



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:47 AM UTC

PDB ID : 7NPH / pdb_00007nph
Title : Crystal structure of Mycobacterium tuberculosis ArgC in complex with 5-methoxy-1,3-benzoxazole-2-carboxylic acid
Authors : Gupta, P.; Mendes, V.; Blundell, T.L.
Deposited on : 2021-02-26
Resolution : 2.57 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

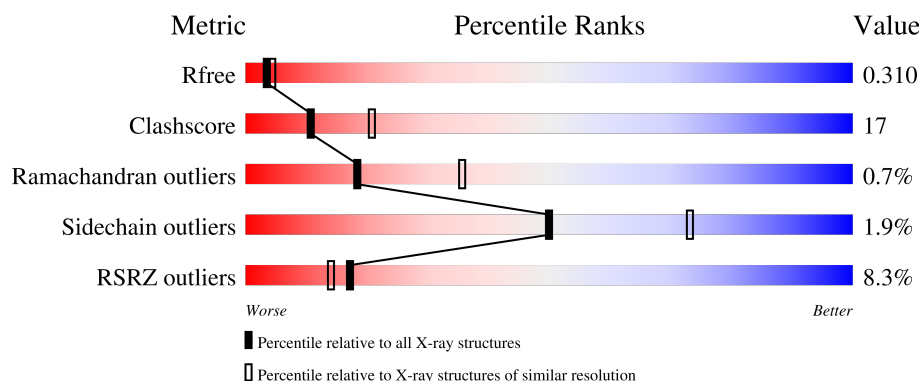
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	354	5% 73% 24% .
1	B	354	3% 72% 25% .
1	C	354	3% 70% 27% ..
1	D	354	5% 67% 28% ..
1	E	354	19% 66% 30% ..

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Mol	Chain	Length	Quality of chain
1	F	354	3% 69% 27% • •
1	G	354	8% 62% 34% • •
1	H	354	20% 66% 30% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19239 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 N-acetyl-gamma-glutamyl-phosphate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2396	1506	426	459	5			
1	B	344	Total	C	N	O	S	0	0	0
			2399	1518	428	448	5			
1	C	344	Total	C	N	O	S	0	0	0
			2423	1537	422	459	5			
1	D	344	Total	C	N	O	S	0	0	0
			2450	1551	429	465	5			
1	E	344	Total	C	N	O	S	0	0	0
			2343	1477	417	444	5			
1	F	344	Total	C	N	O	S	0	0	0
			2473	1563	440	465	5			
1	G	344	Total	C	N	O	S	0	0	0
			2437	1538	432	462	5			
1	H	344	Total	C	N	O	S	0	0	0
			2281	1420	415	441	5			

There are 16 discrepancies between the modelled and reference sequences:

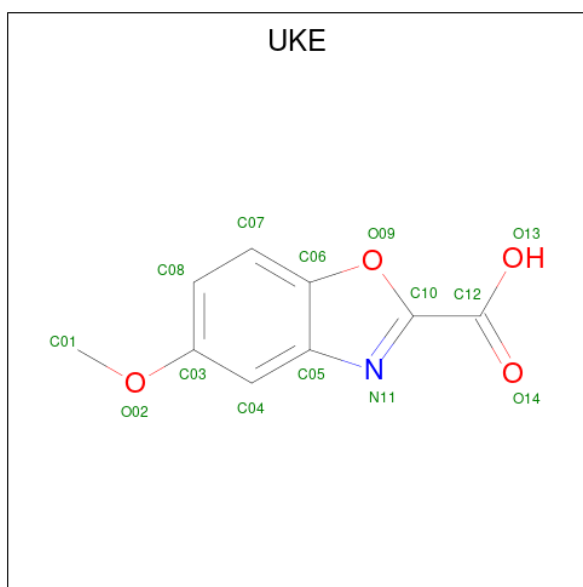
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P9WPZ9
A	0	SER	-	expression tag	UNP P9WPZ9
B	-1	GLY	-	expression tag	UNP P9WPZ9
B	0	SER	-	expression tag	UNP P9WPZ9
C	-1	GLY	-	expression tag	UNP P9WPZ9
C	0	SER	-	expression tag	UNP P9WPZ9
D	-1	GLY	-	expression tag	UNP P9WPZ9
D	0	SER	-	expression tag	UNP P9WPZ9
E	-1	GLY	-	expression tag	UNP P9WPZ9
E	0	SER	-	expression tag	UNP P9WPZ9
F	-1	GLY	-	expression tag	UNP P9WPZ9
F	0	SER	-	expression tag	UNP P9WPZ9
G	-1	GLY	-	expression tag	UNP P9WPZ9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	SER	-	expression tag	UNP P9WPZ9
H	-1	GLY	-	expression tag	UNP P9WPZ9
H	0	SER	-	expression tag	UNP P9WPZ9

- Molecule 2 is 5-methoxy-1,3-benzoxazole-2-carboxylic acid (CCD ID: UKE) (formula: $C_9H_7NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			14	9	1	4		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	P	0	0
			5	4	1		

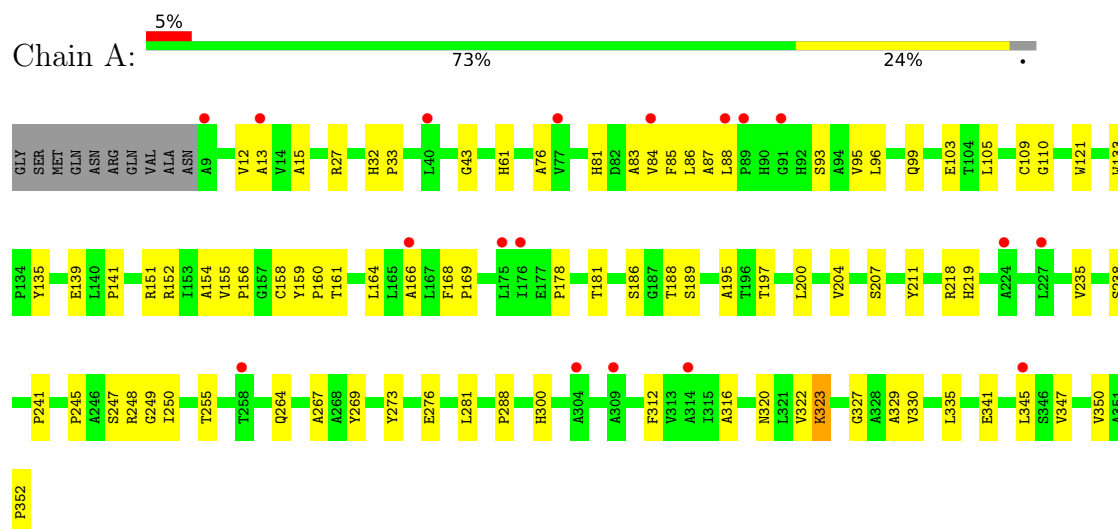
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	O	0	0
			3	3		
4	C	3	Total	O	0	0
			3	3		
4	D	2	Total	O	0	0
			2	2		
4	E	1	Total	O	0	0
			1	1		
4	F	7	Total	O	0	0
			7	7		
4	G	1	Total	O	0	0
			1	1		
4	H	1	Total	O	0	0
			1	1		

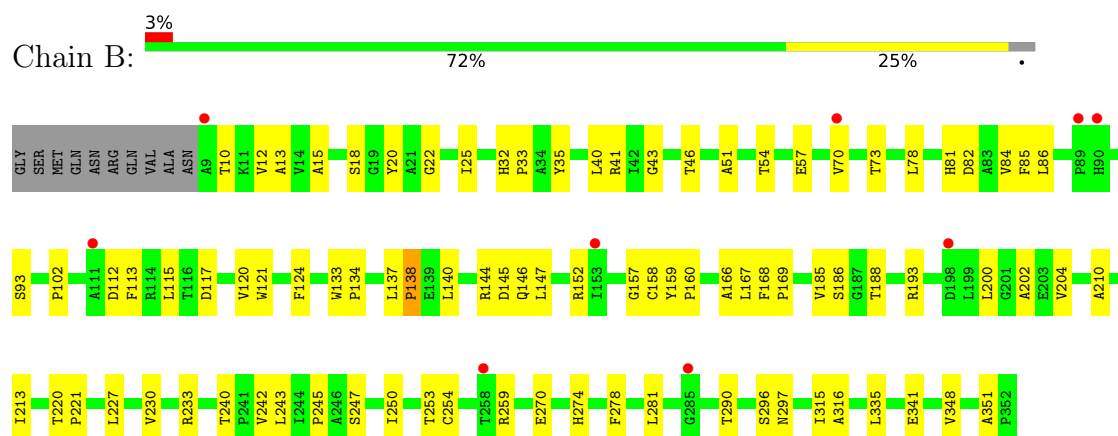
3 Residue-property plots [i](#)

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.

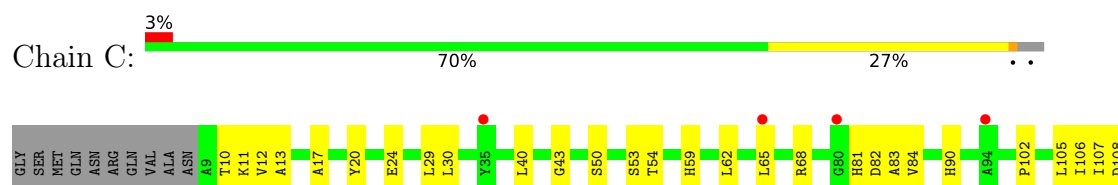
- Molecule 1: N-acetyl-gamma-glutamyl-phosphate reductase

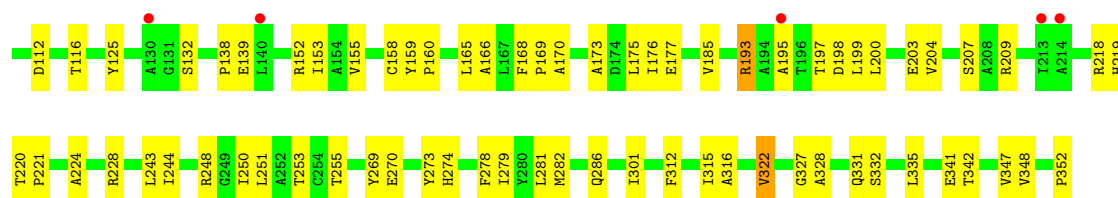


- Molecule 1: N-acetyl-gamma-glutamyl-phosphate reductase

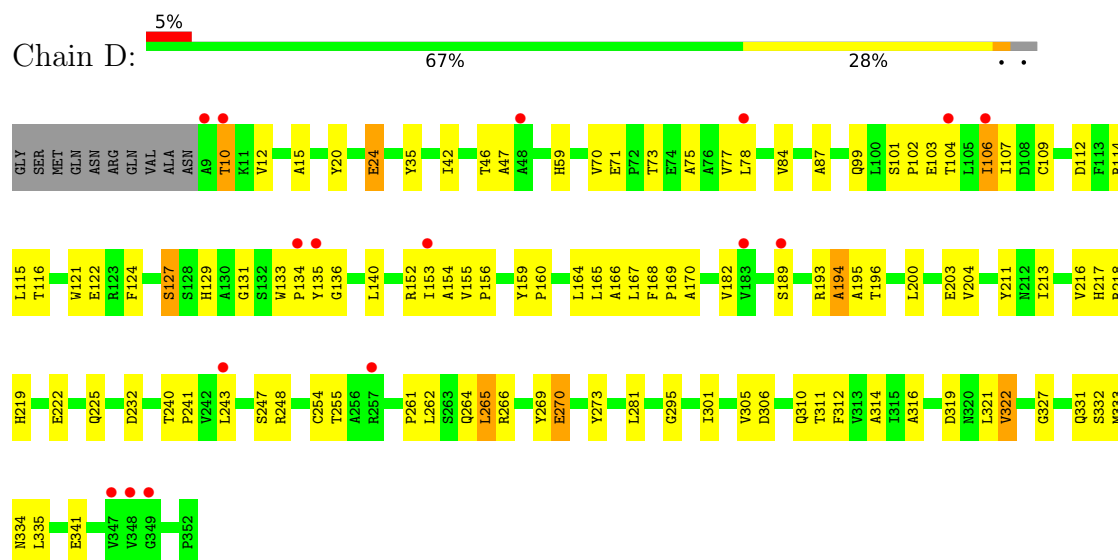


- Molecule 1: N-acetyl-gamma-glutamyl-phosphate reductase

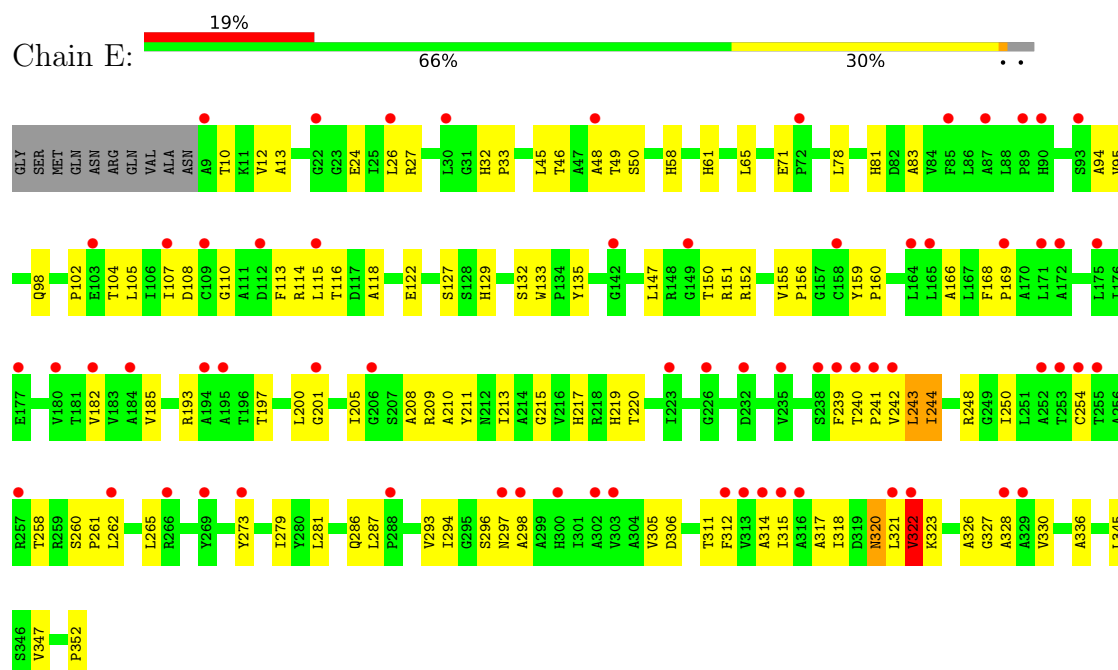




● Molecule 1: N-acetyl-gamma-glutamyl-phosphate reductase

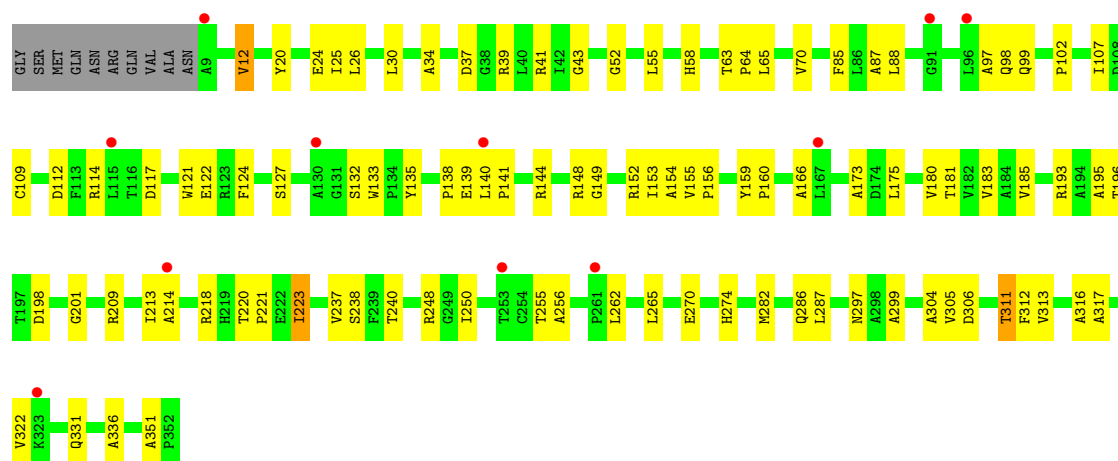


● Molecule 1: N-acetyl-gamma-glutamyl-phosphate reductase

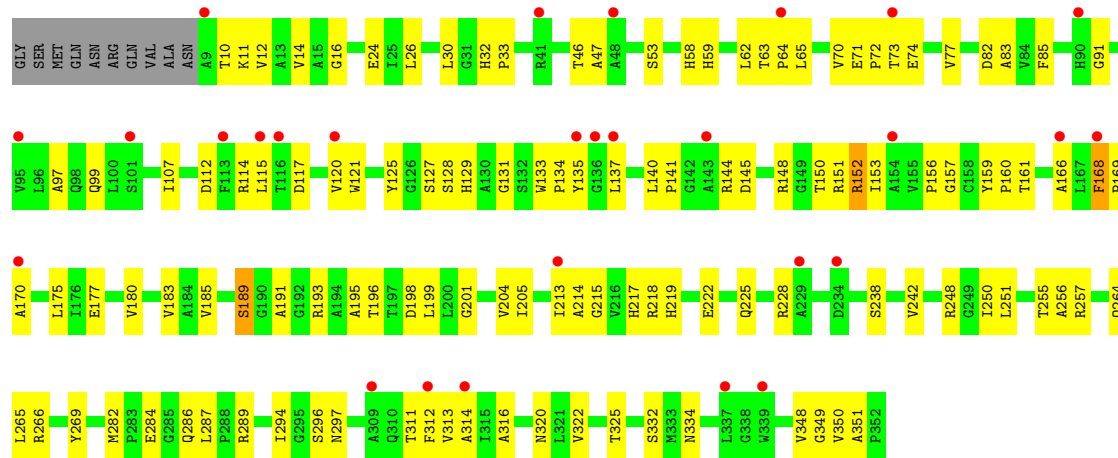


● Molecule 1: N-acetyl-gamma-glutamyl-phosphate reductase

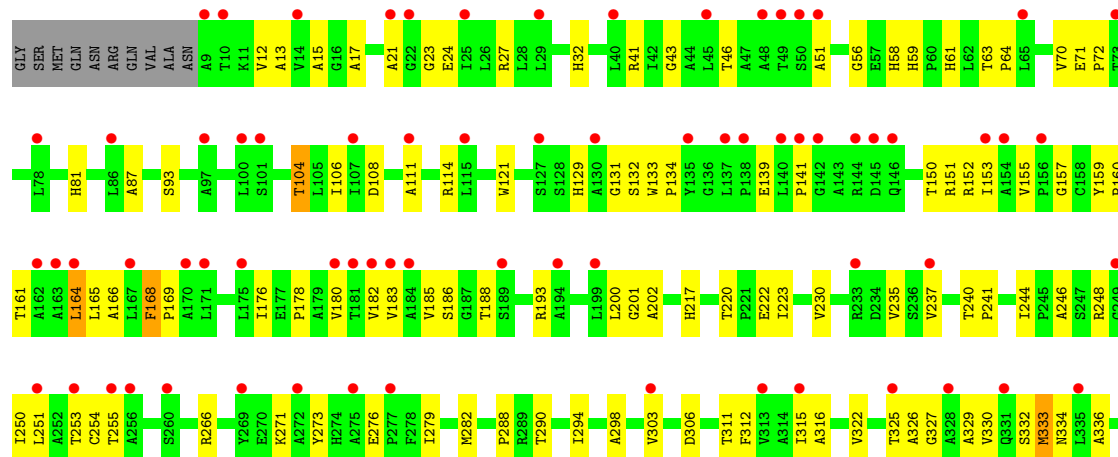


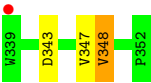


• Molecule 1: N-acetyl-gamma-glutamyl-phosphate reductase



• Molecule 1: N-acetyl-gamma-glutamyl-phosphate reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.29Å 132.78Å 122.82Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	69.59 – 2.57 69.59 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.8 (69.59-2.57) 99.9 (69.59-2.57)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.239 , 0.314 0.259 , 0.310	Depositor DCC
R_{free} test set	4226 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19239	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, UKE

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	0.71	0/2451	0.91	1/3367 (0.0%)
1	B	0.77	1/2454 (0.0%)	1.00	1/3373 (0.0%)
1	C	0.64	0/2478	0.81	1/3405 (0.0%)
1	D	0.55	0/2506	0.80	0/3440
1	E	0.57	0/2394	0.81	0/3295
1	F	0.61	0/2529	0.85	0/3468
1	G	0.50	0/2490	0.74	2/3417 (0.1%)
1	H	0.57	0/2333	0.84	0/3214
All	All	0.62	1/19635 (0.0%)	0.85	5/26979 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	169	PRO	C-O	-5.04	1.18	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	THR	CB-CA-C	-6.38	100.20	110.79
1	B	138	PRO	CB-CA-C	-5.72	102.12	111.56
1	G	189	SER	CA-C-N	5.06	126.50	120.13
1	G	189	SER	C-N-CA	5.06	126.50	120.13
1	C	347	VAL	N-CA-C	-5.01	108.09	112.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2396	0	2279	67	0
1	B	2399	0	2312	88	0
1	C	2423	0	2373	66	0
1	D	2450	0	2409	87	0
1	E	2343	0	2211	94	0
1	F	2473	0	2451	79	0
1	G	2437	0	2396	106	0
1	H	2281	0	2037	92	0
2	C	14	0	0	0	0
3	C	5	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	7	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
All	All	19239	0	18468	628	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 17.

All (628) 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:F:63:THR:OG1	1:F:64:PRO:HD3	1.27	1.31
1:D:102:PRO:HA	1:D:152:ARG:NH2	1.58	1.19
1:H:168:PHE:CD1	1:H:169:PRO:HD3	1.79	1.17
1:B:137:LEU:HD23	1:B:140:LEU:HG	1.21	1.13
1:B:12:VAL:HG21	1:B:40:LEU:HD21	1.32	1.11
1:B:12:VAL:CG2	1:B:40:LEU:HD21	1.82	1.10
1:G:137:LEU:HD23	1:G:140:LEU:HD12	1.43	1.01
1:B:124:PHE:CE2	1:B:221:PRO:HG3	1.96	1.00
1:F:63:THR:OG1	1:F:64:PRO:CD	2.11	0.97
1:H:150:THR:O	1:H:336:ALA:HB1	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:CYS:HB2	1:A:250:ILE:CD1	1.97	0.93
1:B:137:LEU:CD2	1:B:140:LEU:HG	1.97	0.93
1:D:102:PRO:HA	1:D:152:ARG:HH22	1.17	0.90
1:B:137:LEU:HD23	1:B:140:LEU:CG	2.02	0.90
1:G:175:LEU:HD21	1:G:264:GLN:HG2	1.55	0.88
1:D:107:ILE:HD11	1:D:333:MET:HB3	1.55	0.88
1:B:15:ALA:HA	1:B:46:THR:OG1	1.74	0.87
1:B:12:VAL:CG2	1:B:40:LEU:CD2	2.52	0.87
1:D:101:SER:O	1:D:104:THR:HG22	1.75	0.86
1:H:165:LEU:HD23	1:H:279:ILE:CD1	2.05	0.86
1:A:13:ALA:HB3	1:A:84:VAL:HG22	1.60	0.84
1:H:180:VAL:HG22	1:H:237:VAL:HA	1.56	0.84
1:H:141:PRO:HG2	1:H:230:VAL:HG12	1.58	0.83
1:E:114:ARG:HD3	1:E:156:PRO:HA	1.57	0.83
1:A:158:CYS:HB2	1:A:250:ILE:HD11	1.59	0.82
1:B:102:PRO:HA	1:B:152:ARG:HH22	1.43	0.82
1:D:153:ILE:HD13	1:D:332:SER:HB3	1.62	0.82
1:H:150:THR:HG22	1:H:336:ALA:HB2	1.61	0.81
1:C:10:THR:HA	1:C:82:ASP:OD2	1.80	0.80
1:B:12:VAL:HG23	1:B:40:LEU:CD2	2.12	0.79
1:H:168:PHE:HD1	1:H:169:PRO:HD3	1.44	0.79
1:B:32:HIS:ND1	1:B:33:PRO:HD2	1.97	0.79
1:F:63:THR:HG1	1:F:64:PRO:HD3	1.43	0.79
1:D:121:TRP:HE1	1:D:127:SER:HB2	1.44	0.79
1:E:243:LEU:HD12	1:E:243:LEU:O	1.84	0.78
1:E:306:ASP:HB3	1:E:311:THR:HB	1.66	0.77
1:H:166:ALA:HB2	1:H:316:ALA:HB2	1.65	0.77
1:H:330:VAL:HA	1:H:333:MET:HB3	1.67	0.77
1:F:26:LEU:O	1:F:30:LEU:HD12	1.85	0.76
1:H:165:LEU:HD23	1:H:279:ILE:HD11	1.65	0.76
1:D:116:THR:HG23	1:D:225:GLN:HE22	1.50	0.76
1:B:22:GLY:HA2	1:B:25:ILE:HD12	1.68	0.76
1:H:164:LEU:N	1:H:164:LEU:HD23	2.00	0.75
1:D:115:LEU:HD12	1:D:121:TRP:HE3	1.52	0.75
1:E:46:THR:HG22	1:E:71:GLU:HB2	1.68	0.75
1:G:255:THR:HG22	1:G:313:VAL:HG12	1.68	0.74
1:E:243:LEU:HD12	1:E:243:LEU:C	2.13	0.74
1:F:181:THR:HG23	1:F:238:SER:HB3	1.69	0.74
1:G:256:ALA:O	1:G:312:PHE:N	2.20	0.74
1:H:165:LEU:CD2	1:H:279:ILE:HD11	2.17	0.73
1:F:305:VAL:HG23	1:F:305:VAL:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:TYR:HB2	1:E:281:LEU:HD21	1.69	0.73
1:D:109:CYS:HA	1:D:155:VAL:HG22	1.71	0.72
1:G:156:PRO:HB2	1:G:161:THR:HG22	1.71	0.72
1:D:129:HIS:NE2	1:D:131:GLY:O	2.22	0.72
1:F:139:GLU:N	1:F:139:GLU:OE1	2.23	0.71
1:E:24:GLU:HG2	1:E:321:LEU:HB3	1.71	0.71
1:H:151:ARG:NH1	1:H:336:ALA:O	2.21	0.71
1:F:12:VAL:HG23	1:F:41:ARG:O	1.90	0.71
1:A:32:HIS:CG	1:A:33:PRO:HD2	2.26	0.71
1:A:13:ALA:HB2	1:A:81:HIS:CD2	2.26	0.70
1:B:12:VAL:HG23	1:B:40:LEU:HD21	1.67	0.70
1:D:24:GLU:CD	1:D:248:ARG:HH22	1.98	0.70
1:E:322:VAL:O	1:E:327:GLY:N	2.24	0.70
1:C:138:PRO:HG2	1:C:331:GLN:NE2	2.06	0.70
1:B:124:PHE:CZ	1:B:221:PRO:HG3	2.26	0.70
1:G:137:LEU:HD23	1:G:140:LEU:CD1	2.19	0.70
1:A:87:ALA:O	1:A:88:LEU:HD12	1.91	0.70
1:G:144:ARG:HD3	1:G:148:ARG:HH12	1.56	0.69
1:C:139:GLU:OE1	1:C:139:GLU:N	2.24	0.69
1:E:273:TYR:HD2	1:E:281:LEU:HD11	1.57	0.69
1:D:24:GLU:OE1	1:D:24:GLU:HA	1.91	0.69
1:A:87:ALA:C	1:A:88:LEU:HD12	2.18	0.69
1:A:335:LEU:HG	1:A:341:GLU:HG3	1.76	0.69
1:C:282:MET:HE3	1:C:286:GLN:HB3	1.75	0.68
1:B:46:THR:HG21	1:B:78:LEU:CD1	2.24	0.68
1:E:12:VAL:HG22	1:E:83:ALA:HB3	1.76	0.68
1:B:10:THR:HG23	1:B:82:ASP:HB2	1.76	0.67
1:E:240:THR:HG21	1:H:253:THR:HG21	1.76	0.67
1:G:137:LEU:CD2	1:G:140:LEU:HD12	2.23	0.67
1:D:102:PRO:CA	1:D:152:ARG:HH22	2.00	0.67
1:G:137:LEU:HD23	1:G:140:LEU:HB2	1.77	0.67
1:D:121:TRP:NE1	1:D:127:SER:HB2	2.09	0.66
1:E:213:ILE:HG21	1:H:315:ILE:HD11	1.76	0.66
1:A:160:PRO:HD3	1:A:219:HIS:ND1	2.09	0.66
1:F:220:THR:HB	1:F:221:PRO:CD	2.25	0.66
1:F:313:VAL:HG11	1:G:213:ILE:HD12	1.78	0.66
1:D:107:ILE:CD1	1:D:333:MET:HB3	2.24	0.65
1:G:168:PHE:CD2	1:G:169:PRO:HD3	2.31	0.65
1:F:195:ALA:HA	1:H:200:LEU:HD21	1.77	0.65
1:G:140:LEU:HD23	1:G:141:PRO:HD2	1.77	0.64
1:C:107:ILE:HG12	1:C:153:ILE:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:VAL:HG11	1:G:183:VAL:HB	1.80	0.64
1:H:139:GLU:N	1:H:139:GLU:OE1	2.28	0.64
1:B:158:CYS:HB2	1:B:250:ILE:CD1	2.29	0.63
1:B:46:THR:HG21	1:B:78:LEU:HD11	1.79	0.63
1:C:270:GLU:O	1:C:274:HIS:HB3	1.99	0.63
1:H:322:VAL:HG13	1:H:327:GLY:HA3	1.81	0.63
1:B:51:ALA:HA	1:B:70:VAL:O	1.99	0.63
1:F:138:PRO:HG2	1:F:331:GLN:NE2	2.14	0.63
1:B:54:THR:OG1	1:B:57:GLU:HG3	1.99	0.63
1:D:189:SER:OG	1:D:321:LEU:HD11	1.98	0.63
1:A:159:TYR:HB2	1:A:160:PRO:HD3	1.81	0.63
1:E:323:LYS:O	1:E:328:ALA:HB2	1.98	0.63
1:E:262:LEU:HA	1:E:265:LEU:HD12	1.80	0.63
1:C:13:ALA:HB2	1:C:81:HIS:CD2	2.35	0.62
1:G:58:HIS:O	1:G:193:ARG:NH2	2.20	0.62
1:A:96:LEU:N	1:A:96:LEU:HD22	2.14	0.62
1:A:189:SER:HB3	1:A:247:SER:O	2.00	0.62
1:G:135:TYR:CZ	1:G:156:PRO:HB3	2.34	0.62
1:G:30:LEU:HD11	1:G:65:LEU:HD13	1.82	0.61
1:H:217:HIS:HD2	1:H:241:PRO:HG3	1.65	0.61
1:A:109:CYS:HA	1:A:155:VAL:HB	1.82	0.61
1:G:71:GLU:HG2	1:G:72:PRO:HD2	1.82	0.61
1:G:137:LEU:CD2	1:G:140:LEU:HB2	2.30	0.61
1:G:217:HIS:ND1	1:G:219:HIS:HB2	2.14	0.61
1:E:293:VAL:HG11	1:E:318:ILE:HA	1.80	0.61
1:G:129:HIS:NE2	1:G:131:GLY:O	2.34	0.61
1:E:209:ARG:HA	1:H:251:LEU:CD1	2.31	0.61
1:E:24:GLU:HB2	1:E:321:LEU:HD23	1.83	0.60
1:A:27:ARG:NH1	1:A:27:ARG:HG2	2.17	0.60
1:B:270:GLU:O	1:B:274:HIS:HB3	2.01	0.60
1:E:104:THR:O	1:E:152:ARG:NH1	2.35	0.60
1:H:217:HIS:CD2	1:H:241:PRO:HG3	2.36	0.60
1:E:352:PRO:HG3	1:F:20:TYR:CE1	2.37	0.59
1:F:262:LEU:HD13	1:F:305:VAL:HG13	1.84	0.59
1:E:185:VAL:HA	1:E:242:VAL:O	2.03	0.59
1:C:173:ALA:HB3	1:C:175:LEU:HD12	1.82	0.59
1:E:135:TYR:CZ	1:E:156:PRO:HB3	2.37	0.59
1:F:213:ILE:HG12	1:G:287:LEU:HD11	1.83	0.59
1:G:63:THR:OG1	1:H:347:VAL:HG23	2.02	0.59
1:B:78:LEU:O	1:B:81:HIS:ND1	2.25	0.59
1:D:102:PRO:HA	1:D:152:ARG:HH21	1.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:223:ILE:HG22	1:F:237:VAL:HG21	1.85	0.58
1:H:141:PRO:HG2	1:H:230:VAL:CG1	2.32	0.58
1:H:178:PRO:O	1:H:235:VAL:HA	2.03	0.58
1:F:12:VAL:O	1:F:43:GLY:N	2.33	0.58
1:F:25:ILE:HD12	1:F:87:ALA:HB2	1.85	0.58
1:F:299:ALA:HA	1:F:317:ALA:O	2.03	0.58
1:B:159:TYR:HB2	1:B:160:PRO:HD3	1.85	0.58
1:D:124:PHE:HB3	1:D:218:ARG:HG2	1.85	0.58
1:E:215:GLY:HA2	1:E:220:THR:HG21	1.85	0.58
1:G:85:PHE:CE1	1:G:107:ILE:HD12	2.37	0.58
1:A:15:ALA:HB3	1:A:86:LEU:HD23	1.85	0.58
1:D:46:THR:OG1	1:D:73:THR:HG22	2.04	0.58
1:B:220:THR:HB	1:B:221:PRO:HD3	1.84	0.58
1:E:115:LEU:O	1:E:129:HIS:NE2	2.31	0.58
1:G:153:ILE:HD13	1:G:332:SER:HB3	1.84	0.58
1:E:168:PHE:CD2	1:E:169:PRO:HD3	2.39	0.58
1:G:127:SER:OG	1:G:128:SER:N	2.36	0.57
1:H:17:ALA:O	1:H:59:HIS:NE2	2.28	0.57
1:F:262:LEU:HD22	1:F:305:VAL:HG22	1.86	0.57
1:G:16:GLY:N	1:G:46:THR:O	2.32	0.57
1:C:278:PHE:CZ	1:C:342:THR:HG22	2.39	0.57
1:D:213:ILE:HG22	1:D:240:THR:HG23	1.86	0.57
1:F:102:PRO:HA	1:F:152:ARG:HH22	1.67	0.57
1:E:273:TYR:CD2	1:E:281:LEU:HD11	2.39	0.57
1:E:320:ASN:OD1	1:E:320:ASN:N	2.38	0.57
1:A:85:PHE:HE1	1:A:329:ALA:HB1	1.68	0.57
1:H:168:PHE:CD1	1:H:169:PRO:CD	2.71	0.57
1:C:54:THR:HA	1:C:68:ARG:O	2.05	0.57
1:G:166:ALA:HB2	1:G:316:ALA:HB2	1.86	0.57
1:E:94:ALA:O	1:E:98:GLN:HG2	2.03	0.57
1:E:254:CYS:HB2	1:E:314:ALA:HB3	1.86	0.57
1:G:348:VAL:CG1	1:H:27:ARG:HG3	2.35	0.57
1:G:32:HIS:NE2	1:G:334:ASN:OD1	2.35	0.57
1:G:133:TRP:CE2	1:G:152:ARG:HG3	2.40	0.57
1:C:20:TYR:CE2	1:C:193:ARG:HG2	2.40	0.56
1:C:159:TYR:HB2	1:C:219:HIS:ND1	2.19	0.56
1:E:244:ILE:HG21	1:H:244:ILE:HG21	1.86	0.56
1:G:46:THR:OG1	1:G:73:THR:HG22	2.05	0.56
1:C:160:PRO:HD3	1:C:219:HIS:CG	2.40	0.56
1:A:166:ALA:HB2	1:A:316:ALA:HB2	1.87	0.56
1:E:209:ARG:HA	1:H:251:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:PRO:HG2	1:F:331:GLN:HE21	1.71	0.56
1:D:112:ASP:HA	1:D:121:TRP:CH2	2.41	0.56
1:A:269:TYR:HB3	1:A:281:LEU:HD21	1.87	0.56
1:E:217:HIS:O	1:E:220:THR:HG23	2.06	0.56
1:D:102:PRO:CA	1:D:152:ARG:NH2	2.51	0.56
1:A:139:GLU:HG3	1:A:276:GLU:OE1	2.07	0.55
1:C:102:PRO:HA	1:C:152:ARG:HH22	1.72	0.55
1:B:124:PHE:CE2	1:B:221:PRO:CG	2.82	0.55
1:G:168:PHE:CG	1:G:169:PRO:HD3	2.42	0.55
1:E:118:ALA:HA	1:E:129:HIS:CG	2.41	0.55
1:E:122:GLU:HB3	1:E:127:SER:O	2.07	0.55
1:B:124:PHE:CD2	1:B:221:PRO:HG3	2.42	0.55
1:E:201:GLY:HA3	1:G:204:VAL:HG21	1.89	0.54
1:A:323:LYS:HD2	1:A:323:LYS:O	2.07	0.54
1:D:262:LEU:HD13	1:D:305:VAL:HG23	1.89	0.54
1:D:266:ARG:HG3	1:D:270:GLU:OE1	2.06	0.54
1:D:135:TYR:OH	1:D:222:GLU:OE2	2.22	0.54
1:G:196:THR:HG22	1:G:198:ASP:H	1.72	0.54
1:C:50:SER:O	1:C:53:SER:OG	2.21	0.54
1:C:269:TYR:HB3	1:C:281:LEU:HD21	1.89	0.54
1:F:209:ARG:HB3	1:G:289:ARG:HB3	1.90	0.54
1:A:350:VAL:HG12	1:A:350:VAL:O	2.07	0.54
1:H:51:ALA:HA	1:H:70:VAL:HG13	1.90	0.54
1:H:326:ALA:O	1:H:329:ALA:HB3	2.07	0.54
1:G:133:TRP:HB3	1:G:134:PRO:HD2	1.88	0.54
1:B:15:ALA:HB3	1:B:86:LEU:HD23	1.88	0.54
1:F:140:LEU:HD12	1:F:141:PRO:HD2	1.91	0.53
1:G:11:LYS:O	1:G:82:ASP:N	2.40	0.53
1:D:194:ALA:O	1:D:196:THR:HG23	2.08	0.53
1:A:158:CYS:CB	1:A:250:ILE:HD11	2.37	0.53
1:A:27:ARG:CG	1:A:27:ARG:HH11	2.22	0.53
1:H:129:HIS:NE2	1:H:131:GLY:O	2.41	0.53
1:D:255:THR:HB	1:D:311:THR:CG2	2.38	0.53
1:H:159:TYR:OH	1:H:186:SER:HB3	2.09	0.53
1:D:78:LEU:HD22	1:D:84:VAL:HG13	1.89	0.53
1:G:10:THR:HA	1:G:82:ASP:OD2	2.07	0.53
1:B:158:CYS:HB2	1:B:250:ILE:HD11	1.91	0.53
1:E:133:TRP:CD2	1:E:152:ARG:HB3	2.44	0.53
1:F:26:LEU:C	1:F:30:LEU:HD12	2.34	0.53
1:F:122:GLU:HG3	1:F:127:SER:O	2.09	0.53
1:A:105:LEU:HD13	1:A:151:ARG:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:GLU:OE2	1:D:77:VAL:HG13	2.10	0.52
1:G:140:LEU:HD23	1:G:141:PRO:CD	2.39	0.52
1:F:107:ILE:HG12	1:F:153:ILE:HD12	1.90	0.52
1:A:15:ALA:O	1:A:87:ALA:N	2.40	0.52
1:F:144:ARG:O	1:F:148:ARG:HG3	2.09	0.52
1:E:352:PRO:HB2	1:H:202:ALA:O	2.09	0.52
1:F:133:TRP:HB2	1:F:154:ALA:HB2	1.91	0.52
1:H:106:ILE:HB	1:H:152:ARG:HD3	1.92	0.52
1:F:24:GLU:OE1	1:F:248:ARG:NH2	2.42	0.52
1:G:115:LEU:HD12	1:G:121:TRP:HB2	1.92	0.52
1:H:153:ILE:HG21	1:H:332:SER:HB3	1.91	0.52
1:A:96:LEU:N	1:A:96:LEU:CD2	2.73	0.52
1:B:220:THR:N	1:B:221:PRO:CD	2.72	0.52
1:E:61:HIS:CG	1:F:351:ALA:HB3	2.44	0.52
1:E:182:VAL:HG12	1:E:254:CYS:SG	2.49	0.52
1:E:197:THR:HA	1:E:200:LEU:HG	1.92	0.52
1:H:114:ARG:HD3	1:H:222:GLU:OE2	2.10	0.52
1:C:335:LEU:HD21	1:C:341:GLU:HB2	1.91	0.52
1:E:298:ALA:HB2	1:E:347:VAL:HG13	1.92	0.52
1:G:157:GLY:O	1:G:161:THR:HG23	2.09	0.52
1:A:200:LEU:HD23	1:C:199:LEU:HB2	1.93	0.51
1:C:116:THR:HA	1:C:132:SER:OG	2.10	0.51
1:D:170:ALA:HB2	1:D:269:TYR:HE1	1.74	0.51
1:F:34:ALA:HB1	1:F:39:ARG:HG3	1.91	0.51
1:F:85:PHE:CE1	1:F:107:ILE:HD12	2.45	0.51
1:H:133:TRP:HB3	1:H:134:PRO:CD	2.40	0.51
1:D:133:TRP:CZ2	1:D:152:ARG:HD2	2.45	0.51
1:D:265:LEU:HD22	1:D:312:PHE:CD1	2.46	0.51
1:E:135:TYR:OH	1:E:156:PRO:HB3	2.10	0.51
1:G:351:ALA:HB3	1:H:61:HIS:CG	2.45	0.51
1:C:11:LYS:O	1:C:82:ASP:N	2.40	0.51
1:G:59:HIS:CE1	1:G:193:ARG:NH1	2.78	0.51
1:H:223:ILE:HG22	1:H:237:VAL:HG11	1.91	0.51
1:A:322:VAL:O	1:A:327:GLY:N	2.41	0.51
1:B:278:PHE:CE1	1:B:297:ASN:HB3	2.45	0.51
1:E:254:CYS:O	1:E:314:ALA:N	2.37	0.51
1:B:124:PHE:CD2	1:B:221:PRO:CG	2.93	0.51
1:B:186:SER:HB2	1:B:250:ILE:HG12	1.92	0.51
1:G:62:LEU:HD23	1:H:348:VAL:CG1	2.40	0.51
1:H:71:GLU:HB3	1:H:72:PRO:HD2	1.91	0.51
1:D:334:ASN:HB3	1:D:341:GLU:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:VAL:HG11	1:B:85:PHE:HE1	1.75	0.51
1:F:138:PRO:HG2	1:F:331:GLN:HG2	1.93	0.51
1:F:196:THR:OG1	1:F:198:ASP:OD1	2.29	0.51
1:H:176:ILE:HG21	1:H:312:PHE:CD2	2.46	0.51
1:C:159:TYR:HD2	1:C:219:HIS:HD1	1.59	0.51
1:D:261:PRO:HG2	1:D:264:GLN:HB2	1.92	0.51
1:G:74:GLU:HG2	1:G:77:VAL:HG23	1.94	0.50
1:F:270:GLU:O	1:F:274:HIS:HB3	2.11	0.50
1:B:115:LEU:HD12	1:B:121:TRP:HE3	1.77	0.50
1:D:211:TYR:CE1	1:D:243:LEU:HG	2.46	0.50
1:G:189:SER:HB2	1:G:320:ASN:HD21	1.77	0.50
1:H:322:VAL:CG1	1:H:327:GLY:HA3	2.41	0.50
1:G:145:ASP:OD1	1:G:148:ARG:NH1	2.44	0.50
1:D:87:ALA:HA	1:D:109:CYS:HB2	1.93	0.50
1:B:12:VAL:HG23	1:B:40:LEU:HD22	1.91	0.50
1:C:125:TYR:CE1	1:C:218:ARG:HD3	2.47	0.50
1:D:295:GLY:N	1:D:319:ASP:OD2	2.25	0.50
1:H:164:LEU:HD23	1:H:164:LEU:H	1.74	0.50
1:B:253:THR:HA	1:B:315:ILE:HD13	1.93	0.50
1:D:135:TYR:OH	1:D:156:PRO:HB3	2.12	0.50
1:D:20:TYR:CE2	1:D:193:ARG:HG3	2.46	0.49
1:F:311:THR:HG21	1:G:238:SER:OG	2.12	0.49
1:H:58:HIS:O	1:H:193:ARG:NH2	2.34	0.49
1:A:12:VAL:HG22	1:A:83:ALA:HB3	1.93	0.49
1:A:347:VAL:HG12	1:A:347:VAL:O	2.12	0.49
1:B:145:ASP:C	1:B:147:LEU:H	2.19	0.49
1:E:273:TYR:CB	1:E:281:LEU:HD21	2.41	0.49
1:G:169:PRO:HB2	1:G:269:TYR:CZ	2.47	0.49
1:A:61:HIS:CG	1:B:351:ALA:HB3	2.48	0.49
1:B:200:LEU:HD21	1:D:195:ALA:HA	1.94	0.49
1:F:183:VAL:HA	1:F:240:THR:O	2.11	0.49
1:G:59:HIS:CE1	1:G:193:ARG:HH12	2.31	0.49
1:G:85:PHE:CZ	1:G:107:ILE:HD12	2.47	0.49
1:G:191:ALA:HB3	1:G:199:LEU:HD21	1.94	0.49
1:E:220:THR:HG22	1:E:239:PHE:CB	2.43	0.49
1:F:58:HIS:O	1:F:193:ARG:NH2	2.41	0.49
1:H:165:LEU:O	1:H:273:TYR:OH	2.28	0.49
1:D:115:LEU:HD12	1:D:121:TRP:CE3	2.40	0.49
1:F:109:CYS:HA	1:F:155:VAL:HB	1.94	0.49
1:A:88:LEU:O	1:A:110:GLY:CA	2.61	0.49
1:B:113:PHE:CD1	1:B:133:TRP:NE1	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:266:ARG:NH2	1:G:266:ARG:HB3	2.28	0.49
1:G:282:MET:HE2	1:G:286:GLN:HB3	1.94	0.49
1:D:182:VAL:HG22	1:D:254:CYS:SG	2.53	0.49
1:F:304:ALA:HB1	1:G:214:ALA:HB2	1.95	0.49
1:G:156:PRO:HB2	1:G:161:THR:CG2	2.42	0.49
1:G:191:ALA:CB	1:G:199:LEU:HD21	2.42	0.49
1:B:240:THR:HG21	1:C:253:THR:HG21	1.93	0.49
1:E:205:ILE:HG12	1:G:205:ILE:HD11	1.95	0.49
1:A:248:ARG:HH21	1:B:351:ALA:C	2.20	0.48
1:E:24:GLU:OE2	1:E:27:ARG:NH2	2.34	0.48
1:E:258:THR:HG21	1:E:312:PHE:HB2	1.95	0.48
1:F:255:THR:HA	1:F:312:PHE:O	2.12	0.48
1:E:297:ASN:O	1:E:297:ASN:ND2	2.45	0.48
1:G:150:THR:O	1:G:151:ARG:HD2	2.12	0.48
1:D:322:VAL:O	1:D:327:GLY:N	2.46	0.48
1:D:59:HIS:CE1	1:D:193:ARG:NH1	2.81	0.48
1:D:306:ASP:O	1:D:310:GLN:N	2.46	0.48
1:B:137:LEU:HD23	1:B:140:LEU:CD1	2.44	0.48
1:G:30:LEU:HD21	1:G:65:LEU:CD1	2.43	0.48
1:G:121:TRP:O	1:G:125:TYR:HB2	2.13	0.48
1:H:134:PRO:HD2	1:H:152:ARG:O	2.12	0.48
1:A:168:PHE:CD2	1:A:169:PRO:HD3	2.48	0.48
1:B:20:TYR:OH	1:D:203:GLU:HG2	2.14	0.48
1:E:95:VAL:HA	1:E:98:GLN:NE2	2.28	0.48
1:H:159:TYR:CZ	1:H:241:PRO:HB2	2.48	0.48
1:B:46:THR:HB	1:B:73:THR:HA	1.95	0.48
1:C:83:ALA:HA	1:C:105:LEU:HB3	1.96	0.48
1:C:328:ALA:O	1:C:332:SER:OG	2.28	0.48
1:E:213:ILE:HD13	1:H:315:ILE:HD12	1.96	0.48
1:A:141:PRO:HD3	1:A:168:PHE:CE1	2.48	0.48
1:E:159:TYR:N	1:E:160:PRO:HD2	2.29	0.48
1:A:86:LEU:HD13	1:A:93:SER:HB2	1.95	0.48
1:H:185:VAL:O	1:H:250:ILE:HA	2.14	0.48
1:H:290:THR:O	1:H:294:ILE:HG12	2.14	0.47
1:D:165:LEU:HB3	1:D:301:ILE:HD11	1.96	0.47
1:G:257:ARG:HA	1:G:311:THR:HA	1.96	0.47
1:A:27:ARG:HG2	1:A:27:ARG:HH11	1.79	0.47
1:C:30:LEU:HD11	1:C:65:LEU:HD12	1.97	0.47
1:B:233:ARG:HH21	1:B:259:ARG:HH12	1.61	0.47
1:E:159:TYR:HB2	1:E:219:HIS:ND1	2.29	0.47
1:G:85:PHE:CD1	1:G:107:ILE:HB	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ARG:O	1:B:147:LEU:HB2	2.15	0.47
1:D:182:VAL:HG22	1:D:254:CYS:CB	2.44	0.47
1:F:135:TYR:CZ	1:F:156:PRO:HB3	2.49	0.47
1:G:63:THR:OG1	1:G:64:PRO:HD3	2.14	0.47
1:A:195:ALA:HA	1:C:200:LEU:HD21	1.96	0.47
1:C:139:GLU:HG2	1:C:279:ILE:HD11	1.95	0.47
1:C:273:TYR:HD2	1:C:281:LEU:HD11	1.80	0.47
1:D:15:ALA:HA	1:D:46:THR:OG1	2.15	0.47
1:D:47:ALA:HB3	1:D:70:VAL:HG11	1.96	0.47
1:D:104:THR:HG23	1:D:104:THR:O	2.14	0.47
1:D:114:ARG:HD3	1:D:155:VAL:O	2.15	0.47
1:D:232:ASP:OD1	1:D:232:ASP:N	2.42	0.47
1:E:211:TYR:O	1:E:241:PRO:HG2	2.14	0.47
1:E:243:LEU:C	1:E:243:LEU:CD1	2.85	0.47
1:B:117:ASP:HB3	1:B:120:VAL:HB	1.95	0.47
1:E:293:VAL:O	1:E:296:SER:OG	2.30	0.47
1:F:133:TRP:CD2	1:F:152:ARG:HB3	2.50	0.47
1:C:43:GLY:O	1:C:68:ARG:NH2	2.48	0.47
1:G:47:ALA:O	1:G:73:THR:HG23	2.14	0.47
1:B:144:ARG:HA	1:B:147:LEU:HD12	1.97	0.47
1:E:58:HIS:O	1:E:193:ARG:NH2	2.40	0.47
1:G:185:VAL:HA	1:G:242:VAL:HG23	1.96	0.47
1:C:24:GLU:CD	1:C:248:ARG:HH22	2.23	0.46
1:G:135:TYR:OH	1:G:156:PRO:HB3	2.15	0.46
1:H:63:THR:OG1	1:H:64:PRO:HD3	2.15	0.46
1:H:188:THR:HG22	1:H:246:ALA:O	2.15	0.46
1:E:208:ALA:HB2	1:E:244:ILE:HG22	1.98	0.46
1:F:282:MET:HE2	1:F:287:LEU:O	2.14	0.46
1:H:132:SER:O	1:H:132:SER:OG	2.23	0.46
1:A:96:LEU:CD2	1:A:96:LEU:H	2.28	0.46
1:A:200:LEU:HD21	1:C:195:ALA:HA	1.97	0.46
1:E:95:VAL:HA	1:E:98:GLN:HE21	1.80	0.46
1:F:140:LEU:HD12	1:F:141:PRO:CD	2.46	0.46
1:A:188:THR:HG21	1:A:204:VAL:HG21	1.98	0.46
1:D:134:PRO:HD2	1:D:152:ARG:O	2.14	0.46
1:A:178:PRO:O	1:A:235:VAL:HG13	2.15	0.46
1:C:159:TYR:HD2	1:C:219:HIS:ND1	2.13	0.46
1:D:200:LEU:O	1:D:204:VAL:HG13	2.16	0.46
1:G:177:GLU:HG2	1:G:257:ARG:O	2.15	0.46
1:G:152:ARG:HD3	1:G:152:ARG:HA	1.36	0.46
1:A:181:THR:HG23	1:A:238:SER:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:ALA:HB2	1:D:99:GLN:OE1	2.16	0.46
1:D:270:GLU:OE2	1:D:281:LEU:CD1	2.64	0.46
1:E:26:LEU:HD21	1:E:45:LEU:HD21	1.97	0.46
1:E:240:THR:HG21	1:H:253:THR:CG2	2.45	0.46
1:A:250:ILE:HG13	1:A:320:ASN:HB3	1.97	0.46
1:G:248:ARG:HB2	1:G:294:ILE:HD12	1.97	0.46
1:G:296:SER:HB3	1:G:349:GLY:HA2	1.98	0.46
1:B:15:ALA:CB	1:B:86:LEU:HD23	2.45	0.46
1:B:46:THR:CG2	1:B:78:LEU:HD11	2.46	0.46
1:C:20:TYR:CZ	1:C:193:ARG:HG2	2.51	0.46
1:C:138:PRO:HG2	1:C:331:GLN:HE21	1.80	0.46
1:E:24:GLU:CG	1:E:321:LEU:HB3	2.44	0.46
1:E:210:ALA:HB2	1:E:242:VAL:HG22	1.98	0.46
1:F:173:ALA:HB3	1:F:175:LEU:HG	1.97	0.46
1:D:135:TYR:CZ	1:D:156:PRO:HB3	2.51	0.46
1:D:312:PHE:CZ	1:D:314:ALA:HB2	2.51	0.46
1:B:167:LEU:HD21	1:B:254:CYS:HB3	1.99	0.45
1:C:224:ALA:O	1:C:228:ARG:HG3	2.16	0.45
1:F:37:ASP:OD1	1:F:39:ARG:HG2	2.15	0.45
1:G:175:LEU:HD23	1:G:265:LEU:HG	1.98	0.45
1:G:185:VAL:HG22	1:G:251:LEU:HB3	1.97	0.45
1:C:198:ASP:HB3	1:C:209:ARG:NH2	2.31	0.45
1:E:13:ALA:HB2	1:E:81:HIS:CD2	2.51	0.45
1:F:220:THR:HB	1:F:221:PRO:HD3	1.96	0.45
1:F:305:VAL:O	1:F:305:VAL:CG2	2.58	0.45
1:G:297:ASN:OD1	1:G:322:VAL:HG12	2.17	0.45
1:A:207:SER:O	1:A:245:PRO:HD3	2.17	0.45
1:B:12:VAL:HG11	1:B:85:PHE:CE1	2.51	0.45
1:B:213:ILE:HG21	1:C:315:ILE:HD11	1.99	0.45
1:F:201:GLY:HA2	1:H:201:GLY:HA2	1.98	0.45
1:H:32:HIS:NE2	1:H:343:ASP:HB3	2.31	0.45
1:H:255:THR:CG2	1:H:311:THR:HG21	2.46	0.45
1:H:15:ALA:HA	1:H:46:THR:OG1	2.17	0.45
1:B:18:SER:O	1:B:193:ARG:NH1	2.50	0.45
1:E:150:THR:O	1:E:336:ALA:HB1	2.17	0.45
1:F:265:LEU:HD22	1:F:312:PHE:CE1	2.52	0.45
1:B:35:TYR:O	1:B:35:TYR:CG	2.69	0.45
1:D:101:SER:C	1:D:103:GLU:H	2.24	0.45
1:A:135:TYR:CZ	1:A:156:PRO:HB3	2.52	0.45
1:E:330:VAL:HG12	1:E:345:LEU:HD21	1.98	0.45
1:F:282:MET:HE3	1:F:286:GLN:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:THR:HG21	1:B:204:VAL:HG11	1.99	0.45
1:B:213:ILE:HD13	1:C:315:ILE:HD11	1.98	0.45
1:F:112:ASP:HA	1:F:121:TRP:CH2	2.52	0.45
1:F:180:VAL:HG12	1:F:256:ALA:HB2	1.99	0.45
1:G:14:VAL:HG21	1:G:26:LEU:HD21	1.98	0.45
1:A:352:PRO:O	1:B:247:SER:CB	2.65	0.44
1:C:159:TYR:HB2	1:C:160:PRO:HD3	1.99	0.44
1:C:165:LEU:HB3	1:C:301:ILE:HD11	1.98	0.44
1:H:168:PHE:HD2	1:H:230:VAL:HG11	1.82	0.44
1:B:335:LEU:HG	1:B:341:GLU:HG3	1.99	0.44
1:D:47:ALA:HB3	1:D:70:VAL:CG1	2.48	0.44
1:D:213:ILE:O	1:D:216:VAL:HG22	2.18	0.44
1:E:151:ARG:O	1:E:152:ARG:HD3	2.17	0.44
1:F:121:TRP:CD1	1:F:121:TRP:C	2.94	0.44
1:A:32:HIS:ND1	1:A:33:PRO:HD2	2.32	0.44
1:A:186:SER:HA	1:A:249:GLY:O	2.18	0.44
1:F:306:ASP:OD2	1:G:215:GLY:HA3	2.17	0.44
1:H:276:GLU:OE1	1:H:276:GLU:HA	2.16	0.44
1:E:108:ASP:CG	1:E:110:GLY:H	2.26	0.44
1:H:255:THR:HG23	1:H:311:THR:HG21	2.00	0.44
1:D:159:TYR:HB2	1:D:160:PRO:HD3	1.98	0.44
1:E:286:GLN:C	1:E:287:LEU:HD12	2.43	0.44
1:F:132:SER:O	1:F:133:TRP:HD1	2.00	0.44
1:B:202:ALA:O	1:C:352:PRO:HB2	2.17	0.44
1:B:245:PRO:HD2	1:C:244:ILE:HD12	2.00	0.44
1:D:35:TYR:CE1	1:D:42:ILE:HG13	2.53	0.44
1:E:13:ALA:HB1	1:E:78:LEU:HD12	1.99	0.44
1:F:306:ASP:OD2	1:G:215:GLY:CA	2.65	0.44
1:G:115:LEU:HD13	1:G:120:VAL:HG12	1.99	0.44
1:B:35:TYR:O	1:B:35:TYR:CD2	2.70	0.44
1:B:290:THR:OG1	1:C:207:SER:HA	2.17	0.44
1:B:296:SER:HB3	1:B:348:VAL:O	2.18	0.44
1:D:170:ALA:HB2	1:D:269:TYR:CE1	2.53	0.44
1:D:255:THR:HB	1:D:311:THR:HG21	1.99	0.44
1:D:335:LEU:HG	1:D:341:GLU:HG3	2.00	0.44
1:F:213:ILE:HG22	1:F:240:THR:HG23	1.99	0.44
1:G:53:SER:O	1:G:70:VAL:HG12	2.17	0.44
1:G:64:PRO:C	1:G:65:LEU:HD12	2.43	0.44
1:C:197:THR:O	1:C:203:GLU:HG3	2.17	0.44
1:E:273:TYR:CG	1:E:279:ILE:HG21	2.53	0.44
1:G:12:VAL:HG23	1:G:83:ALA:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:GLY:C	1:B:160:PRO:HD2	2.42	0.44
1:D:255:THR:HA	1:D:312:PHE:O	2.18	0.44
1:E:115:LEU:HD12	1:E:115:LEU:N	2.33	0.44
1:E:201:GLY:HA2	1:G:201:GLY:HA2	2.00	0.44
1:E:250:ILE:O	1:E:317:ALA:HA	2.18	0.44
1:A:133:TRP:HB2	1:A:154:ALA:HB2	1.99	0.43
1:E:200:LEU:HD21	1:G:195:ALA:HA	2.00	0.43
1:E:248:ARG:HB2	1:E:294:ILE:HD12	1.99	0.43
1:A:168:PHE:HE2	1:A:273:TYR:OH	2.01	0.43
1:A:330:VAL:CG1	1:A:345:LEU:HD21	2.48	0.43
1:B:93:SER:N	1:B:112:ASP:OD2	2.50	0.43
1:B:270:GLU:HA	1:B:281:LEU:HD11	2.00	0.43
1:F:183:VAL:HG23	1:F:240:THR:O	2.18	0.43
1:H:21:ALA:HB3	1:H:87:ALA:HB1	2.00	0.43
1:C:352:PRO:HG3	1:D:20:TYR:CE1	2.54	0.43
1:D:270:GLU:OE2	1:D:281:LEU:HD12	2.17	0.43
1:E:213:ILE:HD13	1:H:315:ILE:CD1	2.49	0.43
1:H:306:ASP:N	1:H:311:THR:O	2.48	0.43
1:H:322:VAL:O	1:H:327:GLY:N	2.51	0.43
1:A:95:VAL:O	1:A:99:GLN:HG3	2.18	0.43
1:A:197:THR:HA	1:A:200:LEU:HD12	2.01	0.43
1:A:211:TYR:O	1:A:241:PRO:HG2	2.18	0.43
1:C:59:HIS:HB3	1:C:62:LEU:HG	2.00	0.43
1:D:166:ALA:HB2	1:D:316:ALA:HB2	1.99	0.43
1:E:260:SER:HB3	1:E:261:PRO:HD2	1.99	0.43
1:G:32:HIS:ND1	1:G:33:PRO:HD2	2.34	0.43
1:G:133:TRP:HB3	1:G:134:PRO:CD	2.48	0.43
1:B:296:SER:HB3	1:B:348:VAL:C	2.44	0.43
1:D:116:THR:HG23	1:D:225:GLN:NE2	2.26	0.43
1:F:135:TYR:OH	1:F:156:PRO:HB3	2.17	0.43
1:G:170:ALA:HB2	1:G:269:TYR:HE1	1.84	0.43
1:B:40:LEU:HD22	1:B:41:ARG:H	1.83	0.43
1:B:227:LEU:O	1:B:230:VAL:HG22	2.17	0.43
1:D:189:SER:HB3	1:D:247:SER:O	2.18	0.43
1:E:49:THR:OG1	1:E:50:SER:N	2.52	0.43
1:E:320:ASN:ND2	1:E:321:LEU:HD12	2.33	0.43
1:F:297:ASN:OD1	1:F:322:VAL:HG12	2.19	0.43
1:G:250:ILE:HG13	1:G:320:ASN:HB3	2.01	0.43
1:A:12:VAL:HA	1:A:83:ALA:O	2.19	0.43
1:E:113:PHE:O	1:E:132:SER:HA	2.18	0.43
1:H:217:HIS:O	1:H:220:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:298:ALA:HB2	1:H:347:VAL:HB	2.01	0.43
1:B:210:ALA:HB3	1:C:315:ILE:HD13	2.01	0.43
1:E:321:LEU:O	1:E:326:ALA:HB3	2.18	0.43
1:H:58:HIS:HB3	1:H:193:ARG:HH12	1.84	0.43
1:B:138:PRO:O	1:B:144:ARG:CZ	2.66	0.43
1:E:135:TYR:O	1:E:147:LEU:HD21	2.19	0.43
1:H:266:ARG:HE	1:H:303:VAL:CG2	2.32	0.43
1:H:273:TYR:CG	1:H:279:ILE:HG21	2.54	0.43
1:A:288:PRO:HB3	1:A:300:HIS:CB	2.48	0.43
1:D:106:ILE:HG22	1:D:133:TRP:HZ3	1.84	0.43
1:E:116:THR:HA	1:E:132:SER:OG	2.18	0.43
1:G:91:GLY:H	1:G:112:ASP:CG	2.27	0.43
1:B:188:THR:HG21	1:B:204:VAL:HG21	2.00	0.42
1:F:97:ALA:C	1:F:99:GLN:N	2.76	0.42
1:H:23:GLY:HA3	1:H:59:HIS:CE1	2.54	0.42
1:B:15:ALA:HA	1:B:46:THR:HG1	1.78	0.42
1:B:133:TRP:HB3	1:B:134:PRO:CD	2.49	0.42
1:B:138:PRO:HB2	1:B:144:ARG:NH2	2.34	0.42
1:B:140:LEU:HD23	1:B:140:LEU:HA	1.87	0.42
1:C:166:ALA:HB2	1:C:316:ALA:HB2	2.01	0.42
1:E:166:ALA:O	1:E:314:ALA:HB1	2.19	0.42
1:G:225:GLN:HA	1:G:228:ARG:HD2	2.01	0.42
1:H:93:SER:HG	1:H:108:ASP:CG	2.26	0.42
1:H:93:SER:OG	1:H:108:ASP:CG	2.62	0.42
1:B:166:ALA:HB2	1:B:316:ALA:HB2	2.01	0.42
1:C:176:ILE:HD12	1:C:177:GLU:O	2.19	0.42
1:G:24:GLU:CD	1:G:248:ARG:HH22	2.26	0.42
1:D:211:TYR:O	1:D:241:PRO:HD2	2.18	0.42
1:E:32:HIS:CG	1:E:33:PRO:HD2	2.54	0.42
1:H:220:THR:O	1:H:237:VAL:HG21	2.19	0.42
1:F:109:CYS:O	1:F:114:ARG:NH2	2.52	0.42
1:G:114:ARG:HD3	1:G:222:GLU:OE1	2.20	0.42
1:G:133:TRP:CG	1:G:152:ARG:HB3	2.55	0.42
1:A:160:PRO:CD	1:A:219:HIS:ND1	2.81	0.42
1:B:46:THR:CG2	1:B:78:LEU:CD1	2.96	0.42
1:E:320:ASN:ND2	1:E:321:LEU:CD1	2.82	0.42
1:H:161:THR:O	1:H:165:LEU:HD13	2.19	0.42
1:A:264:GLN:O	1:A:267:ALA:HB3	2.20	0.42
1:C:158:CYS:HB2	1:C:250:ILE:CD1	2.50	0.42
1:E:46:THR:HG21	1:E:78:LEU:HD21	2.02	0.42
1:E:244:ILE:HG21	1:H:244:ILE:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:306:ASP:CB	1:E:311:THR:HB	2.44	0.42
1:F:185:VAL:O	1:F:250:ILE:HA	2.20	0.42
1:H:155:VAL:HG11	1:H:325:THR:O	2.20	0.42
1:A:330:VAL:HG12	1:A:345:LEU:HD21	2.01	0.42
1:B:43:GLY:HA3	1:B:81:HIS:NE2	2.35	0.42
1:C:29:LEU:HD22	1:C:40:LEU:HD21	2.01	0.42
1:D:101:SER:O	1:D:103:GLU:N	2.53	0.42
1:F:117:ASP:OD1	1:F:117:ASP:C	2.63	0.42
1:G:135:TYR:CE2	1:G:156:PRO:HG3	2.55	0.42
1:B:133:TRP:HB3	1:B:134:PRO:HD2	2.02	0.42
1:C:170:ALA:HB2	1:C:269:TYR:HE1	1.84	0.42
1:D:104:THR:O	1:D:152:ARG:NH1	2.51	0.42
1:D:122:GLU:HG3	1:D:127:SER:O	2.20	0.42
1:D:167:LEU:HD23	1:D:167:LEU:HA	1.85	0.42
1:F:214:ALA:HB2	1:G:313:VAL:HG21	2.01	0.42
1:H:183:VAL:HG13	1:H:240:THR:HG23	2.01	0.42
1:C:255:THR:HA	1:C:312:PHE:O	2.20	0.41
1:H:13:ALA:HB2	1:H:81:HIS:ND1	2.34	0.41
1:B:113:PHE:CD1	1:B:133:TRP:CE2	3.09	0.41
1:C:12:VAL:HA	1:C:83:ALA:O	2.19	0.41
1:D:273:TYR:HD2	1:D:281:LEU:HD21	1.85	0.41
1:E:46:THR:HA	1:E:71:GLU:O	2.20	0.41
1:H:12:VAL:HG12	1:H:41:ARG:O	2.20	0.41
1:H:334:ASN:ND2	1:H:343:ASP:HB2	2.35	0.41
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.94	0.41
1:C:108:ASP:O	1:C:155:VAL:HG23	2.20	0.41
1:C:168:PHE:CG	1:C:169:PRO:HD3	2.55	0.41
1:F:114:ARG:NE	1:F:155:VAL:O	2.47	0.41
1:G:117:ASP:HB3	1:G:120:VAL:HB	2.00	0.41
1:H:81:HIS:O	1:H:104:THR:HG22	2.20	0.41
1:A:255:THR:HA	1:A:312:PHE:O	2.19	0.41
1:C:17:ALA:O	1:C:59:HIS:NE2	2.52	0.41
1:C:322:VAL:O	1:C:327:GLY:N	2.53	0.41
1:D:217:HIS:ND1	1:D:219:HIS:HB2	2.35	0.41
1:F:149:GLY:HA2	1:F:336:ALA:O	2.20	0.41
1:G:140:LEU:HD23	1:G:141:PRO:N	2.36	0.41
1:G:282:MET:CE	1:G:286:GLN:HB3	2.50	0.41
1:A:95:VAL:HG12	1:A:96:LEU:HD22	2.02	0.41
1:B:245:PRO:CD	1:C:244:ILE:HD12	2.51	0.41
1:G:166:ALA:HB1	1:G:314:ALA:HB1	2.02	0.41
1:A:121:TRP:CD1	1:A:121:TRP:C	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:PHE:CD2	1:B:221:PRO:HG2	2.55	0.41
1:C:90:HIS:HA	1:C:112:ASP:OD1	2.20	0.41
1:D:164:LEU:O	1:D:168:PHE:HD2	2.03	0.41
1:D:262:LEU:CD1	1:D:305:VAL:HG23	2.50	0.41
1:E:265:LEU:CD1	1:E:305:VAL:HG21	2.50	0.41
1:G:159:TYR:HB2	1:G:160:PRO:HD3	2.02	0.41
1:G:284:GLU:OE1	1:G:284:GLU:HA	2.15	0.41
1:H:24:GLU:CD	1:H:248:ARG:HH22	2.28	0.41
1:H:111:ALA:O	1:H:121:TRP:CZ3	2.73	0.41
1:D:114:ARG:HG2	1:D:154:ALA:HB1	2.03	0.41
1:D:169:PRO:HG2	1:D:269:TYR:CE2	2.56	0.41
1:E:105:LEU:HG	1:E:107:ILE:HD11	2.03	0.41
1:F:166:ALA:HB2	1:F:316:ALA:HB2	2.02	0.41
1:A:152:ARG:HD3	1:A:152:ARG:HA	1.86	0.41
1:A:32:HIS:CD2	1:A:33:PRO:HD2	2.56	0.41
1:C:159:TYR:HD2	1:C:219:HIS:CE1	2.39	0.41
1:E:26:LEU:HD22	1:E:65:LEU:HD13	2.01	0.41
1:F:34:ALA:CB	1:F:39:ARG:HG3	2.51	0.41
1:F:52:GLY:N	1:F:70:VAL:O	2.47	0.41
1:F:55:LEU:HD12	1:F:55:LEU:HA	1.95	0.41
1:G:169:PRO:HB2	1:G:269:TYR:CE2	2.56	0.41
1:G:286:GLN:NE2	1:H:56:GLY:O	2.53	0.41
1:H:157:GLY:C	1:H:160:PRO:HD2	2.46	0.41
1:H:282:MET:SD	1:H:288:PRO:HA	2.61	0.41
1:A:103:GLU:O	1:A:151:ARG:NH2	2.48	0.41
1:D:133:TRP:CD2	1:D:152:ARG:HB3	2.55	0.41
1:F:30:LEU:HD21	1:F:65:LEU:HG	2.03	0.41
1:F:124:PHE:CD2	1:F:221:PRO:HG3	2.56	0.41
1:H:182:VAL:HG22	1:H:254:CYS:SG	2.61	0.41
1:B:240:THR:HG21	1:C:253:THR:CG2	2.51	0.40
1:E:102:PRO:HA	1:E:152:ARG:NH2	2.36	0.40
1:D:327:GLY:O	1:D:331:GLN:HB2	2.21	0.40
1:F:133:TRP:CZ2	1:F:152:ARG:HD2	2.55	0.40
1:G:350:VAL:HG12	1:H:27:ARG:CZ	2.51	0.40
1:B:13:ALA:HB3	1:B:84:VAL:HG22	2.04	0.40
1:G:97:ALA:C	1:G:99:GLN:H	2.29	0.40
1:G:282:MET:HE3	1:G:282:MET:HB3	1.89	0.40
1:C:185:VAL:HG22	1:C:251:LEU:HB3	2.02	0.40
1:C:220:THR:N	1:C:221:PRO:HD2	2.36	0.40
1:F:159:TYR:HB2	1:F:160:PRO:HD3	2.04	0.40
1:H:141:PRO:HG3	1:H:168:PHE:HE2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:VAL:HA	1:B:242:VAL:O	2.22	0.40
1:C:84:VAL:HG13	1:C:106:ILE:HA	2.03	0.40
1:G:141:PRO:HD3	1:G:168:PHE:CE1	2.57	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	342/354 (97%)	316 (92%)	23 (7%)	3 (1%)	14	29
1	B	342/354 (97%)	316 (92%)	25 (7%)	1 (0%)	36	56
1	C	342/354 (97%)	320 (94%)	21 (6%)	1 (0%)	36	56
1	D	342/354 (97%)	315 (92%)	22 (6%)	5 (2%)	8	16
1	E	342/354 (97%)	318 (93%)	22 (6%)	2 (1%)	21	39
1	F	342/354 (97%)	325 (95%)	15 (4%)	2 (1%)	21	39
1	G	342/354 (97%)	323 (94%)	17 (5%)	2 (1%)	21	39
1	H	342/354 (97%)	315 (92%)	25 (7%)	2 (1%)	21	39
All	All	2736/2832 (97%)	2548 (93%)	170 (6%)	18 (1%)	18	36

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	48	ALA
1	A	218	ARG
1	F	218	ARG
1	G	218	ARG
1	B	146	GLN
1	F	98	GLN
1	A	76	ALA

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Mol	Chain	Res	Type
1	D	127	SER
1	D	10	THR
1	G	325	THR
1	H	43	GLY
1	D	194	ALA
1	H	271	LYS
1	D	136	GLY
1	D	322	VAL
1	E	322	VAL
1	A	43	GLY
1	C	322	VAL

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	221/255 (87%)	220 (100%)	1 (0%)	81	91
1	B	220/255 (86%)	218 (99%)	2 (1%)	70	85
1	C	232/255 (91%)	228 (98%)	4 (2%)	53	76
1	D	238/255 (93%)	231 (97%)	7 (3%)	37	63
1	E	207/255 (81%)	200 (97%)	7 (3%)	32	58
1	F	242/255 (95%)	238 (98%)	4 (2%)	53	76
1	G	234/255 (92%)	231 (99%)	3 (1%)	61	81
1	H	187/255 (73%)	182 (97%)	5 (3%)	39	65
All	All	1781/2040 (87%)	1748 (98%)	33 (2%)	50	73

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	LYS
1	B	168	PHE
1	B	243	LEU
1	C	193	ARG

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Mol	Chain	Res	Type
1	C	204	VAL
1	C	243	LEU
1	C	348	VAL
1	D	10	THR
1	D	12	VAL
1	D	24	GLU
1	D	106	ILE
1	D	140	LEU
1	D	265	LEU
1	D	270	GLU
1	E	10	THR
1	E	155	VAL
1	E	243	LEU
1	E	244	ILE
1	E	315	ILE
1	E	320	ASN
1	E	322	VAL
1	F	12	VAL
1	F	88	LEU
1	F	223	ILE
1	F	311	THR
1	G	152	ARG
1	G	168	PHE
1	G	180	VAL
1	H	104	THR
1	H	164	LEU
1	H	168	PHE
1	H	333	MET
1	H	348	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	D	286	GLN
1	E	98	GLN
1	G	67	HIS
1	G	92	HIS
1	G	264	GLN

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	UKE	C	401	-	15,15,15	2.18	3 (20%)	19,21,21	2.64	9 (47%)
3	PO4	C	402	-	4,4,4	1.30	0	6,6,6	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UKE	C	401	-	-	0/5/6/6	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	UKE	O09-C10	-5.65	1.27	1.37
2	C	401	UKE	O09-C06	-5.15	1.30	1.38
2	C	401	UKE	O13-C12	-2.45	1.23	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	UKE	C06-O09-C10	4.97	110.47	104.12
2	C	401	UKE	O14-C12-C10	-4.86	115.94	122.44
2	C	401	UKE	O13-C12-C10	4.40	123.52	113.83
2	C	401	UKE	O09-C10-N11	-3.44	110.74	115.68
2	C	401	UKE	C04-C05-N11	3.27	136.35	129.31
2	C	401	UKE	C06-C05-N11	-2.93	105.88	108.60
2	C	401	UKE	C04-C05-C06	-2.85	117.77	120.27
2	C	401	UKE	O09-C06-C07	2.45	131.63	126.49
2	C	401	UKE	C01-O02-C03	-2.32	112.52	117.50

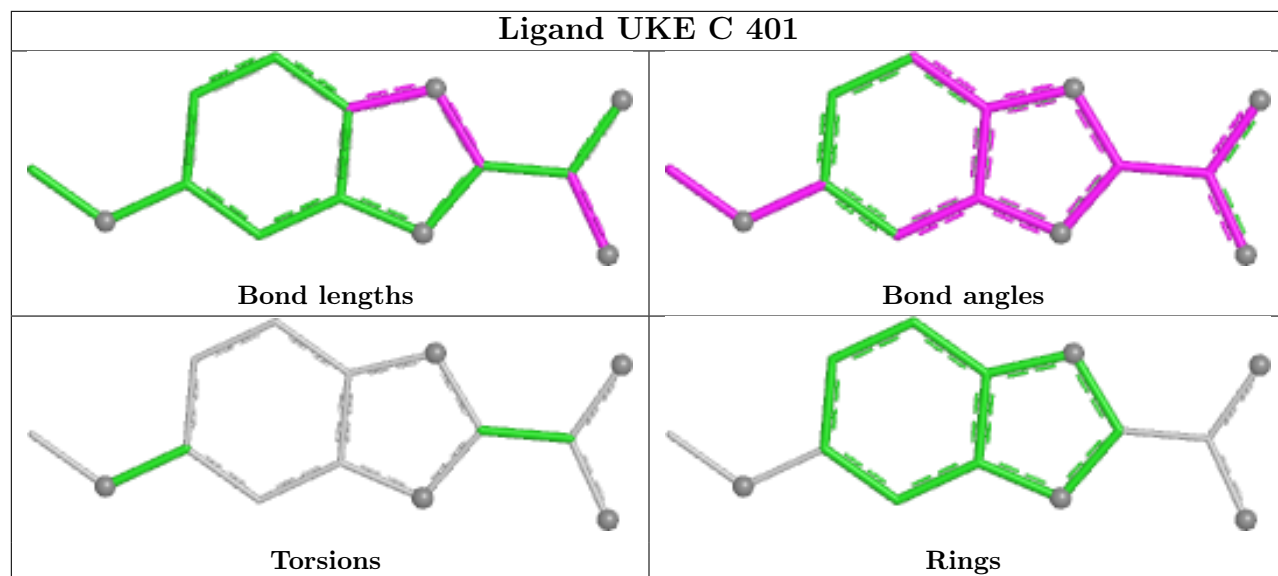
There are no chirality outliers.

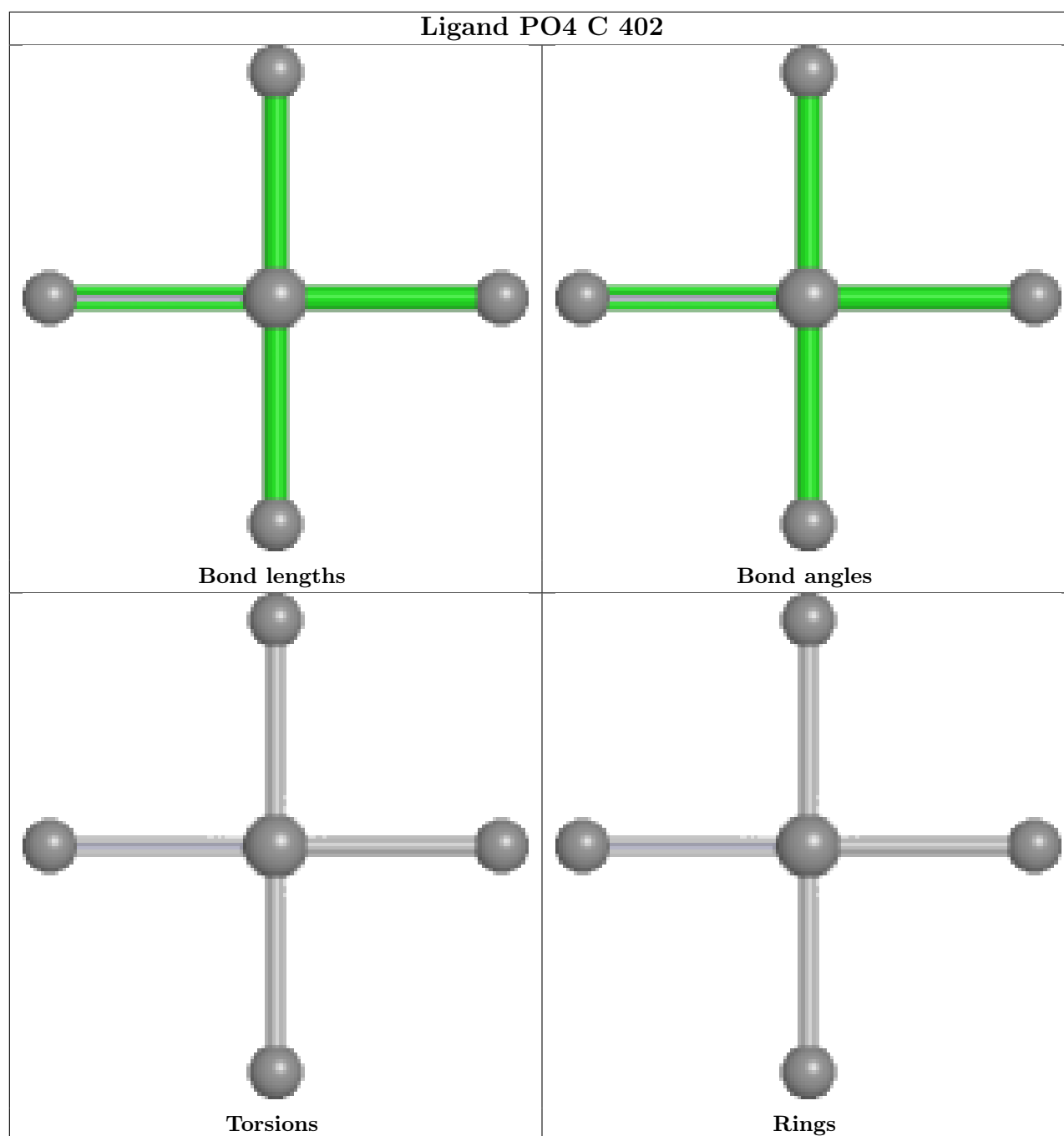
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	344/354 (97%)	0.54	18 (5%) 33 28	30, 69, 91, 100	0
1	B	344/354 (97%)	0.54	9 (2%) 57 52	30, 69, 95, 123	0
1	C	344/354 (97%)	0.47	9 (2%) 57 52	30, 69, 94, 102	0
1	D	344/354 (97%)	0.80	16 (4%) 36 32	30, 79, 106, 115	0
1	E	344/354 (97%)	1.21	66 (19%) 3 2	30, 95, 110, 121	0
1	F	344/354 (97%)	0.60	11 (3%) 50 45	59, 80, 97, 111	0
1	G	344/354 (97%)	0.92	28 (8%) 18 15	30, 89, 105, 112	0
1	H	344/354 (97%)	1.28	72 (20%) 2 2	30, 103, 120, 130	0
All	All	2752/2832 (97%)	0.79	229 (8%) 17 14	30, 82, 109, 130	0

All (229) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	165	LEU	5.8
1	E	87	ALA	5.5
1	H	73	THR	4.9
1	H	9	ALA	4.7
1	H	141	PRO	4.6
1	E	314	ALA	4.5
1	G	9	ALA	4.5
1	E	239	PHE	4.4
1	E	112	ASP	4.3
1	A	314	ALA	4.2
1	B	111	ALA	4.0
1	H	251	LEU	4.0
1	E	288	PRO	4.0
1	G	135	TYR	3.9
1	H	269	TYR	3.8
1	G	137	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	10	THR	3.6
1	E	164	LEU	3.6
1	H	181	THR	3.5
1	E	235	VAL	3.5
1	H	145	ASP	3.4
1	E	252	ALA	3.4
1	H	233	ARG	3.3
1	B	90	HIS	3.3
1	H	142	GLY	3.3
1	A	227	LEU	3.2
1	H	303	VAL	3.2
1	G	101	SER	3.2
1	E	115	LEU	3.2
1	H	140	LEU	3.2
1	D	9	ALA	3.2
1	G	312	PHE	3.1
1	E	195	ALA	3.1
1	H	328	ALA	3.1
1	H	253	THR	3.1
1	H	315	ILE	3.1
1	E	107	ILE	3.0
1	E	313	VAL	3.0
1	E	85	PHE	3.0
1	E	302	ALA	3.0
1	H	107	ILE	3.0
1	G	116	THR	3.0
1	D	257	ARG	3.0
1	H	130	ALA	2.9
1	E	158	CYS	2.9
1	H	137	LEU	2.9
1	E	22	GLY	2.9
1	E	9	ALA	2.9
1	B	153	ILE	2.8
1	F	96	LEU	2.8
1	E	90	HIS	2.8
1	A	176	ILE	2.8
1	E	223	ILE	2.8
1	D	243	LEU	2.8
1	E	240	THR	2.8
1	F	140	LEU	2.7
1	H	170	ALA	2.7
1	E	93	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	224	ALA	2.7
1	H	97	ALA	2.7
1	H	331	GLN	2.7
1	F	130	ALA	2.7
1	E	177	GLU	2.7
1	H	275	ALA	2.7
1	G	309	ALA	2.6
1	E	238	SER	2.6
1	D	10	THR	2.6
1	E	184	ALA	2.6
1	E	300	HIS	2.6
1	B	198	ASP	2.6
1	E	149	GLY	2.6
1	E	297	ASN	2.6
1	G	154	ALA	2.6
1	E	232	ASP	2.6
1	D	153	ILE	2.6
1	H	48	ALA	2.6
1	D	135	TYR	2.6
1	E	169	PRO	2.5
1	F	91	GLY	2.5
1	C	213	ILE	2.5
1	E	26	LEU	2.5
1	E	262	LEU	2.5
1	D	348	VAL	2.5
1	H	184	ALA	2.5
1	H	144	ARG	2.5
1	D	134	PRO	2.5
1	G	166	ALA	2.5
1	A	88	LEU	2.5
1	G	115	LEU	2.5
1	H	45	LEU	2.5
1	H	78	LEU	2.5
1	C	94	ALA	2.5
1	C	195	ALA	2.5
1	F	253	THR	2.5
1	G	73	THR	2.5
1	G	337	LEU	2.5
1	G	168	PHE	2.5
1	H	51	ALA	2.5
1	H	138	PRO	2.4
1	F	323	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	213	ILE	2.4
1	H	25	ILE	2.4
1	A	345	LEU	2.4
1	H	164	LEU	2.4
1	F	9	ALA	2.4
1	B	258	THR	2.4
1	H	101	SER	2.4
1	B	89	PRO	2.4
1	E	103	GLU	2.4
1	H	22	GLY	2.4
1	H	40	LEU	2.4
1	G	41	ARG	2.4
1	A	258	THR	2.4
1	H	65	LEU	2.4
1	H	167	LEU	2.4
1	H	335	LEU	2.4
1	E	257	ARG	2.4
1	A	304	ALA	2.4
1	B	285	GLY	2.4
1	H	249	GLY	2.4
1	G	90	HIS	2.4
1	G	113	PHE	2.4
1	D	347	VAL	2.4
1	G	120	VAL	2.4
1	E	48	ALA	2.4
1	G	48	ALA	2.4
1	G	229	ALA	2.4
1	C	140	LEU	2.3
1	E	254	CYS	2.3
1	B	70	VAL	2.3
1	H	182	VAL	2.3
1	H	313	VAL	2.3
1	A	166	ALA	2.3
1	H	325	THR	2.3
1	G	136	GLY	2.3
1	A	40	LEU	2.3
1	E	30	LEU	2.3
1	E	321	LEU	2.3
1	H	115	LEU	2.3
1	H	183	VAL	2.3
1	B	9	ALA	2.3
1	E	329	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	226	GLY	2.3
1	E	322	VAL	2.3
1	A	91	GLY	2.3
1	H	146	GLN	2.3
1	H	127	SER	2.3
1	F	167	LEU	2.3
1	G	234	ASP	2.3
1	E	312	PHE	2.3
1	D	48	ALA	2.2
1	E	269	TYR	2.3
1	G	170	ALA	2.2
1	G	95	VAL	2.2
1	H	163	ALA	2.2
1	E	255	THR	2.2
1	C	80	GLY	2.2
1	H	50	SER	2.2
1	H	339	TRP	2.2
1	G	64	PRO	2.2
1	H	156	PRO	2.2
1	A	9	ALA	2.2
1	H	194	ALA	2.2
1	C	35	TYR	2.2
1	C	65	LEU	2.2
1	E	206	GLY	2.2
1	H	100	LEU	2.2
1	D	183	VAL	2.2
1	H	14	VAL	2.2
1	H	237	VAL	2.2
1	E	175	LEU	2.2
1	E	201	GLY	2.2
1	E	273	TYR	2.2
1	H	175	LEU	2.2
1	E	266	ARG	2.2
1	E	89	PRO	2.2
1	A	13	ALA	2.1
1	E	142	GLY	2.1
1	H	260	SER	2.1
1	A	89	PRO	2.1
1	E	303	VAL	2.1
1	E	194	ALA	2.1
1	E	316	ALA	2.1
1	E	328	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	214	ALA	2.1
1	G	143	ALA	2.1
1	H	154	ALA	2.1
1	H	86	LEU	2.1
1	H	135	TYR	2.1
1	H	277	PRO	2.1
1	A	77	VAL	2.1
1	A	84	VAL	2.1
1	E	298	ALA	2.1
1	G	339	TRP	2.1
1	H	162	ALA	2.1
1	H	255	THR	2.1
1	D	106	ILE	2.1
1	H	189	SER	2.1
1	E	180	VAL	2.1
1	E	242	VAL	2.1
1	C	130	ALA	2.1
1	G	314	ALA	2.1
1	H	21	ALA	2.1
1	H	256	ALA	2.1
1	D	78	LEU	2.1
1	F	115	LEU	2.1
1	H	49	THR	2.1
1	D	189	SER	2.1
1	E	72	PRO	2.1
1	E	241	PRO	2.1
1	E	172	ALA	2.0
1	H	111	ALA	2.0
1	H	171	LEU	2.0
1	D	104	THR	2.0
1	H	153	ILE	2.0
1	F	261	PRO	2.0
1	E	109	CYS	2.0
1	E	182	VAL	2.0
1	H	180	VAL	2.0
1	A	175	LEU	2.0
1	A	309	ALA	2.0
1	C	214	ALA	2.0
1	E	171	LEU	2.0
1	H	29	LEU	2.0
1	H	199	LEU	2.0
1	H	272	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	349	GLY	2.0
1	E	253	THR	2.0
1	E	315	ILE	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](#)

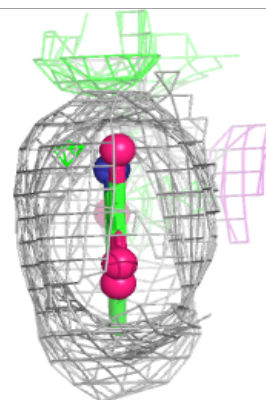
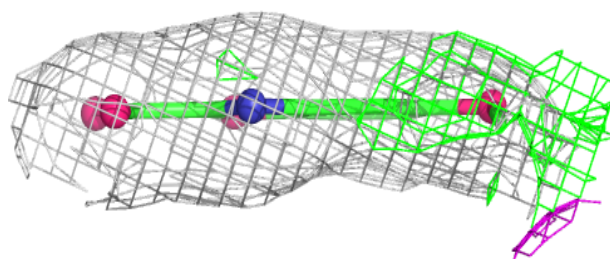
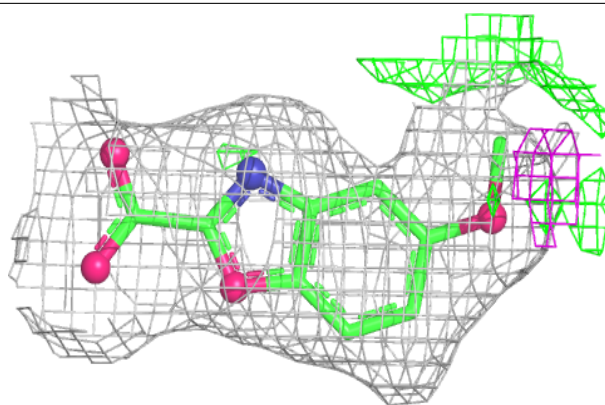
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	UKE	C	401	14/14	0.80	0.15	62,74,82,121	0
3	PO4	C	402	5/5	0.96	0.23	20,20,20,20	0

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

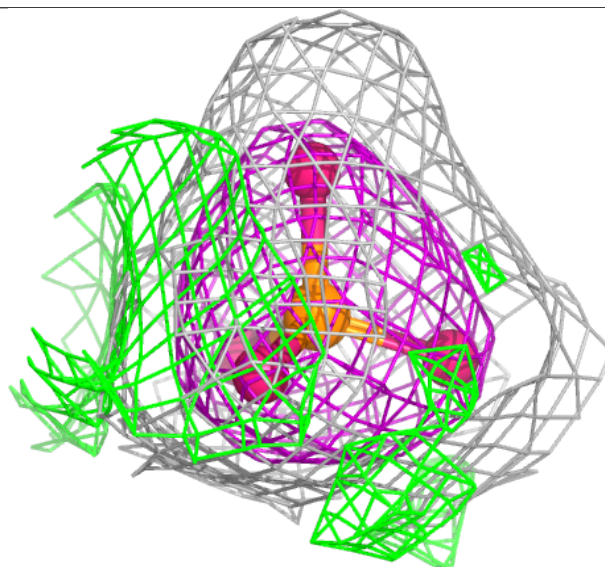
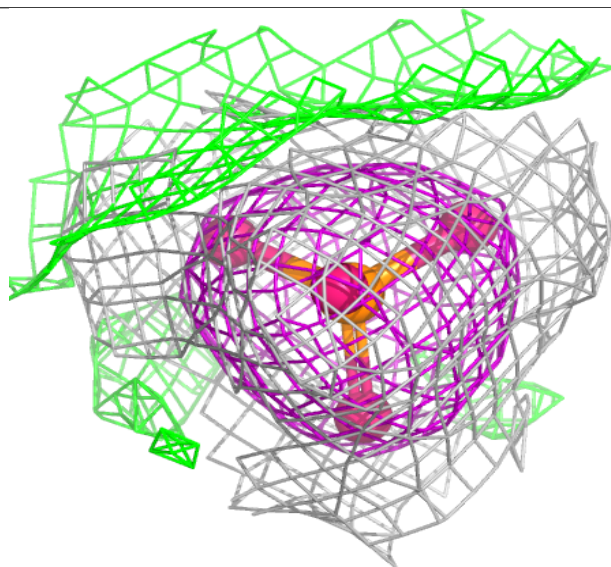
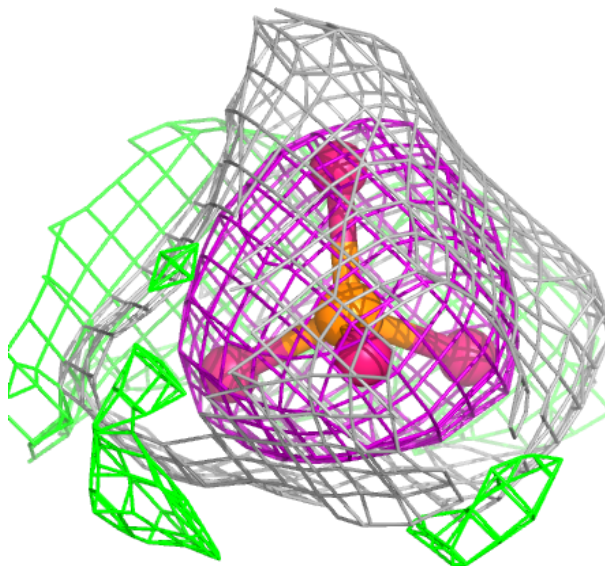
Electron density around UKE C 401:

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



Electron density around PO4 C 402:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.