Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2023 – 10:39 PM JST

PDB ID	:	7C11
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 (i) 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 (i)) were used in the production of this report:

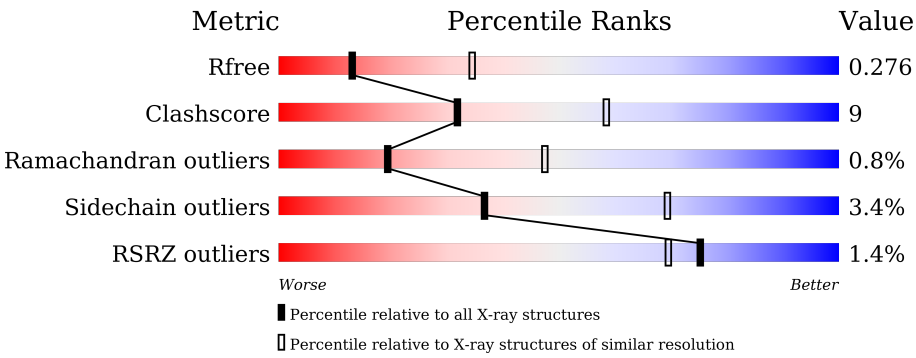
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (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 <=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	84% 14% •
1	B	568	80% 17% •
1	C	568	76% 21% • •
1	D	568	81% 17% •
1	M	568	2% 74% 22% • •
1	N	568	2% 76% 21% • •

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Mol	Chain	Length	Quality of chain
1	O	568	2% 73% 23%
1	P	568	4% 67% 25%

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	TLA	D	601	-	X	-	-
4	FLC	N	601	-	-	X	-

2 Entry composition (i)

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

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

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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

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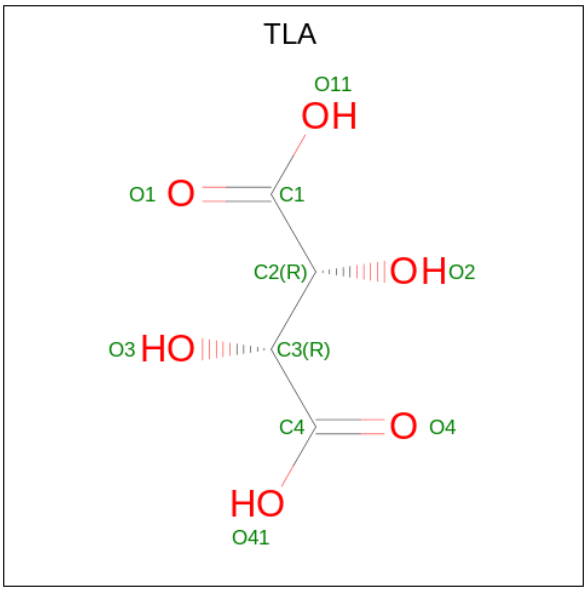
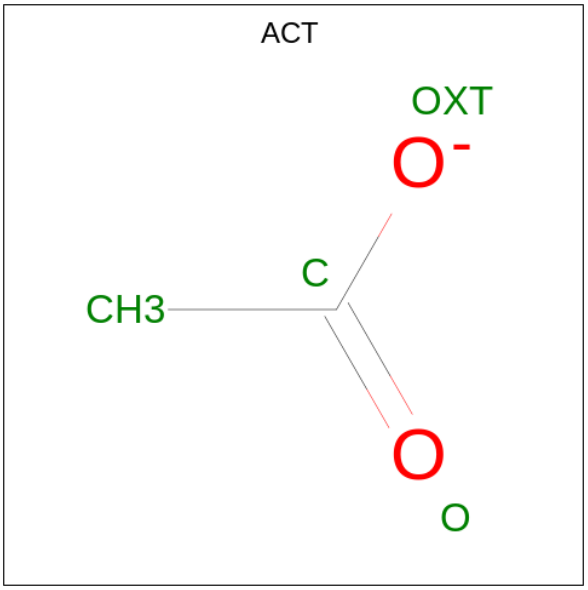
Chain	Residue	Modelled	Actual	Comment	Reference
N	558	ALA	-	expression tag	UNP B7L0A5
N	559	ALA	-	expression tag	UNP B7L0A5
N	560	ALA	-	expression tag	UNP B7L0A5
N	561	LEU	-	expression tag	UNP B7L0A5
N	562	GLU	-	expression tag	UNP B7L0A5
N	563	HIS	-	expression tag	UNP B7L0A5
N	564	HIS	-	expression tag	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 (three-letter code: TLA) (formula: $C_4H_6O_6$).



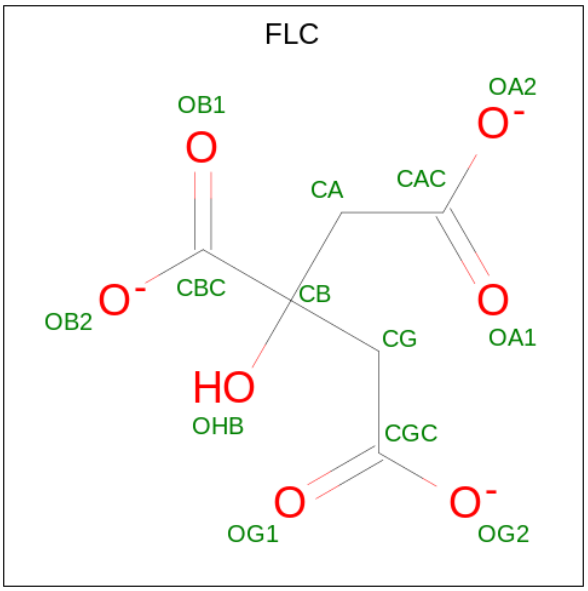
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	D	1	10	4	6	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



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

- Molecule 5 is water.

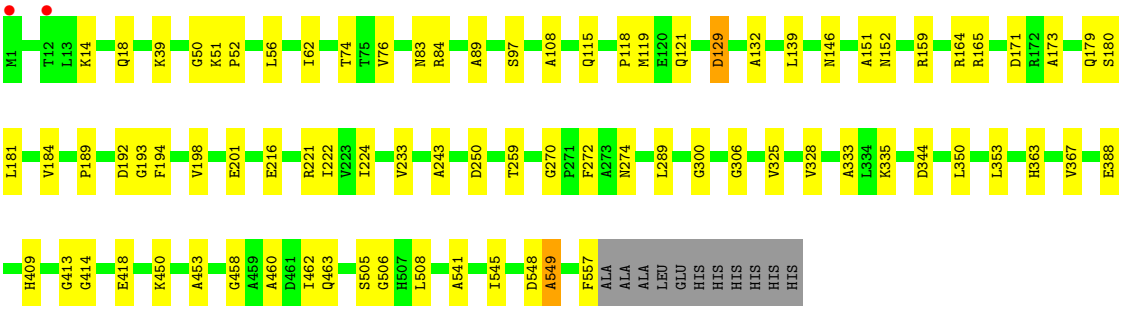
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	67	Total O 67 67	0	0
5	B	73	Total O 73 73	0	0
5	C	51	Total O 51 51	0	0
5	D	58	Total O 58 58	0	0
5	M	37	Total O 37 37	0	0
5	N	42	Total O 42 42	0	0
5	O	31	Total O 31 31	0	0
5	P	21	Total O 21 21	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

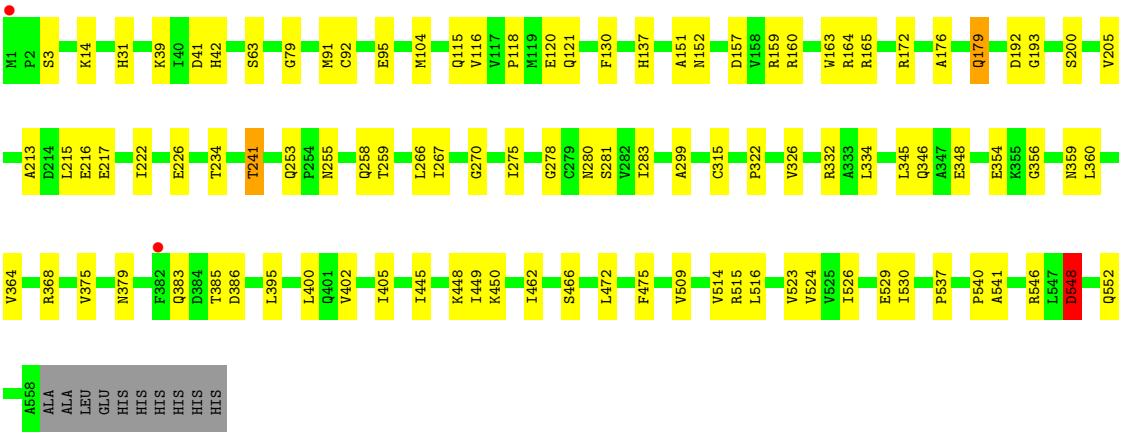
• Molecule 1: Formate-tetrahydrofolate ligase

Chain A: 84% 14% •



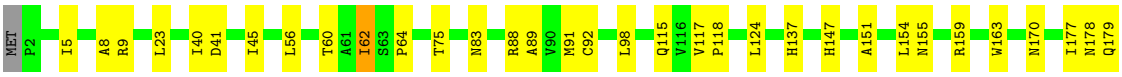
• Molecule 1: Formate-tetrahydrofolate ligase

Chain B: 80% 17% •



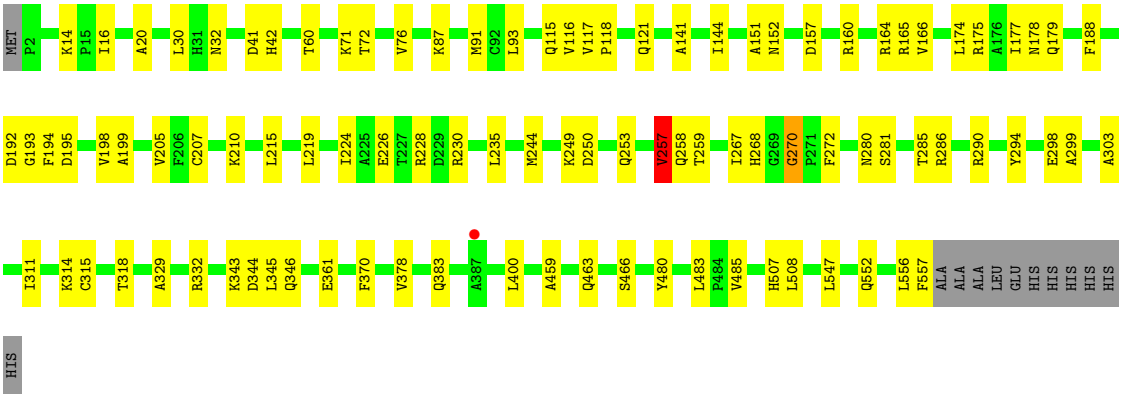
• Molecule 1: Formate-tetrahydrofolate ligase

Chain C: 76% 21% ••



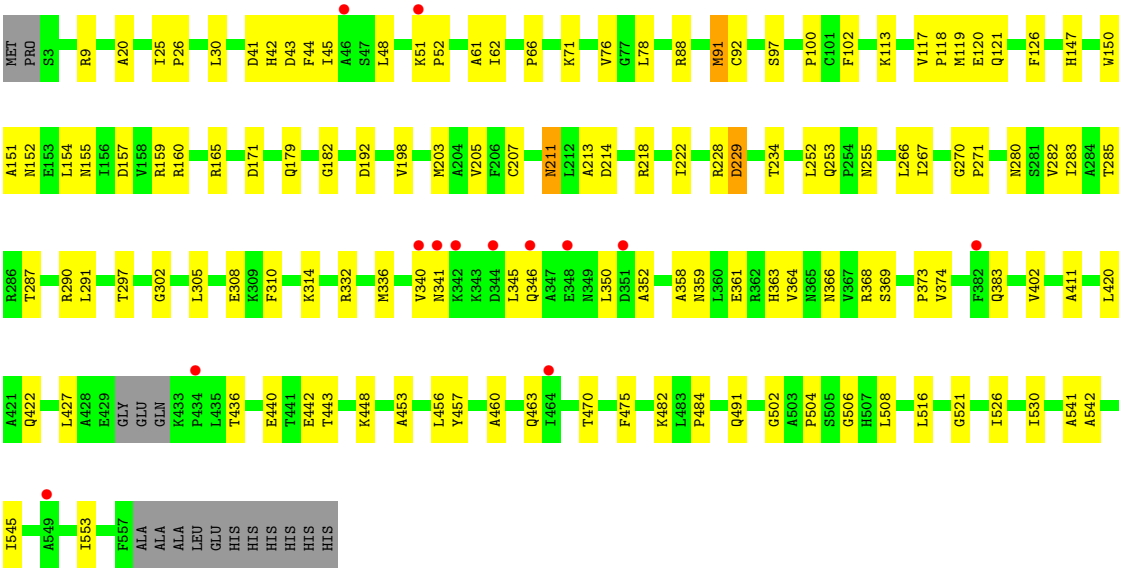
• Molecule 1: Formate-tetrahydrofolate ligase

Chain D:



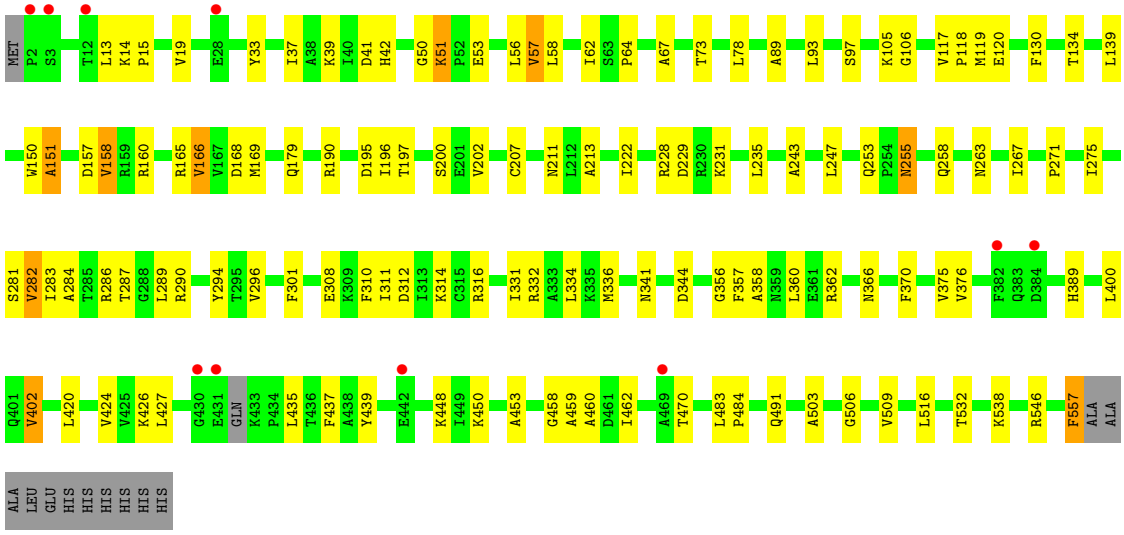
• Molecule 1: Formate-tetrahydrofolate ligase

Chain M:



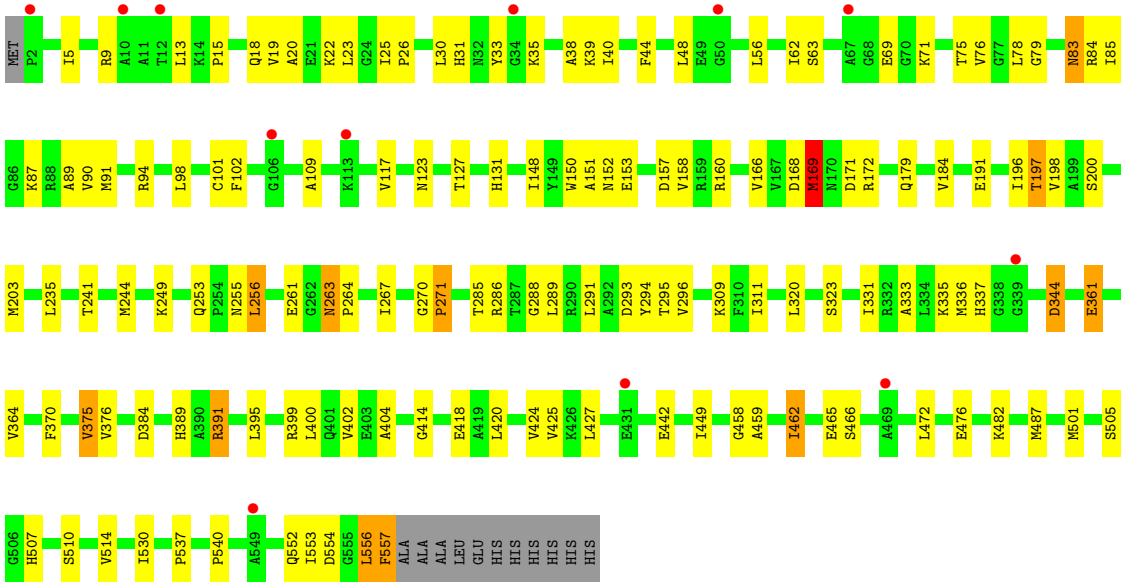
• Molecule 1: Formate-tetrahydrofolate ligase

Chain N:



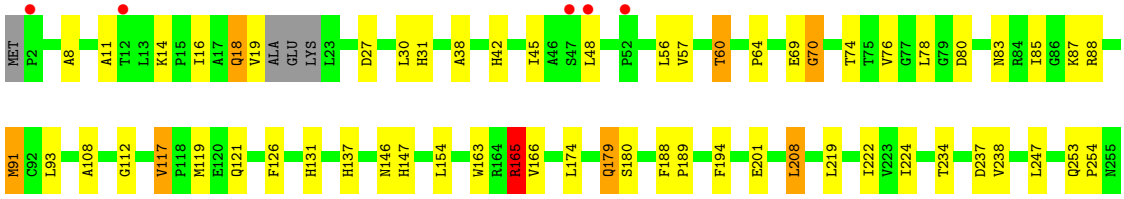
• Molecule 1: Formate-tetrahydrofolate ligase

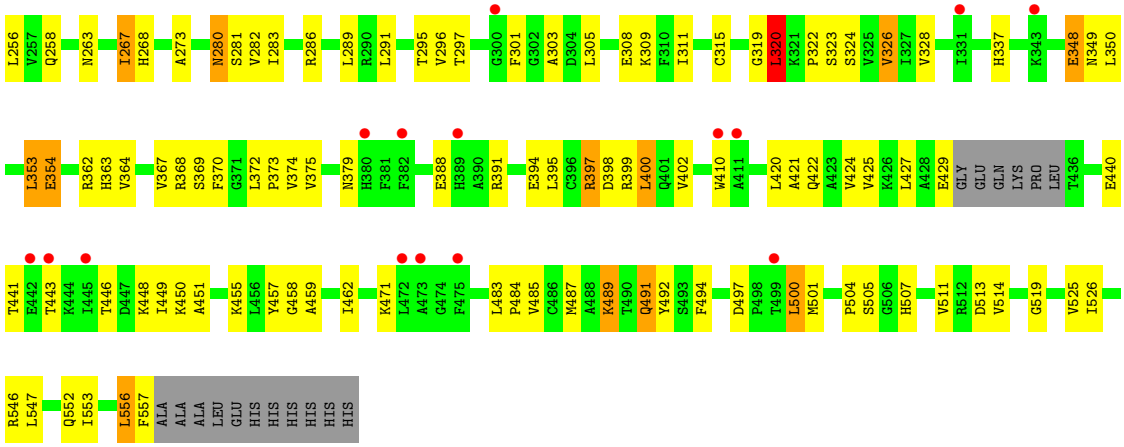
Chain O:



• Molecule 1: Formate-tetrahydrofolate ligase

Chain P:




L256 V257 Q258 N263 I267 H268 A273 N280 S281 V282 I283 R286 L289 R290 L291 T295 V296 T297 G300 F301 G302 A303 D304 L305 E308 K309 F310 I311 C315 G319 L330 K321 P322 S323 S324 V325 V326 I327 V328 I331 H337 K343 E348 N349 L350
L353 E354 R362 H363 V364 V367 R368 S369 F370 G371 L372 P373 V374 V375 N379 H380 F381 F382 E388 H389 A390 R391 E394 L395 C396 R397 D398 R399 L400 Q401 V402 W410 A411 L420 A421 Q422 A423 V424 V425 K426 L427 A428 E429 GLY GLU GLN LYS PRO LEU T436 E440
T441 E442 T443 K444 I445 T446 D447 K448 I449 K450 A451 K455 L456 Y457 G458 A459 I462 K471 L472 A473 G474 F475 L483 P484 V485 C486 M487 A488 K489 T490 Q491 Y492 S493 F494 D497 P498 T499 L500 M501 P504 S505 G506 H507 V511 R512 D513 V514 G519 V525 I526
R546 L547 Q552 I553 L556 F557 ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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 36.58 – 2.82	Depositor EDS
% Data completeness (in resolution range)	97.4 (36.60-2.81) 97.5 (36.58-2.82)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (4.98%)	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)	0.35 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: TLA, FLC, ACT

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	0.75	0/4254	0.92	1/5759 (0.0%)
1	B	0.76	0/4251	0.91	0/5755
1	C	0.76	0/4238	0.92	2/5737 (0.0%)
1	D	0.74	0/4238	0.91	0/5737
1	M	0.73	0/4207	0.87	0/5694
1	N	0.74	0/4228	0.88	0/5722
1	O	0.72	0/4238	0.89	0/5737
1	P	0.72	0/4166	0.87	1/5638 (0.0%)
All	All	0.74	0/33820	0.90	4/45779 (0.0%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	548	ASP	CB-CA-C	-5.71	98.99	110.40
1	C	190	ARG	CB-CA-C	-5.57	99.27	110.40
1	P	165	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	221	ARG	NE-CZ-NH1	5.06	122.83	120.30

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	48	0
1	B	4181	0	4257	66	0
1	C	4168	0	4241	80	0
1	D	4168	0	4241	65	0
1	M	4139	0	4215	78	0
1	N	4159	0	4232	87	0
1	O	4168	0	4241	86	0
1	P	4099	0	4167	110	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	597	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 (597) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:203:MET:HE1	1:M:270:GLY:H	1.48	0.77
1:C:348:GLU:HB2	1:C:385:THR:HG21	1.68	0.76
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
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:N:462:ILE:HD13	1:N:509:VAL:HB	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:ARG:NH1	1:D:318:THR:O	2.33	0.62
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
1:B:346:GLN:HG3	1:B:383:GLN:OE1	2.02	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: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: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: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:C:343:LYS:O	1:C:346:GLN:NE2	2.38	0.57
1:A:119:MET:HE2	1:A:557:PHE:CE1	2.40	0.57
1:C:329:ALA:O	1:C:378:VAL:HA	2.05	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:44:PHE:O	1:O:48:LEU:HD13	2.06	0.56
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:A:108:ALA:HA	1:A:119:MET:HE3	1.88	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:367:VAL:HG12	1:P:374:VAL:HG12	1.88	0.54
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:50:GLY:O	1:N:51:LYS:C	2.46	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:B:39:LYS:HZ1	1:B:255:ASN:HD21	1.56	0.53
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:M:422:GLN:HA	1:M:422:GLN:NE2	2.23	0.53
1:A:350:LEU:O	1:A:353:LEU:HB3	2.09	0.53
1:C:346:GLN:CD	1:C:346:GLN:H	2.12	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: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:P:179:GLN:HE21	1:P:179:GLN:C	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:P:309:LYS:NZ	1:P:487:MET:O	2.28	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:C:285:THR:HG21	1:C:314:LYS:HZ1	1.74	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: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: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: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:C:203:MET:HE2	1:C:270:GLY:H	1.76	0.50

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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: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: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:N:169:MET:HE3	1:N:169:MET:HA	1.94	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:P:76:VAL:HG13	1:P:91:MET:HE1	1.96	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: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: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:O:127:THR:HG21	1:O:255:ASN:OD1	2.14	0.47
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:D:157:ASP:CG	1:D:160:ARG:HG3	2.35	0.47
1:N:13:LEU:HD12	1:N:13:LEU:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:288:GLY:C	1:O:295:THR:HG21	2.35	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:P:471:LYS:NZ	1:P:513:ASP:OD1	2.43	0.46
1:A:84:ARG:HD3	1:A:418:GLU:OE2	2.16	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:119:MET:HE1	1:N:557:PHE:CD2	2.51	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:151:ALA:O	1:D:152:ASN:C	2.55	0.45
1:M:151:ALA:O	1:M:152:ASN:C	2.55	0.45
1:P:425:VAL:O	1:P:429:GLU:HG2	2.16	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:235:LEU:HD13	1:D:244:MET:CE	2.47	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:O:344:ASP:OD1	1:O:344:ASP:N	2.50	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
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: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
4:N:601:FLC:OG2	4:N:601:FLC:HA2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:M:346:GLN:HG3	1:M:383:GLN:OE1	2.18	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
1:P:117:VAL:HG12	1:P:119:MET:N	2.33	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:A:51:LYS:CG	1:A:52:PRO:HD2	2.49	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:91:MET:HE3	1:C:264:PRO:O	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:C:210:LYS:C	1:C:283:ILE:HD11	2.39	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:491:GLN:NE2	1:P:492:TYR:CZ	2.88	0.42
1:B:405:ILE:HA	5:B:640:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:D:235:LEU:HD13	1:D:244:MET:HE3	2.03	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: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:N:106:GLY:O	1:N:557:PHE:HD2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:219:LEU:HD22	1:C:244:MET:CE	2.51	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
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:O:169:MET:CE	1:O:169:MET:HA	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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%)	29 59
1	B	556/568 (98%)	516 (93%)	36 (6%)	4 (1%)	22 51
1	C	554/568 (98%)	513 (93%)	38 (7%)	3 (0%)	29 59
1	D	554/568 (98%)	522 (94%)	30 (5%)	2 (0%)	34 64
1	M	548/568 (96%)	498 (91%)	48 (9%)	2 (0%)	34 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	551/568 (97%)	473 (86%)	71 (13%)	7 (1%)	12	34
1	O	554/568 (98%)	507 (92%)	43 (8%)	4 (1%)	22	51
1	P	541/568 (95%)	484 (90%)	48 (9%)	9 (2%)	9	27
All	All	4414/4544 (97%)	4040 (92%)	340 (8%)	34 (1%)	19	47

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
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

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Mol	Chain	Res	Type
1	O	271	PRO

5.3.2 Protein sidechains (i)

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%)	429 (99%)	5 (1%)	71	91
1	B	433/441 (98%)	424 (98%)	9 (2%)	53	82
1	C	432/441 (98%)	424 (98%)	8 (2%)	57	84
1	D	432/441 (98%)	425 (98%)	7 (2%)	62	87
1	M	429/441 (97%)	418 (97%)	11 (3%)	46	78
1	N	431/441 (98%)	416 (96%)	15 (4%)	36	68
1	O	432/441 (98%)	405 (94%)	27 (6%)	18	44
1	P	425/441 (96%)	390 (92%)	35 (8%)	11	31
All	All	3448/3528 (98%)	3331 (97%)	117 (3%)	37	69

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ASP
1	A	152	ASN
1	A	180	SER
1	A	216	GLU
1	A	344	ASP
1	B	3	SER
1	B	120	GLU
1	B	179	GLN
1	B	241	THR
1	B	280	ASN
1	B	386	ASP
1	B	466	SER
1	B	529	GLU
1	B	548	ASP

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Mol	Chain	Res	Type
1	C	179	GLN
1	C	255	ASN
1	C	323	SER
1	C	344	ASP
1	C	346	GLN
1	C	446	THR
1	C	461	ASP
1	C	552	GLN
1	D	41	ASP
1	D	210	LYS
1	D	226	GLU
1	D	257	VAL
1	D	344	ASP
1	D	466	SER
1	D	485	VAL
1	M	43	ASP
1	M	91	MET
1	M	119	MET
1	M	179	GLN
1	M	211	ASN
1	M	229	ASP
1	M	287	THR
1	M	436	THR
1	M	442	GLU
1	M	470	THR
1	M	482	LYS
1	N	57	VAL
1	N	73	THR
1	N	158	VAL
1	N	166	VAL
1	N	179	GLN
1	N	255	ASN
1	N	282	VAL
1	N	283	ILE
1	N	316	ARG
1	N	402	VAL
1	N	426	LYS
1	N	470	THR
1	N	516	LEU
1	N	546	ARG
1	N	557	PHE
1	O	71	LYS

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Mol	Chain	Res	Type
1	O	83	ASN
1	O	85	ILE
1	O	158	VAL
1	O	169	MET
1	O	179	GLN
1	O	197	THR
1	O	241	THR
1	O	249	LYS
1	O	256	LEU
1	O	263	ASN
1	O	285	THR
1	O	293	ASP
1	O	323	SER
1	O	344	ASP
1	O	361	GLU
1	O	375	VAL
1	O	391	ARG
1	O	442	GLU
1	O	462	ILE
1	O	466	SER
1	O	476	GLU
1	O	530	ILE
1	O	552	GLN
1	O	554	ASP
1	O	556	LEU
1	O	557	PHE
1	P	19	VAL
1	P	27	ASP
1	P	45	ILE
1	P	60	THR
1	P	85	ILE
1	P	91	MET
1	P	117	VAL
1	P	165	ARG
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

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Mol	Chain	Res	Type
1	P	305	LEU
1	P	320	LEU
1	P	324	SER
1	P	326	VAL
1	P	348	GLU
1	P	353	LEU
1	P	354	GLU
1	P	369	SER
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	514	VAL
1	P	526	ILE
1	P	546	ARG
1	P	556	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	83	ASN
1	A	123	ASN
1	A	152	ASN
1	A	178	ASN
1	A	179	GLN
1	A	280	ASN
1	A	346	GLN
1	A	363	HIS
1	B	83	ASN
1	B	137	HIS
1	B	253	GLN
1	B	255	ASN
1	B	258	GLN
1	B	263	ASN
1	B	280	ASN
1	B	379	ASN
1	B	463	GLN
1	C	115	GLN

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Mol	Chain	Res	Type
1	C	123	ASN
1	C	155	ASN
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	147	HIS
1	M	155	ASN
1	M	179	GLN
1	M	211	ASN
1	M	280	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	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
1	O	178	ASN
1	O	211	ASN
1	O	258	GLN
1	O	337	HIS
1	O	379	ASN
1	O	401	GLN

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Mol	Chain	Res	Type
1	O	432	GLN
1	P	18	GLN
1	P	147	HIS
1	P	179	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 monosaccharides 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	$\#\|Z\| > 2$
3	ACT	D	602	-	3,3,3	1.19	0	3,3,3	0.66	0
4	FLC	N	601	-	12,12,12	1.41	2 (16%)	17,17,17	1.63	5 (29%)
2	TLA	D	601	-	9,9,9	1.30	1 (11%)	12,12,12	2.81	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	-	-	7/12/12/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	601	FLC	CB-CBC	3.02	1.56	1.53
2	D	601	TLA	C2-C1	-2.08	1.49	1.52
4	N	601	FLC	OG2-CGC	-2.03	1.23	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	TLA	C2-C3-C4	4.42	119.74	109.87
2	D	601	TLA	O41-C4-C3	4.03	124.17	113.27
2	D	601	TLA	O41-C4-O4	-3.89	115.26	124.09
2	D	601	TLA	O1-C1-C2	-3.78	111.70	121.63
4	N	601	FLC	OB1-CBC-CB	-3.60	117.15	122.25
2	D	601	TLA	O3-C3-C2	-3.29	103.70	110.23
2	D	601	TLA	O11-C1-C2	2.73	120.66	113.27
4	N	601	FLC	CB-CA-CAC	2.67	120.29	113.81
4	N	601	FLC	OB2-CBC-CB	2.67	117.68	113.05
2	D	601	TLA	O2-C2-C3	2.31	114.83	110.23
4	N	601	FLC	OA2-CAC-CA	2.21	121.46	114.35
4	N	601	FLC	OA1-CAC-CA	-2.16	116.64	122.94

There are no chirality outliers.

All (17) 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
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

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Mol	Chain	Res	Type	Atoms
4	N	601	FLC	CA-CB-CG-CGC
2	D	601	TLA	C2-C3-C4-O4
4	N	601	FLC	CAC-CA-CB-OHB
4	N	601	FLC	CB-CG-CGC-OG1
2	D	601	TLA	O3-C3-C4-O4
2	D	601	TLA	C2-C3-C4-O41
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%)	-0.55	2 (0%)	92	91	17, 28, 48, 84	0
1	B	558/568 (98%)	-0.43	2 (0%)	92	91	18, 29, 46, 76	0
1	C	556/568 (97%)	-0.31	0	100	100	18, 33, 55, 71	0
1	D	556/568 (97%)	-0.41	1 (0%)	95	94	18, 30, 49, 69	0
1	M	552/568 (97%)	-0.06	13 (2%)	59	49	21, 51, 75, 97	0
1	N	555/568 (97%)	-0.02	10 (1%)	68	61	24, 55, 79, 95	0
1	O	556/568 (97%)	-0.13	12 (2%)	62	52	23, 49, 73, 92	0
1	P	547/568 (96%)	0.16	20 (3%)	41	31	22, 59, 83, 112	0
All	All	4437/4544 (97%)	-0.22	60 (1%)	75	69	17, 39, 74, 112	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	2	PRO	4.2
1	P	499	THR	4.1
1	M	341	ASN	3.8
1	N	469	ALA	3.7
1	P	389	HIS	3.7
1	P	411	ALA	3.5
1	P	331	ILE	3.4
1	P	382	PHE	3.4
1	M	346	GLN	3.2
1	D	387	ALA	3.1
1	M	351	ASP	3.1
1	M	464	ILE	3.1
1	M	46	ALA	3.0
1	O	549	ALA	3.0
1	P	380	HIS	2.9
1	O	339	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	P	52	PRO	2.7
1	P	12	THR	2.6
1	M	344	ASP	2.6
1	M	340	VAL	2.6
1	O	2	PRO	2.6
1	M	549	ALA	2.6
1	N	430	GLY	2.6
1	O	12	THR	2.5
1	P	442	GLU	2.5
1	P	410	TRP	2.5
1	P	473	ALA	2.5
1	O	106	GLY	2.4
1	P	343	LYS	2.4
1	B	1	MET	2.4
1	N	431	GLU	2.4
1	P	472	LEU	2.4
1	O	431	GLU	2.3
1	N	382	PHE	2.3
1	M	382	PHE	2.3
1	O	67	ALA	2.3
1	P	47	SER	2.3
1	M	348	GLU	2.3
1	P	443	THR	2.2
1	M	342	LYS	2.2
1	N	442	GLU	2.2
1	A	12	THR	2.2
1	N	12	THR	2.2
1	O	34	GLY	2.2
1	O	113	LYS	2.2
1	M	434	PRO	2.2
1	O	50	GLY	2.2
1	M	51	LYS	2.2
1	P	2	PRO	2.2
1	N	28	GLU	2.1
1	P	445	ILE	2.1
1	A	1	MET	2.1
1	N	384	ASP	2.1
1	O	469	ALA	2.1
1	P	300	GLY	2.1
1	P	475	PHE	2.1
1	B	382	PHE	2.1
1	O	10	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	N	3	SER	2.0
1	P	48	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	0.81	0.51	52,55,60,61	0
2	TLA	D	601	10/10	0.89	0.17	41,46,47,50	0
4	FLC	N	601	13/13	0.93	0.17	39,46,49,50	0

6.5 Other polymers (i)

There are no such residues in this entry.