



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:51 PM UTC

PDB ID : 7C11 / pdb_00007c11
Title : Formate--tetrahydrofolate ligase from Methylobacterium extorquens CM4 strain
Authors : Kim, K.-J.; Kim, S.; Seo, H.; Lee, S.
Deposited on : 2020-05-02
Resolution : 2.81 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

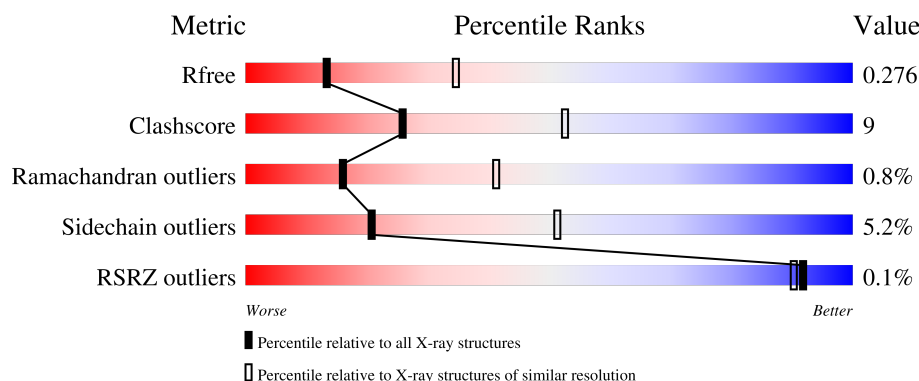
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	568	
1	B	568	
1	C	568	
1	D	568	
1	M	568	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	N	568	
1	O	568	
1	P	568	

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
4	FLC	N	601	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33673 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 Formate-tetrahydrofolate ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	1	0
			4184	2637	745	781	21			
1	B	558	Total	C	N	O	S	0	0	0
			4181	2634	745	781	21			
1	C	556	Total	C	N	O	S	0	0	0
			4168	2626	743	779	20			
1	D	556	Total	C	N	O	S	0	0	0
			4168	2626	743	779	20			
1	M	552	Total	C	N	O	S	0	0	0
			4139	2609	738	772	20			
1	N	555	Total	C	N	O	S	0	0	0
			4159	2621	741	777	20			
1	O	556	Total	C	N	O	S	0	0	0
			4168	2626	743	779	20			
1	P	547	Total	C	N	O	S	0	0	0
			4099	2583	731	765	20			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	558	ALA	-	expression tag	UNP B7L0A5
A	559	ALA	-	expression tag	UNP B7L0A5
A	560	ALA	-	expression tag	UNP B7L0A5
A	561	LEU	-	expression tag	UNP B7L0A5
A	562	GLU	-	expression tag	UNP B7L0A5
A	563	HIS	-	expression tag	UNP B7L0A5
A	564	HIS	-	expression tag	UNP B7L0A5
A	565	HIS	-	expression tag	UNP B7L0A5
A	566	HIS	-	expression tag	UNP B7L0A5
A	567	HIS	-	expression tag	UNP B7L0A5
A	568	HIS	-	expression tag	UNP B7L0A5
B	558	ALA	-	expression tag	UNP B7L0A5
B	559	ALA	-	expression tag	UNP B7L0A5

Continued on next page...

Continued from previous page...

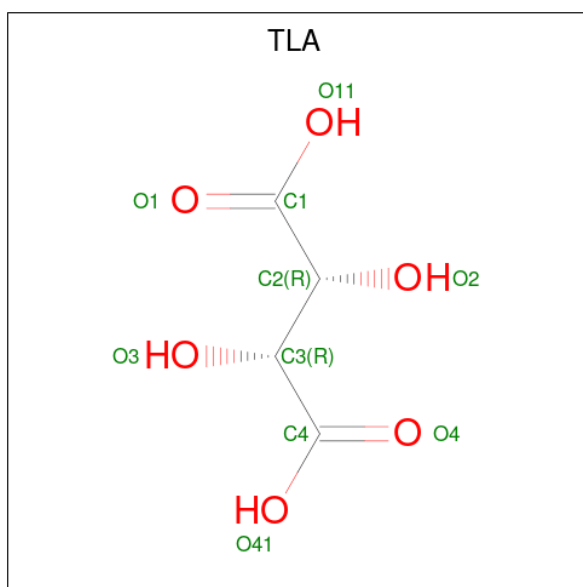
Chain	Residue	Modelled	Actual	Comment	Reference
B	560	ALA	-	expression tag	UNP B7L0A5
B	561	LEU	-	expression tag	UNP B7L0A5
B	562	GLU	-	expression tag	UNP B7L0A5
B	563	HIS	-	expression tag	UNP B7L0A5
B	564	HIS	-	expression tag	UNP B7L0A5
B	565	HIS	-	expression tag	UNP B7L0A5
B	566	HIS	-	expression tag	UNP B7L0A5
B	567	HIS	-	expression tag	UNP B7L0A5
B	568	HIS	-	expression tag	UNP B7L0A5
C	558	ALA	-	expression tag	UNP B7L0A5
C	559	ALA	-	expression tag	UNP B7L0A5
C	560	ALA	-	expression tag	UNP B7L0A5
C	561	LEU	-	expression tag	UNP B7L0A5
C	562	GLU	-	expression tag	UNP B7L0A5
C	563	HIS	-	expression tag	UNP B7L0A5
C	564	HIS	-	expression tag	UNP B7L0A5
C	565	HIS	-	expression tag	UNP B7L0A5
C	566	HIS	-	expression tag	UNP B7L0A5
C	567	HIS	-	expression tag	UNP B7L0A5
C	568	HIS	-	expression tag	UNP B7L0A5
D	558	ALA	-	expression tag	UNP B7L0A5
D	559	ALA	-	expression tag	UNP B7L0A5
D	560	ALA	-	expression tag	UNP B7L0A5
D	561	LEU	-	expression tag	UNP B7L0A5
D	562	GLU	-	expression tag	UNP B7L0A5
D	563	HIS	-	expression tag	UNP B7L0A5
D	564	HIS	-	expression tag	UNP B7L0A5
D	565	HIS	-	expression tag	UNP B7L0A5
D	566	HIS	-	expression tag	UNP B7L0A5
D	567	HIS	-	expression tag	UNP B7L0A5
D	568	HIS	-	expression tag	UNP B7L0A5
M	558	ALA	-	expression tag	UNP B7L0A5
M	559	ALA	-	expression tag	UNP B7L0A5
M	560	ALA	-	expression tag	UNP B7L0A5
M	561	LEU	-	expression tag	UNP B7L0A5
M	562	GLU	-	expression tag	UNP B7L0A5
M	563	HIS	-	expression tag	UNP B7L0A5
M	564	HIS	-	expression tag	UNP B7L0A5
M	565	HIS	-	expression tag	UNP B7L0A5
M	566	HIS	-	expression tag	UNP B7L0A5
M	567	HIS	-	expression tag	UNP B7L0A5
M	568	HIS	-	expression tag	UNP B7L0A5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
N	558	ALA	-	expression tag	UNP B7L0A5
N	559	ALA	-	expression tag	UNP B7L0A5
N	560	ALA	-	expression tag	UNP B7L0A5
N	561	LEU	-	expression tag	UNP B7L0A5
N	562	GLU	-	expression tag	UNP B7L0A5
N	563	HIS	-	expression tag	UNP B7L0A5
N	564	HIS	-	expression tag	UNP B7L0A5
N	565	HIS	-	expression tag	UNP B7L0A5
N	566	HIS	-	expression tag	UNP B7L0A5
N	567	HIS	-	expression tag	UNP B7L0A5
N	568	HIS	-	expression tag	UNP B7L0A5
O	558	ALA	-	expression tag	UNP B7L0A5
O	559	ALA	-	expression tag	UNP B7L0A5
O	560	ALA	-	expression tag	UNP B7L0A5
O	561	LEU	-	expression tag	UNP B7L0A5
O	562	GLU	-	expression tag	UNP B7L0A5
O	563	HIS	-	expression tag	UNP B7L0A5
O	564	HIS	-	expression tag	UNP B7L0A5
O	565	HIS	-	expression tag	UNP B7L0A5
O	566	HIS	-	expression tag	UNP B7L0A5
O	567	HIS	-	expression tag	UNP B7L0A5
O	568	HIS	-	expression tag	UNP B7L0A5
P	558	ALA	-	expression tag	UNP B7L0A5
P	559	ALA	-	expression tag	UNP B7L0A5
P	560	ALA	-	expression tag	UNP B7L0A5
P	561	LEU	-	expression tag	UNP B7L0A5
P	562	GLU	-	expression tag	UNP B7L0A5
P	563	HIS	-	expression tag	UNP B7L0A5
P	564	HIS	-	expression tag	UNP B7L0A5
P	565	HIS	-	expression tag	UNP B7L0A5
P	566	HIS	-	expression tag	UNP B7L0A5
P	567	HIS	-	expression tag	UNP B7L0A5
P	568	HIS	-	expression tag	UNP B7L0A5

- Molecule 2 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



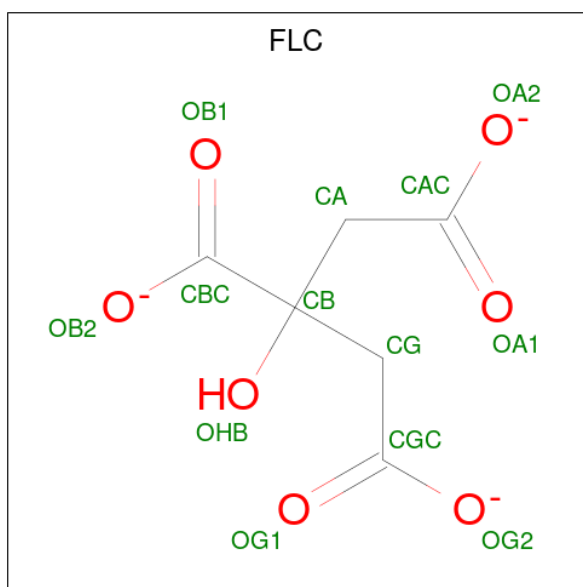
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			10	4	6		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 4 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	N	1	Total	C	O	0	0
			13	6	7		

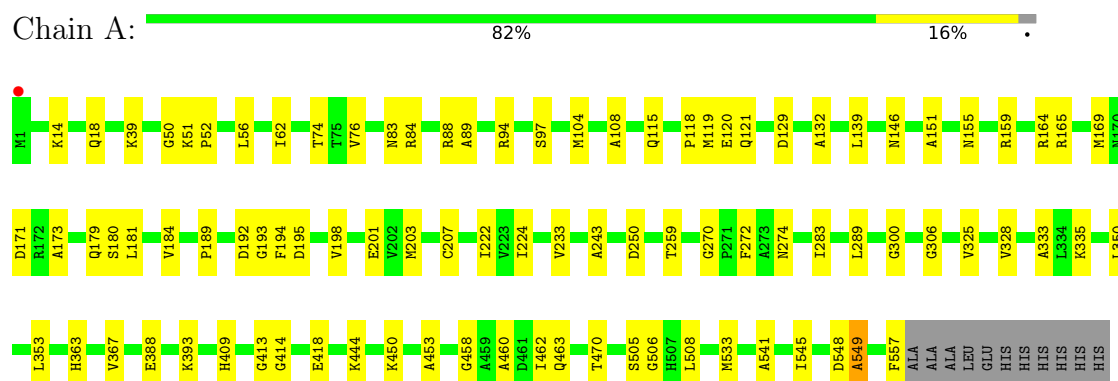
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	67	Total	O	0	0
			67	67		
5	B	73	Total	O	0	0
			73	73		
5	C	51	Total	O	0	0
			51	51		
5	D	58	Total	O	0	0
			58	58		
5	M	37	Total	O	0	0
			37	37		
5	N	42	Total	O	0	0
			42	42		
5	O	31	Total	O	0	0
			31	31		
5	P	21	Total	O	0	0
			21	21		

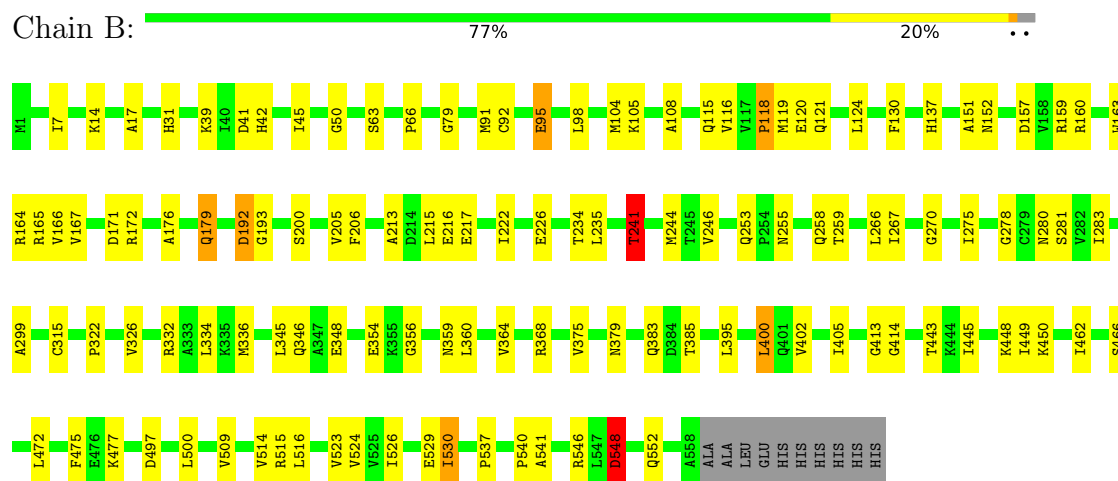
3 Residue-property plots

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.

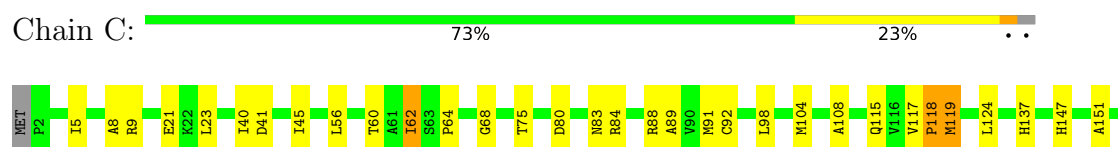
• Molecule 1: Formate-tetrahydrofolate ligase



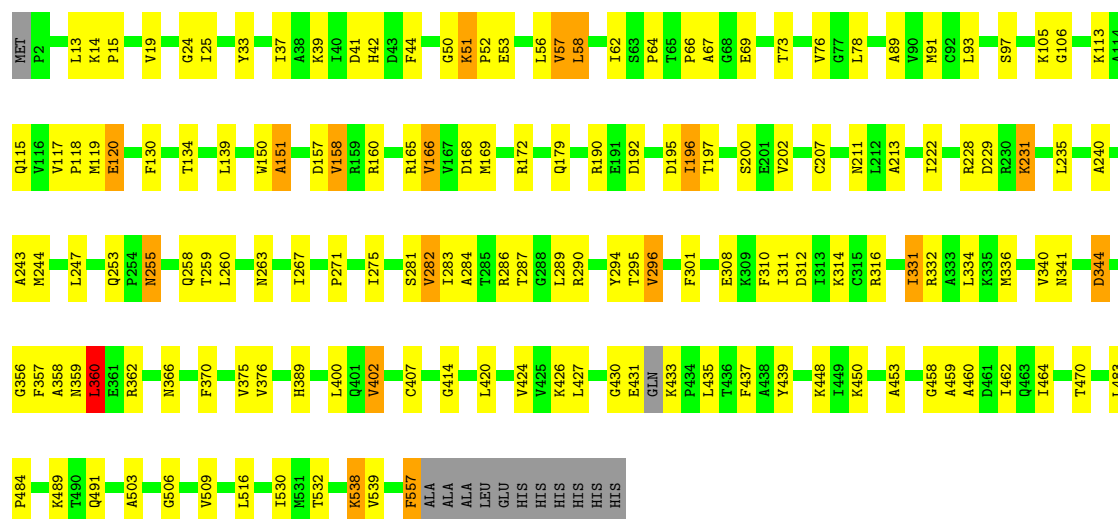
• Molecule 1: Formate-tetrahydrofolate ligase



• Molecule 1: Formate-tetrahydrofolate ligase

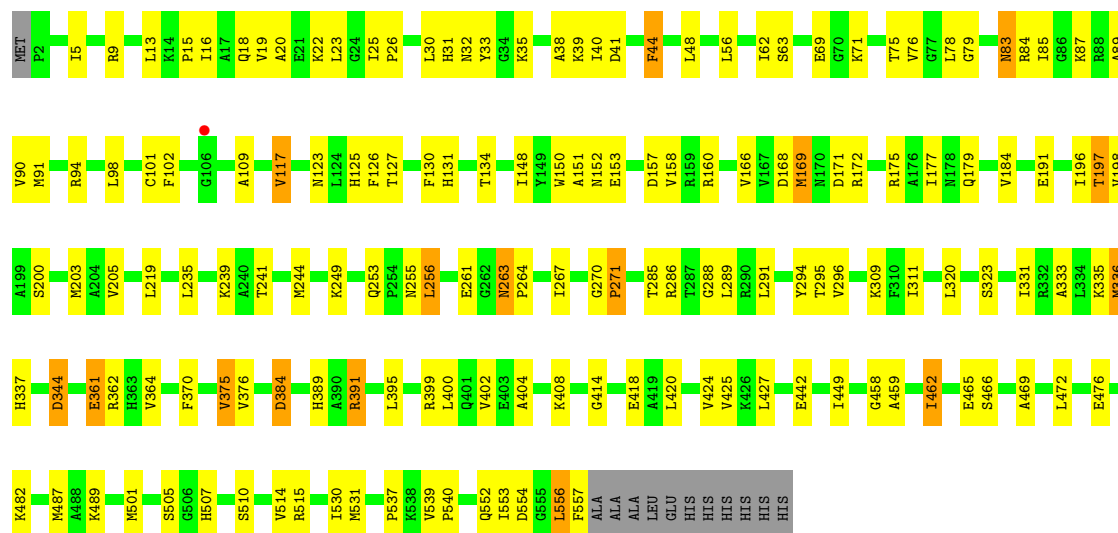


Chain N:  71% 24% • •



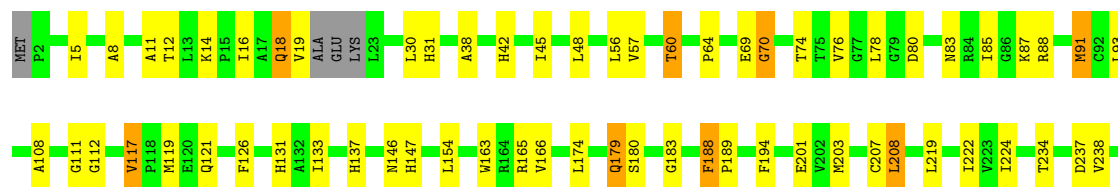
• Molecule 1: Formate-tetrahydrofolate ligase

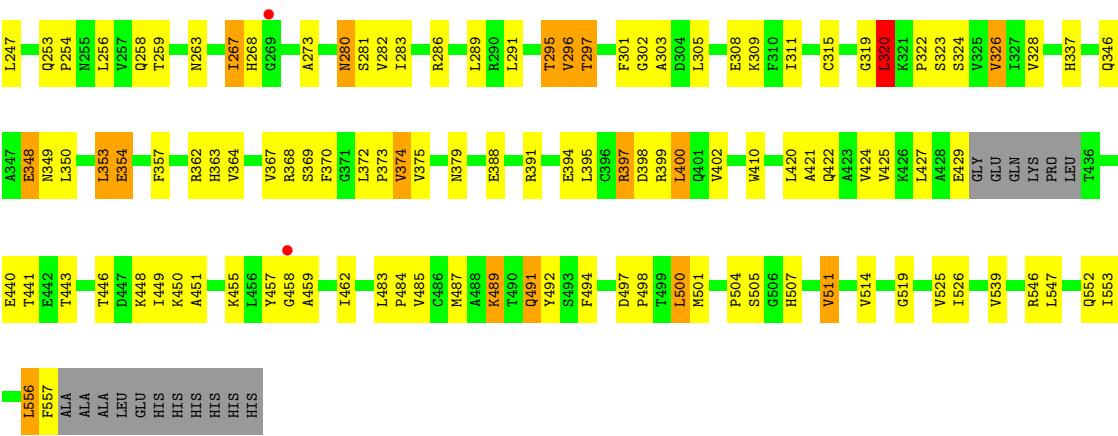
Chain O:  70% 25% • •



• Molecule 1: Formate-tetrahydrofolate ligase

Chain P:  65% 26% • •





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.56Å 168.74Å 126.99Å 90.00° 100.62° 90.00°	Depositor
Resolution (Å)	36.60 – 2.81 36.60 – 2.81	Depositor EDS
% Data completeness (in resolution range)	97.4 (36.60-2.81) 97.4 (36.60-2.81)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.180 , 0.276 0.183 , 0.276	Depositor DCC
R_{free} test set	5124 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33673	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.73% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, TLA, FLC

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	1.13	0/4254	1.59	5/5759 (0.1%)
1	B	1.13	0/4251	1.56	20/5755 (0.3%)
1	C	1.14	1/4238 (0.0%)	1.60	18/5737 (0.3%)
1	D	1.11	0/4238	1.59	26/5737 (0.5%)
1	M	1.12	1/4207 (0.0%)	1.57	6/5694 (0.1%)
1	N	1.12	1/4228 (0.0%)	1.55	10/5722 (0.2%)
1	O	1.09	0/4238	1.56	11/5737 (0.2%)
1	P	1.09	0/4166	1.56	11/5638 (0.2%)
All	All	1.12	3/33820 (0.0%)	1.57	107/45779 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	119	MET	C-O	5.40	1.30	1.24
1	M	25	ILE	N-CA	5.36	1.50	1.46
1	N	25	ILE	N-CA	5.31	1.50	1.45

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	299	ALA	CA-C-N	8.99	128.65	120.10
1	C	299	ALA	C-N-CA	8.99	128.65	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	241	THR	CB-CA-C	8.59	124.27	110.95
1	M	304	ASP	CA-CB-CG	7.28	119.88	112.60
1	P	188	PHE	CB-CA-C	7.12	118.26	110.08
1	N	192	ASP	CA-CB-CG	6.87	119.47	112.60
1	B	167	VAL	CA-C-O	-6.58	115.43	120.96
1	D	167	VAL	CA-C-O	-6.29	115.67	120.96
1	C	206	PHE	CA-CB-CG	6.16	119.96	113.80
1	O	469	ALA	CA-C-N	5.96	128.59	120.54
1	O	469	ALA	C-N-CA	5.96	128.59	120.54
1	C	84	ARG	CB-CA-C	-5.91	100.98	110.79
1	D	117	VAL	CB-CA-C	5.90	115.11	109.33
1	P	183	GLY	CA-C-N	5.90	127.99	120.56
1	P	183	GLY	C-N-CA	5.90	127.99	120.56
1	M	232	PRO	N-CA-C	5.89	120.11	111.03
1	A	88	ARG	CB-CA-C	5.88	119.61	110.67
1	O	219	LEU	CA-C-N	5.83	127.48	120.13
1	O	219	LEU	C-N-CA	5.83	127.48	120.13
1	B	118	PRO	CA-C-N	5.77	127.94	120.44
1	B	118	PRO	C-N-CA	5.77	127.94	120.44
1	O	362	ARG	CB-CA-C	-5.74	101.79	110.92
1	B	7	ILE	CA-C-N	5.72	127.95	120.28
1	B	7	ILE	C-N-CA	5.72	127.95	120.28
1	C	118	PRO	CA-C-N	5.72	128.41	120.29
1	C	118	PRO	C-N-CA	5.72	128.41	120.29
1	O	205	VAL	CA-C-N	5.72	128.21	120.38
1	O	205	VAL	C-N-CA	5.72	128.21	120.38
1	P	302	GLY	CA-C-O	-5.71	117.66	122.29
1	B	17	ALA	CA-C-N	5.70	127.85	120.44
1	B	17	ALA	C-N-CA	5.70	127.85	120.44
1	C	480	TYR	CA-C-N	5.67	126.24	120.00
1	C	480	TYR	C-N-CA	5.67	126.24	120.00
1	N	360	LEU	CA-C-N	5.64	128.16	120.54
1	N	360	LEU	C-N-CA	5.64	128.16	120.54
1	B	443	THR	CA-C-O	-5.61	115.34	120.95
1	N	24	GLY	CA-C-N	5.58	127.70	122.85
1	N	24	GLY	C-N-CA	5.58	127.70	122.85
1	P	12	THR	CB-CA-C	5.53	118.70	110.62
1	D	19	VAL	N-CA-C	-5.53	104.97	111.00
1	C	548	ASP	CB-CA-C	-5.52	98.99	111.30
1	D	193	GLY	CA-C-O	-5.50	115.84	121.61
1	O	41	ASP	CA-C-N	5.49	127.58	120.44
1	O	41	ASP	C-N-CA	5.49	127.58	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	384	ASP	CA-CB-CG	5.48	118.08	112.60
1	D	168	ASP	CA-CB-CG	5.45	118.05	112.60
1	D	493	SER	CA-C-O	-5.42	114.93	120.89
1	D	188	PHE	CB-CA-C	5.39	116.28	110.08
1	C	104	MET	CA-C-O	-5.39	115.79	121.88
1	P	357	PHE	CA-C-N	5.38	127.75	120.38
1	P	357	PHE	C-N-CA	5.38	127.75	120.38
1	A	155	ASN	CA-C-N	5.37	127.77	120.63
1	A	155	ASN	C-N-CA	5.37	127.77	120.63
1	C	167	VAL	CA-C-O	-5.36	115.67	121.19
1	M	476	GLU	CA-C-N	5.35	128.23	120.79
1	M	476	GLU	C-N-CA	5.35	128.23	120.79
1	O	44	PHE	CA-CB-CG	-5.31	108.49	113.80
1	C	80	ASP	CA-C-N	5.28	127.35	120.28
1	C	80	ASP	C-N-CA	5.28	127.35	120.28
1	A	393	LYS	CA-C-N	5.28	127.30	120.44
1	A	393	LYS	C-N-CA	5.28	127.30	120.44
1	B	50	GLY	CA-C-N	5.27	127.98	120.49
1	B	50	GLY	C-N-CA	5.27	127.98	120.49
1	D	384	ASP	CA-CB-CG	5.27	117.87	112.60
1	D	213	ALA	CA-C-N	5.26	127.33	120.28
1	D	213	ALA	C-N-CA	5.26	127.33	120.28
1	D	78	LEU	CA-C-N	5.24	125.76	119.94
1	D	78	LEU	C-N-CA	5.24	125.76	119.94
1	C	68	GLY	CA-C-O	-5.22	117.69	122.24
1	C	171	ASP	CA-C-N	5.22	127.80	120.28
1	C	171	ASP	C-N-CA	5.22	127.80	120.28
1	D	423	ALA	CA-C-N	5.21	127.13	120.56
1	D	423	ALA	C-N-CA	5.21	127.13	120.56
1	B	192	ASP	CA-CB-CG	5.21	117.81	112.60
1	N	344	ASP	CA-CB-CG	5.21	117.81	112.60
1	P	498	PRO	CA-C-N	5.16	127.46	120.44
1	P	498	PRO	C-N-CA	5.16	127.46	120.44
1	D	345	LEU	CA-C-N	5.16	127.15	120.44
1	D	345	LEU	C-N-CA	5.16	127.15	120.44
1	B	95	GLU	N-CA-C	-5.14	103.18	109.65
1	B	171	ASP	CA-C-N	5.13	127.67	120.28
1	B	171	ASP	C-N-CA	5.13	127.67	120.28
1	C	190	ARG	CB-CA-C	-5.13	99.27	109.79
1	B	166	VAL	CA-C-N	5.13	128.83	121.96
1	B	166	VAL	C-N-CA	5.13	128.83	121.96
1	D	76	VAL	CA-C-N	5.12	125.66	119.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	76	VAL	C-N-CA	5.12	125.66	119.98
1	D	322	PRO	CA-C-N	5.10	127.11	120.28
1	D	322	PRO	C-N-CA	5.10	127.11	120.28
1	C	104	MET	N-CA-C	-5.09	103.32	110.35
1	N	359	ASN	CA-C-N	5.07	127.32	120.38
1	N	359	ASN	C-N-CA	5.07	127.32	120.38
1	B	124	LEU	CA-C-N	5.07	128.01	120.31
1	B	124	LEU	C-N-CA	5.07	128.01	120.31
1	B	206	PHE	CA-CB-CG	5.06	118.86	113.80
1	N	414	GLY	CA-C-N	5.05	127.30	120.38
1	N	414	GLY	C-N-CA	5.05	127.30	120.38
1	D	211	ASN	CA-C-N	5.04	127.04	120.28
1	D	211	ASN	C-N-CA	5.04	127.04	120.28
1	D	66	PRO	CA-C-N	5.03	127.96	120.31
1	D	66	PRO	C-N-CA	5.03	127.96	120.31
1	M	419	ALA	CA-C-N	5.02	127.28	120.65
1	M	419	ALA	C-N-CA	5.02	127.28	120.65
1	D	94	ARG	CA-C-N	5.02	127.39	120.67
1	D	94	ARG	C-N-CA	5.02	127.39	120.67
1	P	111	GLY	CA-C-N	5.00	126.07	120.42
1	P	111	GLY	C-N-CA	5.00	126.07	120.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	50	GLY	Peptide

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	4184	0	4262	51	0
1	B	4181	0	4257	72	0
1	C	4168	0	4241	82	0
1	D	4168	0	4241	68	0
1	M	4139	0	4215	82	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4159	0	4232	97	0
1	O	4168	0	4241	91	0
1	P	4099	0	4167	116	0
2	D	10	0	4	0	0
3	D	4	0	3	0	0
4	N	13	0	5	4	0
5	A	67	0	0	0	0
5	B	73	0	0	2	0
5	C	51	0	0	0	0
5	D	58	0	0	1	0
5	M	37	0	0	0	0
5	N	42	0	0	0	0
5	O	31	0	0	0	0
5	P	21	0	0	0	0
All	All	33673	0	33868	636	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (636) 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:O:78:LEU:HD13	1:O:420:LEU:HD23	1.53	0.89
1:N:53:GLU:OE2	1:N:286:ARG:NH2	2.04	0.89
1:N:420:LEU:O	1:N:424:VAL:HG23	1.73	0.88
1:A:83:ASN:HD21	1:A:89:ALA:H	1.22	0.87
1:D:235:LEU:HD13	1:D:244:MET:HE1	1.59	0.85
1:N:229:ASP:HB2	1:N:231:LYS:HE3	1.60	0.84
1:O:83:ASN:HB2	1:O:263:ASN:HD22	1.42	0.83
1:P:179:GLN:NE2	1:P:180:SER:OG	2.13	0.82
1:P:60:THR:HG21	1:P:303:ALA:HA	1.63	0.80
1:B:216:GLU:HG2	1:B:241:THR:HG23	1.65	0.78
1:C:348:GLU:HB2	1:C:385:THR:HG21	1.68	0.76
1:B:235:LEU:HD13	1:B:244:MET:HE1	1.67	0.75
1:A:179:GLN:NE2	1:A:192:ASP:OD2	2.20	0.75
1:M:61:ALA:HB2	1:M:71:LYS:HG2	1.69	0.74
1:N:117:VAL:HG22	1:N:118:PRO:HA	1.72	0.72
1:O:171:ASP:OD2	1:P:165:ARG:NH1	2.23	0.71
1:A:453:ALA:CB	1:A:462:ILE:HD11	2.21	0.71
1:B:79:GLY:HA3	1:B:91:MET:SD	2.32	0.70
1:P:422:GLN:O	1:P:425:VAL:HG22	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:LEU:HB3	1:B:402:VAL:HG23	1.72	0.69
1:M:157:ASP:OD2	1:M:160:ARG:HD2	1.90	0.69
1:A:453:ALA:HB3	1:A:462:ILE:HD11	1.75	0.69
1:D:240:ALA:HB1	1:D:244:MET:HE2	1.73	0.69
1:N:462:ILE:HD13	1:N:509:VAL:HB	1.75	0.68
1:O:169:MET:HE3	1:O:169:MET:HA	1.75	0.68
1:C:210:LYS:O	1:C:283:ILE:HD11	1.92	0.67
1:O:83:ASN:CB	1:O:263:ASN:HD22	2.08	0.67
1:D:205:VAL:HG12	1:D:215:LEU:HD12	1.76	0.66
1:M:198:VAL:HA	1:M:203:MET:HG3	1.76	0.66
1:D:164:ARG:NH2	1:D:195:ASP:OD1	2.26	0.66
1:P:301:PHE:CE1	1:P:491:GLN:HG2	2.30	0.66
1:O:130:PHE:CE1	1:O:203:MET:HE1	2.31	0.65
1:P:301:PHE:CD1	1:P:491:GLN:HG2	2.31	0.65
1:P:78:LEU:HD13	1:P:420:LEU:HD12	1.78	0.65
1:A:83:ASN:ND2	1:A:89:ALA:H	1.94	0.64
1:O:83:ASN:HB2	1:O:263:ASN:ND2	2.12	0.64
1:O:375:VAL:HG22	1:O:427:LEU:HD12	1.79	0.64
1:D:463:GLN:HE21	1:D:508:LEU:HD21	1.62	0.64
1:D:286:ARG:HD2	1:D:290:ARG:HH21	1.62	0.63
1:M:440:GLU:O	1:M:443:THR:HG22	1.98	0.63
1:D:164:ARG:NH1	1:D:175:ARG:O	2.28	0.63
1:N:362:ARG:HH12	1:N:458:GLY:HA3	1.64	0.63
1:M:120:GLU:HG2	1:M:553:ILE:HD12	1.79	0.63
1:N:362:ARG:O	1:N:366:ASN:N	2.31	0.63
1:P:362:ARG:NH1	1:P:504:PRO:O	2.30	0.63
1:B:548:ASP:HB2	1:B:552:GLN:O	1.98	0.63
1:M:366:ASN:O	1:M:369:SER:HB3	1.98	0.63
1:B:216:GLU:HG2	1:B:241:THR:CG2	2.29	0.62
1:M:364:VAL:HG13	1:M:374:VAL:HG11	1.81	0.62
1:M:336:MET:HE2	1:M:342:LYS:HG3	1.80	0.62
1:D:286:ARG:NH1	1:D:318:THR:O	2.33	0.62
1:D:240:ALA:CB	1:D:244:MET:HE2	2.30	0.62
1:O:337:HIS:CD2	1:O:501:MET:HE3	2.36	0.61
1:C:9:ARG:HD2	1:C:552:GLN:NE2	2.14	0.61
1:A:181:LEU:HD23	1:A:189:PRO:HB3	1.81	0.61
1:C:257:VAL:HG21	1:C:267:ILE:HD12	1.83	0.61
1:B:115:GLN:O	1:B:259:THR:HA	2.01	0.61
1:P:322:PRO:HG2	1:P:372:LEU:HD21	1.83	0.61
1:M:205:VAL:HG13	1:M:218:ARG:HD3	1.83	0.60
1:P:280:ASN:HD21	1:P:297:THR:HG23	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:GLN:HG3	1:B:383:GLN:OE1	2.02	0.60
1:A:108:ALA:HA	1:A:119:MET:HE3	1.84	0.60
1:O:196:ILE:HG23	1:O:198:VAL:HG12	1.84	0.59
1:P:364:VAL:HG22	1:P:374:VAL:HG21	1.83	0.59
1:C:64:PRO:HD2	1:C:491:GLN:O	2.02	0.59
1:O:148:ILE:HA	1:O:152:ASN:HB2	1.84	0.59
1:N:362:ARG:HD2	1:N:503:ALA:HB1	1.85	0.59
1:O:151:ALA:HB3	1:O:153:GLU:HG3	1.84	0.59
1:C:285:THR:HG21	1:C:314:LYS:NZ	2.17	0.59
1:O:255:ASN:HB2	1:O:267:ILE:O	2.03	0.59
1:P:311:ILE:HA	1:P:315:CYS:HB2	1.85	0.59
1:B:332:ARG:HB3	1:B:345:LEU:HD13	1.85	0.58
1:O:175:ARG:NH2	1:O:531:MET:HE2	2.18	0.58
1:D:198:VAL:HB	1:D:270:GLY:O	2.03	0.58
1:M:358:ALA:O	1:M:361:GLU:HB3	2.03	0.58
1:N:50:GLY:O	1:N:51:LYS:C	2.46	0.58
1:O:364:VAL:HG11	1:O:402:VAL:HG21	1.86	0.58
1:A:325:VAL:HG11	1:A:367:VAL:HG11	1.86	0.58
1:B:450:LYS:HA	1:B:462:ILE:HG13	1.85	0.58
1:P:147:HIS:HE1	1:P:154:LEU:H	1.51	0.58
1:M:310:PHE:O	1:M:314:LYS:HB3	2.04	0.58
1:P:373:PRO:HB2	1:P:427:LEU:HD22	1.84	0.58
1:C:346:GLN:CD	1:C:346:GLN:H	2.12	0.58
1:M:252:LEU:HG	1:M:283:ILE:HD12	1.86	0.58
1:A:146:ASN:OD1	1:B:172:ARG:NH2	2.37	0.57
1:M:203:MET:HE1	1:M:270:GLY:H	1.68	0.57
1:C:343:LYS:O	1:C:346:GLN:NE2	2.38	0.57
1:P:91:MET:HE1	1:P:259:THR:HG22	1.85	0.57
1:C:329:ALA:O	1:C:378:VAL:HA	2.05	0.57
1:P:179:GLN:HE21	1:P:179:GLN:C	2.12	0.57
1:A:184:VAL:HA	1:C:159:ARG:HD2	1.87	0.56
1:C:354:GLU:OE2	1:C:391:ARG:NH2	2.38	0.56
1:P:441:THR:O	1:P:448:LYS:NZ	2.38	0.56
1:A:119:MET:HE2	1:A:557:PHE:CE1	2.40	0.56
1:N:207:CYS:O	1:N:282:VAL:N	2.38	0.56
1:C:170:ASN:OD1	1:C:534:PRO:HG2	2.05	0.56
1:C:210:LYS:O	1:C:283:ILE:CD1	2.53	0.56
1:C:538:LYS:HE3	1:O:482:LYS:CE	2.35	0.56
1:M:88:ARG:O	1:M:88:ARG:HG3	2.05	0.56
1:N:158:VAL:HG22	1:N:190:ARG:HD2	1.87	0.56
1:O:44:PHE:O	1:O:48:LEU:HD13	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556:LEU:HD23	1:D:557:PHE:CE2	2.40	0.56
1:M:484:PRO:HD2	1:M:521:GLY:O	2.06	0.56
1:N:376:VAL:HG23	1:N:402:VAL:HG11	1.88	0.56
1:O:5:ILE:HD12	1:O:557:PHE:CE2	2.40	0.56
1:O:361:GLU:HG2	1:O:400:LEU:HD21	1.87	0.56
1:N:64:PRO:HD2	1:N:491:GLN:O	2.05	0.56
1:P:500:LEU:HB3	1:P:504:PRO:CG	2.36	0.56
1:B:515:ARG:HD2	1:B:526:ILE:HD11	1.87	0.55
1:C:60:THR:HG21	1:C:303:ALA:HB2	1.88	0.55
1:P:108:ALA:HA	1:P:119:MET:SD	2.47	0.55
1:O:90:VAL:HG12	1:O:295:THR:HG22	1.88	0.55
1:A:460:ALA:HB2	1:A:506:GLY:HA2	1.89	0.55
1:B:104:MET:O	1:B:541:ALA:HB2	2.06	0.55
1:B:42:HIS:H	1:B:253:GLN:HE21	1.54	0.55
1:N:42:HIS:H	1:N:253:GLN:HE21	1.53	0.55
1:O:20:ALA:CB	1:O:30:LEU:HD11	2.37	0.55
1:A:201:GLU:OE2	1:A:222:ILE:HG12	2.07	0.55
1:B:39:LYS:NZ	1:B:255:ASN:HD21	2.04	0.55
1:B:159:ARG:NH1	1:D:188:PHE:CZ	2.74	0.55
1:D:165:ARG:NH1	1:D:179:GLN:HE22	2.04	0.55
1:N:435:LEU:HD22	1:N:437:PHE:CE1	2.41	0.55
1:O:472:LEU:HD21	1:O:514:VAL:HG11	1.89	0.55
1:P:547:LEU:HA	1:P:552:GLN:O	2.06	0.55
1:C:409:HIS:HA	1:C:413:GLY:O	2.06	0.55
1:N:166:VAL:HG22	1:N:197:THR:HA	1.88	0.55
1:P:309:LYS:NZ	1:P:487:MET:O	2.28	0.55
1:A:14:LYS:HG2	1:A:18:GLN:HE21	1.72	0.55
1:C:8:ALA:HB2	1:C:115:GLN:HE22	1.72	0.55
1:C:177:ILE:HD13	1:D:179:GLN:HA	1.88	0.55
1:N:117:VAL:CG2	1:N:118:PRO:HA	2.37	0.55
1:B:281:SER:HB2	1:B:283:ILE:HG22	1.89	0.55
1:B:546:ARG:NH1	5:B:605:HOH:O	2.40	0.55
1:D:71:LYS:HE3	1:D:299:ALA:O	2.07	0.55
1:N:57:VAL:HG22	1:N:296:VAL:HG12	1.89	0.55
1:N:286:ARG:O	1:N:290:ARG:HG3	2.07	0.55
1:O:101:CYS:SG	1:O:123:ASN:HB3	2.47	0.55
1:O:337:HIS:HA	1:O:501:MET:HB3	1.88	0.54
1:C:9:ARG:CD	1:C:552:GLN:NE2	2.71	0.54
1:C:385:THR:OG1	1:C:388:GLU:HG3	2.06	0.54
1:N:78:LEU:HD11	1:N:424:VAL:HG21	1.90	0.54
1:P:367:VAL:HG12	1:P:374:VAL:HG12	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:LYS:HG2	1:D:294:TYR:CE1	2.42	0.54
1:M:165:ARG:NH1	1:M:192:ASP:OD2	2.40	0.54
1:N:150:TRP:O	1:N:151:ALA:HB3	2.08	0.54
1:P:57:VAL:CG1	1:P:296:VAL:HG12	2.38	0.54
1:A:164:ARG:HH11	1:A:193:GLY:HA3	1.73	0.54
1:P:80:ASP:HA	1:P:263:ASN:HD22	1.73	0.54
1:A:463:GLN:HB2	1:A:508[A]:LEU:HD11	1.90	0.54
1:M:66:PRO:HD2	1:M:336:MET:SD	2.47	0.54
1:N:91:MET:HE1	1:N:259:THR:CG2	2.37	0.54
1:A:409:HIS:HA	1:A:413:GLY:O	2.07	0.54
1:M:76:VAL:HA	1:M:91:MET:SD	2.48	0.54
1:O:69:GLU:HG2	1:O:69:GLU:O	2.08	0.54
1:M:332:ARG:HG2	1:M:345:LEU:HB3	1.91	0.53
1:M:453:ALA:O	1:M:457:TYR:HB2	2.07	0.53
1:N:89:ALA:HA	1:N:294:TYR:O	2.08	0.53
1:B:364:VAL:HG11	1:B:402:VAL:HG21	1.89	0.53
1:A:350:LEU:O	1:A:353:LEU:HB3	2.09	0.53
1:O:198:VAL:HG23	1:O:270:GLY:O	2.09	0.53
1:B:179:GLN:NE2	1:B:192:ASP:OD2	2.41	0.53
1:M:422:GLN:HA	1:M:422:GLN:NE2	2.23	0.53
1:C:207:CYS:SG	1:C:271:PRO:HD3	2.49	0.53
1:M:530:ILE:N	1:M:530:ILE:HD12	2.24	0.53
1:B:354:GLU:HG3	1:B:395:LEU:HD11	1.90	0.53
1:C:462:ILE:HG22	1:C:509:VAL:HB	1.91	0.52
1:D:215:LEU:O	1:D:219:LEU:HG	2.10	0.52
1:O:391:ARG:HA	1:O:391:ARG:NE	2.24	0.52
1:P:112:GLY:HA3	1:P:410:TRP:CD1	2.44	0.52
1:O:336:MET:HG3	1:O:501:MET:HE2	1.91	0.52
1:D:44:PHE:O	1:D:47:SER:OG	2.20	0.52
1:B:475:PHE:HE2	1:B:514:VAL:HG12	1.74	0.52
1:A:97:SER:HB3	1:A:198:VAL:HG11	1.91	0.52
1:P:368:ARG:HH21	1:P:402:VAL:HG12	1.75	0.52
1:B:368:ARG:NH1	1:B:402:VAL:HG22	2.24	0.52
1:D:42:HIS:H	1:D:253:GLN:HE21	1.57	0.52
1:N:93:LEU:HB2	1:N:267:ILE:HD13	1.91	0.52
1:P:295:THR:HG22	1:P:295:THR:O	2.09	0.52
1:A:224:ILE:HG13	1:A:233:VAL:O	2.10	0.52
1:C:472:LEU:HD21	1:C:514:VAL:HG11	1.91	0.52
1:D:117:VAL:CG2	1:D:118:PRO:HA	2.39	0.52
1:N:56:LEU:HB2	1:N:289:LEU:HD21	1.91	0.52
1:N:450:LYS:HA	1:N:462:ILE:HG13	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:89:ALA:HA	1:O:294:TYR:O	2.10	0.52
1:P:268:HIS:O	1:P:281:SER:OG	2.27	0.52
1:N:334:LEU:O	1:N:356:GLY:HA3	2.10	0.52
1:P:179:GLN:O	1:P:189:PRO:HA	2.10	0.52
1:D:157:ASP:CG	1:D:160:ARG:HG3	2.35	0.52
1:M:340:VAL:HG11	1:M:345:LEU:HD23	1.92	0.52
1:N:211:ASN:HD22	1:N:213:ALA:H	1.58	0.52
1:M:118:PRO:HB2	1:M:121:GLN:OE1	2.10	0.51
1:N:41:ASP:HA	1:N:253:GLN:NE2	2.25	0.51
1:N:196:ILE:HG22	1:N:532:THR:O	2.10	0.51
1:D:224:ILE:HG21	1:D:235:LEU:HD23	1.92	0.51
1:D:343:LYS:HG2	5:D:737:HOH:O	2.10	0.51
1:N:39:LYS:HE2	1:N:255:ASN:HD21	1.75	0.51
1:P:78:LEU:HD12	1:P:78:LEU:O	2.09	0.51
1:C:199:ALA:HB2	1:C:272:PHE:HE2	1.75	0.51
1:P:16:ILE:HD11	1:P:256:LEU:HG	1.91	0.51
1:P:174:LEU:HB3	1:P:194:PHE:CD1	2.46	0.51
1:C:324:SER:HA	1:C:373:PRO:HG2	1.91	0.51
1:M:460:ALA:HB2	1:M:506:GLY:HA2	1.92	0.51
1:O:288:GLY:C	1:O:295:THR:HG21	2.35	0.51
1:C:407:CYS:HB3	1:C:409:HIS:ND1	2.26	0.51
1:C:98:LEU:HD13	1:C:124:LEU:HA	1.92	0.51
1:M:92:CYS:HA	1:M:266:LEU:O	2.10	0.51
1:O:19:VAL:O	1:O:22:LYS:HB2	2.11	0.51
1:O:203:MET:HG3	1:O:271:PRO:HB3	1.92	0.51
1:B:360:LEU:HD23	1:B:364:VAL:HG23	1.93	0.51
1:A:56:LEU:HB2	1:A:289:LEU:HD21	1.92	0.51
1:N:130:PHE:O	1:N:134:THR:HG22	2.11	0.51
1:A:300:GLY:O	1:A:306:GLY:HA3	2.11	0.51
1:B:116:VAL:HG11	1:B:267:ILE:HD11	1.92	0.51
1:D:207:CYS:HA	1:D:281:SER:HA	1.91	0.51
1:B:213:ALA:HB3	1:N:344:ASP:HB3	1.91	0.50
1:C:219:LEU:HD22	1:C:244:MET:HE2	1.93	0.50
1:C:480:TYR:HB3	1:C:483:LEU:HD12	1.93	0.50
1:M:117:VAL:HB	1:M:118:PRO:HA	1.93	0.50
1:M:147:HIS:HE1	1:M:154:LEU:H	1.58	0.50
1:N:166:VAL:HA	1:N:195:ASP:O	2.11	0.50
1:B:66:PRO:HG2	1:B:336:MET:HE1	1.93	0.50
1:D:117:VAL:HG23	1:D:118:PRO:HA	1.92	0.50
1:B:41:ASP:HA	1:B:253:GLN:NE2	2.26	0.50
1:M:336:MET:HE3	1:M:345:LEU:HD11	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:39:LYS:CE	1:N:255:ASN:ND2	2.75	0.50
1:P:440:GLU:HB3	1:P:443:THR:HG23	1.94	0.50
1:P:8:ALA:HB1	1:P:117:VAL:HG11	1.94	0.50
1:M:113:LYS:HD3	1:M:411:ALA:O	2.11	0.50
1:N:39:LYS:HE2	1:N:255:ASN:ND2	2.26	0.50
1:N:228:ARG:NH2	4:N:601:FLC:OA1	2.44	0.50
1:N:308:GLU:O	1:N:312:ASP:HB2	2.11	0.50
1:P:76:VAL:HA	1:P:91:MET:HE3	1.92	0.50
1:O:289:LEU:N	1:O:295:THR:HG21	2.27	0.50
1:P:303:ALA:HB3	1:P:363:HIS:CD2	2.47	0.50
1:P:500:LEU:HB3	1:P:504:PRO:HG2	1.93	0.50
1:M:542:ALA:HA	1:M:545:ILE:HD12	1.93	0.50
1:B:449:ILE:HG22	1:B:462:ILE:HD12	1.94	0.50
1:C:304:ASP:HB3	1:C:494:PHE:CE1	2.47	0.50
1:M:151:ALA:O	1:M:152:ASN:C	2.55	0.50
1:D:151:ALA:O	1:D:152:ASN:C	2.55	0.49
1:D:311:ILE:HG21	1:D:370:PHE:CD1	2.47	0.49
1:D:547:LEU:HA	1:D:552:GLN:O	2.12	0.49
1:O:78:LEU:HD21	1:O:424:VAL:HG21	1.94	0.49
1:P:87:LYS:HE3	1:P:425:VAL:HG11	1.94	0.49
1:P:315:CYS:HA	1:P:320:LEU:CD1	2.42	0.49
1:C:198:VAL:HG13	1:C:270:GLY:O	2.11	0.49
1:O:311:ILE:HG21	1:O:370:PHE:CD2	2.46	0.49
1:P:80:ASP:HA	1:P:263:ASN:ND2	2.27	0.49
1:P:83:ASN:ND2	1:P:88:ARG:HH11	2.10	0.49
1:A:203:MET:HE2	1:A:207:CYS:SG	2.52	0.49
1:D:480:TYR:O	1:D:483:LEU:HB2	2.12	0.49
1:B:41:ASP:HA	1:B:253:GLN:HE21	1.77	0.49
1:B:157:ASP:OD1	1:B:159:ARG:HD3	2.12	0.49
1:O:395:LEU:O	1:O:399:ARG:HB2	2.12	0.49
1:C:89:ALA:HA	1:C:294:TYR:O	2.12	0.49
1:P:64:PRO:HA	1:P:69:GLU:OE1	2.13	0.49
1:C:56:LEU:HB2	1:C:289:LEU:HD21	1.94	0.49
1:D:329:ALA:O	1:D:378:VAL:HA	2.12	0.49
1:P:70:GLY:O	1:P:74:THR:HG23	2.13	0.49
1:D:268:HIS:O	1:D:280:ASN:HB2	2.13	0.49
1:N:460:ALA:HB2	1:N:506:GLY:HA2	1.95	0.49
1:P:137:HIS:CD2	1:P:166:VAL:HG13	2.48	0.49
1:C:40:ILE:HB	1:C:45:ILE:HD11	1.94	0.49
1:M:62:ILE:HB	1:M:359:ASN:OD1	2.12	0.49
1:N:169:MET:HE3	1:N:169:MET:HA	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:13:LEU:HD21	1:O:117:VAL:HG12	1.94	0.49
1:O:157:ASP:HB3	1:O:160:ARG:HB2	1.95	0.49
1:P:363:HIS:NE2	1:P:494:PHE:CZ	2.81	0.49
1:P:450:LYS:HA	1:P:462:ILE:HG21	1.95	0.49
1:N:158:VAL:HG13	1:N:190:ARG:HB3	1.95	0.49
1:C:92:CYS:HA	1:C:266:LEU:O	2.13	0.48
1:C:547:LEU:HA	1:C:552:GLN:O	2.14	0.48
1:D:20:ALA:CB	1:D:30:LEU:HD11	2.43	0.48
1:O:23:LEU:HD11	1:O:264:PRO:HB2	1.95	0.48
1:P:326:VAL:HG13	1:P:375:VAL:HG13	1.95	0.48
1:N:66:PRO:HG2	1:N:336:MET:HE1	1.95	0.48
1:P:208:LEU:HA	1:P:282:VAL:CG2	2.44	0.48
1:B:205:VAL:HG12	1:B:215:LEU:HD12	1.96	0.48
1:D:332:ARG:HB3	1:D:345:LEU:HD13	1.95	0.48
1:M:62:ILE:HA	1:M:363:HIS:CD2	2.49	0.48
1:C:41:ASP:O	1:C:45:ILE:HG12	2.14	0.48
1:D:165:ARG:NH1	1:D:192:ASP:OD2	2.45	0.48
1:N:14:LYS:H	1:N:258:GLN:HE22	1.60	0.48
1:P:553:ILE:HG21	1:P:556:LEU:HD12	1.96	0.48
1:C:364:VAL:HG11	1:C:400:LEU:HD13	1.96	0.48
1:O:294:TYR:OH	1:O:425:VAL:HG13	2.13	0.48
1:P:222:ILE:HG13	1:P:519:GLY:HA3	1.95	0.48
1:B:108:ALA:N	1:B:119:MET:HE3	2.28	0.48
1:C:5:ILE:HG13	1:C:9:ARG:HD3	1.95	0.48
1:M:182:GLY:N	1:O:191:GLU:OE2	2.42	0.48
1:P:93:LEU:HB2	1:P:267:ILE:HD13	1.96	0.48
1:A:115:GLN:O	1:A:259:THR:HA	2.14	0.47
1:O:131:HIS:ND1	1:P:131:HIS:HB3	2.29	0.47
1:P:78:LEU:HD13	1:P:420:LEU:CD1	2.44	0.47
1:D:219:LEU:O	1:D:235:LEU:HD12	2.14	0.47
1:O:309:LYS:NZ	1:O:487:MET:O	2.36	0.47
1:N:97:SER:HB2	1:N:168:ASP:OD1	2.15	0.47
4:N:601:FLC:OG2	4:N:601:FLC:CA	2.63	0.47
1:P:203:MET:HE2	1:P:207:CYS:SG	2.54	0.47
1:P:350:LEU:N	1:P:350:LEU:HD23	2.30	0.47
1:O:449:ILE:HG22	1:O:462:ILE:HG12	1.95	0.47
1:P:421:ALA:O	1:P:425:VAL:HG13	2.13	0.47
1:A:458:GLY:O	1:A:505:SER:HA	2.14	0.47
1:M:255:ASN:HB2	1:M:267:ILE:O	2.13	0.47
1:N:235:LEU:HD13	1:N:244:MET:HE1	1.95	0.47
1:O:127:THR:HG21	1:O:255:ASN:OD1	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:273:ALA:HB3	1:P:301:PHE:CD2	2.49	0.47
1:D:160:ARG:CZ	1:D:230:ARG:HD3	2.44	0.47
1:O:56:LEU:HB2	1:O:289:LEU:HD21	1.96	0.47
1:C:210:LYS:HE2	1:C:286:ARG:CZ	2.44	0.47
1:C:315:CYS:HB3	1:C:320:LEU:O	2.14	0.47
1:N:13:LEU:HD12	1:N:13:LEU:HA	1.80	0.47
1:O:375:VAL:HG22	1:O:427:LEU:CD1	2.44	0.47
1:A:76:VAL:HG13	1:A:259:THR:HG22	1.97	0.47
1:D:16:ILE:HD11	1:D:32:ASN:ND2	2.29	0.47
1:P:201:GLU:HG2	1:P:222:ILE:HD11	1.96	0.47
1:C:210:LYS:C	1:C:283:ILE:HD11	2.39	0.47
1:P:337:HIS:HA	1:P:501:MET:HB3	1.96	0.47
1:M:270:GLY:H	1:M:271:PRO:HD3	1.80	0.47
1:M:541:ALA:O	1:M:545:ILE:HG13	2.15	0.47
1:N:139:LEU:HD21	1:N:243:ALA:HB3	1.97	0.47
1:A:84:ARG:HE	1:A:414:GLY:HA3	1.80	0.46
1:A:450:LYS:HA	1:A:462:ILE:HG13	1.97	0.46
1:M:42:HIS:CE1	1:M:253:GLN:HG3	2.50	0.46
1:O:400:LEU:HB3	1:O:402:VAL:HG23	1.98	0.46
1:P:163:TRP:CE3	1:P:224:ILE:HG22	2.50	0.46
1:D:463:GLN:NE2	1:D:508:LEU:HD21	2.29	0.46
1:B:537:PRO:HG2	1:B:540:PRO:HA	1.97	0.46
1:C:88:ARG:HB3	1:C:293:ASP:OD2	2.16	0.46
1:O:261:GLU:OE2	1:O:414:GLY:N	2.33	0.46
1:B:515:ARG:HB2	1:B:524:VAL:HB	1.98	0.46
1:M:305:LEU:CD1	1:M:491:GLN:HA	2.44	0.46
1:O:35:LYS:CE	1:P:30:LEU:O	2.63	0.46
1:A:548:ASP:O	1:A:549:ALA:CB	2.64	0.46
1:M:270:GLY:N	1:M:271:PRO:HD3	2.30	0.46
1:N:166:VAL:CG2	1:N:197:THR:HA	2.46	0.46
1:P:31:HIS:O	1:P:38:ALA:HA	2.15	0.46
1:P:500:LEU:HD13	1:P:504:PRO:HB3	1.97	0.46
1:B:222:ILE:O	1:B:234:THR:HA	2.16	0.46
1:B:348:GLU:HB2	1:B:385:THR:HG21	1.97	0.46
1:B:445:ILE:O	1:B:448:LYS:N	2.49	0.46
1:N:275:ILE:O	1:N:275:ILE:HG22	2.15	0.46
1:A:84:ARG:HD3	1:A:418:GLU:OE2	2.16	0.46
1:A:104:MET:HA	1:A:104:MET:HE3	1.97	0.46
1:A:108:ALA:HA	1:A:119:MET:CE	2.45	0.46
1:M:211:ASN:HD21	1:M:213:ALA:HB3	1.81	0.46
1:N:240:ALA:HB1	1:N:244:MET:HE2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:35:LYS:HE2	1:P:30:LEU:O	2.16	0.46
1:P:254:PRO:HA	1:P:268:HIS:CD2	2.51	0.46
1:A:62:ILE:HA	1:A:363:HIS:CD2	2.51	0.46
1:A:165:ARG:NH1	1:A:179:GLN:HE22	2.14	0.46
1:M:41:ASP:O	1:M:45:ILE:HG13	2.15	0.46
1:M:51:LYS:HD2	1:M:52:PRO:HD2	1.98	0.46
1:N:13:LEU:HD11	1:N:117:VAL:HG13	1.98	0.46
1:P:375:VAL:HG13	1:P:375:VAL:O	2.16	0.46
1:P:497:ASP:HB3	1:P:500:LEU:HG	1.98	0.46
1:P:147:HIS:HE1	1:P:154:LEU:N	2.12	0.46
1:B:514:VAL:HG13	1:B:523:VAL:CG1	2.46	0.46
1:C:442:GLU:O	1:C:442:GLU:HG2	2.16	0.46
1:M:9:ARG:NH1	1:M:120:GLU:OE2	2.35	0.46
1:P:289:LEU:HD23	1:P:295:THR:HB	1.98	0.46
1:P:42:HIS:NE2	1:P:253:GLN:HG3	2.31	0.45
1:A:139:LEU:CD2	1:A:243:ALA:HB1	2.46	0.45
1:B:217:GLU:OE1	1:N:341:ASN:HB2	2.16	0.45
1:M:211:ASN:ND2	1:M:213:ALA:HB3	2.31	0.45
1:N:439:TYR:CD1	1:N:448:LYS:HD3	2.51	0.45
1:P:5:ILE:HD13	1:P:119:MET:HE2	1.97	0.45
1:P:91:MET:HE1	1:P:259:THR:CG2	2.46	0.45
1:P:394:GLU:HA	1:P:397:ARG:HB3	1.98	0.45
1:B:165:ARG:NH1	1:B:192:ASP:OD2	2.49	0.45
1:C:40:ILE:HD11	1:C:256:LEU:HB2	1.98	0.45
1:C:83:ASN:ND2	1:C:263:ASN:HB3	2.32	0.45
1:D:285:THR:HG21	1:D:314:LYS:NZ	2.30	0.45
1:O:286:ARG:HG3	1:O:320:LEU:HD11	1.98	0.45
1:D:72:THR:HA	1:D:298:GLU:OE1	2.16	0.45
1:D:346:GLN:HG3	1:D:383:GLN:OE1	2.16	0.45
1:M:207:CYS:O	1:M:282:VAL:N	2.42	0.45
1:P:364:VAL:HG11	1:P:400:LEU:HD22	1.98	0.45
1:D:116:VAL:CG1	1:D:257:VAL:HG13	2.46	0.45
1:N:119:MET:HE2	1:N:557:PHE:CE2	2.51	0.45
1:N:157:ASP:HB3	1:N:160:ARG:HD2	1.98	0.45
1:P:457:TYR:CE2	1:P:489:LYS:HE2	2.51	0.45
1:A:159:ARG:HD2	1:C:184:VAL:HA	1.98	0.45
1:O:40:ILE:HD11	1:O:256:LEU:HB2	1.99	0.45
1:P:56:LEU:O	1:P:323:SER:N	2.42	0.45
1:P:448:LYS:HE3	1:P:483:LEU:O	2.16	0.45
1:B:95:GLU:HB3	1:B:130:PHE:CE1	2.52	0.45
1:P:425:VAL:O	1:P:429:GLU:HG2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:HIS:CE1	1:D:253:GLN:HG3	2.52	0.45
1:A:118:PRO:HB2	1:A:121:GLN:OE1	2.17	0.45
1:B:63:SER:HB2	1:B:359:ASN:HD21	1.81	0.45
1:B:152:ASN:HB2	1:D:228:ARG:HH12	1.82	0.45
1:N:222:ILE:HD12	1:N:235:LEU:HD12	1.98	0.45
1:P:74:THR:HG22	1:P:379:ASN:OD1	2.17	0.45
1:B:164:ARG:HB3	1:B:193:GLY:O	2.17	0.45
1:B:497:ASP:C	1:B:497:ASP:OD1	2.59	0.45
1:C:62:ILE:HA	1:C:363:HIS:CD2	2.52	0.45
1:M:222:ILE:O	1:M:234:THR:HA	2.17	0.45
1:N:44:PHE:CD1	1:N:44:PHE:C	2.95	0.45
1:P:354:GLU:OE2	1:P:391:ARG:NH1	2.49	0.45
1:P:373:PRO:HB2	1:P:427:LEU:HB3	1.98	0.45
1:A:195:ASP:C	1:A:533:MET:HE2	2.42	0.44
1:C:117:VAL:HB	1:C:118:PRO:HA	1.99	0.44
1:C:155:ASN:O	1:C:227:THR:HA	2.17	0.44
1:C:178:ASN:HB2	1:D:178:ASN:HB2	1.99	0.44
1:M:61:ALA:HB3	1:M:71:LYS:HE3	1.98	0.44
1:N:78:LEU:HD11	1:N:424:VAL:CG2	2.46	0.44
1:P:451:ALA:O	1:P:455:LYS:HG3	2.16	0.44
1:A:139:LEU:HD21	1:A:243:ALA:HB1	1.98	0.44
1:A:272:PHE:HB3	1:A:274:ASN:OD1	2.17	0.44
1:B:462:ILE:HD13	1:B:509:VAL:HB	1.99	0.44
1:C:332:ARG:HD2	1:C:381:PHE:CD2	2.52	0.44
1:D:14:LYS:H	1:D:258:GLN:HE22	1.64	0.44
1:D:311:ILE:HA	1:D:315:CYS:HB2	1.99	0.44
1:M:340:VAL:HG23	1:M:352:ALA:HB1	1.98	0.44
1:N:357:PHE:HZ	1:N:400:LEU:HD23	1.81	0.44
1:O:75:THR:HG23	1:O:296:VAL:HG12	1.99	0.44
1:B:118:PRO:HB2	1:B:121:GLN:OE1	2.17	0.44
1:C:242:GLY:O	1:C:246:VAL:HG23	2.17	0.44
1:D:60:THR:CG2	1:D:303:ALA:HB2	2.47	0.44
1:O:537:PRO:HG2	1:O:540:PRO:HA	1.98	0.44
1:A:181:LEU:O	1:B:176:ALA:HB3	2.18	0.44
1:M:25:ILE:HD11	1:M:291:LEU:HD13	2.00	0.44
1:M:463:GLN:HB2	1:M:508:LEU:HD11	2.00	0.44
1:P:48:LEU:HD21	1:P:291:LEU:HD21	1.98	0.44
1:P:83:ASN:ND2	1:P:263:ASN:OD1	2.50	0.44
1:P:375:VAL:HB	1:P:427:LEU:CD1	2.48	0.44
1:D:459:ALA:HB2	1:D:507:HIS:CE1	2.52	0.44
1:M:44:PHE:O	1:M:48:LEU:HD13	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:207:CYS:HA	1:N:281:SER:HA	1.99	0.44
1:O:15:PRO:HG2	1:O:18:GLN:HG3	1.99	0.44
1:B:275:ILE:HG23	1:B:530:ILE:HG21	1.98	0.44
1:M:9:ARG:HH12	1:M:120:GLU:CD	2.24	0.44
1:M:102:PHE:CZ	1:N:247:LEU:HD21	2.53	0.44
1:N:139:LEU:HD21	1:N:243:ALA:CB	2.47	0.44
1:B:278:GLY:O	1:B:299:ALA:HA	2.18	0.44
1:C:251:ALA:O	1:C:268:HIS:NE2	2.45	0.44
1:N:113:LYS:C	1:N:260:LEU:HD12	2.42	0.44
4:N:601:FLC:OG2	4:N:601:FLC:HA2	2.17	0.44
1:O:94:ARG:HB3	1:O:270:GLY:HA3	1.99	0.44
1:B:31:HIS:HB2	1:B:39:LYS:HB2	1.98	0.44
1:C:303:ALA:HA	1:C:307:ALA:HB3	1.99	0.44
1:D:20:ALA:HB2	1:D:30:LEU:HD11	2.00	0.44
1:M:341:ASN:O	1:M:345:LEU:HG	2.17	0.44
1:M:475:PHE:CZ	1:M:516:LEU:HB2	2.52	0.44
1:O:87:LYS:H	1:O:87:LYS:HD2	1.81	0.44
1:O:553:ILE:CG2	1:O:556:LEU:HD23	2.48	0.44
1:A:74:THR:HG21	1:A:328:VAL:CG2	2.48	0.44
1:M:97:SER:HB3	1:M:100:PRO:HG2	1.99	0.44
1:M:308:GLU:HG3	1:M:456:LEU:HD13	2.00	0.44
1:M:502:GLY:O	1:M:504:PRO:HD3	2.18	0.44
1:O:102:PHE:CZ	1:P:247:LEU:HD21	2.53	0.44
1:O:376:VAL:HB	1:O:404:ALA:HA	2.00	0.44
1:C:335:LYS:O	1:C:340:VAL:HG23	2.17	0.43
1:N:229:ASP:HB2	1:N:231:LYS:CE	2.41	0.43
1:O:25:ILE:HD11	1:O:291:LEU:HD13	1.99	0.43
1:O:344:ASP:OD1	1:O:344:ASP:N	2.50	0.43
1:O:458:GLY:O	1:O:505:SER:HA	2.18	0.43
1:B:334:LEU:O	1:B:356:GLY:HA3	2.17	0.43
1:C:310:PHE:O	1:C:314:LYS:HB3	2.18	0.43
1:D:164:ARG:NH1	1:D:193:GLY:HA3	2.33	0.43
1:N:284:ALA:O	1:N:287:THR:HG22	2.18	0.43
1:O:63:SER:HB2	1:O:337:HIS:CE1	2.53	0.43
1:P:399:ARG:O	1:P:400:LEU:HG	2.18	0.43
1:A:129:ASP:O	1:A:132:ALA:HB3	2.18	0.43
1:N:76:VAL:HG11	1:N:115:GLN:C	2.43	0.43
1:M:346:GLN:HG3	1:M:383:GLN:OE1	2.18	0.43
1:N:51:LYS:O	1:N:52:PRO:C	2.61	0.43
1:N:310:PHE:O	1:N:314:LYS:HB3	2.17	0.43
1:P:56:LEU:HB3	1:P:322:PRO:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:117:VAL:HG12	1:P:119:MET:N	2.33	0.43
1:P:491:GLN:CD	1:P:491:GLN:H	2.25	0.43
1:A:165:ARG:O	1:A:194:PHE:HA	2.18	0.43
1:M:350:LEU:N	1:M:350:LEU:HD12	2.34	0.43
1:O:172:ARG:NH2	1:P:146:ASN:OD1	2.51	0.43
1:B:160:ARG:HB3	1:B:226:GLU:HB2	2.01	0.43
1:C:420:LEU:O	1:C:424:VAL:HG23	2.18	0.43
1:D:249:LYS:HG3	1:D:250:ASP:N	2.34	0.43
1:M:159:ARG:HD2	1:O:184:VAL:HA	2.00	0.43
1:C:23:LEU:HB3	1:C:291:LEU:HB3	2.00	0.43
1:C:75:THR:HG23	1:C:296:VAL:HG12	2.01	0.43
1:C:108:ALA:N	1:C:119:MET:HE3	2.33	0.43
1:P:234:THR:O	1:P:237:ASP:HB2	2.19	0.43
1:B:275:ILE:CG2	1:B:530:ILE:HG21	2.49	0.43
1:D:144:ILE:HG12	1:D:224:ILE:HD12	2.01	0.43
1:D:199:ALA:HB2	1:D:272:PHE:CE2	2.54	0.43
1:M:340:VAL:CG1	1:M:345:LEU:HD23	2.49	0.43
1:N:453:ALA:O	1:N:459:ALA:HB3	2.19	0.43
1:B:98:LEU:HD23	1:B:98:LEU:C	2.44	0.43
1:N:67:ALA:HB2	1:N:336:MET:SD	2.59	0.43
1:O:5:ILE:HD13	1:O:9:ARG:NH2	2.33	0.43
1:O:83:ASN:HA	1:O:87:LYS:O	2.18	0.43
1:O:125:HIS:O	1:O:126:PHE:C	2.62	0.43
1:C:83:ASN:OD1	1:C:88:ARG:NH2	2.52	0.43
1:D:141:ALA:HB1	1:D:165:ARG:CZ	2.48	0.43
1:P:14:LYS:HB3	1:P:18:GLN:NE2	2.34	0.43
1:P:57:VAL:HG13	1:P:296:VAL:HG12	2.00	0.43
1:M:20:ALA:CB	1:M:30:LEU:HD11	2.48	0.42
1:O:39:LYS:HE2	1:O:253:GLN:O	2.18	0.42
1:C:272:PHE:O	1:C:276:ALA:HB3	2.18	0.42
1:M:280:ASN:OD1	1:M:297:THR:OG1	2.37	0.42
1:N:42:HIS:N	1:N:253:GLN:HE21	2.16	0.42
1:N:207:CYS:SG	1:N:271:PRO:HG3	2.59	0.42
1:P:367:VAL:CG1	1:P:374:VAL:HG12	2.48	0.42
1:D:157:ASP:OD2	1:D:160:ARG:HD2	2.20	0.42
1:D:361:GLU:HA	1:D:400:LEU:HD11	2.00	0.42
1:M:368:ARG:NH2	1:M:402:VAL:HG13	2.34	0.42
1:P:219:LEU:HD23	1:P:219:LEU:HA	1.86	0.42
1:C:217:GLU:O	1:C:221:ARG:HG3	2.19	0.42
1:N:263:ASN:HD22	1:N:263:ASN:HA	1.66	0.42
1:N:375:VAL:CG2	1:N:427:LEU:HD22	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LYS:CG	1:A:52:PRO:HD2	2.49	0.42
1:C:203:MET:HE2	1:C:270:GLY:H	1.85	0.42
1:M:26:PRO:HD2	1:M:44:PHE:CE2	2.54	0.42
1:O:400:LEU:CB	1:O:402:VAL:HG23	2.50	0.42
1:A:335:LYS:HE3	1:A:388:GLU:OE2	2.20	0.42
1:C:147:HIS:CD2	1:C:154:LEU:HD12	2.54	0.42
1:C:318:THR:HG21	1:C:320:LEU:HD12	2.01	0.42
1:C:364:VAL:HG22	1:C:374:VAL:HG11	2.01	0.42
1:N:78:LEU:HD13	1:N:420:LEU:HD23	2.00	0.42
1:B:39:LYS:HD3	1:B:253:GLN:HB2	2.01	0.42
1:B:472:LEU:HD21	1:B:514:VAL:HG21	2.00	0.42
1:M:340:VAL:HG12	1:M:341:ASN:O	2.20	0.42
1:M:373:PRO:HB2	1:M:427:LEU:HB3	2.02	0.42
1:O:83:ASN:CB	1:O:263:ASN:ND2	2.76	0.42
1:P:420:LEU:C	1:P:420:LEU:HD13	2.45	0.42
1:P:491:GLN:NE2	1:P:492:TYR:CZ	2.88	0.42
1:B:39:LYS:HZ3	1:B:255:ASN:HD21	1.67	0.42
1:B:405:ILE:HA	5:B:640:HOH:O	2.20	0.42
1:C:537:PRO:HD2	1:C:540:PRO:HB3	2.01	0.42
1:O:384:ASP:HB3	1:O:389:HIS:CD2	2.54	0.42
1:B:159:ARG:HD2	1:D:188:PHE:CD1	2.55	0.42
1:C:91:MET:HE3	1:C:264:PRO:O	2.19	0.42
1:N:430:GLY:O	1:N:431:GLU:C	2.63	0.42
1:P:353:LEU:O	1:P:353:LEU:HD22	2.19	0.42
1:P:368:ARG:NH1	1:P:373:PRO:HA	2.35	0.42
1:M:443:THR:O	1:M:448:LYS:HE2	2.19	0.42
1:M:526:ILE:HG23	1:M:530:ILE:HD13	2.02	0.42
1:N:53:GLU:HB3	1:N:289:LEU:HB3	2.01	0.42
1:N:62:ILE:CG2	1:N:360:LEU:HD12	2.49	0.42
1:O:62:ILE:HD11	1:O:333:ALA:HB3	2.02	0.42
1:O:331:ILE:HG22	1:O:335:LYS:HE2	2.02	0.42
1:P:311:ILE:HG21	1:P:370:PHE:HD2	1.85	0.42
1:N:14:LYS:HB2	1:N:258:GLN:HE22	1.84	0.41
1:P:511:VAL:HG22	1:P:525:VAL:HG12	2.01	0.41
1:B:137:HIS:CD2	1:B:163:TRP:CZ2	3.08	0.41
1:D:121:GLN:N	1:D:121:GLN:OE1	2.53	0.41
1:P:348:GLU:HA	1:P:388:GLU:OE2	2.20	0.41
1:A:62:ILE:HD11	1:A:333:ALA:CB	2.50	0.41
1:B:137:HIS:HD2	1:B:200:SER:OG	2.03	0.41
1:C:318:THR:HG23	1:C:320:LEU:HG	2.03	0.41
1:D:115:GLN:O	1:D:259:THR:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:69:GLU:N	1:N:69:GLU:CD	2.78	0.41
1:N:311:ILE:HG21	1:N:370:PHE:CD1	2.56	0.41
1:B:472:LEU:CD2	1:B:514:VAL:HG11	2.50	0.41
1:C:483:LEU:HD22	1:C:521:GLY:C	2.45	0.41
1:D:413:GLY:O	1:D:414:GLY:C	2.64	0.41
1:M:150:TRP:CD1	1:N:538:LYS:HA	2.56	0.41
1:A:39:LYS:CE	1:A:250:ASP:O	2.69	0.41
1:B:472:LEU:HD21	1:B:514:VAL:HG11	2.02	0.41
1:M:48:LEU:HD23	1:M:290:ARG:HB2	2.02	0.41
1:M:78:LEU:HD13	1:M:420:LEU:HD12	2.02	0.41
1:M:229:ASP:OD1	1:M:229:ASP:N	2.52	0.41
1:O:25:ILE:HA	1:O:26:PRO:HD2	1.97	0.41
1:P:289:LEU:HG	1:P:295:THR:HG21	2.02	0.41
1:B:42:HIS:N	1:B:253:GLN:HE21	2.17	0.41
1:C:538:LYS:HE3	1:O:482:LYS:HE2	2.03	0.41
1:D:76:VAL:HA	1:D:91:MET:SD	2.60	0.41
1:D:166:VAL:HA	1:D:195:ASP:O	2.21	0.41
1:N:362:ARG:NH1	1:N:458:GLY:HA3	2.32	0.41
1:O:465:GLU:OE2	1:O:510:SER:OG	2.38	0.41
1:P:91:MET:HE2	1:P:91:MET:HB2	1.89	0.41
1:P:147:HIS:CE1	1:P:154:LEU:H	2.35	0.41
1:C:373:PRO:HB2	1:C:427:LEU:HD22	2.02	0.41
1:M:203:MET:C	1:M:203:MET:HE3	2.46	0.41
1:N:106:GLY:O	1:N:557:PHE:HD2	2.04	0.41
1:N:200:SER:OG	1:N:202:VAL:HB	2.20	0.41
1:O:333:ALA:O	1:O:336:MET:HB3	2.20	0.41
1:P:121:GLN:O	1:P:126:PHE:HB2	2.21	0.41
1:P:459:ALA:HB2	1:P:507:HIS:CE1	2.55	0.41
1:A:541:ALA:O	1:A:545:ILE:HG13	2.21	0.41
1:B:14:LYS:H	1:B:258:GLN:HE22	1.68	0.41
1:N:483:LEU:HD23	1:N:483:LEU:HA	1.83	0.41
1:O:31:HIS:O	1:O:38:ALA:HA	2.21	0.41
1:O:168:ASP:HB2	1:O:197:THR:CG2	2.51	0.41
1:P:137:HIS:NE2	1:P:166:VAL:HG13	2.36	0.41
1:P:556:LEU:HB3	1:P:557:PHE:CE2	2.56	0.41
1:A:171:ASP:OD1	1:A:173:ALA:HB3	2.20	0.41
1:B:92:CYS:HA	1:B:266:LEU:O	2.21	0.41
1:B:413:GLY:O	1:B:414:GLY:C	2.62	0.41
1:C:303:ALA:HA	1:C:307:ALA:CB	2.51	0.41
1:D:224:ILE:HG21	1:D:235:LEU:CD2	2.51	0.41
1:M:171:ASP:OD2	1:N:165:ARG:NH1	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:285:THR:HG21	1:M:314:LYS:NZ	2.36	0.41
1:N:222:ILE:HB	1:N:235:LEU:HD12	2.02	0.41
1:N:275:ILE:O	1:N:275:ILE:CG2	2.69	0.41
4:N:601:FLC:HA1	1:P:188:PHE:CD2	2.55	0.41
1:O:84:ARG:NE	1:O:418:GLU:OE2	2.49	0.41
1:O:98:LEU:O	1:O:101:CYS:HB2	2.21	0.41
1:P:319:GLY:O	1:P:320:LEU:O	2.39	0.41
1:P:458:GLY:O	1:P:505:SER:HA	2.20	0.41
1:P:483:LEU:HA	1:P:484:PRO:HD3	1.92	0.41
1:B:315:CYS:SG	1:B:322:PRO:HD3	2.61	0.41
1:B:326:VAL:HA	1:B:375:VAL:O	2.21	0.41
1:M:155:ASN:HD21	1:M:228:ARG:CZ	2.33	0.41
1:N:301:PHE:CG	1:N:491:GLN:HG2	2.56	0.41
1:O:235:LEU:HD13	1:O:244:MET:SD	2.60	0.41
1:O:459:ALA:HB2	1:O:507:HIS:NE2	2.37	0.41
1:P:74:THR:OG1	1:P:328:VAL:HG21	2.21	0.41
1:D:93:LEU:O	1:D:267:ILE:HA	2.21	0.40
1:D:174:LEU:O	1:D:194:PHE:N	2.52	0.40
1:N:15:PRO:O	1:N:19:VAL:HG23	2.21	0.40
1:N:58:LEU:HG	1:N:310:PHE:CD1	2.56	0.40
1:C:60:THR:CG2	1:C:303:ALA:HB2	2.50	0.40
1:C:363:HIS:CE1	1:C:494:PHE:CZ	3.10	0.40
1:M:211:ASN:ND2	1:M:214:ASP:H	2.19	0.40
1:N:331:ILE:HD13	1:N:389:HIS:CE1	2.56	0.40
1:O:76:VAL:HA	1:O:91:MET:SD	2.62	0.40
1:O:166:VAL:HG11	1:O:200:SER:HB2	2.03	0.40
1:P:485:VAL:HG13	1:P:525:VAL:HG21	2.02	0.40
1:C:178:ASN:O	1:D:177:ILE:HA	2.21	0.40
1:C:201:GLU:CD	1:C:222:ILE:HG12	2.47	0.40
1:C:361:GLU:OE2	1:C:399:ARG:NH2	2.54	0.40
1:D:249:LYS:HG3	1:D:250:ASP:H	1.86	0.40
1:N:33:TYR:O	1:N:37:ILE:HB	2.21	0.40
1:N:334:LEU:HD23	1:N:334:LEU:HA	1.97	0.40
1:O:78:LEU:HD12	1:O:78:LEU:HA	1.90	0.40
1:A:39:LYS:HE2	1:A:250:ASP:O	2.21	0.40
1:B:475:PHE:CZ	1:B:516:LEU:HB2	2.56	0.40
1:C:137:HIS:CE1	1:C:163:TRP:CZ2	3.10	0.40
1:C:345:LEU:HD23	1:C:345:LEU:HA	1.93	0.40
1:N:150:TRP:O	1:N:151:ALA:CB	2.68	0.40
1:O:33:TYR:CE1	1:O:39:LYS:HG3	2.56	0.40
1:O:79:GLY:HA3	1:O:91:MET:SD	2.62	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:373:PRO:HB3	1:M:427:LEU:HD22	2.04	0.40
1:N:301:PHE:CD2	1:N:491:GLN:HG2	2.56	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	556/568 (98%)	527 (95%)	26 (5%)	3 (0%)	24	53
1	B	556/568 (98%)	516 (93%)	36 (6%)	4 (1%)	18	45
1	C	554/568 (98%)	513 (93%)	38 (7%)	3 (0%)	24	53
1	D	554/568 (98%)	522 (94%)	30 (5%)	2 (0%)	30	58
1	M	548/568 (96%)	498 (91%)	48 (9%)	2 (0%)	30	58
1	N	551/568 (97%)	473 (86%)	71 (13%)	7 (1%)	9	29
1	O	554/568 (98%)	507 (92%)	43 (8%)	4 (1%)	18	45
1	P	541/568 (95%)	484 (90%)	48 (9%)	9 (2%)	7	23
All	All	4414/4544 (97%)	4040 (92%)	340 (8%)	34 (1%)	16	41

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	548	ASP
1	P	18	GLN
1	P	320	LEU
1	A	151	ALA
1	A	549	ALA
1	M	126	PHE
1	N	105	LYS
1	O	150	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	400	LEU
1	C	151	ALA
1	N	120	GLU
1	N	358	ALA
1	P	70	GLY
1	P	349	ASN
1	P	500	LEU
1	B	379	ASN
1	N	51	LYS
1	N	151	ALA
1	N	332	ARG
1	O	169	MET
1	P	449	ILE
1	B	151	ALA
1	O	109	ALA
1	P	11	ALA
1	P	308	GLU
1	B	270	GLY
1	D	270	GLY
1	N	484	PRO
1	C	270	GLY
1	M	302	GLY
1	C	62	ILE
1	D	257	VAL
1	A	270	GLY
1	O	271	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	434/441 (98%)	427 (98%)	7 (2%)	55	82
1	B	433/441 (98%)	419 (97%)	14 (3%)	34	68
1	C	432/441 (98%)	418 (97%)	14 (3%)	34	68
1	D	432/441 (98%)	413 (96%)	19 (4%)	25	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	429/441 (97%)	412 (96%)	17 (4%)	28	61
1	N	431/441 (98%)	400 (93%)	31 (7%)	13	37
1	O	432/441 (98%)	397 (92%)	35 (8%)	11	32
1	P	425/441 (96%)	384 (90%)	41 (10%)	8	24
All	All	3448/3528 (98%)	3270 (95%)	178 (5%)	21	51

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ARG
1	A	120	GLU
1	A	169	MET
1	A	180	SER
1	A	283	ILE
1	A	444	LYS
1	A	470	THR
1	B	45	ILE
1	B	105	LYS
1	B	120	GLU
1	B	179	GLN
1	B	241	THR
1	B	246	VAL
1	B	280	ASN
1	B	400	LEU
1	B	466	SER
1	B	477	LYS
1	B	500	LEU
1	B	529	GLU
1	B	530	ILE
1	B	548	ASP
1	C	21	GLU
1	C	167	VAL
1	C	179	GLN
1	C	184	VAL
1	C	323	SER
1	C	340	VAL
1	C	344	ASP
1	C	346	GLN
1	C	374	VAL
1	C	441	THR
1	C	445	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	446	THR
1	C	485	VAL
1	C	552	GLN
1	D	16	ILE
1	D	41	ASP
1	D	69	GLU
1	D	71	LYS
1	D	113	LYS
1	D	125	HIS
1	D	167	VAL
1	D	180	SER
1	D	210	LYS
1	D	226	GLU
1	D	257	VAL
1	D	275	ILE
1	D	283	ILE
1	D	344	ASP
1	D	355	LYS
1	D	466	SER
1	D	485	VAL
1	D	526	ILE
1	D	539	VAL
1	M	12	THR
1	M	45	ILE
1	M	119	MET
1	M	179	GLN
1	M	229	ASP
1	M	283	ILE
1	M	287	THR
1	M	321	LYS
1	M	355	LYS
1	M	378	VAL
1	M	436	THR
1	M	442	GLU
1	M	444	LYS
1	M	470	THR
1	M	482	LYS
1	M	501	MET
1	M	514	VAL
1	N	57	VAL
1	N	58	LEU
1	N	73	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	120	GLU
1	N	158	VAL
1	N	166	VAL
1	N	172	ARG
1	N	179	GLN
1	N	196	ILE
1	N	231	LYS
1	N	255	ASN
1	N	282	VAL
1	N	283	ILE
1	N	295	THR
1	N	296	VAL
1	N	316	ARG
1	N	331	ILE
1	N	340	VAL
1	N	360	LEU
1	N	402	VAL
1	N	407	CYS
1	N	426	LYS
1	N	433	LYS
1	N	464	ILE
1	N	470	THR
1	N	489	LYS
1	N	516	LEU
1	N	530	ILE
1	N	538	LYS
1	N	539	VAL
1	N	557	PHE
1	O	16	ILE
1	O	32	ASN
1	O	71	LYS
1	O	83	ASN
1	O	85	ILE
1	O	117	VAL
1	O	134	THR
1	O	158	VAL
1	O	177	ILE
1	O	179	GLN
1	O	197	THR
1	O	239	LYS
1	O	241	THR
1	O	249	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	256	LEU
1	O	263	ASN
1	O	285	THR
1	O	323	SER
1	O	336	MET
1	O	344	ASP
1	O	361	GLU
1	O	375	VAL
1	O	391	ARG
1	O	408	LYS
1	O	442	GLU
1	O	462	ILE
1	O	466	SER
1	O	476	GLU
1	O	489	LYS
1	O	515	ARG
1	O	530	ILE
1	O	539	VAL
1	O	552	GLN
1	O	554	ASP
1	O	556	LEU
1	P	19	VAL
1	P	45	ILE
1	P	60	THR
1	P	85	ILE
1	P	91	MET
1	P	117	VAL
1	P	133	ILE
1	P	179	GLN
1	P	208	LEU
1	P	238	VAL
1	P	258	GLN
1	P	267	ILE
1	P	280	ASN
1	P	283	ILE
1	P	286	ARG
1	P	295	THR
1	P	296	VAL
1	P	297	THR
1	P	305	LEU
1	P	320	LEU
1	P	324	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	326	VAL
1	P	346	GLN
1	P	348	GLU
1	P	353	LEU
1	P	354	GLU
1	P	369	SER
1	P	374	VAL
1	P	395	LEU
1	P	397	ARG
1	P	398	ASP
1	P	424	VAL
1	P	446	THR
1	P	489	LYS
1	P	491	GLN
1	P	511	VAL
1	P	514	VAL
1	P	526	ILE
1	P	539	VAL
1	P	546	ARG
1	P	556	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	83	ASN
1	A	152	ASN
1	A	170	ASN
1	A	178	ASN
1	A	179	GLN
1	A	346	GLN
1	A	363	HIS
1	A	422	GLN
1	B	83	ASN
1	B	137	HIS
1	B	162	HIS
1	B	253	GLN
1	B	255	ASN
1	B	379	ASN
1	B	380	HIS
1	B	389	HIS
1	B	463	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	18	GLN
1	C	115	GLN
1	C	123	ASN
1	C	155	ASN
1	C	162	HIS
1	C	253	GLN
1	C	255	ASN
1	C	258	GLN
1	C	363	HIS
1	C	365	ASN
1	C	552	GLN
1	D	32	ASN
1	D	36	HIS
1	D	178	ASN
1	D	179	GLN
1	D	253	GLN
1	D	258	GLN
1	D	463	GLN
1	M	32	ASN
1	M	147	HIS
1	M	155	ASN
1	M	179	GLN
1	M	211	ASN
1	M	263	ASN
1	M	349	ASN
1	M	463	GLN
1	N	31	HIS
1	N	137	HIS
1	N	147	HIS
1	N	178	ASN
1	N	179	GLN
1	N	186	ASN
1	N	211	ASN
1	N	253	GLN
1	N	255	ASN
1	N	258	GLN
1	N	359	ASN
1	N	379	ASN
1	N	409	HIS
1	O	36	HIS
1	O	115	GLN
1	O	155	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	178	ASN
1	O	211	ASN
1	O	258	GLN
1	O	337	HIS
1	O	379	ASN
1	O	401	GLN
1	O	432	GLN
1	P	18	GLN
1	P	147	HIS
1	P	179	GLN
1	P	253	GLN
1	P	280	ASN
1	P	363	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
4	FLC	N	601	-	12,12,12	1.43	2 (16%)	17,17,17	1.44	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	D	602	-	3,3,3	1.26	0	3,3,3	0.67	0
2	TLA	D	601	-	9,9,9	1.31	0	12,12,12	2.77	7 (58%)

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
4	FLC	N	601	-	-	10/16/16/16	-
2	TLA	D	601	-	-	5/12/12/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	601	FLC	CB-CBC	2.97	1.56	1.53
4	N	601	FLC	OG2-CGC	-2.09	1.23	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	TLA	C2-C3-C4	4.48	119.74	109.82
2	D	601	TLA	O41-C4-C3	3.91	124.17	113.31
2	D	601	TLA	O41-C4-O4	-3.89	115.26	124.08
2	D	601	TLA	O1-C1-C2	-3.72	111.70	121.62
2	D	601	TLA	O3-C3-C2	-3.17	103.70	110.17
2	D	601	TLA	O11-C1-C2	2.65	120.66	113.31
4	N	601	FLC	OB1-CBC-CB	-2.55	117.15	122.09
4	N	601	FLC	OB2-CBC-CB	2.37	117.68	113.14
4	N	601	FLC	CB-CA-CAC	2.33	120.29	113.92
2	D	601	TLA	O2-C2-C3	2.29	114.83	110.17
4	N	601	FLC	OA2-CAC-CA	2.25	121.46	114.35
4	N	601	FLC	OA1-CAC-CA	-2.23	116.64	122.95

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	TLA	C1-C2-C3-C4
2	D	601	TLA	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	601	TLA	O2-C2-C3-C4
4	N	601	FLC	CG-CB-CBC-OB1
4	N	601	FLC	CG-CB-CBC-OB2
4	N	601	FLC	OHB-CB-CBC-OB1
4	N	601	FLC	OHB-CB-CBC-OB2
2	D	601	TLA	C1-C2-C3-O3
4	N	601	FLC	CB-CA-CAC-OA2
4	N	601	FLC	CB-CA-CAC-OA1
2	D	601	TLA	C2-C3-C4-O4
4	N	601	FLC	CA-CB-CG-CGC
4	N	601	FLC	CAC-CA-CB-OHB
4	N	601	FLC	CB-CG-CGC-OG1
4	N	601	FLC	CB-CG-CGC-OG2

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	601	FLC	4	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, 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	557/568 (98%)	-0.62	1 (0%) 91 89	13, 28, 48, 84	1 (0%)
1	B	558/568 (98%)	-0.61	0 100 100	18, 29, 46, 76	0
1	C	556/568 (97%)	-0.51	1 (0%) 91 89	18, 33, 55, 71	0
1	D	556/568 (97%)	-0.61	0 100 100	18, 30, 49, 69	0
1	M	552/568 (97%)	-0.19	1 (0%) 91 89	21, 51, 75, 97	0
1	N	555/568 (97%)	-0.10	0 100 100	24, 55, 79, 95	0
1	O	556/568 (97%)	-0.18	1 (0%) 91 89	23, 49, 73, 92	0
1	P	547/568 (96%)	0.01	2 (0%) 88 84	22, 59, 83, 112	0
All	All	4437/4544 (97%)	-0.35	6 (0%) 92 90	13, 39, 74, 112	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	350	LEU	3.4
1	P	269	GLY	2.4
1	A	1	MET	2.2
1	O	106	GLY	2.1
1	P	458	GLY	2.1
1	M	89	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	ACT	D	602	4/4	0.64	0.20	52,55,60,61	0
2	TLA	D	601	10/10	0.89	0.11	41,46,47,50	0
4	FLC	N	601	13/13	0.91	0.09	39,46,49,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.