB	2.41	0.51
1:A:355:SER:O	1:A:356:ALA:O	2.28	0.51
1:B:110:VAL:HG12	1:B:113:GLY:HA3	1.93	0.51
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:THR:N	1:D:367:PRO:HD3	2.26	0.50
1:D:399(C):PHE:C	1:D:399(C):PHE:HD2	2.19	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:207:LEU:HB3	1:D:213:VAL:HG22	1.94	0.50
1:D:310:VAL:HG21	1:D:320:LEU:HD23	1.92	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:318:LEU:HD12	1:C:318:LEU:C	2.36	0.50
1:B:384[B]:HIS:HD2	6:B:836:HOH:O	1.94	0.50
1:C:321:VAL:O	1:C:361:GLY:HA2	2.12	0.50
1:B:94:GLN:N	1:B:95:PRO:CD	2.75	0.50
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:A:369:LEU:O	1:A:372:ARG:HB2	2.13	0.49
1:C:97:SER:C	1:C:100:PRO:HD2	2.37	0.49
1:C:110:VAL:CG1	1:C:113:GLY:HA3	2.41	0.49
1:D:4:GLN:HE21	1:D:11:SER:HA	1.78	0.49
1:B:167:PRO:O	1:B:195:ALA:HB2	2.12	0.49
1:B:399(B):GLU:C	1:B:399(D):LYS:H	2.20	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:A:310:VAL:C	1:A:311:THR:HG23	2.38	0.49
1:D:122:PRO:HA	1:D:348:THR:HB	1.95	0.48
1:B:169:LEU:HD23	1:B:169:LEU:C	2.38	0.48
1:B:412:ARG:O	1:B:415(A):GLU:HG3	2.13	0.48
1:A:108:ALA:HB2	1:A:255:ALA:HB2	1.94	0.48
1:B:268:ALA:O	1:B:272:VAL:HG23	2.12	0.48
1:A:169:LEU:C	1:A:169:LEU:HD23	2.38	0.48
1:B:178:SER:HB2	1:B:314:SER:CB	2.44	0.48
1:B:329:ASP:HB2	1:B:359:PRO:O	2.12	0.48
1:A:115:ARG:HA	1:A:141:GLU:O	2.14	0.48
1:D:396(B):PRO:C	1:D:397:ALA:N	2.69	0.48
1:A:318:LEU:HD12	1:A:318:LEU:C	2.39	0.48
1:B:121:LEU:CB	1:B:122:PRO:HD3	2.44	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:134(A):LYS:HD2	1:D:134(A):LYS:C	2.39	0.48
1:D:366:THR:H	1:D:367:PRO:HD3	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:399(B):GLU:O	1:D:400:GLU:N	2.45	0.48
1:A:94:GLN:N	1:A:95:PRO:CD	2.76	0.48
1:B:126:HIS:HE1	1:B:128:THR:HG23	1.78	0.48
1:B:207:LEU:HB3	1:B:213:VAL:HG22	1.94	0.48
1:D:356:ALA:HB1	4:D:420(F)[B]:TGF:O12	2.14	0.48
1:C:2:LEU:HA	1:D:40:SER:HB2	1.96	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:B:318:LEU:C	1:B:318:LEU:HD12	2.39	0.48
1:D:94:GLN:N	1:D:95:PRO:CD	2.77	0.48
1:A:-9:LEU:O	1:A:-7:SER:N	2.47	0.47
1:A:366:THR:N	1:A:367:PRO:HD3	2.28	0.47
1:C:398:THR:HG22	1:C:399(B):GLU:CB	2.44	0.47
1:D:346:LYS:HD3	1:D:346:LYS:H	1.79	0.47
1:D:397:ALA:C	1:D:399:LEU:H	2.22	0.47
1:B:34:ALA:HA	1:B:365:GLY:HA3	1.95	0.47
1:C:178:SER:HB2	1:C:314:SER:HB2	1.96	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: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:12:ASP:HA	1:B:277:LYS:HZ3	1.80	0.47
1:D:167:PRO:O	1:D:195:ALA:HB2	2.14	0.47
1:B:-8:TRP:CD1	1:B:-8:TRP:H3	2.33	0.47
1:D:4:GLN:HE21	1:D:11:SER:CA	2.28	0.47
1:A:3:ALA:O	1:B:41:ARG:HD3	2.15	0.47
1:A:244(A):VAL:O	1:A:244(A):VAL:HG23	2.15	0.47
1:B:32:LEU:HB2	1:B:343:ALA:O	2.14	0.47
1:B:418(H):PRO:C	1:B:418(J):PHE:H	2.22	0.47
1:C:98:GLY:HA3	1:C:226:THR:HG22	1.97	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:D:115:ARG:HA	1:D:141:GLU:O	2.14	0.47
1:D:324:ARG:O	1:D:324:ARG:HG2	2.12	0.47
1:A:86:TYR:CE2	1:A:209:VAL:HG23	2.50	0.47
1:A:97:SER:C	1:A:100:PRO:HD2	2.39	0.47
1:D:169:LEU:C	1:D:169:LEU:HD23	2.40	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:B:104:ALA:HA	1:B:260:LEU:CD1	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:VAL:O	1:C:415(A):GLU:HA	2.16	0.46
1:D:336:VAL:HG23	1:D:337:LEU:N	2.29	0.46
1:B:145:TYR:CD2	1:B:158:LEU:HD13	2.50	0.46
1:A:332:ARG:NH2	1:A:398:THR:CB	2.78	0.46
1:B:-5:HIS:HE1	1:B:2:LEU:HD11	1.79	0.46
1:B:357:LEU:HD23	1:B:357:LEU:O	2.15	0.46
1:D:122:PRO:HA	1:D:348:THR:CB	2.45	0.46
1:D:135:ILE:HG13	1:D:136:SER:H	1.78	0.46
1:A:28:VAL:O	1:A:415(A):GLU:HA	2.16	0.46
1:C:152:TYR:CE1	1:C:179:ARG:HG3	2.50	0.46
1:C:309:ILE:CD1	1:C:321:VAL:HG22	2.45	0.46
1:D:126:HIS:HE1	1:D:128:THR:HG23	1.80	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:C:345:ASN:HB2	6:C:555:HOH:O	2.16	0.46
1:D:228:HIS:CD2	1:D:235:ARG:HA	2.50	0.46
1:B:404(B):GLU:C	1:B:406:HIS:N	2.74	0.46
1:C:32:LEU:HD13	1:C:386:ILE:HD11	1.98	0.46
1:C:279:ALA:HA	1:C:284:PHE:CG	2.51	0.46
1:A:152:TYR:CE1	1:A:179:ARG:HG3	2.51	0.46
1:A:343:ALA:HB3	6:A:776:HOH:O	2.15	0.46
1:C:-9:LEU:HD11	1:D:283:GLU:HG3	1.97	0.46
1:D:323:LEU:O	1:D:324:ARG:HB3	2.15	0.46
1:A:204:ILE:O	1:A:208:VAL:HG23	2.16	0.45
1:D:207:LEU:HD23	1:D:288:GLN:OE1	2.16	0.45
1:B:388:ARG:HH22	1:B:414:GLU:CD	2.25	0.45
1:C:-9:LEU:HD13	1:C:-8:TRP:N	2.29	0.45
1:B:146:LYS:HD2	1:D:164:LEU:HD21	1.98	0.45
1:B:207:LEU:HD22	1:B:212:VAL:HG21	1.97	0.45
1:C:92:ASN:OD1	1:C:95:PRO:HD3	2.17	0.45
1:A:294:ASN:HB3	1:A:377:PHE:CD2	2.51	0.45
1:B:117:MET:HG3	1:B:167:PRO:HB3	1.97	0.45
1:C:55:TYR:N	1:D:36:GLU:OE2	2.44	0.45
1:C:395:ASP:O	1:C:396:THR:C	2.60	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
1:A:48:GLY:O	1:B:44:LEU:HD23	2.15	0.45
1:B:137:ALA:HA	1:B:139:ILE:HD12	1.98	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:C:246:GLU:O	1:C:247:ILE:CB	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:THR:C	1:D:399(A):LYS:N	2.75	0.45
1:A:99:SER:HA	1:A:128:THR:HG21	1.98	0.45
1:D:322:ASP:O	1:D:323:LEU:O	2.34	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:A:355:SER:O	1:A:356:ALA:C	2.60	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:A:-9:LEU:C	1:A:-7:SER:N	2.75	0.44
1:A:147:VAL:HA	1:A:153:ILE:HA	1.99	0.44
1:B:55:TYR:CE1	1:B:263:GLY:HA3	2.53	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:D:28:VAL:HG11	6:D:514:HOH:O	2.16	0.44
1:D:268:ALA:O	1:D:272:VAL:HG23	2.17	0.44
1:D:418(G):LEU:O	1:D:418(H):PRO:O	2.35	0.44
1:A:323:LEU:HB2	1:A:360:SER:O	2.17	0.44
1:B:134(A):LYS:CD	1:B:134(B):LYS:N	2.75	0.44
1:B:340:CYS:O	1:B:341:SER:HB2	2.16	0.44
1:C:99:SER:HA	1:C:128:THR:HG21	1.99	0.44
1:D:392:THR:C	1:D:394:GLN:N	2.73	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:D:187:ARG:NH1	1:D:219:HIS:O	2.49	0.44
1:A:199:ALA:HB3	1:A:223:VAL:HG22	1.98	0.44
1:B:91(A):VAL:CG2	1:B:92:ASN:N	2.81	0.44
1:B:91(A):VAL:HG22	1:B:92:ASN:N	2.33	0.44
1:A:126:HIS:HE1	1:A:128:THR:HG23	1.83	0.44
1:A:137:ALA:CB	1:B:260:LEU:HD23	2.47	0.44
1:A:244(A):VAL:HA	1:A:248:LEU:HA	2.00	0.44
1:B:28:VAL:HB	1:B:415(A):GLU:HB3	1.99	0.44
1:C:309:ILE:HD13	1:C:321:VAL:HG22	1.99	0.44
1:D:404(A):ASP:OD1	1:D:405:LYS:HB3	2.17	0.44
1:A:-8:TRP:CZ2	1:B:290:GLN:HG2	2.53	0.44
1:A:132:MET:HE2	1:C:166:HIS:CD2	2.53	0.44
1:B:316:ASN:HB2	1:B:317:HIS:H	1.65	0.44
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:A:123:ASP:HB3	1:A:147:VAL:HG13	2.00	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:ASN:HB3	1:D:377:PHE:CD2	2.52	0.44
1:B:131:PHE:O	1:B:135:ILE:HG12	2.18	0.43
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:A:203:HIS:HD2	1:A:317:HIS:NE2	2.05	0.43
1:A:376:ASP:O	1:A:382:VAL:HG23	2.18	0.43
1:B:322:ASP:C	1:B:324:ARG:N	2.76	0.43
1:B:336:VAL:HG23	1:B:337:LEU:H	1.83	0.43
1:D:399(B):GLU:C	1:D:400:GLU:H	2.26	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:A:329:ASP:HB2	1:A:359:PRO:O	2.18	0.43
1:A:406:HIS:O	1:A:408:ALA:HB3	2.18	0.43
1:D:178:SER:HB2	1:D:314:SER:CB	2.49	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:307:TYR:HE1	1:D:387:HIS:HD1	1.65	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
1:C:110:VAL:HG13	1:C:113:GLY:HA3	2.01	0.43
1:D:316:ASN:HB2	1:D:317:HIS:H	1.60	0.43
4:D:420(F)[A]:TGF:HG3	4:D:420(F)[A]:TGF:HB21	1.44	0.43
1:A:123:ASP:OD1	1:A:146:LYS:HB3	2.18	0.43
1:A:250:ASN:CG	1:A:250:ASN:O	2.61	0.43
1:B:57:GLU:HB3	1:B:257:PHE:CZ	2.53	0.43
1:D:104:ALA:HA	1:D:260:LEU:CD1	2.48	0.43
1:D:108:ALA:HB2	1:D:255:ALA:CB	2.47	0.43
1:C:310:VAL:C	1:C:311:THR:HG23	2.44	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:A:369:LEU:HB3	1:A:374:LEU:HD22	2.01	0.42
1:B:32:LEU:HD13	1:B:386:ILE:HD11	2.01	0.42
1:D:244(A):VAL:CA	1:D:249:TYR:HD2	2.30	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:213:VAL:O	1:C:214:PRO:C	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:GLY:O	1:C:352:ASP:C	2.61	0.42
1:D:397:ALA:C	1:D:399:LEU:N	2.77	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:HD2	1:D:335:LYS:HA	1.86	0.42
1:A:31:GLU:HA	6:A:776:HOH:O	2.18	0.42
1:B:86:TYR:CE2	1:B:209:VAL:HG23	2.54	0.42
1:D:145:TYR:CD2	1:D:158:LEU:HD13	2.54	0.42
1:D:226:THR:HB	1:D:228:HIS:CD2	2.55	0.42
1:B:204:ILE:O	1:B:208:VAL:HG23	2.19	0.42
1:B:418(D):LEU:HD12	1:B:418(D):LEU:HA	1.90	0.42
1:C:108:ALA:HB2	1:C:255:ALA:CB	2.49	0.42
1:A:57:GLU:HB3	1:A:257:PHE:CZ	2.55	0.42
1:A:108:ALA:HB2	1:A:255:ALA:CB	2.50	0.42
1:A:411(A):LEU:O	1:A:412:ARG:C	2.62	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:D:399(B):GLU:O	1:D:401:LYS:N	2.52	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:131:PHE:H	1:D:138(A):SER:HB2	1.85	0.42
4:D:420(F)[B]:TGF:HG3	4:D:420(F)[B]:TGF:HB21	1.73	0.42
1:A:121:LEU:HD21	1:A:127:LEU:HD23	2.01	0.42
1:B:226:THR:HB	1:B:228:HIS:CD2	2.55	0.42
1:C:260:LEU:HD23	1:D:137:ALA:CB	2.50	0.42
1:D:336:VAL:O	1:D:339:ALA:N	2.52	0.42
1:A:115:ARG:HH21	1:C:141:GLU:HB3	1.84	0.42
1:A:168:LYS:HE2	1:A:168:LYS:HB3	1.88	0.42
1:B:339:ALA:HB1	1:B:409:VAL:HG11	2.01	0.42
1:B:108:ALA:HB2	1:B:255:ALA:CB	2.49	0.41
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:A:358:ARG:N	1:A:359:PRO:HD3	2.34	0.41
1:B:121:LEU:HB3	1:B:122:PRO:HD3	2.02	0.41
1:C:155:TYR:CE2	1:C:182:ASP:HB3	2.55	0.41
1:C:369:LEU:HB3	1:C:374:LEU:HD22	2.02	0.41
1:A:13:ALA:O	1:A:14:GLU:C	2.64	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:C:316:ASN:HB2	1:C:317:HIS:H	1.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404(C):GLU:CD	1:C:404(C):GLU:C	2.88	0.41
1:D:314:SER:HB2	1:D:319:ILE:HG22	2.03	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:B:295:CYS:SG	1:B:319:ILE:HG23	2.59	0.41
1:C:38:PHE:CE2	1:C:418(D):LEU:HD11	2.55	0.41
1:C:169:LEU:HD23	1:C:169:LEU:C	2.45	0.41
1:C:265:HIS:HB3	1:C:267:HIS:CE1	2.55	0.41
1:A:356:ALA:C	1:A:358:ARG:N	2.78	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:C:391(A):LEU:HD13	1:C:391(A):LEU:C	2.46	0.41
1:D:133:THR:OG1	1:D:134:ASP:N	2.51	0.41
1:A:137:ALA:HA	1:A:139:ILE:HD12	2.02	0.41
1:B:228:HIS:CD2	1:B:228:HIS:N	2.88	0.41
1:D:328:THR:OG1	1:D:329:ASP:N	2.53	0.41
1:B:399(A):LYS:C	1:B:399(C):PHE:N	2.79	0.41
1:D:355:SER:C	1:D:357:LEU:H	2.29	0.41
1:A:295:CYS:SG	1:A:319:ILE:HG23	2.61	0.41
1:B:4:GLN:HA	1:B:5:PRO:HD3	1.89	0.41
1:B:153:ILE:HB	1:B:155:TYR:CE1	2.56	0.41
1:B:357:LEU:HG	4:B:420(C)[A]:TGF:CG3	2.44	0.41
1:C:-5:HIS:CD2	1:D:287:TYR:HB2	2.56	0.41
1:C:171:ILE:HA	1:C:198:MET:O	2.21	0.41
1:C:295:CYS:SG	1:C:319:ILE:HG23	2.60	0.41
1:D:152:TYR:CE1	1:D:179:ARG:HG3	2.56	0.41
1:D:163:ARG:NE	1:D:192:GLU:OE2	2.42	0.41
1:A:178:SER:HB2	1:A:314:SER:CB	2.50	0.41
1:A:418(F):GLY:C	1:A:418(H):PRO:N	2.79	0.41
1:D:110:VAL:HG12	1:D:113:GLY:HA3	2.03	0.41
1:C:203:HIS:HD2	1:C:317:HIS:NE2	2.04	0.40
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:391(A):LEU:HD13	1:C:391(A):LEU:O	2.21	0.40
1:A:4:GLN:HA	1:A:5:PRO:HD3	1.97	0.40
1:D:32:LEU:HB2	1:D:343:ALA:O	2.21	0.40
1:D:132:MET:HB3	1:D:138(A):SER:OG	2.22	0.40
1:A:398:THR:HG23	1:A:399:LEU:CD2	2.52	0.40
1:B:134(A):LYS:CD	1:B:134(B):LYS:H	2.33	0.40
1:B:418(B):PHE:HA	1:B:418(C):PRO:HD3	1.80	0.40
1:C:12:ASP:OD1	1:C:12:ASP:C	2.65	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:418(G):LEU:HB3	1:D:418(H):PRO:HD2	2.03	0.40
1:A:104:ALA:HA	1:A:260:LEU:CD1	2.50	0.40
1:A:307:TYR:HE1	1:A:387:HIS:HD1	1.68	0.40
1:A:404(C):GLU:C	1:A:406:HIS:H	2.29	0.40
1:B:199:ALA:HB2	1:B:220:CYS:SG	2.62	0.40
1:C:117:MET:HA	1:C:143:MET:O	2.21	0.40
1:C:323:LEU:N	1:C:360:SER:O	2.55	0.40
1:C:342:ILE:HD11	1:C:415:VAL:HG21	2.04	0.40
1:D:404(A):ASP:OD1	1:D:404(A):ASP:C	2.64	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%)	4	12
1	B	447/483 (92%)	404 (90%)	34 (8%)	9 (2%)	6	16
1	C	461/483 (95%)	427 (93%)	31 (7%)	3 (1%)	18	41
1	D	452/483 (94%)	404 (89%)	36 (8%)	12 (3%)	4	10
All	All	1822/1932 (94%)	1647 (90%)	140 (8%)	35 (2%)	6	17

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	418(H)	PRO
1	B	244(E)	ASP
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%)	339 (97%)	11 (3%)	35 65
1	B	335/391 (86%)	321 (96%)	14 (4%)	26 55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	345/391 (88%)	337 (98%)	8 (2%)	44	73
1	D	333/391 (85%)	322 (97%)	11 (3%)	33	63
All	All	1363/1564 (87%)	1319 (97%)	44 (3%)	34	64

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	TYR
1	A	97	SER
1	A	121	LEU
1	A	203	HIS
1	A	207	LEU
1	A	228	HIS
1	A	347	ASN
1	A	352	ASP
1	A	396(B)	PRO
1	A	396(C)	ARG
1	A	411(A)	LEU
1	B	55	TYR
1	B	97	SER
1	B	121	LEU
1	B	134	ASP
1	B	134(A)	LYS
1	B	134(B)	LYS
1	B	134(C)	LYS
1	B	203	HIS
1	B	207	LEU
1	B	228	HIS
1	B	372	ARG
1	B	399(B)	GLU
1	B	399(D)	LYS
1	B	404(B)	GLU
1	C	-9	LEU
1	C	55	TYR
1	C	97	SER
1	C	121	LEU
1	C	203	HIS
1	C	207	LEU
1	C	228	HIS
1	C	347	ASN
1	D	36	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	55	TYR
1	D	97	SER
1	D	203	HIS
1	D	207	LEU
1	D	228	HIS
1	D	244(A)	VAL
1	D	285	LYS
1	D	324	ARG
1	D	335	LYS
1	D	372	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	180	ASN
1	A	203	HIS
1	A	228	HIS
1	A	250	ASN
1	A	347	ASN
1	A	378	GLN
1	A	394	GLN
1	A	394(B)	GLN
1	B	203	HIS
1	B	228	HIS
1	C	4	GLN
1	C	166	HIS
1	C	180	ASN
1	C	203	HIS
1	C	228	HIS
1	C	347	ASN
1	D	-3	GLN
1	D	4	GLN
1	D	180	ASN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	GLY	A	420(B)	2	4,4,4	0.96	0	3,4,4	1.06	0
2	PLP	D	419(A)	1	15,15,16	1.50	3 (20%)	21,22,23	2.84	11 (52%)
3	GLY	C	420(B)	2	4,4,4	0.92	0	3,4,4	1.01	0
5	GOL	C	421	-	5,5,5	0.97	0	5,5,5	0.20	0
2	PLP	A	419(A)	1,3	15,15,16	1.59	4 (26%)	21,22,23	2.70	9 (42%)
2	PLP	C	419(A)	1,3	15,15,16	1.44	3 (20%)	21,22,23	2.75	8 (38%)
4	TGF	D	420(F)[B]	-	51,54,54	2.31	10 (19%)	59,74,74	2.24	13 (22%)
4	TGF	B	420(C)[B]	-	51,54,54	2.42	10 (19%)	59,74,74	2.17	13 (22%)
5	GOL	D	421	-	5,5,5	0.68	0	5,5,5	0.28	0
2	PLP	B	419(A)	1	15,15,16	1.63	5 (33%)	21,22,23	2.83	11 (52%)
5	GOL	B	422	-	5,5,5	0.84	0	5,5,5	0.23	0
5	GOL	B	421	-	5,5,5	0.61	0	5,5,5	0.27	0
4	TGF	D	420(F)[A]	-	51,54,54	2.32	11 (21%)	59,74,74	2.28	14 (23%)
4	TGF	B	420(C)[A]	-	51,54,54	2.42	10 (19%)	59,74,74	2.17	13 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLY	A	420(B)	2	-	2/2/2/2	-
2	PLP	D	419(A)	1	-	3/6/6/8	0/1/1/1
3	GLY	C	420(B)	2	-	2/2/2/2	-
5	GOL	C	421	-	-	0/4/4/4	-
2	PLP	A	419(A)	1,3	-	0/6/6/8	0/1/1/1
2	PLP	C	419(A)	1,3	-	0/6/6/8	0/1/1/1
4	TGF	D	420(F)[B]	-	-	21/50/63/63	0/3/3/3
4	TGF	B	420(C)[B]	-	-	18/50/63/63	0/3/3/3
5	GOL	D	421	-	-	0/4/4/4	-
2	PLP	B	419(A)	1	-	3/6/6/8	0/1/1/1
5	GOL	B	422	-	-	0/4/4/4	-
5	GOL	B	421	-	-	0/4/4/4	-
4	TGF	D	420(F)[A]	-	-	20/50/63/63	0/3/3/3
4	TGF	B	420(C)[A]	-	-	18/50/63/63	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	420(C)[A]	TGF	C4A-N5	9.00	1.52	1.38
4	B	420(C)[B]	TGF	C4A-N5	9.00	1.52	1.38
4	D	420(F)[A]	TGF	C4A-N5	8.65	1.51	1.38
4	D	420(F)[B]	TGF	C4A-N5	8.65	1.51	1.38
4	B	420(C)[A]	TGF	C13-C14	6.16	1.49	1.39
4	B	420(C)[B]	TGF	C13-C14	6.16	1.49	1.39
4	B	420(C)[A]	TGF	C12-C11	6.12	1.48	1.39
4	B	420(C)[B]	TGF	C12-C11	6.12	1.48	1.39
4	D	420(F)[A]	TGF	C7-N8	-5.87	1.40	1.46
4	D	420(F)[B]	TGF	C7-N8	-5.87	1.40	1.46
4	B	420(C)[A]	TGF	C7-N8	-5.70	1.40	1.46
4	B	420(C)[B]	TGF	C7-N8	-5.70	1.40	1.46
4	D	420(F)[A]	TGF	C13-C14	5.35	1.48	1.39
4	D	420(F)[B]	TGF	C13-C14	5.35	1.48	1.39
4	D	420(F)[A]	TGF	C12-C11	5.20	1.47	1.39
4	D	420(F)[B]	TGF	C12-C11	5.20	1.47	1.39
4	B	420(C)[A]	TGF	C9-N10	4.25	1.53	1.45
4	B	420(C)[B]	TGF	C9-N10	4.25	1.53	1.45
4	D	420(F)[A]	TGF	C16-C15	4.01	1.45	1.38
4	D	420(F)[B]	TGF	C16-C15	4.01	1.45	1.38
4	B	420(C)[A]	TGF	C16-C15	3.89	1.45	1.38
4	B	420(C)[B]	TGF	C16-C15	3.89	1.45	1.38
4	B	420(C)[A]	TGF	C8A-N1	3.78	1.42	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	420(C)[B]	TGF	C8A-N1	3.78	1.42	1.36
4	D	420(F)[A]	TGF	C8A-N1	3.72	1.41	1.36
4	D	420(F)[B]	TGF	C8A-N1	3.72	1.41	1.36
4	D	420(F)[A]	TGF	C9-N10	3.36	1.51	1.45
4	D	420(F)[B]	TGF	C9-N10	3.36	1.51	1.45
2	A	419(A)	PLP	C3-C2	3.14	1.44	1.41
4	D	420(F)[A]	TGF	C4A-C4	3.09	1.51	1.43
4	D	420(F)[B]	TGF	C4A-C4	3.09	1.51	1.43
2	B	419(A)	PLP	C4A-C4	-3.06	1.45	1.51
4	B	420(C)[A]	TGF	C4A-C4	3.05	1.51	1.43
4	B	420(C)[B]	TGF	C4A-C4	3.05	1.51	1.43
2	D	419(A)	PLP	C4A-C4	-2.89	1.45	1.51
2	C	419(A)	PLP	C3-C2	2.60	1.43	1.41
2	C	419(A)	PLP	C6-C5	2.57	1.42	1.37
2	A	419(A)	PLP	C6-C5	2.56	1.42	1.37
2	B	419(A)	PLP	C6-C5	2.49	1.42	1.37
2	B	419(A)	PLP	C3-C2	2.49	1.43	1.41
2	D	419(A)	PLP	C3-C4	2.33	1.44	1.40
2	C	419(A)	PLP	O3-C3	-2.28	1.31	1.36
4	B	420(C)[A]	TGF	O4-C4	2.22	1.27	1.23
4	B	420(C)[B]	TGF	O4-C4	2.22	1.27	1.23
4	D	420(F)[A]	TGF	CA2-NG2	2.20	1.50	1.45
2	D	419(A)	PLP	O3-C3	-2.16	1.31	1.36
4	D	420(F)[A]	TGF	C7-C6	-2.15	1.49	1.52
4	D	420(F)[B]	TGF	C7-C6	-2.15	1.49	1.52
2	B	419(A)	PLP	C3-C4	2.07	1.44	1.40
4	D	420(F)[A]	TGF	O4-C4	2.07	1.27	1.23
4	D	420(F)[B]	TGF	O4-C4	2.07	1.27	1.23
2	A	419(A)	PLP	C3-C4	2.02	1.44	1.40
2	B	419(A)	PLP	O3-C3	-2.02	1.32	1.36
4	B	420(C)[A]	TGF	CA1-NG1	2.01	1.50	1.45
4	B	420(C)[B]	TGF	CA1-NG1	2.01	1.50	1.45
2	A	419(A)	PLP	O3-C3	-2.00	1.32	1.36

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	419(A)	PLP	O4P-C5A-C5	7.04	122.56	109.36
2	B	419(A)	PLP	O4P-C5A-C5	6.84	122.18	109.36
2	D	419(A)	PLP	O4P-C5A-C5	6.48	121.51	109.36
4	B	420(C)[A]	TGF	NA2-C2-N1	6.43	132.21	119.67
4	B	420(C)[B]	TGF	NA2-C2-N1	6.43	132.21	119.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	420(F)[A]	TGF	C2-N1-C8A	6.31	124.50	113.36
4	D	420(F)[B]	TGF	C2-N1-C8A	6.31	124.50	113.36
4	B	420(C)[A]	TGF	C2-N1-C8A	6.31	124.49	113.36
4	B	420(C)[B]	TGF	C2-N1-C8A	6.31	124.49	113.36
4	D	420(F)[A]	TGF	NA2-C2-N1	6.22	131.82	119.67
4	D	420(F)[B]	TGF	NA2-C2-N1	6.22	131.82	119.67
2	A	419(A)	PLP	O4P-C5A-C5	6.14	120.87	109.36
4	D	420(F)[A]	TGF	C15-C14-C13	5.35	126.15	119.04
4	D	420(F)[B]	TGF	C15-C14-C13	5.35	126.15	119.04
4	B	420(C)[A]	TGF	N3-C2-N1	-5.17	113.85	123.32
4	B	420(C)[B]	TGF	N3-C2-N1	-5.17	113.85	123.32
2	A	419(A)	PLP	C2A-C2-C3	5.17	126.85	120.80
4	D	420(F)[A]	TGF	N3-C2-N1	-5.11	113.97	123.32
4	D	420(F)[B]	TGF	N3-C2-N1	-5.11	113.97	123.32
2	B	419(A)	PLP	C2A-C2-C3	5.03	126.69	120.80
4	B	420(C)[A]	TGF	C15-C14-C13	5.01	125.70	119.04
4	B	420(C)[B]	TGF	C15-C14-C13	5.01	125.70	119.04
2	D	419(A)	PLP	C2A-C2-C3	4.85	126.48	120.80
2	C	419(A)	PLP	C2A-C2-C3	4.82	126.44	120.80
4	D	420(F)[A]	TGF	C16-C15-C14	-4.71	114.87	120.30
4	D	420(F)[B]	TGF	C16-C15-C14	-4.71	114.87	120.30
2	C	419(A)	PLP	C5A-C5-C6	-4.40	112.19	119.36
2	D	419(A)	PLP	C5A-C5-C4	4.31	131.14	122.64
2	A	419(A)	PLP	C5A-C5-C6	-4.30	112.35	119.36
2	B	419(A)	PLP	C5A-C5-C4	4.26	131.04	122.64
4	B	420(C)[A]	TGF	C16-C15-C14	-4.19	115.48	120.30
4	B	420(C)[B]	TGF	C16-C15-C14	-4.19	115.48	120.30
2	D	419(A)	PLP	C5A-C5-C6	-4.19	112.54	119.36
2	C	419(A)	PLP	C5A-C5-C4	4.13	130.78	122.64
2	B	419(A)	PLP	C5A-C5-C6	-4.12	112.65	119.36
2	A	419(A)	PLP	C5A-C5-C4	4.11	130.76	122.64
4	D	420(F)[A]	TGF	CG1-CB1-CA1	4.11	120.74	113.16
4	D	420(F)[B]	TGF	CG1-CB1-CA1	4.11	120.74	113.16
4	B	420(C)[A]	TGF	O5B-C5A-N5	-4.07	117.79	124.67
4	B	420(C)[B]	TGF	O5B-C5A-N5	-4.07	117.79	124.67
4	D	420(F)[A]	TGF	O5B-C5A-N5	-3.89	118.10	124.67
4	D	420(F)[B]	TGF	O5B-C5A-N5	-3.89	118.10	124.67
2	D	419(A)	PLP	C6-N1-C2	3.83	126.14	119.20
4	B	420(C)[A]	TGF	C12-C13-C14	-3.68	116.06	120.30
4	B	420(C)[B]	TGF	C12-C13-C14	-3.68	116.06	120.30
2	B	419(A)	PLP	C6-N1-C2	3.66	125.84	119.20
4	D	420(F)[A]	TGF	CB1-CA1-NG1	3.61	118.06	110.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	420(F)[B]	TGF	CB1-CA1-NG1	3.61	118.06	110.91
2	A	419(A)	PLP	C6-N1-C2	3.55	125.64	119.20
4	D	420(F)[A]	TGF	C12-C13-C14	-3.53	116.23	120.30
4	D	420(F)[B]	TGF	C12-C13-C14	-3.53	116.23	120.30
2	B	419(A)	PLP	C3-C2-N1	-3.52	116.52	120.96
4	B	420(C)[A]	TGF	C11-C-NG1	3.51	123.54	117.04
4	B	420(C)[B]	TGF	C11-C-NG1	3.51	123.54	117.04
2	D	419(A)	PLP	C3-C2-N1	-3.49	116.56	120.96
4	D	420(F)[A]	TGF	CA1-NG1-C	3.47	129.89	121.56
4	D	420(F)[B]	TGF	CA1-NG1-C	3.47	129.89	121.56
2	C	419(A)	PLP	C6-N1-C2	3.42	125.39	119.20
2	C	419(A)	PLP	C3-C2-N1	-3.32	116.77	120.96
2	D	419(A)	PLP	O3P-P-O4P	3.28	115.23	106.67
2	A	419(A)	PLP	C3-C2-N1	-3.13	117.01	120.96
2	A	419(A)	PLP	O3P-P-O4P	2.90	114.24	106.67
4	D	420(F)[A]	TGF	C13-C14-N10	-2.87	114.48	120.96
4	D	420(F)[B]	TGF	C13-C14-N10	-2.87	114.48	120.96
2	B	419(A)	PLP	C3-C4-C5	2.86	122.02	118.59
4	B	420(C)[A]	TGF	C4A-C4-N3	2.77	115.82	110.94
4	B	420(C)[B]	TGF	C4A-C4-N3	2.77	115.82	110.94
4	D	420(F)[A]	TGF	C4A-C4-N3	2.70	115.70	110.94
4	D	420(F)[B]	TGF	C4A-C4-N3	2.70	115.70	110.94
2	D	419(A)	PLP	C3-C4-C5	2.69	121.81	118.59
4	B	420(C)[A]	TGF	CA3-NG3-CD2	2.59	128.17	121.68
4	B	420(C)[B]	TGF	CA3-NG3-CD2	2.59	128.17	121.68
2	B	419(A)	PLP	O3P-P-O4P	2.54	113.29	106.67
2	C	419(A)	PLP	O3P-P-O4P	2.51	113.21	106.67
2	B	419(A)	PLP	C6-C5-C4	-2.42	116.11	118.10
4	D	420(F)[A]	TGF	CA2-NG2-CD1	2.40	127.69	121.68
4	B	420(C)[A]	TGF	CA1-NG1-C	2.36	127.23	121.56
4	B	420(C)[B]	TGF	CA1-NG1-C	2.36	127.23	121.56
4	D	420(F)[A]	TGF	OEB-CD1-CG1	-2.35	117.77	122.02
2	D	419(A)	PLP	C6-C5-C4	-2.35	116.17	118.10
4	B	420(C)[A]	TGF	C15-C16-C11	2.33	123.28	120.80
4	B	420(C)[B]	TGF	C15-C16-C11	2.33	123.28	120.80
2	D	419(A)	PLP	C5-C6-N1	-2.32	120.05	123.83
2	B	419(A)	PLP	C5-C6-N1	-2.22	120.22	123.83
2	D	419(A)	PLP	C4A-C4-C3	-2.20	116.86	120.52
2	B	419(A)	PLP	C4A-C4-C3	-2.19	116.87	120.52
2	A	419(A)	PLP	C5-C6-N1	-2.19	120.27	123.83
4	D	420(F)[B]	TGF	CG2-CB2-CA2	2.09	117.02	113.16
2	C	419(A)	PLP	C5-C6-N1	-2.09	120.43	123.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	420(C)[A]	TGF	O-C-C11	-2.02	116.89	120.90
4	B	420(C)[B]	TGF	O-C-C11	-2.02	116.89	120.90
2	A	419(A)	PLP	C3-C4-C5	2.01	121.00	118.59

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	419(A)	PLP	C5A-O4P-P-O3P
2	D	419(A)	PLP	C5A-O4P-P-O1P
2	D	419(A)	PLP	C5A-O4P-P-O2P
2	D	419(A)	PLP	C5A-O4P-P-O3P
3	A	420(B)	GLY	O-C-CA-N
3	A	420(B)	GLY	OXT-C-CA-N
3	C	420(B)	GLY	O-C-CA-N
3	C	420(B)	GLY	OXT-C-CA-N
4	B	420(C)[A]	TGF	O5B-C5A-N5-C4A
4	B	420(C)[A]	TGF	O5B-C5A-N5-C6
4	B	420(C)[A]	TGF	C11-C-NG1-CA1
4	B	420(C)[B]	TGF	O5B-C5A-N5-C4A
4	B	420(C)[B]	TGF	O5B-C5A-N5-C6
4	B	420(C)[B]	TGF	C11-C-NG1-CA1
4	D	420(F)[A]	TGF	O5B-C5A-N5-C4A
4	D	420(F)[A]	TGF	O5B-C5A-N5-C6
4	D	420(F)[A]	TGF	CB1-CA1-NG1-C
4	D	420(F)[B]	TGF	O5B-C5A-N5-C4A
4	D	420(F)[B]	TGF	O5B-C5A-N5-C6
4	D	420(F)[B]	TGF	CB1-CA1-NG1-C
4	B	420(C)[A]	TGF	O-C-NG1-CA1
4	B	420(C)[B]	TGF	O-C-NG1-CA1
4	D	420(F)[B]	TGF	CB2-CA2-NG2-CD1
4	D	420(F)[A]	TGF	CT2-CA2-NG2-CD1
4	D	420(F)[A]	TGF	OEB-CD1-NG2-CA2
4	D	420(F)[B]	TGF	OEB-CD1-NG2-CA2
4	B	420(C)[A]	TGF	OEB-CD1-NG2-CA2
4	B	420(C)[B]	TGF	OEB-CD1-NG2-CA2
4	D	420(F)[B]	TGF	CG2-CD2-NG3-CA3
4	D	420(F)[B]	TGF	OEC-CD2-NG3-CA3
4	B	420(C)[A]	TGF	CA2-CB2-CG2-CD2
4	B	420(C)[B]	TGF	CA2-CB2-CG2-CD2
4	D	420(F)[A]	TGF	CA1-CB1-CG1-CD1
4	D	420(F)[A]	TGF	CA2-CB2-CG2-CD2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	420(C)[A]	TGF	OEC-CD2-NG3-CA3
4	B	420(C)[B]	TGF	OEC-CD2-NG3-CA3
4	D	420(F)[B]	TGF	CA2-CB2-CG2-CD2
4	B	420(C)[A]	TGF	CG2-CD2-NG3-CA3
4	B	420(C)[B]	TGF	CG2-CD2-NG3-CA3
4	B	420(C)[A]	TGF	NG3-CD2-CG2-CB2
4	B	420(C)[B]	TGF	NG3-CD2-CG2-CB2
4	B	420(C)[A]	TGF	OEC-CD2-CG2-CB2
4	B	420(C)[B]	TGF	OEC-CD2-CG2-CB2
4	D	420(F)[A]	TGF	OEC-CD2-CG2-CB2
4	D	420(F)[A]	TGF	NG3-CD2-CG2-CB2
4	B	420(C)[A]	TGF	CB3-CA3-NG3-CD2
4	D	420(F)[B]	TGF	NG3-CD2-CG2-CB2
4	D	420(F)[B]	TGF	OEC-CD2-CG2-CB2
4	D	420(F)[A]	TGF	C11-C-NG1-CA1
4	D	420(F)[B]	TGF	C11-C-NG1-CA1
4	D	420(F)[B]	TGF	CA1-CB1-CG1-CD1
4	B	420(C)[A]	TGF	CT3-CA3-CB3-CG3
4	D	420(F)[A]	TGF	O-C-NG1-CA1
4	D	420(F)[B]	TGF	O-C-NG1-CA1
4	D	420(F)[A]	TGF	C13-C14-N10-C9
4	D	420(F)[B]	TGF	C13-C14-N10-C9
4	B	420(C)[A]	TGF	CB2-CA2-CT2-O12
4	B	420(C)[B]	TGF	CB2-CA2-CT2-O12
4	D	420(F)[B]	TGF	CG1-CD1-NG2-CA2
4	B	420(C)[A]	TGF	CB2-CA2-CT2-O22
4	B	420(C)[B]	TGF	CB2-CA2-CT2-O22
4	D	420(F)[A]	TGF	C15-C14-N10-C9
4	D	420(F)[B]	TGF	C15-C14-N10-C9
2	B	419(A)	PLP	C5A-O4P-P-O2P
4	D	420(F)[A]	TGF	NG2-CA2-CT2-O12
4	D	420(F)[A]	TGF	NG2-CA2-CT2-O22
4	B	420(C)[B]	TGF	CA3-CB3-CG3-CD3
4	D	420(F)[B]	TGF	CB3-CA3-CT3-O13
2	B	419(A)	PLP	C5A-O4P-P-O1P
4	D	420(F)[A]	TGF	CT2-CA2-CB2-CG2
4	D	420(F)[A]	TGF	CA3-CB3-CG3-CD3
4	D	420(F)[B]	TGF	CB3-CA3-CT3-O23
4	D	420(F)[B]	TGF	OED-CD3-CG3-CB3
4	B	420(C)[A]	TGF	OEN-CD3-CG3-CB3
4	D	420(F)[B]	TGF	OEN-CD3-CG3-CB3
4	B	420(C)[B]	TGF	OEN-CD3-CG3-CB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	420(C)[A]	TGF	OED-CD3-CG3-CB3
4	B	420(C)[B]	TGF	OED-CD3-CG3-CB3
4	D	420(F)[A]	TGF	CG1-CD1-NG2-CA2
4	D	420(F)[A]	TGF	OED-CD3-CG3-CB3
4	D	420(F)[A]	TGF	OEN-CD3-CG3-CB3
4	B	420(C)[A]	TGF	C6-C9-N10-C14
4	B	420(C)[B]	TGF	C6-C9-N10-C14
4	D	420(F)[B]	TGF	CT3-CA3-CB3-CG3
4	B	420(C)[A]	TGF	NG1-CA1-CT1-O11
4	B	420(C)[B]	TGF	NG1-CA1-CT1-O11
4	B	420(C)[B]	TGF	CT3-CA3-CB3-CG3

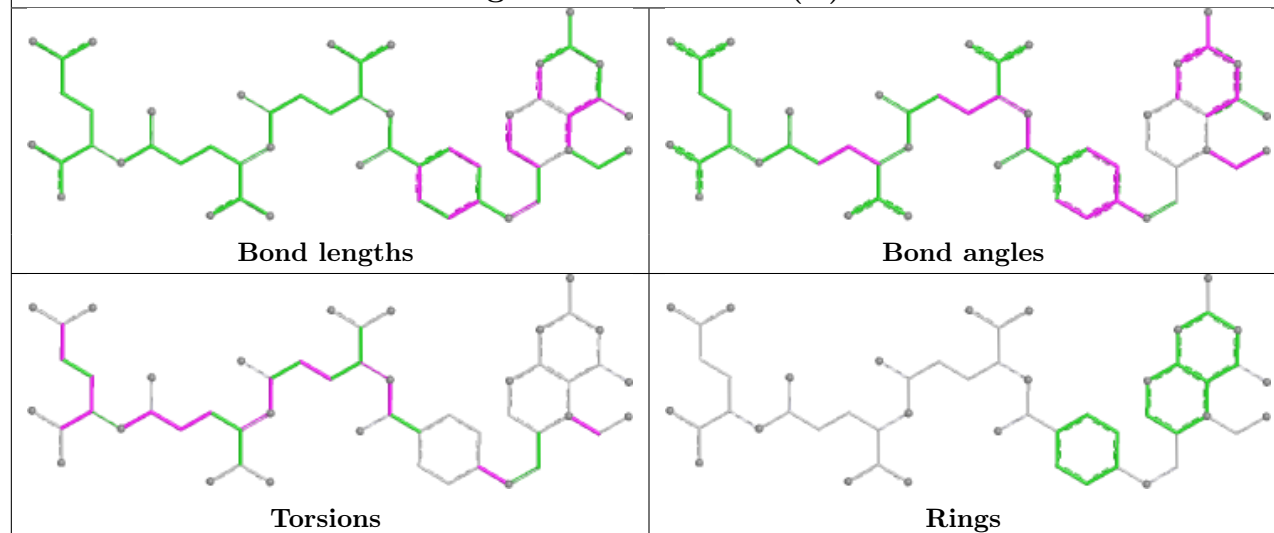
There are no ring outliers.

5 monomers are involved in 9 short contacts:

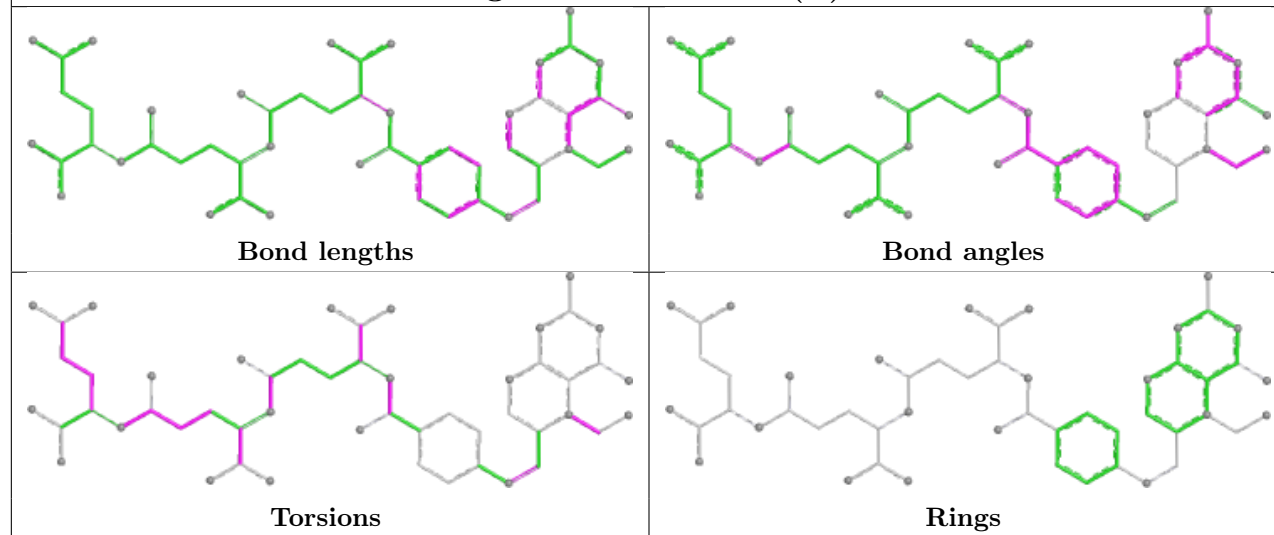
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	420(B)	GLY	2	0
4	D	420(F)[B]	TGF	2	0
5	B	422	GOL	1	0
4	D	420(F)[A]	TGF	2	0
4	B	420(C)[A]	TGF	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

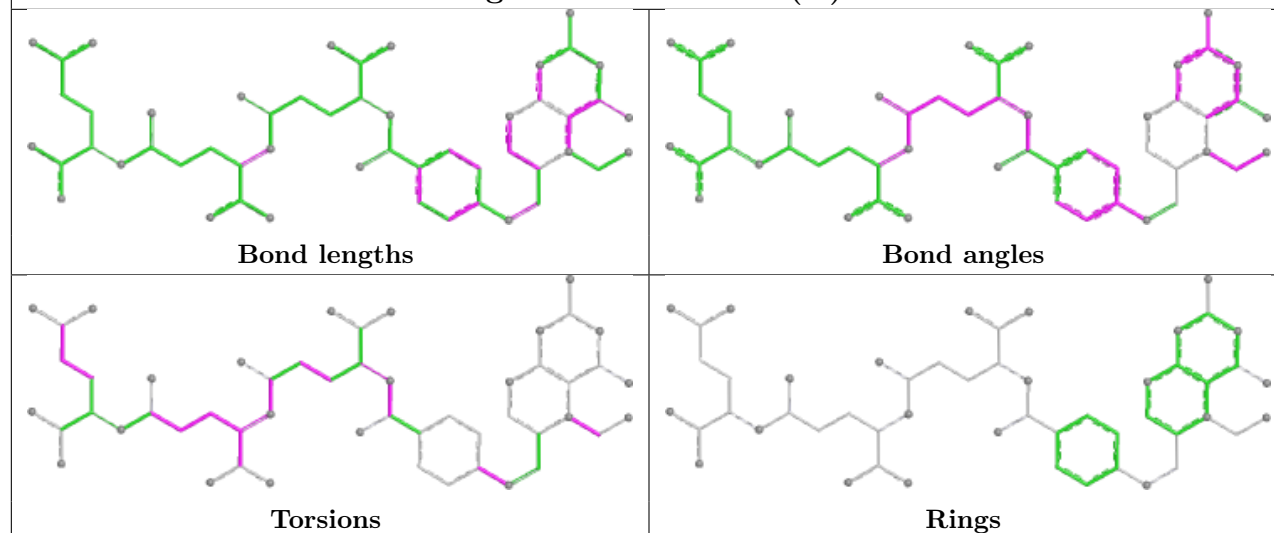
Ligand TGF D 420F (B)

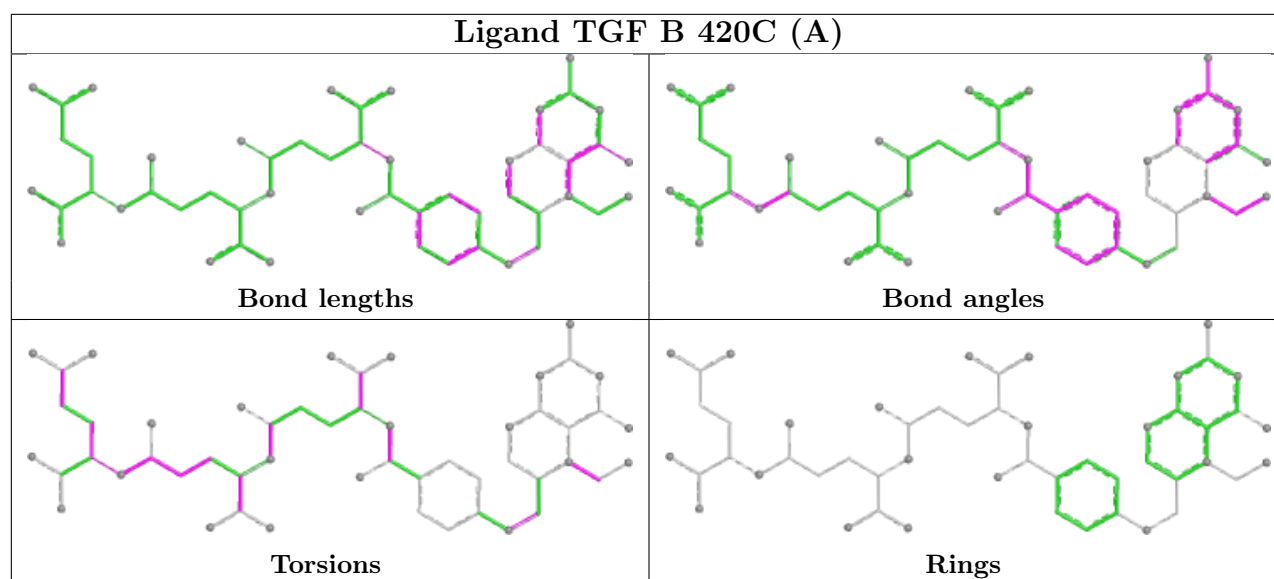


Ligand TGF B 420C (B)



Ligand TGF D 420F (A)





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, 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	465/483 (96%)	-1.52	0 100 100	22, 44, 78, 153	1 (0%)
1	B	455/483 (94%)	-1.48	0 100 100	16, 45, 92, 155	3 (0%)
1	C	465/483 (96%)	-1.53	0 100 100	22, 43, 73, 125	0
1	D	456/483 (94%)	-1.48	0 100 100	20, 46, 94, 156	0
All	All	1841/1932 (95%)	-1.50	0 100 100	16, 44, 83, 156	4 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	C	421	6/6	0.97	0.05	75,75,75,75	0
4	TGF	B	420(C)[B]	52/52	0.98	0.05	24,61,107,122	52
4	TGF	D	420(F)[A]	52/52	0.98	0.07	8,54,92,99	52
4	TGF	D	420(F)[B]	52/52	0.98	0.07	20,59,94,99	52

Continued on next page...

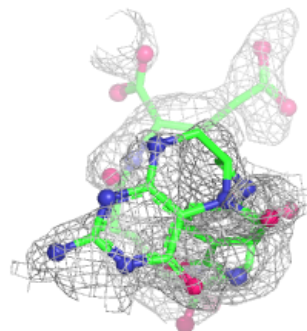
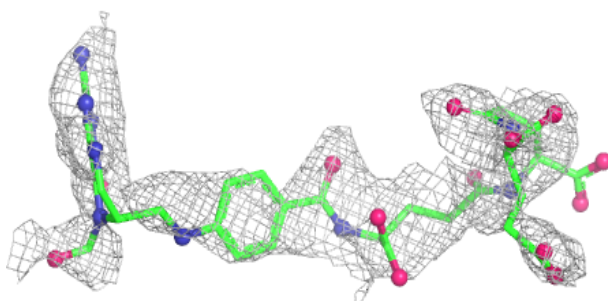
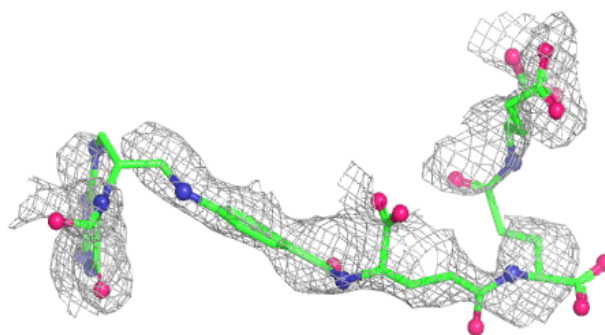
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	B	421	6/6	0.98	0.05	58,58,58,58	0
5	GOL	B	422	6/6	0.98	0.05	77,77,77,77	0
4	TGF	B	420(C)[A]	52/52	0.98	0.05	20,58,107,122	52
5	GOL	D	421	6/6	0.98	0.04	56,56,56,56	0
2	PLP	B	419(A)	15/16	0.99	0.04	45,45,45,45	0
2	PLP	D	419(A)	15/16	0.99	0.03	37,37,37,37	0
3	GLY	A	420(B)	5/5	0.99	0.03	67,67,67,67	0
3	GLY	C	420(B)	5/5	0.99	0.04	51,51,51,51	0
2	PLP	C	419(A)	15/16	1.00	0.03	36,36,36,36	0
2	PLP	A	419(A)	15/16	1.00	0.03	37,37,37,37	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

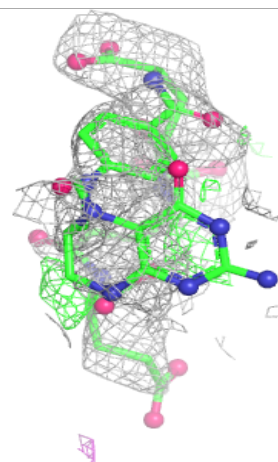
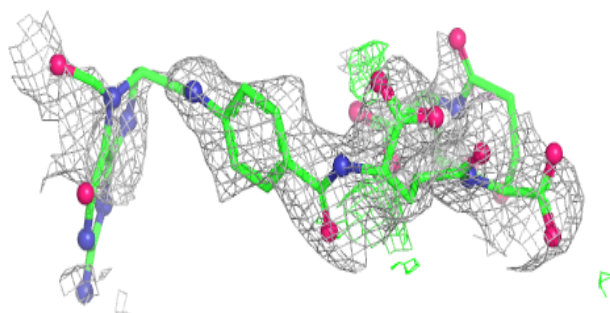
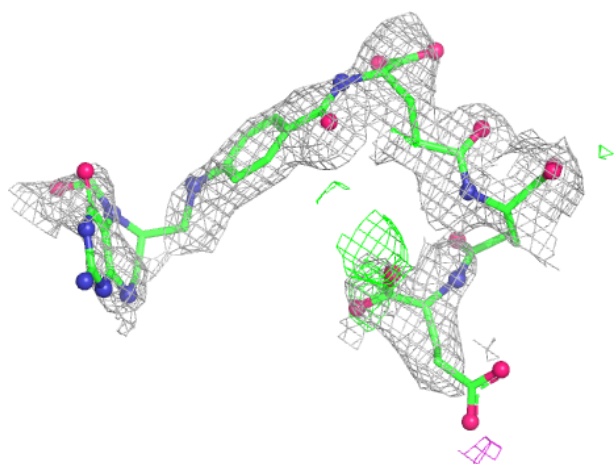
Electron density around TGF B 420C (B):

2mF_o-DF_c (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
 and green (positive)



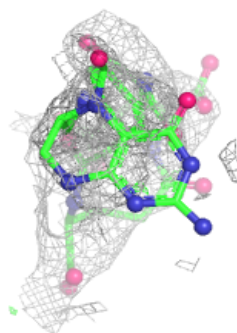
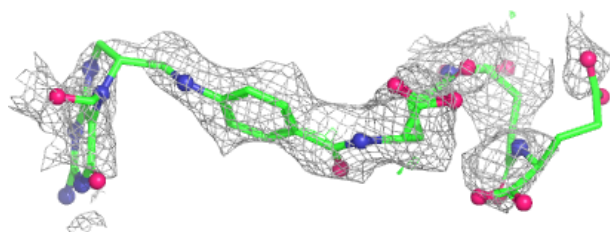
Electron density around TGF D 420F (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

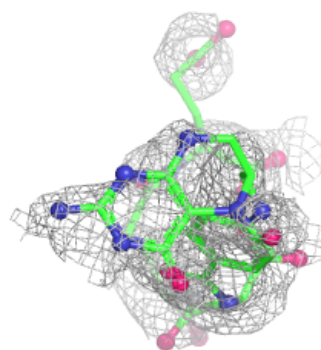
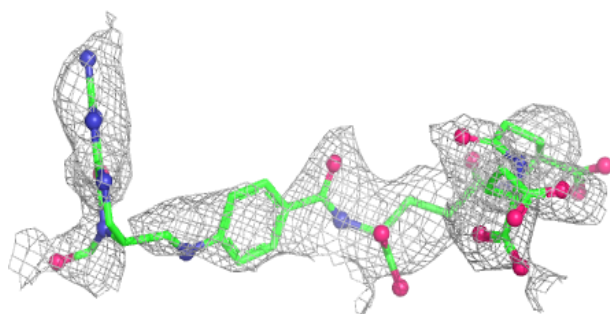
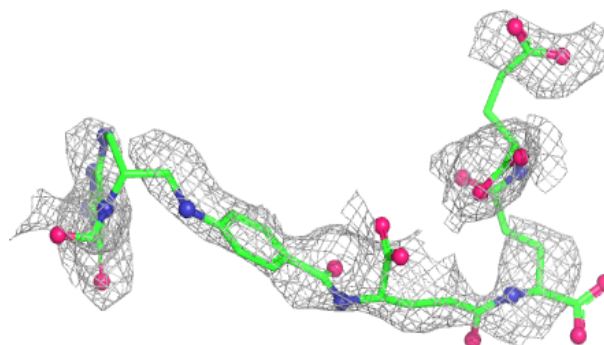


Electron density around TGF D 420F (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around TGF B 420C (A):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.