W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 02:21 AM EDT

PDB ID	:	7TDV
Title	:	Crystal structure of S. aureus glutamine synthetase in Met-Sox-P/ADP transition state complex
Authors	:	Schumacher, M.A.
Deposited on	:	2022-01-03
Resolution	:	2.92 Å(reported)

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

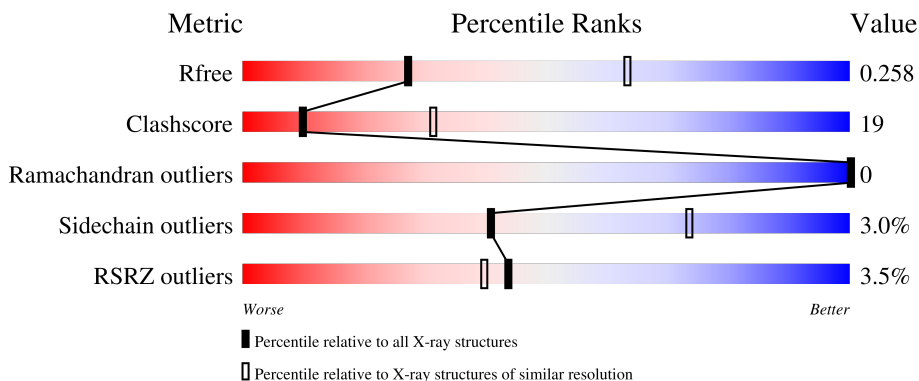|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.92 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.
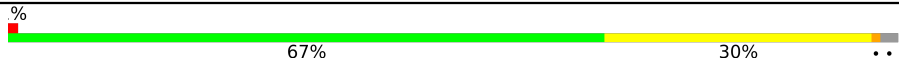
Metric	Percentile Ranks	Value
Rfree		0.258
Clashscore		19
Ramachandran outliers		0
Sidechain outliers		3.0%
RSRZ outliers		3.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_free	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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	449	3% / 65% / 32% / ..
1	B	449	% / 69% / 29% / .
1	C	449	% / 69% / 29% / ..
1	D	449	6% / 56% / 39% / ..
1	E	449	7% / 60% / 37% / ..

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Mol	Chain	Length	Quality of chain
1	H	449	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	E	505	-	-	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 21932 atoms, of which 132 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 Glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total 3531	C 2249	N 591	O 674	S 17	0	0	0
1	C	443	Total 3546	C 2258	N 596	O 675	S 17	0	0	0
1	D	442	Total 3537	C 2252	N 591	O 677	S 17	0	0	0
1	E	442	Total 3533	C 2251	N 592	O 673	S 17	1	0	0
1	B	443	Total 3536	C 2252	N 592	O 675	S 17	0	0	0
1	H	442	Total 3533	C 2251	N 592	O 673	S 17	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP E3VXC2
A	-1	SER	-	expression tag	UNP E3VXC2
A	0	HIS	-	expression tag	UNP E3VXC2
A	15	VAL	ALA	conflict	UNP E3VXC2
C	-2	GLY	-	expression tag	UNP E3VXC2
C	-1	SER	-	expression tag	UNP E3VXC2
C	0	HIS	-	expression tag	UNP E3VXC2
C	15	VAL	ALA	conflict	UNP E3VXC2
D	-2	GLY	-	expression tag	UNP E3VXC2
D	-1	SER	-	expression tag	UNP E3VXC2
D	0	HIS	-	expression tag	UNP E3VXC2
D	15	VAL	ALA	conflict	UNP E3VXC2
E	-2	GLY	-	expression tag	UNP E3VXC2
E	-1	SER	-	expression tag	UNP E3VXC2
E	0	HIS	-	expression tag	UNP E3VXC2
E	15	VAL	ALA	conflict	UNP E3VXC2
B	-2	GLY	-	expression tag	UNP E3VXC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	expression tag	UNP E3VXC2
B	0	HIS	-	expression tag	UNP E3VXC2
B	15	VAL	ALA	conflict	UNP E3VXC2
H	-2	GLY	-	expression tag	UNP E3VXC2
H	-1	SER	-	expression tag	UNP E3VXC2
H	0	HIS	-	expression tag	UNP E3VXC2
H	15	VAL	ALA	conflict	UNP E3VXC2

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
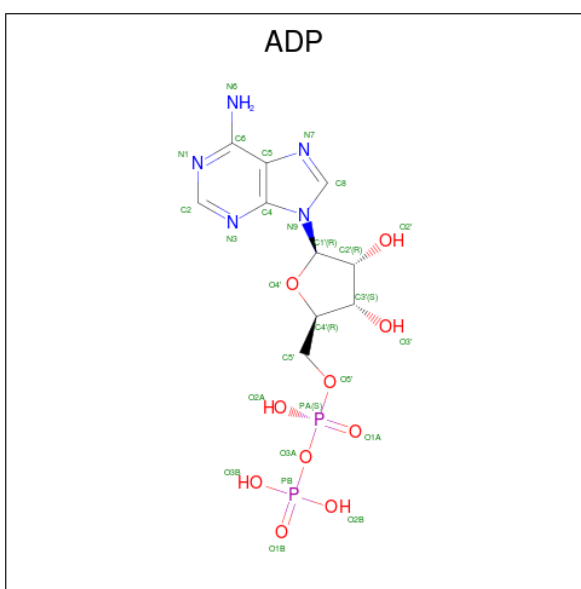
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	C	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	D	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	E	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	B	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	H	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		

- Molecule 3 is L-METHIONINE-S-SULFOXIMINE PHOSPHATE (three-letter code: P3S) (formula: $C_5H_{13}N_2O_6PS$) (labeled as "Ligand of Interest" by depositor).
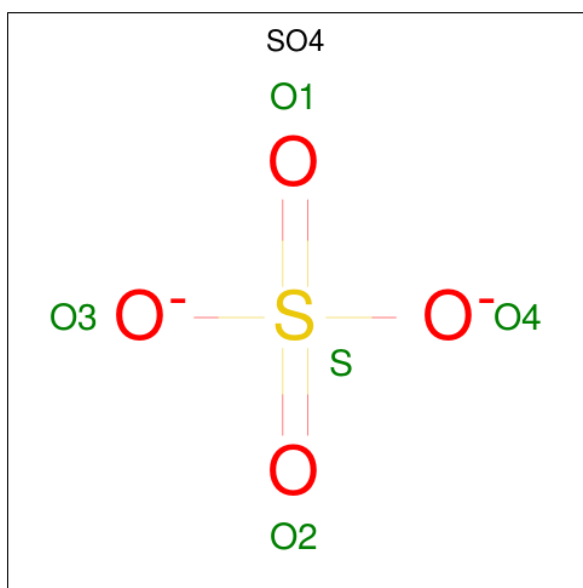
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	S	0	0
			25	5	10	2	6	1	1		
3	C	1	Total	C	H	N	O	P	S	0	0
			25	5	10	2	6	1	1		
3	D	1	Total	C	H	N	O	P	S	0	0
			25	5	10	2	6	1	1		
3	E	1	Total	C	H	N	O	P	S	0	0
			25	5	10	2	6	1	1		
3	B	1	Total	C	H	N	O	P	S	0	0
			25	5	10	2	6	1	1		
3	H	1	Total	C	H	N	O	P	S	0	0
			25	5	10	2	6	1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	C	5	Total	Mg	0	0
			5	5		
4	D	3	Total	Mg	0	0
			3	3		
4	E	4	Total	Mg	0	0
			4	4		
4	B	5	Total	Mg	0	0
			5	5		
4	H	2	Total	Mg	0	0
			2	2		

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total 5	O 4	S 1	0	0

• Molecule 6 is water.

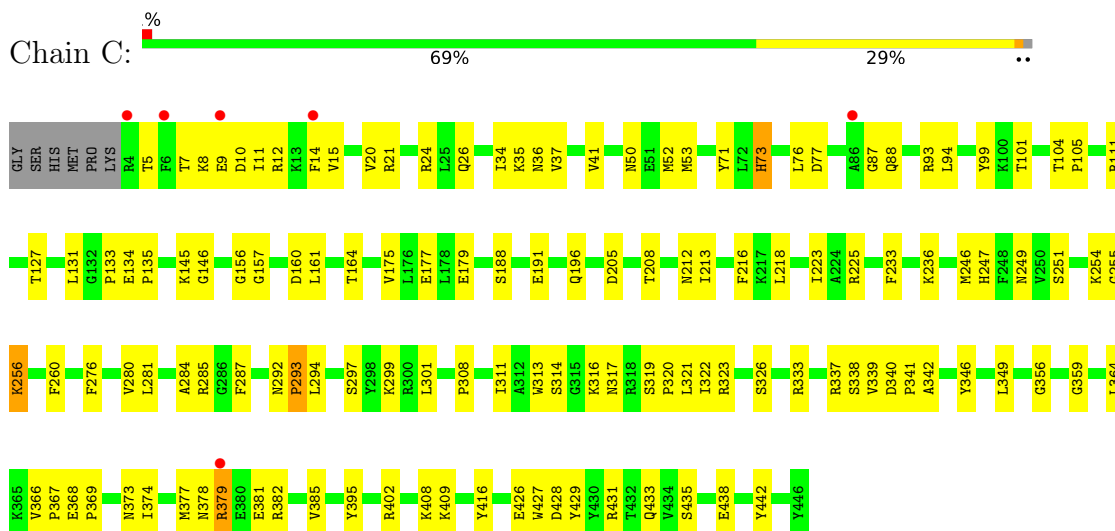| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	50	Total 50	O 50	0	0
6	C	77	Total 77	O 77	0	0
6	D	30	Total 30	O 30	0	0
6	E	26	Total 26	O 26	0	0
6	B	56	Total 56	O 56	0	0
6	H	67	Total 67	O 67	0	0

3 Residue-property plots ⓘ

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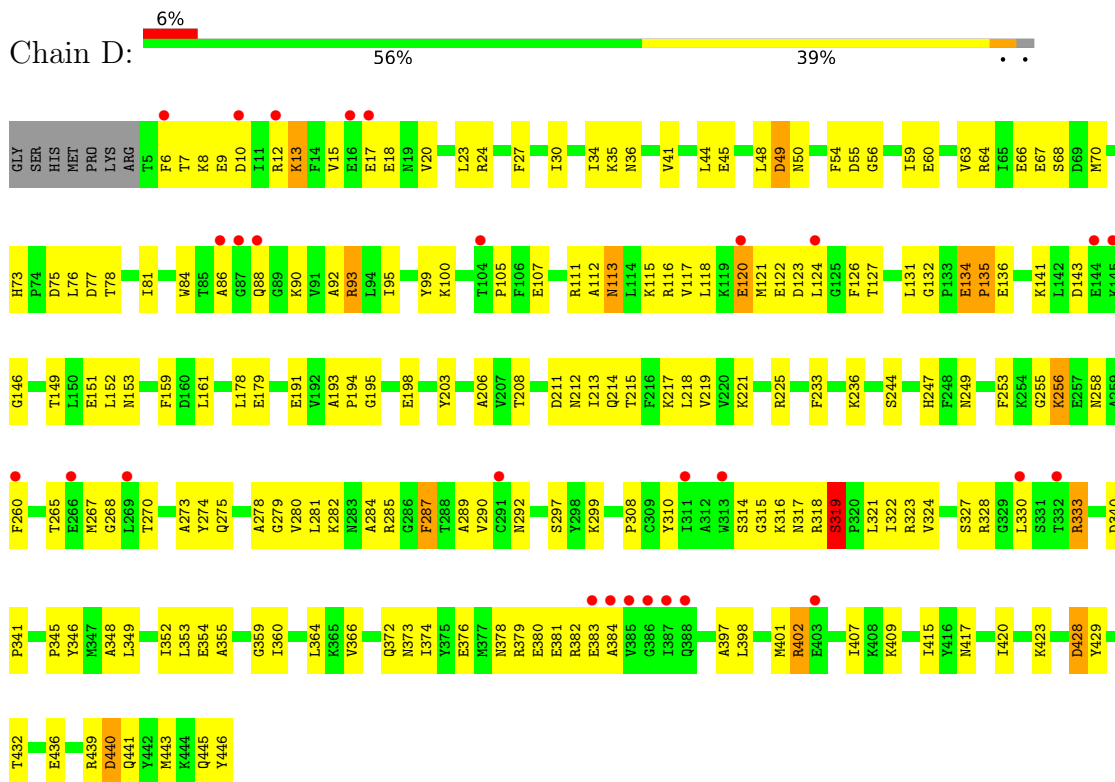
• Molecule 1: Glutamine synthetase

• Molecule 1: Glutamine synthetase

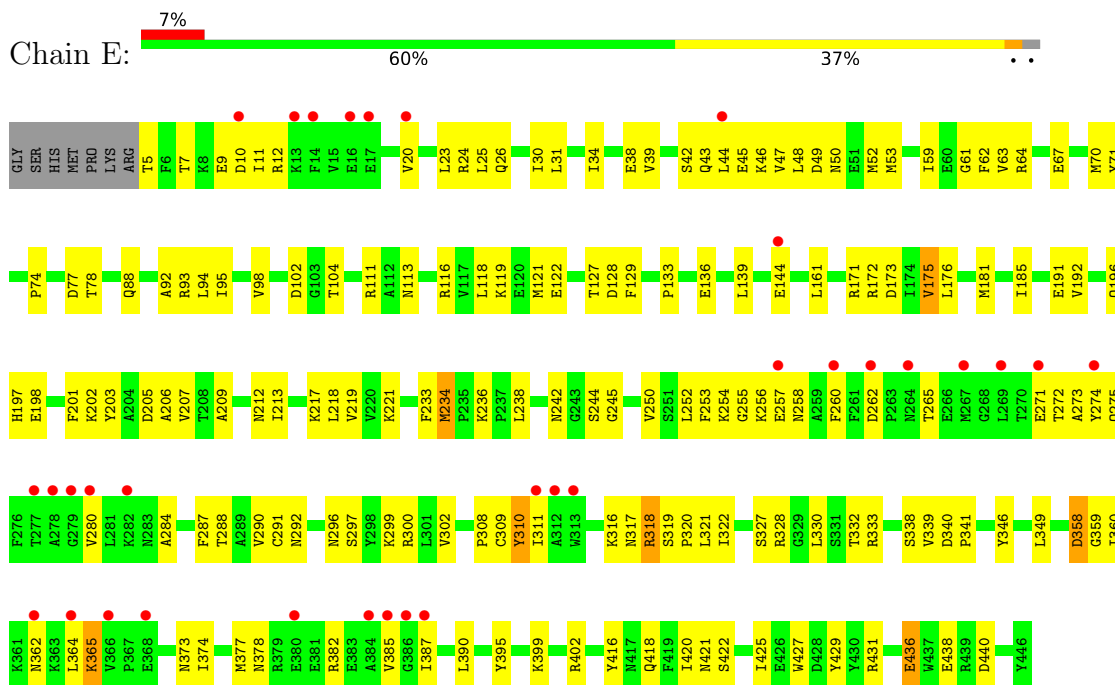• Molecule 1: Glutamine synthetase

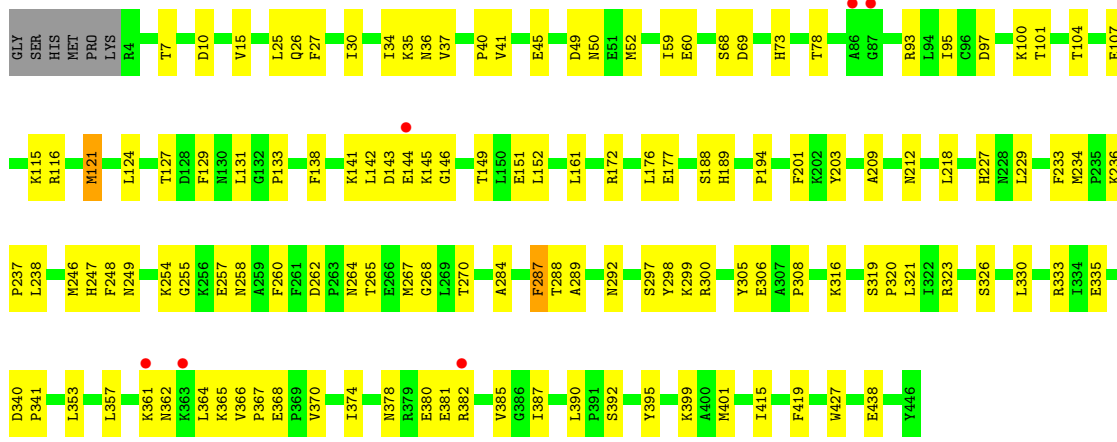Chain D:

• Molecule 1: Glutamine synthetase

Chain E:

• Molecule 1: Glutamine synthetase

Chain B:

GLY SER HIS MET PRO LYS R4 T7 D10 V15 L25 Q26 F27 I30 I34 K35 N36 V37 P40 V41 E45 D49 N50 E51 M52 I59 E60 S68 D69 H73 T78 A86 G87 R93 L94 I95 C96 D97 K100 T101 T104 E107

K115 R116 M121 L124 T127 D128 F129 N130 L131 G132 P133 F138 K141 L142 D143 E144 K145 G146 T149 L150 E151 L152 L161 R172 L176 E177 S188 H189 P194 F201 K202 Y203 A209 N212 L218 H227 N228 L229 F233 M234 P235 K236

P237 L238 M246 H247 F248 N249 K254 G255 K256 E257 N258 A259 F260 F261 D262 P263 N264 T265 E266 M267 G268 L269 T270 A284 F287 T288 A289 N292 S297 Y298 K299 R300 Y305 E306 A307 P308 K316 S319 P320 L321 I322 R323 S326 L330 R333 I334 E335

D340 P341 L353 L357 K361 N362 K363 L364 K365 V366 P367 E368 P369 V370 I374 N378 R379 E380 E381 R382 V385 G386 I387 L390 P391 S392 Y395 K399 A400 M401 I415 F419 W427 E438 Y446

• Molecule 1: Glutamine synthetase

Chain H:

GLY SER HIS MET PRO LYS ARG T5 F6 I7 K8 E9 D10 I11 R12 K13 F14 E18 N19 V20 R21 Y22 L23 R24 L25 I34 K35 N36 S42 K46 E51 M52 G56 V63 R64 I65 E66 E67 S68 D69 M70 H73 L76 D77 T78 W79 V80 I81 F82 P83

K90 R93 L94 T101 R111 E122 D123 L124 G125 F126 T127 D128 L131 E134 P135 E136 F140 K141 L142 D143 E144 E147 P148 N153 F159 D160 L161 D180 I185 S188 H189 H190 E191 G195 E198 A209 C210 D211 N212 I213 H230 A231 T232

F233 M234 P235 K236 S244 G245 M246 H247 F248 F253 K254 G255 F261 D262 G268 Y274 Q275 F276 V280 L281 A284 F287 T288 C291 N292 S297 Y298 K299 K316 N317 R318 S319 P320 L321 I322 R323 R328 G329 I334 E335 D340 P341 P345 Y346 M347

A348 A351 G359 I360 K361 N362 K363 L364 K365 V366 I374 M377 N378 E381 R382 I387 L390 P391 S392 T393 L394 Y395 M401 R402 E403 I407 K408 K409 A410 L411 I420 E426 W427 Y430 Q433 V434 S435 E438 Y442 Y446

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	154.62Å 154.62Å 299.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.89 – 2.92 48.89 – 2.92	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.89-2.92) 100.0 (48.89-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.198 , 0.256 0.200 , 0.258	Depositor DCC
R_{free} test set	1880 reflections (2.37%)	wwPDB-VP
Wilson B-factor (Å^2)	69.5	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.8	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21932	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, SO4, MG, P3S

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	0.56	2/3613 (0.1%)	0.64	0/4894
1	B	0.57	0/3618	0.66	0/4901
1	C	0.63	1/3628 (0.0%)	0.69	1/4912 (0.0%)
1	D	0.62	3/3619 (0.1%)	0.65	1/4901 (0.0%)
1	E	0.52	1/3615 (0.0%)	0.61	0/4895
1	H	0.62	0/3615	0.67	1/4895 (0.0%)
All	All	0.59	7/21708 (0.0%)	0.65	3/29398 (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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	135	PRO	N-CA	12.97	1.69	1.47
1	D	319	SER	C-N	8.71	1.50	1.34
1	A	324	VAL	C-N	8.39	1.50	1.34
1	E	302	VAL	C-N	7.90	1.49	1.34
1	A	251	SER	CA-CB	-5.77	1.44	1.52
1	C	146	GLY	C-N	5.44	1.46	1.34
1	D	134	GLU	C-N	5.26	1.44	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	135	PRO	CA-N-CD	-7.58	100.88	111.50
1	C	337	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	H	24	ARG	NE-CZ-NH1	-5.17	117.72	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	LYS	Mainchain

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	3531	0	3431	133	0
1	B	3536	0	3433	126	2
1	C	3546	0	3455	102	2
1	D	3537	0	3432	184	0
1	E	3533	0	3437	167	1
1	H	3533	0	3437	142	2
2	A	27	12	12	3	0
2	B	27	12	12	2	0
2	C	27	12	12	0	0
2	D	27	12	12	4	0
2	E	27	12	12	0	0
2	H	27	12	12	2	0
3	A	15	10	10	3	0
3	B	15	10	10	1	0
3	C	15	10	10	0	0
3	D	15	10	10	1	0
3	E	15	10	10	1	0
3	H	15	10	10	1	0
4	A	2	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	3	0	0	0	0
4	E	4	0	0	0	0
4	H	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	5	0	0	1	0
6	A	50	0	0	1	0
6	B	56	0	0	0	0
6	C	77	0	0	3	0
6	D	30	0	0	1	0
6	E	26	0	0	0	0
6	H	67	0	0	2	0
All	All	21800	132	20757	808	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (808) 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:D:135:PRO:CA	1:D:135:PRO:N	1.69	1.36
1:C:255:GLY:O	1:C:256:LYS:HD3	1.07	1.24
1:C:7:THR:HG22	1:C:10:ASP:OD2	1.40	1.19
1:E:172:ARG:O	1:E:175:VAL:HG23	1.46	1.14
1:B:234:MET:HE1	1:B:237:PRO:HA	1.23	1.13
1:D:136:GLU:OE1	3:D:502:P3S:N	1.83	1.10
1:D:213:ILE:HD11	1:D:345:PRO:HG3	1.29	1.09
1:C:255:GLY:O	1:C:256:LYS:CD	2.00	1.08
1:A:280:VAL:CG2	1:A:322:ILE:HD11	1.85	1.07
1:B:234:MET:CE	1:B:237:PRO:HA	1.85	1.06
1:E:171:ARG:O	1:E:175:VAL:HG22	1.59	1.01
1:E:359:GLY:HA2	1:E:364:LEU:HD12	1.39	1.00
1:C:7:THR:CG2	1:C:10:ASP:OD2	2.12	0.97
1:C:377:MET:HE2	1:C:382:ARG:HG2	1.46	0.97
1:D:354:GLU:OE2	1:D:409:LYS:HD3	1.67	0.94
1:E:11:ILE:HD11	1:E:48:LEU:HD21	1.48	0.94
1:E:196:GLN:HE21	1:E:244:SER:HB3	1.30	0.94
1:D:319:SER:HB3	1:D:374:ILE:HD13	1.51	0.93
1:D:141:LYS:O	1:D:149:THR:HG22	1.71	0.90
1:A:323:ARG:NH1	2:A:501:ADP:O1B	2.04	0.90
1:A:56:GLY:C	1:A:63:VAL:HG12	1.94	0.88
1:E:288:THR:HG21	1:E:390:LEU:HD22	1.54	0.87
1:D:127:THR:HG21	1:D:255:GLY:H	1.38	0.87
1:C:24:ARG:HD3	1:C:36:ASN:ND2	1.90	0.87
1:D:118:LEU:HD11	1:D:206:ALA:HB3	1.56	0.87
1:C:377:MET:CE	1:C:382:ARG:HG2	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:ARG:O	1:E:175:VAL:CG2	2.23	0.86
1:B:34:ILE:HG23	1:H:161:LEU:HD21	1.57	0.85
1:H:401:MET:HE2	1:H:420:ILE:CG1	2.04	0.85
1:H:323:ARG:NH2	2:H:501:ADP:O3B	2.10	0.85
1:H:281:LEU:CD2	1:H:322:ILE:HD12	2.07	0.85
1:H:288:THR:HG21	1:H:390:LEU:HD22	1.59	0.84
1:A:275:GLN:HE22	1:A:363:LYS:HE2	1.43	0.84
1:D:213:ILE:HD11	1:D:345:PRO:CG	2.08	0.83
1:A:280:VAL:HG21	1:A:322:ILE:HD11	1.58	0.83
1:D:127:THR:CG2	1:D:255:GLY:H	1.92	0.82
1:D:63:VAL:HG21	1:D:67:GLU:O	1.77	0.82
1:A:378:ASN:ND2	1:A:381:GLU:H	1.78	0.81
1:B:284:ALA:O	1:B:288:THR:HG23	1.79	0.81
1:E:196:GLN:NE2	1:E:244:SER:HB3	1.96	0.81
1:E:359:GLY:HA2	1:E:364:LEU:CD1	2.10	0.81
1:C:218:LEU:HD13	1:B:161:LEU:HD13	1.63	0.81
1:H:378:ASN:HB2	1:H:381:GLU:CG	2.11	0.80
1:H:401:MET:HE2	1:H:420:ILE:HG12	1.63	0.80
1:D:233:PHE:HB3	1:D:341:PRO:HB2	1.63	0.80
1:E:26:GLN:OE1	1:E:93:ARG:HD2	1.80	0.80
1:A:258:ASN:HB2	1:A:330:LEU:HD23	1.64	0.80
1:D:120:GLU:HA	1:D:123:ASP:HB2	1.63	0.79
1:E:205:ASP:OD1	1:E:207:VAL:HG12	1.82	0.79
1:H:11:ILE:HD11	1:H:76:LEU:HB3	1.63	0.79
1:E:61:GLY:HA2	1:E:418:GLN:HG2	1.63	0.79
1:E:172:ARG:HA	1:E:175:VAL:CG2	2.12	0.79
1:H:378:ASN:HB2	1:H:381:GLU:HG3	1.65	0.79
1:C:378:ASN:HB3	1:C:381:GLU:HG3	1.65	0.79
1:H:281:LEU:HD21	1:H:322:ILE:HD12	1.64	0.78
1:D:63:VAL:HB	1:D:70:MET:HE1	1.64	0.78
1:B:34:ILE:CG2	1:H:161:LEU:HD21	2.14	0.78
1:D:225:ARG:HD3	6:D:603:HOH:O	1.83	0.78
1:D:118:LEU:HD22	1:D:121:MET:HE2	1.65	0.77
1:E:254:LYS:O	1:E:257:GLU:HB2	1.84	0.77
1:E:11:ILE:HD11	1:E:48:LEU:HD11	1.66	0.77
1:C:218:LEU:HD13	1:B:161:LEU:CD1	2.15	0.77
1:H:236:LYS:HD2	1:H:299:LYS:O	1.85	0.77
1:B:236:LYS:HD3	1:B:299:LYS:O	1.84	0.77
1:B:401:MET:HE1	1:B:419:PHE:HE2	1.47	0.76
1:E:340:ASP:HB2	1:E:341:PRO:HD2	1.66	0.76
1:E:5:THR:HA	1:E:77:ASP:OD1	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:HD12	1:A:34:ILE:H	1.51	0.76
1:H:46:LYS:HE2	1:H:51:GLU:O	1.86	0.76
1:H:319:SER:HB2	1:H:374:ILE:HG22	1.69	0.75
1:B:362:ASN:HB3	1:B:364:LEU:HD21	1.69	0.75
1:D:63:VAL:HG22	1:D:64:ARG:O	1.87	0.74
1:E:127:THR:HG22	1:E:128:ASP:OD2	1.84	0.74
1:H:233:PHE:HB3	1:H:341:PRO:HB2	1.69	0.74
1:A:271:GLU:O	1:A:275:GLN:HG3	1.87	0.74
1:D:265:THR:HG23	1:D:268:GLY:H	1.52	0.73
1:D:127:THR:HG21	1:D:255:GLY:N	2.03	0.73
1:B:292:ASN:HB3	1:B:297:SER:HB3	1.70	0.73
1:B:124:LEU:HD11	1:B:361:LYS:HG3	1.71	0.73
1:B:401:MET:HE1	1:B:419:PHE:CE2	2.24	0.73
1:D:379:ARG:O	1:D:383:GLU:HG2	1.89	0.73
1:E:288:THR:CG2	1:E:390:LEU:HD22	2.18	0.73
1:H:142:LEU:HD21	1:H:230:HIS:HB2	1.70	0.73
1:D:86:ALA:O	1:D:90:LYS:HB2	1.89	0.73
1:E:262:ASP:OD1	1:E:265:THR:HG23	1.87	0.73
1:D:120:GLU:O	1:D:124:LEU:HD23	1.89	0.72
1:E:11:ILE:CD1	1:E:48:LEU:HD21	2.18	0.72
1:H:7:THR:HG22	1:H:10:ASP:OD2	1.89	0.72
1:A:136:GLU:OE1	3:A:502:P3S:N	2.22	0.72
1:D:373:ASN:N	1:H:66:GLU:OE2	2.23	0.72
1:B:36:ASN:HD21	1:H:161:LEU:HB3	1.54	0.72
1:A:340:ASP:HB2	1:A:341:PRO:HD2	1.70	0.71
1:D:292:ASN:HB3	1:D:297:SER:HB3	1.71	0.71
1:D:118:LEU:HD22	1:D:121:MET:CE	2.21	0.71
1:E:377:MET:HE2	1:E:382:ARG:HB3	1.73	0.71
1:A:323:ARG:NH2	1:A:335:GLU:OE2	2.23	0.70
1:A:378:ASN:ND2	1:A:381:GLU:N	2.39	0.70
1:C:101:THR:HG21	1:B:316:LYS:HD3	1.73	0.70
1:D:373:ASN:O	1:D:376:GLU:HG2	1.91	0.70
1:A:39:VAL:CG1	1:A:43:GLN:HB2	2.22	0.70
1:D:64:ARG:HD3	1:D:66:GLU:OE1	1.92	0.70
1:H:147:GLU:OE1	1:H:148:PRO:O	2.09	0.69
1:D:374:ILE:HD12	1:D:374:ILE:H	1.56	0.69
1:D:359:GLY:HA2	1:D:364:LEU:HG	1.75	0.69
1:E:284:ALA:HB3	1:E:311:ILE:HD13	1.75	0.69
1:H:147:GLU:OE1	1:H:148:PRO:N	2.26	0.69
1:D:111:ARG:HG3	1:D:346:TYR:CE1	2.28	0.69
1:D:217:LYS:O	1:D:221:LYS:HG3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:147:GLU:HG2	1:H:148:PRO:HD2	1.74	0.68
1:A:218:LEU:O	1:A:222:THR:HG23	1.93	0.68
1:D:267:MET:HG2	1:D:328:ARG:HH21	1.57	0.68
1:E:7:THR:OG1	1:E:10:ASP:N	2.26	0.68
1:H:275:GLN:HE22	1:H:363:LYS:HD3	1.58	0.68
1:D:63:VAL:CG2	1:D:67:GLU:HB2	2.24	0.68
1:H:323:ARG:HD3	1:H:335:GLU:OE1	1.94	0.68
1:A:66:GLU:OE1	1:C:373:ASN:HB2	1.94	0.68
1:A:319:SER:CB	1:A:374:ILE:HG22	2.24	0.67
1:C:111:ARG:HG3	1:C:346:TYR:CE1	2.30	0.67
1:H:401:MET:CE	1:H:420:ILE:CG1	2.72	0.67
1:C:246:MET:O	1:C:339:VAL:HB	1.95	0.67
1:C:292:ASN:HB3	1:C:297:SER:HB3	1.76	0.67
1:H:111:ARG:HG3	1:H:346:TYR:CE1	2.30	0.67
1:A:34:ILE:HB	1:C:161:LEU:CD1	2.25	0.67
1:E:308:PRO:HB3	1:E:321:LEU:HA	1.75	0.67
1:B:34:ILE:HG23	1:H:161:LEU:CD2	2.24	0.66
1:C:175:VAL:O	1:C:179:GLU:HG3	1.94	0.66
1:A:280:VAL:HG23	1:A:322:ILE:HD11	1.74	0.66
1:A:366:VAL:HG22	1:A:367:PRO:O	1.96	0.66
1:H:347:MET:HE3	1:H:411:LEU:HD22	1.77	0.66
1:A:133:PRO:HB3	1:A:213:ILE:HD11	1.76	0.66
1:D:316:LYS:CD	1:H:101:THR:HG21	2.26	0.66
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.60	0.66
1:C:280:VAL:CG1	1:C:322:ILE:HD11	2.26	0.66
1:E:271:GLU:O	1:E:275:GLN:HG3	1.95	0.66
1:A:262:ASP:OD1	1:A:265:THR:HG22	1.95	0.66
1:E:431:ARG:O	1:E:431:ARG:HG3	1.96	0.66
1:A:177:GLU:HG3	1:A:223:ILE:HD11	1.76	0.65
1:E:328:ARG:HD3	1:E:332:THR:HG23	1.78	0.65
1:C:379:ARG:HG2	1:C:379:ARG:HH11	1.61	0.65
1:E:133:PRO:HB3	1:E:213:ILE:HD11	1.78	0.65
1:E:399:LYS:HD2	1:E:402:ARG:HH21	1.61	0.65
1:C:104:THR:HG22	1:C:105:PRO:O	1.96	0.65
1:E:50:ASN:OD1	1:E:74:PRO:HD2	1.97	0.65
1:H:127:THR:HG21	1:H:255:GLY:N	2.12	0.65
1:C:37:VAL:HG23	1:B:189:HIS:HB3	1.78	0.65
1:D:63:VAL:HG12	1:D:70:MET:HE2	1.76	0.65
1:A:161:LEU:HD13	1:E:218:LEU:HD12	1.79	0.65
1:A:378:ASN:O	1:A:382:ARG:HG3	1.97	0.65
1:D:428:ASP:O	1:D:432:THR:HG23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:THR:HA	1:E:275:GLN:NE2	2.12	0.65
1:B:378:ASN:O	1:B:382:ARG:HG2	1.97	0.65
1:C:284:ALA:HA	1:C:287:PHE:CE2	2.32	0.64
1:E:11:ILE:HD11	1:E:48:LEU:CD2	2.23	0.64
1:D:236:LYS:HD2	1:D:299:LYS:O	1.98	0.64
1:A:359:GLY:HA2	1:A:364:LEU:HD12	1.79	0.64
1:D:374:ILE:HD12	1:D:374:ILE:N	2.12	0.64
1:E:362:ASN:HB3	1:E:364:LEU:HD21	1.80	0.64
1:E:436:GLU:O	1:E:440:ASP:HB2	1.96	0.64
1:D:63:VAL:HG23	1:D:67:GLU:HB2	1.79	0.64
1:C:251:SER:HA	1:C:260:PHE:CE2	2.33	0.64
1:D:34:ILE:H	1:D:34:ILE:HD12	1.63	0.63
1:C:359:GLY:HA2	1:C:364:LEU:HD22	1.80	0.63
1:D:319:SER:HB3	1:D:374:ILE:CD1	2.27	0.63
1:E:111:ARG:HG3	1:E:346:TYR:CE1	2.33	0.63
1:E:172:ARG:HA	1:E:175:VAL:HG21	1.78	0.63
1:D:30:ILE:HG22	1:D:60:GLU:O	1.99	0.63
1:B:101:THR:HG21	1:H:316:LYS:HE3	1.80	0.63
1:C:9:GLU:HG2	1:C:12:ARG:HH11	1.63	0.63
1:E:24:ARG:HD3	1:E:38:GLU:OE2	1.98	0.63
1:H:93:ARG:HD2	1:H:94:LEU:N	2.14	0.63
1:H:127:THR:CG2	1:H:255:GLY:H	2.12	0.63
1:A:319:SER:HB2	1:A:374:ILE:HG22	1.79	0.63
1:D:372:GLN:C	1:H:66:GLU:HG2	2.18	0.63
1:A:441:GLN:O	1:A:445:GLN:HG3	1.98	0.63
1:D:113:ASN:HD21	1:D:116:ARG:HH21	1.47	0.63
1:H:401:MET:CE	1:H:420:ILE:HG12	2.29	0.63
1:B:124:LEU:HD11	1:B:361:LYS:CG	2.28	0.62
1:H:322:ILE:CG2	1:H:334:ILE:HG23	2.29	0.62
1:C:379:ARG:HH11	1:C:379:ARG:CG	2.13	0.62
1:E:233:PHE:HB3	1:E:341:PRO:HB2	1.81	0.62
1:C:191:GLU:HB3	1:C:196:GLN:HG2	1.82	0.62
1:B:68:SER:HB2	1:H:318:ARG:HH11	1.65	0.62
1:D:88:GLN:O	1:D:88:GLN:HG2	1.99	0.62
1:D:439:ARG:HG2	1:D:443:MET:CE	2.30	0.62
1:D:24:ARG:HD3	1:D:36:ASN:ND2	2.15	0.62
1:A:292:ASN:HB3	1:A:297:SER:HB3	1.82	0.61
1:H:401:MET:CE	1:H:420:ILE:HG13	2.30	0.61
1:E:172:ARG:CA	1:E:175:VAL:CG2	2.79	0.61
1:H:275:GLN:HB3	1:H:360:ILE:HG22	1.82	0.61
1:C:53:MET:HG2	1:C:71:TYR:CE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:422:SER:O	1:E:425:ILE:CG1	2.49	0.61
1:A:283:ASN:HB3	1:A:404:ASN:HD21	1.66	0.61
1:A:319:SER:OG	1:A:374:ILE:HG22	2.00	0.61
1:C:7:THR:O	1:C:10:ASP:HB2	2.00	0.61
1:D:340:ASP:HB2	1:D:341:PRO:CD	2.31	0.61
1:B:233:PHE:O	1:B:341:PRO:HG2	2.01	0.61
1:B:234:MET:HE2	1:B:237:PRO:HA	1.80	0.61
1:C:280:VAL:HG12	1:C:322:ILE:HD11	1.83	0.60
1:H:127:THR:HG21	1:H:255:GLY:H	1.64	0.60
1:D:315:GLY:HA2	1:D:324:VAL:HG22	1.83	0.60
1:A:283:ASN:OD1	1:A:406:VAL:HG11	1.99	0.60
1:D:161:LEU:HD13	1:H:34:ILE:O	2.01	0.60
1:H:79:TRP:CZ2	1:H:81:ILE:HD11	2.36	0.60
1:H:322:ILE:HG23	1:H:334:ILE:HG23	1.82	0.60
1:C:93:ARG:HG2	1:C:94:LEU:N	2.13	0.60
1:D:13:LYS:O	1:D:17:GLU:HG2	2.01	0.60
1:H:79:TRP:HZ2	1:H:81:ILE:HD11	1.66	0.60
1:D:7:THR:HG22	1:D:10:ASP:OD2	2.02	0.60
1:E:378:ASN:O	1:E:382:ARG:HG2	2.01	0.60
1:E:30:ILE:HG23	1:E:31:LEU:HD23	1.84	0.60
1:D:120:GLU:OE2	1:D:123:ASP:OD2	2.20	0.60
1:D:439:ARG:HG2	1:D:443:MET:HE3	1.83	0.60
1:A:255:GLY:O	1:A:256:LYS:HB2	2.02	0.59
1:A:273:ALA:O	1:A:277:THR:HG22	2.01	0.59
1:A:206:ALA:HB1	1:A:349:LEU:CD2	2.31	0.59
1:B:262:ASP:OD1	1:B:264:ASN:ND2	2.36	0.59
1:H:430:TYR:O	1:H:433:GLN:HG3	2.02	0.59
1:E:191:GLU:CG	1:E:192:VAL:H	2.16	0.59
1:E:275:GLN:HB2	1:E:360:ILE:HG12	1.83	0.59
1:B:288:THR:HG21	1:B:390:LEU:HD22	1.84	0.59
1:D:317:ASN:ND2	1:D:372:GLN:O	2.35	0.59
1:E:209:ALA:O	1:E:212:ASN:HB2	2.02	0.59
1:A:196:GLN:HE21	1:A:244:SER:HB3	1.66	0.59
1:C:281:LEU:HD11	1:C:313:TRP:HB3	1.84	0.59
1:E:308:PRO:CG	1:E:338:SER:HA	2.32	0.59
1:E:133:PRO:CB	1:E:213:ILE:HD11	2.33	0.59
1:D:55:ASP:HB2	1:E:318:ARG:CZ	2.33	0.58
1:A:69:ASP:OD1	1:C:323:ARG:NH2	2.36	0.58
1:H:359:GLY:HA2	1:H:364:LEU:HD12	1.85	0.58
1:A:236:LYS:HD2	1:A:299:LYS:O	2.02	0.58
1:A:272:THR:HG23	1:A:360:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:LEU:N	1:C:294:LEU:HD12	2.17	0.58
1:E:39:VAL:HG12	1:E:43:GLN:HB2	1.84	0.58
1:E:252:LEU:HD12	1:E:260:PHE:HE1	1.68	0.58
1:E:422:SER:O	1:E:425:ILE:HG12	2.02	0.58
1:D:15:VAL:HA	1:D:20:VAL:HG12	1.85	0.58
1:E:202:LYS:HG2	1:E:203:TYR:N	2.19	0.58
1:E:402:ARG:HA	1:E:416:TYR:OH	2.02	0.58
1:E:217:LYS:O	1:E:221:LYS:HG3	2.03	0.58
1:E:272:THR:HA	1:E:275:GLN:HE21	1.67	0.58
1:H:147:GLU:CG	1:H:148:PRO:HD2	2.34	0.58
1:A:93:ARG:O	1:A:93:ARG:HG3	2.03	0.58
1:E:198:GLU:OE1	3:E:502:P3S:O1A	2.22	0.58
1:E:377:MET:CE	1:E:382:ARG:HB3	2.33	0.57
1:B:257:GLU:OE2	1:B:257:GLU:HA	2.04	0.57
1:C:433:GLN:NE2	6:C:604:HOH:O	2.37	0.57
1:E:319:SER:N	1:E:320:PRO:CD	2.68	0.57
1:E:46:LYS:HD3	1:E:52:MET:CE	2.33	0.57
1:H:378:ASN:HB2	1:H:381:GLU:CB	2.35	0.57
1:D:402:ARG:NH2	1:D:420:ILE:HD13	2.20	0.57
1:E:129:PHE:CE1	1:E:250:VAL:HG13	2.39	0.57
1:D:111:ARG:NH2	1:D:211:ASP:OD2	2.38	0.57
1:E:34:ILE:HD12	1:E:34:ILE:H	1.70	0.57
1:H:80:VAL:HG21	1:H:93:ARG:NH2	2.20	0.57
1:C:20:VAL:O	1:C:41:VAL:HG11	2.04	0.56
1:H:318:ARG:HH11	1:H:318:ARG:HG3	1.70	0.56
1:A:39:VAL:HG13	1:A:43:GLN:HB2	1.88	0.56
1:A:318:ARG:NH1	3:A:502:P3S:O3A	2.38	0.56
1:C:21:ARG:C	1:C:41:VAL:HG13	2.24	0.56
1:D:122:GLU:HA	1:D:126:PHE:O	2.06	0.56
1:D:436:GLU:HG3	1:D:440:ASP:OD1	2.06	0.56
1:B:78:THR:HG21	1:B:95:ILE:HB	1.87	0.56
1:B:265:THR:HG23	1:B:268:GLY:N	2.19	0.56
1:H:56:GLY:C	1:H:63:VAL:HG12	2.25	0.56
1:A:152:LEU:HD22	1:A:194:PRO:O	2.06	0.56
1:C:177:GLU:HG3	1:C:223:ILE:HD11	1.87	0.56
1:B:370:VAL:HG21	1:B:387:ILE:HD11	1.86	0.56
1:D:118:LEU:HD23	1:D:353:LEU:CD2	2.36	0.56
1:E:39:VAL:CG1	1:E:43:GLN:HB2	2.36	0.56
1:D:292:ASN:HB3	1:D:297:SER:CB	2.34	0.56
1:E:385:VAL:O	1:E:385:VAL:HG22	2.06	0.56
1:B:36:ASN:ND2	1:H:161:LEU:HB3	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:281:LEU:HD23	1:H:322:ILE:HD12	1.86	0.56
1:H:25:LEU:O	1:H:36:ASN:HA	2.05	0.56
1:H:274:TYR:O	1:H:366:VAL:HG13	2.06	0.56
1:C:254:LYS:HE3	6:C:626:HOH:O	2.05	0.56
1:D:378:ASN:OD1	1:D:381:GLU:HG3	2.06	0.56
1:B:100:LYS:HE2	1:B:107:GLU:OE1	2.06	0.56
1:D:24:ARG:HG3	1:D:36:ASN:HD22	1.70	0.55
1:A:24:ARG:HD2	1:A:36:ASN:ND2	2.21	0.55
1:A:133:PRO:CB	1:A:213:ILE:HD11	2.35	0.55
1:E:291:CYS:HB3	1:E:339:VAL:HG22	1.87	0.55
1:B:267:MET:HG2	1:B:267:MET:O	2.06	0.55
1:A:275:GLN:NE2	1:A:363:LYS:HE2	2.16	0.55
1:D:136:GLU:O	1:D:244:SER:HB3	2.05	0.55
1:D:135:PRO:N	1:D:135:PRO:C	2.57	0.55
1:D:316:LYS:HD3	1:H:101:THR:HG21	1.88	0.55
1:D:12:ARG:NH1	1:D:45:GLU:OE2	2.40	0.55
1:D:315:GLY:C	1:D:317:ASN:H	2.10	0.55
1:E:382:ARG:HB2	1:E:387:ILE:HD11	1.87	0.55
1:B:68:SER:HB2	1:H:318:ARG:NH1	2.21	0.55
1:H:127:THR:HG22	1:H:253:PHE:O	2.07	0.55
1:E:53:MET:HG3	1:E:71:TYR:CE2	2.42	0.55
1:H:161:LEU:HD23	1:H:161:LEU:H	1.72	0.55
1:H:275:GLN:CB	1:H:360:ILE:HG22	2.37	0.55
1:H:378:ASN:HD22	1:H:381:GLU:HG3	1.71	0.55
1:C:53:MET:HG2	1:C:71:TYR:CD2	2.43	0.54
1:C:233:PHE:HB3	1:C:341:PRO:HB2	1.90	0.54
1:D:193:ALA:HB1	1:D:194:PRO:HD2	1.89	0.54
1:E:11:ILE:HD11	1:E:48:LEU:CD1	2.35	0.54
1:D:159:PHE:HB3	1:H:35:LYS:HB3	1.90	0.54
1:D:373:ASN:HB3	1:D:376:GLU:HG2	1.89	0.54
1:A:26:GLN:HG2	1:A:36:ASN:CB	2.37	0.54
1:A:56:GLY:C	1:A:63:VAL:CG1	2.73	0.54
1:H:378:ASN:O	1:H:382:ARG:HG3	2.08	0.54
1:B:37:VAL:HG23	1:H:189:HIS:HB3	1.90	0.54
1:E:308:PRO:HG3	1:E:338:SER:N	2.22	0.54
1:B:385:VAL:HG12	1:B:385:VAL:O	2.08	0.54
1:H:191:GLU:OE2	1:H:198:GLU:OE1	2.26	0.54
1:H:284:ALA:O	1:H:288:THR:HG23	2.08	0.54
1:C:285:ARG:HG3	1:C:311:ILE:CD1	2.38	0.54
1:D:24:ARG:CG	1:D:36:ASN:HD22	2.21	0.54
1:H:46:LYS:HD3	1:H:52:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:LEU:O	1:E:47:VAL:HG13	2.08	0.53
1:E:172:ARG:C	1:E:175:VAL:CG2	2.77	0.53
1:H:136:GLU:HG2	1:H:191:GLU:HG3	1.90	0.53
1:D:260:PHE:CG	1:D:273:ALA:HB2	2.43	0.53
1:E:78:THR:HG21	1:E:95:ILE:HB	1.91	0.53
1:D:55:ASP:OD1	1:E:318:ARG:HD2	2.08	0.53
1:D:99:TYR:CE2	1:D:105:PRO:HD3	2.43	0.53
1:B:233:PHE:HB3	1:B:341:PRO:HB2	1.90	0.53
1:C:379:ARG:CG	1:C:379:ARG:NH1	2.71	0.53
1:C:26:GLN:HA	1:C:35:LYS:O	2.08	0.53
1:A:26:GLN:HG2	1:A:36:ASN:HB3	1.91	0.53
1:D:34:ILE:O	1:D:35:LYS:HD3	2.09	0.53
1:A:325:PRO:HG2	1:A:333:ARG:CZ	2.38	0.53
1:C:135:PRO:HG2	1:C:216:PHE:CE2	2.44	0.53
1:C:236:LYS:HE2	1:C:299:LYS:O	2.09	0.53
1:E:292:ASN:HB3	1:E:297:SER:HB3	1.91	0.53
1:B:308:PRO:HB3	1:B:321:LEU:HA	1.91	0.53
1:H:401:MET:HE2	1:H:420:ILE:HG13	1.84	0.53
1:A:319:SER:N	1:A:320:PRO:CD	2.71	0.52
1:B:15:VAL:HG13	1:B:41:VAL:HG21	1.91	0.52
1:A:267:MET:HG2	1:A:274:TYR:OH	2.10	0.52
1:D:63:VAL:HG21	1:D:67:GLU:C	2.29	0.52
1:D:441:GLN:O	1:D:441:GLN:HG3	2.08	0.52
1:E:382:ARG:CB	1:E:387:ILE:HD11	2.39	0.52
1:H:210:CYS:HB2	1:H:346:TYR:CE1	2.44	0.52
1:C:157:GLY:N	1:C:160:ASP:OD2	2.35	0.52
1:B:246:MET:H	1:B:340:ASP:HA	1.73	0.52
1:A:34:ILE:HB	1:C:161:LEU:HD13	1.92	0.52
1:D:373:ASN:N	1:H:66:GLU:HG2	2.24	0.52
1:A:251:SER:HA	1:A:260:PHE:CE2	2.45	0.52
1:D:340:ASP:HB2	1:D:341:PRO:HD3	1.92	0.52
1:C:99:TYR:CE2	1:C:105:PRO:HD3	2.45	0.52
1:E:319:SER:N	1:E:320:PRO:HD3	2.25	0.52
1:H:213:ILE:HD12	1:H:345:PRO:HB3	1.92	0.52
1:E:321:LEU:HG	1:E:322:ILE:HG13	1.92	0.52
1:A:437:TRP:O	1:A:441:GLN:HG2	2.10	0.52
1:C:11:ILE:O	1:C:15:VAL:HG23	2.10	0.52
1:D:66:GLU:OE2	1:E:373:ASN:HB2	2.10	0.52
1:A:132:GLY:HA3	2:A:501:ADP:H1'	1.91	0.52
1:D:132:GLY:HA3	2:D:501:ADP:H1'	1.90	0.52
1:B:258:ASN:HB2	1:B:330:LEU:HD23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:GLU:OE2	1:B:385:VAL:HG12	2.10	0.52
1:H:395:TYR:HB2	1:H:427:TRP:CE2	2.44	0.52
1:D:36:ASN:OD1	1:E:161:LEU:HG	2.11	0.51
1:B:30:ILE:CD1	1:B:415:ILE:HG23	2.40	0.51
1:C:314:SER:HB3	1:C:317:ASN:HB3	1.91	0.51
1:D:398:LEU:HD23	1:D:401:MET:CE	2.40	0.51
1:E:44:LEU:HA	1:E:47:VAL:HG12	1.91	0.51
1:E:118:LEU:HD11	1:E:206:ALA:HB3	1.91	0.51
1:B:378:ASN:HD21	1:B:380:GLU:HG3	1.74	0.51
1:H:153:ASN:OD1	1:H:195:GLY:HA2	2.10	0.51
1:H:284:ALA:HA	1:H:287:PHE:CE2	2.45	0.51
1:H:435:SER:OG	1:H:438:GLU:HG3	2.10	0.51
1:A:284:ALA:HA	1:A:287:PHE:CZ	2.45	0.51
1:B:30:ILE:HD11	1:B:415:ILE:HG23	1.91	0.51
1:B:141:LYS:NZ	1:B:151:GLU:OE1	2.35	0.51
1:C:285:ARG:HG3	1:C:311:ILE:HD11	1.91	0.51
1:H:161:LEU:HD23	1:H:161:LEU:N	2.25	0.51
1:D:120:GLU:CA	1:D:123:ASP:HB2	2.37	0.51
1:E:317:ASN:OD1	1:E:320:PRO:HD3	2.11	0.51
1:A:437:TRP:O	1:A:441:GLN:CG	2.59	0.51
1:B:144:GLU:HG2	1:B:145:LYS:H	1.75	0.51
1:A:420:ILE:O	1:A:424:SER:OG	2.27	0.51
1:D:161:LEU:HG	1:H:36:ASN:ND2	2.26	0.51
1:A:26:GLN:NE2	1:A:93:ARG:HD3	2.26	0.51
1:A:57:SER:HA	1:A:63:VAL:O	2.11	0.51
1:A:206:ALA:HB1	1:A:349:LEU:HD23	1.92	0.51
1:D:316:LYS:HD2	1:H:101:THR:HG21	1.93	0.51
1:E:25:LEU:HD12	1:E:52:MET:HG2	1.92	0.51
1:A:254:LYS:HD3	6:A:635:HOH:O	2.11	0.50
1:E:234:MET:HG2	1:E:296:ASN:OD1	2.11	0.50
1:D:324:VAL:HG23	1:D:324:VAL:O	2.12	0.50
1:B:262:ASP:HB3	1:B:265:THR:HG22	1.93	0.50
1:A:185:ILE:HD13	1:A:201:PHE:HB3	1.93	0.50
1:E:11:ILE:CD1	1:E:48:LEU:HD11	2.40	0.50
1:E:121:MET:O	1:E:121:MET:HG2	2.10	0.50
1:A:131:LEU:HD22	1:A:349:LEU:HD13	1.93	0.50
1:A:233:PHE:HB3	1:A:341:PRO:HB2	1.93	0.50
1:D:310:TYR:CE1	1:D:382:ARG:NH1	2.79	0.50
1:E:308:PRO:HG2	1:E:338:SER:HA	1.94	0.50
1:B:209:ALA:O	1:B:212:ASN:HB2	2.10	0.50
1:E:300:ARG:O	1:E:300:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:308:PRO:HG3	1:E:338:SER:HA	1.93	0.50
1:C:218:LEU:CD1	1:B:161:LEU:HD13	2.40	0.50
1:A:404:ASN:OD1	1:A:406:VAL:HG12	2.12	0.50
1:D:118:LEU:CD2	1:D:121:MET:HE2	2.37	0.50
1:B:305:TYR:O	1:B:306:GLU:HB2	2.11	0.50
1:H:348:ALA:O	1:H:351:ALA:HB3	2.12	0.50
1:A:331:SER:O	1:A:333:ARG:HD3	2.12	0.50
1:D:436:GLU:O	1:D:440:ASP:HB2	2.10	0.50
1:A:321:LEU:HD23	1:A:390:LEU:HD11	1.94	0.49
1:B:300:ARG:O	1:B:300:ARG:HG2	2.12	0.49
1:B:340:ASP:HB2	1:B:341:PRO:HD2	1.94	0.49
1:H:287:PHE:HD1	1:H:291:CYS:HG	1.59	0.49
1:D:143:ASP:OD1	1:D:146:GLY:N	2.42	0.49
1:D:56:GLY:HA3	1:D:63:VAL:HG12	1.94	0.49
1:D:275:GLN:HG3	1:D:360:ILE:HG12	1.95	0.49
1:B:370:VAL:HG11	1:B:374:ILE:HG12	1.93	0.49
1:D:179:GLU:OE1	1:H:22:TYR:OH	2.20	0.49
1:A:56:GLY:O	1:A:63:VAL:HG12	2.12	0.49
1:D:255:GLY:C	1:D:256:LYS:HD3	2.32	0.49
1:D:274:TYR:HD1	1:D:366:VAL:HG21	1.78	0.49
1:E:236:LYS:HE2	1:E:300:ARG:HA	1.95	0.49
1:B:362:ASN:O	1:B:364:LEU:HD23	2.12	0.49
1:A:43:GLN:O	1:A:47:VAL:HG23	2.12	0.49
1:E:365:LYS:HG2	1:E:365:LYS:O	2.12	0.49
1:C:7:THR:O	1:C:10:ASP:N	2.46	0.49
1:C:9:GLU:HG2	1:C:12:ARG:NH1	2.26	0.49
1:E:127:THR:HB	1:E:255:GLY:H	1.77	0.49
1:B:116:ARG:HG2	1:B:116:ARG:HH11	1.78	0.49
1:E:61:GLY:HA2	1:E:418:GLN:CG	2.41	0.49
1:B:40:PRO:HG2	1:H:185:ILE:O	2.12	0.49
1:C:319:SER:HB2	1:C:374:ILE:HG23	1.95	0.49
1:B:15:VAL:CG1	1:B:41:VAL:HG21	2.42	0.49
1:B:144:GLU:CG	1:B:145:LYS:N	2.76	0.49
1:D:113:ASN:C	1:D:113:ASN:HD22	2.15	0.48
1:H:247:HIS:NE2	3:H:502:P3S:OT	2.32	0.48
1:A:323:ARG:NH2	1:A:335:GLU:CD	2.67	0.48
1:A:353:LEU:O	1:A:357:LEU:HG	2.13	0.48
1:A:404:ASN:OD1	1:A:406:VAL:CG1	2.62	0.48
1:E:25:LEU:CD1	1:E:52:MET:HG2	2.42	0.48
1:E:422:SER:O	1:E:425:ILE:HG13	2.13	0.48
1:A:191:GLU:CG	1:A:192:VAL:H	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:VAL:HG12	1:C:367:PRO:O	2.13	0.48
1:D:17:GLU:HG3	1:D:18:GLU:HG2	1.95	0.48
1:D:372:GLN:O	1:D:374:ILE:HD12	2.13	0.48
1:A:174:ILE:HG23	1:A:219:VAL:HG12	1.94	0.48
1:D:260:PHE:C	1:D:270:THR:HG23	2.33	0.48
1:D:134:GLU:HB2	1:D:247:HIS:HB2	1.95	0.48
1:E:93:ARG:HG2	1:E:94:LEU:N	2.28	0.48
1:E:129:PHE:HE2	1:E:349:LEU:HD22	1.78	0.48
1:A:310:TYR:CD1	1:A:374:ILE:HG12	2.48	0.48
1:D:141:LYS:HD2	1:D:151:GLU:CD	2.34	0.48
1:D:274:TYR:O	1:D:366:VAL:CG1	2.62	0.48
1:E:88:GLN:N	1:E:88:GLN:OE1	2.44	0.48
1:B:395:TYR:O	1:B:399:LYS:HG3	2.14	0.48
1:H:262:ASP:O	1:H:268:GLY:HA2	2.13	0.48
1:H:378:ASN:HB2	1:H:381:GLU:HB2	1.94	0.48
1:A:328:ARG:HG2	1:A:328:ARG:NH1	2.28	0.48
1:C:205:ASP:OD2	1:C:208:THR:HG23	2.14	0.48
1:C:428:ASP:OD1	1:C:431:ARG:HD3	2.14	0.48
1:D:23:LEU:HD11	1:D:41:VAL:HG12	1.94	0.48
1:B:26:GLN:HG2	1:B:36:ASN:HB3	1.95	0.48
1:C:8:LYS:O	1:C:11:ILE:HB	2.14	0.48
1:E:46:LYS:HD3	1:E:52:MET:HE2	1.95	0.48
1:E:287:PHE:O	1:E:290:VAL:HG22	2.14	0.48
1:B:142:LEU:HD22	1:B:146:GLY:O	2.12	0.48
1:A:130:ASN:HA	1:A:204:ALA:O	2.14	0.48
1:E:44:LEU:HA	1:E:47:VAL:CG1	2.44	0.48
1:A:7:THR:HG22	1:A:10:ASP:OD2	2.13	0.48
1:A:18:GLU:O	1:A:90:LYS:NZ	2.44	0.48
1:A:56:GLY:HA3	1:A:63:VAL:HG11	1.96	0.48
1:C:131:LEU:HA	1:C:249:ASN:O	2.14	0.48
1:C:218:LEU:HD13	1:B:161:LEU:HD11	1.92	0.48
1:E:44:LEU:O	1:E:44:LEU:HG	2.12	0.48
1:A:107:GLU:CD	1:A:107:GLU:H	2.17	0.47
1:B:121:MET:O	1:B:121:MET:HG2	2.12	0.47
1:B:218:LEU:HD22	1:B:218:LEU:O	2.14	0.47
1:B:255:GLY:C	1:B:257:GLU:H	2.18	0.47
1:B:366:VAL:CG2	1:B:367:PRO:HD2	2.44	0.47
1:H:340:ASP:HB2	1:H:341:PRO:CD	2.43	0.47
1:H:409:LYS:HE2	6:H:608:HOH:O	2.14	0.47
1:A:233:PHE:O	1:A:341:PRO:HG2	2.14	0.47
1:D:24:ARG:O	1:D:93:ARG:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:324:VAL:O	1:D:324:VAL:CG2	2.62	0.47
1:D:445:GLN:HG2	1:D:446:TYR:CD1	2.49	0.47
1:E:102:ASP:HB3	1:E:104:THR:HG23	1.96	0.47
1:D:55:ASP:OD2	1:D:55:ASP:C	2.52	0.47
1:H:275:GLN:NE2	1:H:363:LYS:HD3	2.27	0.47
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.77	0.47
1:A:314:SER:HB2	1:A:317:ASN:HB3	1.95	0.47
1:C:14:PHE:N	1:C:14:PHE:CD2	2.83	0.47
1:D:333:ARG:HD3	2:D:501:ADP:C5	2.49	0.47
1:E:24:ARG:HG2	1:E:38:GLU:HG3	1.97	0.47
1:B:7:THR:O	1:B:10:ASP:HB2	2.14	0.47
1:B:69:ASP:CG	1:H:323:ARG:HH11	2.17	0.47
1:B:143:ASP:OD1	1:B:145:LYS:N	2.47	0.47
1:C:131:LEU:HD22	1:C:349:LEU:HD22	1.96	0.47
1:E:144:GLU:OE2	1:E:144:GLU:N	2.29	0.47
1:B:69:ASP:OD1	1:H:323:ARG:NH1	2.47	0.47
1:A:23:LEU:HA	1:A:92:ALA:O	2.14	0.47
1:A:321:LEU:CD1	1:A:322:ILE:HG13	2.45	0.47
1:D:178:LEU:HD21	1:D:219:VAL:HG21	1.95	0.47
1:B:121:MET:HB2	1:B:357:LEU:HD11	1.96	0.47
1:A:184:ASP:HB3	1:A:202:LYS:HB2	1.96	0.47
1:E:308:PRO:HG3	1:E:338:SER:CA	2.44	0.47
1:B:45:GLU:HA	1:B:45:GLU:OE2	2.14	0.47
1:B:362:ASN:HB3	1:B:364:LEU:CD2	2.42	0.47
1:H:6:PHE:CE2	1:H:14:PHE:HE2	2.33	0.47
1:H:24:ARG:NE	1:H:36:ASN:ND2	2.63	0.47
1:D:63:VAL:CG1	1:D:70:MET:HE2	2.44	0.47
1:A:321:LEU:HD13	1:A:322:ILE:HG13	1.97	0.47
1:B:144:GLU:CG	1:B:145:LYS:H	2.28	0.47
1:B:395:TYR:CE2	1:B:399:LYS:HD2	2.50	0.47
1:H:11:ILE:CD1	1:H:76:LEU:HB3	2.39	0.47
1:D:136:GLU:HG2	1:D:191:GLU:HG3	1.97	0.47
1:D:24:ARG:CD	1:D:36:ASN:HD22	2.28	0.46
1:D:75:ASP:OD1	1:D:77:ASP:HB2	2.16	0.46
1:E:172:ARG:C	1:E:175:VAL:HG23	2.30	0.46
1:B:246:MET:HG2	1:B:248:PHE:CE1	2.50	0.46
1:B:333:ARG:NH1	2:B:501:ADP:H5'1	2.30	0.46
1:A:313:TRP:CZ2	1:A:369:PRO:HD3	2.50	0.46
1:C:316:LYS:HG2	1:C:326:SER:OG	2.14	0.46
1:D:117:VAL:CG1	1:D:354:GLU:HG3	2.45	0.46
1:E:254:LYS:C	1:E:257:GLU:HB2	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:SER:N	1:B:320:PRO:CD	2.78	0.46
1:C:34:ILE:O	1:C:35:LYS:HD3	2.15	0.46
1:E:119:LYS:HA	1:E:122:GLU:HG2	1.97	0.46
1:E:395:TYR:HB2	1:E:427:TRP:CE2	2.50	0.46
1:D:215:THR:O	1:D:219:VAL:HG22	2.16	0.46
1:E:327:SER:HB2	1:E:333:ARG:NH1	2.31	0.46
1:C:93:ARG:CG	1:C:94:LEU:N	2.77	0.46
1:D:132:GLY:N	1:D:249:ASN:O	2.38	0.46
1:B:227:HIS:O	1:B:229:LEU:HG	2.15	0.46
1:H:140:PHE:HE1	1:H:232:THR:HG21	1.81	0.46
1:A:359:GLY:HA2	1:A:364:LEU:CD1	2.44	0.46
1:D:131:LEU:HA	1:D:249:ASN:O	2.15	0.46
1:A:302:VAL:HG13	1:A:303:PRO:HD2	1.98	0.46
1:C:280:VAL:HG11	1:C:322:ILE:HD11	1.98	0.46
1:E:62:PHE:CD2	1:E:70:MET:HE1	2.51	0.46
1:A:161:LEU:HD21	1:E:24:ARG:HH21	1.81	0.46
1:D:127:THR:HG22	1:D:253:PHE:O	2.16	0.46
1:D:282:LYS:HD2	1:D:364:LEU:HD13	1.98	0.46
1:H:292:ASN:HB3	1:H:297:SER:HB3	1.98	0.46
1:C:319:SER:N	1:C:320:PRO:CD	2.78	0.46
1:C:385:VAL:HG12	1:C:385:VAL:O	2.16	0.46
1:C:429:TYR:N	1:C:429:TYR:CD2	2.84	0.46
1:B:141:LYS:HE2	1:B:151:GLU:CD	2.37	0.46
1:B:260:PHE:C	1:B:270:THR:HG23	2.36	0.46
1:B:316:LYS:HG2	1:B:326:SER:OG	2.16	0.46
1:D:113:ASN:OD1	1:D:415:ILE:HD12	2.15	0.46
1:D:349:LEU:HD23	1:D:349:LEU:HA	1.65	0.46
1:A:116:ARG:NH1	1:A:116:ARG:HG2	2.31	0.45
1:A:272:THR:HG23	1:A:360:ILE:CD1	2.46	0.45
1:A:280:VAL:CG2	1:A:322:ILE:CD1	2.75	0.45
1:D:289:ALA:HB2	1:D:397:ALA:HB1	1.98	0.45
1:D:348:ALA:O	1:D:352:ILE:HG12	2.16	0.45
1:E:258:ASN:HD22	1:E:330:LEU:C	2.19	0.45
1:B:30:ILE:HG22	1:B:60:GLU:HB3	1.97	0.45
1:H:6:PHE:HE2	1:H:14:PHE:CE2	2.34	0.45
1:A:374:ILE:HD11	1:A:387:ILE:HG21	1.97	0.45
1:C:87:GLY:O	1:C:88:GLN:HB3	2.17	0.45
1:B:265:THR:HG23	1:B:268:GLY:H	1.80	0.45
1:A:5:THR:HB	1:A:77:ASP:OD1	2.15	0.45
1:E:327:SER:HB2	1:E:333:ARG:HH12	1.81	0.45
1:E:358:ASP:O	1:E:362:ASN:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:80:VAL:HG21	1:H:93:ARG:HH21	1.81	0.45
1:C:292:ASN:HB3	1:C:297:SER:CB	2.44	0.45
1:D:8:LYS:O	1:D:12:ARG:HG3	2.17	0.45
1:E:420:ILE:HG13	1:E:421:ASN:N	2.31	0.45
1:H:46:LYS:HG2	1:H:51:GLU:HB2	1.98	0.45
1:D:112:ALA:HA	1:D:115:LYS:HG2	1.98	0.45
1:H:374:ILE:O	1:H:377:MET:HB2	2.17	0.45
1:C:8:LYS:O	1:C:11:ILE:N	2.49	0.45
1:D:8:LYS:HD3	1:D:48:LEU:HB3	1.98	0.45
1:E:9:GLU:HA	1:E:12:ARG:HB2	1.98	0.45
1:E:191:GLU:HG3	1:E:192:VAL:H	1.81	0.45
1:B:287:PHE:CD1	1:B:287:PHE:C	2.90	0.45
1:B:366:VAL:HG23	1:B:367:PRO:HD2	1.97	0.45
1:C:284:ALA:HA	1:C:287:PHE:CZ	2.52	0.45
1:E:45:GLU:O	1:E:49:ASP:HB2	2.17	0.45
1:B:26:GLN:OE1	1:B:93:ARG:HD2	2.17	0.45
1:D:76:LEU:N	1:D:76:LEU:HD12	2.32	0.45
1:D:281:LEU:HD21	1:D:322:ILE:HG13	1.99	0.45
1:H:93:ARG:HD2	1:H:93:ARG:C	2.37	0.45
1:H:378:ASN:CB	1:H:381:GLU:HG3	2.41	0.45
1:E:136:GLU:CB	1:E:244:SER:HB2	2.47	0.44
1:D:203:TYR:HB3	2:D:501:ADP:N3	2.32	0.44
1:D:218:LEU:HD13	1:E:161:LEU:HD13	1.99	0.44
1:B:35:LYS:HB3	1:H:159:PHE:HB3	2.00	0.44
1:B:27:PHE:HE2	1:B:59:ILE:CD1	2.31	0.44
1:H:254:LYS:CE	6:H:601:HOH:O	2.65	0.44
1:C:50:ASN:HB3	1:C:73:HIS:CE1	2.53	0.44
1:C:256:LYS:O	1:C:256:LYS:HG2	2.17	0.44
1:D:274:TYR:O	1:D:366:VAL:HG13	2.18	0.44
1:A:398:LEU:O	1:A:401:MET:HB3	2.17	0.44
1:C:374:ILE:CG1	1:C:374:ILE:O	2.65	0.44
1:D:380:GLU:HA	1:D:383:GLU:CG	2.47	0.44
1:E:70:MET:CE	1:E:98:VAL:HG11	2.48	0.44
1:B:50:ASN:HB3	1:B:73:HIS:CD2	2.52	0.44
1:B:262:ASP:O	1:B:268:GLY:HA2	2.17	0.44
1:A:129:PHE:CE2	1:A:353:LEU:HB2	2.52	0.44
1:C:5:THR:HA	1:C:77:ASP:OD2	2.17	0.44
1:D:290:VAL:HG21	1:D:407:ILE:HD11	1.99	0.44
1:D:314:SER:O	1:D:323:ARG:HA	2.18	0.44
1:E:136:GLU:CD	1:E:191:GLU:OE1	2.56	0.44
1:E:399:LYS:HA	1:E:399:LYS:HD3	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:VAL:HG21	1:B:387:ILE:CD1	2.46	0.44
1:C:294:LEU:HD11	1:C:342:ALA:HB1	1.98	0.44
1:D:118:LEU:HD11	1:D:206:ALA:CB	2.38	0.44
1:B:236:LYS:HD2	1:B:300:ARG:HA	2.00	0.44
1:H:19:ASN:OD1	1:H:21:ARG:HD3	2.17	0.44
1:A:206:ALA:HB1	1:A:349:LEU:HD21	2.00	0.44
1:E:129:PHE:CZ	1:E:250:VAL:HG13	2.52	0.44
1:E:362:ASN:HB3	1:E:364:LEU:CD2	2.47	0.44
1:H:122:GLU:HG2	1:H:126:PHE:O	2.18	0.44
1:H:347:MET:HE3	1:H:411:LEU:CD2	2.47	0.44
1:D:23:LEU:CD1	1:D:41:VAL:HG12	2.48	0.44
1:D:208:THR:O	1:D:212:ASN:N	2.50	0.44
1:E:236:LYS:HD2	1:E:238:LEU:O	2.17	0.44
1:B:138:PHE:CD1	1:B:237:PRO:HG3	2.53	0.44
1:B:177:GLU:OE2	1:B:177:GLU:HA	2.18	0.44
1:H:63:VAL:HG22	1:H:67:GLU:HG3	1.99	0.44
1:A:66:GLU:HA	1:C:317:ASN:ND2	2.33	0.43
1:A:203:TYR:N	2:A:501:ADP:O2'	2.50	0.43
1:C:395:TYR:HB2	1:C:427:TRP:CE2	2.53	0.43
1:D:24:ARG:CD	1:D:36:ASN:ND2	2.81	0.43
1:E:139:LEU:HD12	1:E:197:HIS:CD2	2.53	0.43
1:B:35:LYS:HA	1:H:159:PHE:O	2.18	0.43
1:B:176:LEU:HD23	1:B:176:LEU:HA	1.78	0.43
1:H:276:PHE:O	1:H:280:VAL:HG23	2.18	0.43
1:C:293:PRO:C	1:C:294:LEU:HD12	2.38	0.43
1:D:287:PHE:CD1	1:D:287:PHE:C	2.91	0.43
1:H:6:PHE:CE2	1:H:14:PHE:CE2	3.05	0.43
1:H:134:GLU:OE1	2:H:501:ADP:O1B	2.36	0.43
1:C:321:LEU:CD1	1:C:338:SER:HB3	2.48	0.43
1:D:9:GLU:CD	1:D:12:ARG:HE	2.22	0.43
1:D:152:LEU:HD13	1:D:194:PRO:O	2.18	0.43
1:B:116:ARG:HG2	1:B:116:ARG:NH1	2.33	0.43
1:H:63:VAL:HB	1:H:70:MET:CE	2.47	0.43
1:H:209:ALA:O	1:H:212:ASN:HB2	2.17	0.43
1:H:287:PHE:HB3	1:H:407:ILE:HD13	2.00	0.43
1:A:326:SER:HA	1:A:328:ARG:HH12	1.83	0.43
1:E:70:MET:HE3	1:E:98:VAL:HG11	2.01	0.43
1:B:265:THR:HG23	1:B:268:GLY:CA	2.48	0.43
1:H:298:TYR:HB3	1:H:392:SER:O	2.18	0.43
1:D:49:ASP:O	1:D:50:ASN:HB2	2.17	0.43
1:D:136:GLU:OE2	1:D:198:GLU:OE1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:ILE:H	1:D:374:ILE:CD1	2.29	0.43
1:B:27:PHE:CE2	1:B:59:ILE:CD1	3.01	0.43
1:B:141:LYS:CE	1:B:151:GLU:CD	2.87	0.43
1:B:152:LEU:HD13	1:B:194:PRO:O	2.18	0.43
1:B:218:LEU:HD21	1:H:161:LEU:HD12	2.00	0.43
1:H:147:GLU:OE1	1:H:147:GLU:C	2.57	0.43
1:C:368:GLU:HB2	1:C:369:PRO:HD2	1.99	0.43
1:E:113:ASN:OD1	1:E:116:ARG:NH1	2.52	0.43
1:B:247:HIS:HE1	3:B:502:P3S:NE	2.17	0.43
1:H:318:ARG:HH11	1:H:318:ARG:CG	2.31	0.43
1:A:56:GLY:HA3	1:A:63:VAL:CG1	2.48	0.43
1:A:364:LEU:H	1:A:364:LEU:HG	1.71	0.43
1:D:330:LEU:HD23	1:D:330:LEU:HA	1.64	0.43
1:E:185:ILE:HD13	1:E:201:PHE:HB3	2.01	0.43
1:E:280:VAL:HG23	1:E:322:ILE:HD11	2.01	0.43
1:A:316:LYS:HD2	1:A:326:SER:OG	2.19	0.43
1:C:127:THR:OG1	1:C:255:GLY:N	2.48	0.43
1:E:62:PHE:CD2	1:E:70:MET:CE	3.01	0.43
1:A:114:LEU:O	1:A:114:LEU:HD12	2.18	0.43
1:A:161:LEU:HD12	1:E:34:ILE:HB	1.99	0.43
1:C:301:LEU:HD22	1:C:308:PRO:O	2.18	0.43
1:D:280:VAL:CG1	1:D:322:ILE:HD11	2.49	0.43
1:E:20:VAL:HG11	1:E:92:ALA:HB3	2.00	0.43
1:B:319:SER:N	1:B:320:PRO:HD3	2.33	0.43
1:H:298:TYR:CE2	1:H:394:LEU:HB2	2.54	0.43
1:C:435:SER:OG	1:C:438:GLU:HG3	2.19	0.43
1:E:191:GLU:HG3	1:E:192:VAL:HG23	2.00	0.43
1:E:253:PHE:HA	1:E:257:GLU:O	2.19	0.43
1:E:236:LYS:HB2	1:E:300:ARG:HB2	2.00	0.42
1:H:36:ASN:C	1:H:36:ASN:OD1	2.57	0.42
1:A:18:GLU:O	1:A:90:LYS:CE	2.68	0.42
1:D:278:ALA:CB	1:D:364:LEU:HB2	2.50	0.42
1:E:260:PHE:HA	1:E:273:ALA:HB2	2.01	0.42
1:B:97:ASP:OD2	1:B:115:LYS:NZ	2.31	0.42
1:A:319:SER:HB2	1:A:374:ILE:CG2	2.48	0.42
1:C:133:PRO:HB3	1:C:213:ILE:HD11	2.02	0.42
1:D:417:ASN:HA	1:D:420:ILE:HG12	2.02	0.42
1:E:399:LYS:CD	1:E:402:ARG:HH21	2.30	0.42
1:B:30:ILE:O	1:B:30:ILE:HG13	2.19	0.42
1:H:131:LEU:HD11	1:H:248:PHE:CG	2.54	0.42
1:A:184:ASP:HB3	1:A:202:LYS:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:GLY:O	1:A:316:LYS:HB2	2.18	0.42
1:B:323:ARG:HD3	1:B:335:GLU:OE1	2.20	0.42
1:B:340:ASP:OD1	1:B:340:ASP:C	2.58	0.42
1:H:135:PRO:HB3	1:H:246:MET:SD	2.59	0.42
1:D:315:GLY:CA	1:D:324:VAL:HG22	2.48	0.42
1:E:236:LYS:O	1:E:236:LYS:HG3	2.20	0.42
1:H:124:LEU:HD21	1:H:361:LYS:HB3	2.02	0.42
1:A:7:THR:HG23	1:A:10:ASP:H	1.85	0.42
1:C:208:THR:O	1:C:212:ASN:N	2.38	0.42
1:D:100:LYS:HE2	1:D:107:GLU:OE1	2.20	0.42
1:E:218:LEU:C	1:E:218:LEU:HD23	2.39	0.42
1:B:203:TYR:N	2:B:501:ADP:O2'	2.53	0.42
1:B:378:ASN:OD1	1:B:381:GLU:CB	2.68	0.42
1:H:261:PHE:CE2	1:H:329:GLY:HA2	2.54	0.42
1:D:258:ASN:HB2	1:D:330:LEU:HD23	2.02	0.42
1:D:279:GLY:HA3	1:D:355:ALA:O	2.20	0.42
1:E:255:GLY:O	1:E:256:LYS:HB2	2.19	0.42
1:E:284:ALA:HA	1:E:287:PHE:CE2	2.54	0.42
1:H:46:LYS:HD3	1:H:52:MET:CE	2.49	0.42
1:A:142:LEU:HD12	1:A:228:ASN:HA	2.01	0.42
1:C:429:TYR:N	1:C:429:TYR:HD2	2.18	0.42
1:E:136:GLU:HB2	1:E:244:SER:HB2	2.01	0.42
1:E:317:ASN:HB3	1:E:320:PRO:HG3	2.01	0.42
1:E:321:LEU:HD12	1:E:321:LEU:O	2.20	0.42
1:E:340:ASP:HB2	1:E:341:PRO:CD	2.42	0.42
1:A:34:ILE:HB	1:C:161:LEU:HD11	1.99	0.42
1:A:340:ASP:HB2	1:A:341:PRO:CD	2.46	0.42
1:D:20:VAL:HA	1:D:90:LYS:HD2	2.02	0.42
1:D:78:THR:HG21	1:D:95:ILE:HB	2.02	0.42
1:H:127:THR:CG2	1:H:255:GLY:N	2.77	0.42
1:A:202:LYS:HG2	1:A:203:TYR:N	2.34	0.42
1:C:11:ILE:HG13	1:C:76:LEU:HD22	2.02	0.42
1:C:340:ASP:HB2	1:C:341:PRO:CD	2.50	0.42
1:C:408:LYS:NZ	6:C:607:HOH:O	2.53	0.42
1:D:117:VAL:HG11	1:D:354:GLU:HG3	2.02	0.42
1:E:245:GLY:C	1:E:341:PRO:HD3	2.41	0.42
1:E:252:LEU:HD12	1:E:260:PHE:CE1	2.50	0.42
1:E:271:GLU:HA	1:E:274:TYR:HB2	2.01	0.42
1:H:78:THR:O	1:H:80:VAL:HG23	2.20	0.42
1:D:45:GLU:O	1:D:49:ASP:HB2	2.20	0.41
1:B:364:LEU:HD23	1:B:364:LEU:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLY:C	1:A:256:LYS:HD2	2.41	0.41
1:D:429:TYR:N	1:D:429:TYR:CD1	2.88	0.41
1:B:289:ALA:HB3	1:B:401:MET:HE2	2.02	0.41
1:H:82:PHE:HA	1:H:83:PRO:HD3	1.94	0.41
1:A:186:GLU:O	1:A:187:ALA:HB2	2.19	0.41
1:A:198:GLU:OE1	3:A:502:P3S:O2A	2.38	0.41
1:D:214:GLN:OE1	1:D:214:GLN:HA	2.21	0.41
1:E:349:LEU:HD23	1:E:349:LEU:HA	1.77	0.41
1:B:267:MET:O	1:B:267:MET:CG	2.68	0.41
1:B:298:TYR:HB3	1:B:392:SER:O	2.20	0.41
1:H:56:GLY:HA3	1:H:70:MET:HG3	2.02	0.41
1:H:317:ASN:OD1	1:H:320:PRO:HD3	2.20	0.41
1:A:260:PHE:C	1:A:270:THR:HG23	2.41	0.41
1:C:156:GLY:HA2	1:C:164:THR:HG22	2.02	0.41
1:C:349:LEU:HD12	1:C:349:LEU:HA	1.87	0.41
1:D:54:PHE:CE1	1:D:70:MET:HB2	2.56	0.41
1:D:63:VAL:HG22	1:D:64:ARG:N	2.34	0.41
1:H:401:MET:HE3	1:H:420:ILE:HG13	2.03	0.41
1:A:246:MET:H	1:A:340:ASP:HA	1.85	0.41
1:C:276:PHE:CE1	1:C:356:GLY:HA3	2.56	0.41
1:D:27:PHE:CE2	1:D:59:ILE:HD12	2.56	0.41
1:D:84:TRP:CZ3	1:D:219:VAL:HG12	2.56	0.41
1:B:131:LEU:HA	1:B:249:ASN:O	2.21	0.41
1:H:83:PRO:HG3	1:H:180:ASP:O	2.21	0.41
1:H:328:ARG:HA	1:H:328:ARG:HD3	1.66	0.41
1:A:261:PHE:HB2	1:A:332:THR:OG1	2.21	0.41
1:A:404:ASN:O	1:A:407:ILE:HG22	2.21	0.41
1:D:398:LEU:HD23	1:D:401:MET:HE1	2.03	0.41
1:D:423:LYS:HA	1:D:423:LYS:HD3	1.91	0.41
1:E:181:MET:CE	1:E:219:VAL:HG21	2.50	0.41
1:B:100:LYS:NZ	1:B:104:THR:HG21	2.35	0.41
1:H:46:LYS:HG2	1:H:51:GLU:CB	2.50	0.41
1:H:235:PRO:O	1:H:244:SER:N	2.40	0.41
1:D:203:TYR:N	2:D:501:ADP:O2'	2.54	0.41
1:D:402:ARG:NH2	1:D:420:ILE:CD1	2.83	0.41
1:E:23:LEU:HD11	1:E:44:LEU:HD13	2.02	0.41
1:B:141:LYS:O	1:B:149:THR:HG23	2.21	0.41
1:B:255:GLY:O	1:B:257:GLU:N	2.53	0.41
1:B:395:TYR:HB2	1:B:427:TRP:CE2	2.55	0.41
1:A:50:ASN:OD1	1:A:74:PRO:HD2	2.21	0.41
1:D:44:LEU:HD12	1:D:44:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:THR:HG22	1:A:34:ILE:O	2.21	0.41
1:C:134:GLU:HB2	1:C:247:HIS:HB2	2.03	0.41
1:D:127:THR:HG21	1:D:255:GLY:CA	2.51	0.41
1:D:153:ASN:OD1	1:D:195:GLY:HA2	2.20	0.41
1:E:44:LEU:O	1:E:47:VAL:CG1	2.68	0.41
1:E:385:VAL:O	1:E:385:VAL:CG2	2.69	0.41
1:H:18:GLU:OE1	1:H:90:LYS:NZ	2.54	0.41
1:H:402:ARG:NH1	5:H:505:SO4:O2	2.54	0.41
1:A:279:GLY:O	1:A:283:ASN:ND2	2.53	0.41
1:D:258:ASN:HB2	1:D:330:LEU:CD2	2.51	0.41
1:E:20:VAL:HG11	1:E:92:ALA:CB	2.51	0.41
1:E:310:TYR:CD2	1:E:374:ILE:CG2	3.03	0.41
1:B:27:PHE:CZ	1:B:59:ILE:HD11	2.56	0.41
1:B:127:THR:HG23	1:B:254:LYS:HA	2.01	0.41
1:H:394:LEU:O	1:H:394:LEU:HG	2.21	0.41
1:D:270:THR:O	1:D:274:TYR:HD2	2.04	0.40
1:D:281:LEU:HD23	1:D:321:LEU:HD23	2.03	0.40
1:E:63:VAL:HB	1:E:67:GLU:HG3	2.02	0.40
1:C:308:PRO:HB3	1:C:321:LEU:HA	2.02	0.40
1:D:380:GLU:O	1:D:384:ALA:N	2.45	0.40
1:E:23:LEU:HD23	1:E:23:LEU:HA	1.94	0.40
1:E:59:ILE:HG21	1:E:62:PHE:CE2	2.57	0.40
1:B:25:LEU:CD1	1:B:52:MET:HG3	2.51	0.40
1:B:237:PRO:O	1:B:238:LEU:HD23	2.21	0.40
1:A:314:SER:CB	1:A:317:ASN:HB3	2.51	0.40
1:D:63:VAL:HB	1:D:70:MET:CE	2.44	0.40
1:D:284:ALA:HA	1:D:287:PHE:CZ	2.56	0.40
1:D:308:PRO:HB3	1:D:321:LEU:HA	2.03	0.40
1:D:327:SER:C	1:D:328:ARG:HG2	2.42	0.40
1:E:45:GLU:HA	1:E:48:LEU:HB2	2.03	0.40
1:H:322:ILE:HG21	1:H:334:ILE:HG23	2.02	0.40
1:A:108:GLY:HA2	1:A:415:ILE:HG13	2.02	0.40
1:C:15:VAL:HG13	1:C:20:VAL:HG22	2.03	0.40
1:D:81:ILE:HG12	1:D:92:ALA:HB2	2.02	0.40
1:E:287:PHE:HD1	1:E:291:CYS:HG	1.63	0.40
1:E:431:ARG:O	1:E:431:ARG:CG	2.65	0.40
1:B:129:PHE:CE2	1:B:353:LEU:HD13	2.56	0.40
1:A:116:ARG:HG2	1:A:116:ARG:HH11	1.86	0.40
1:C:402:ARG:HA	1:C:416:TYR:OH	2.22	0.40
1:D:63:VAL:H	1:D:70:MET:CE	2.35	0.40
1:D:373:ASN:HD22	1:H:64:ARG:HH12	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:GLU:OE1	1:E:198:GLU:OE1	2.40	0.40
1:B:133:PRO:HG2	1:B:201:PHE:CZ	2.56	0.40
1:H:284:ALA:HA	1:H:287:PHE:CZ	2.57	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:LYS:NZ	1:B:438:GLU:OE2[7_465]	1.39	0.81
1:E:299:LYS:NZ	1:E:438:GLU:OE1[7_465]	1.70	0.50
1:C:442:TYR:OH	1:H:426:GLU:OE1[7_465]	2.02	0.18
1:C:426:GLU:OE2	1:H:442:TYR:OH[7_465]	2.13	0.07
1:B:299:LYS:CE	1:B:438:GLU:OE2[7_465]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	440/449 (98%)	416 (94%)	24 (6%)	0	100	100
1	B	441/449 (98%)	412 (93%)	29 (7%)	0	100	100
1	C	441/449 (98%)	417 (95%)	24 (5%)	0	100	100
1	D	440/449 (98%)	421 (96%)	19 (4%)	0	100	100
1	E	440/449 (98%)	415 (94%)	25 (6%)	0	100	100
1	H	440/449 (98%)	418 (95%)	22 (5%)	0	100	100
All	All	2642/2694 (98%)	2499 (95%)	143 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	381/391 (97%)	371 (97%)	10 (3%)	46	76
1	B	381/391 (97%)	375 (98%)	6 (2%)	62	85
1	C	383/391 (98%)	373 (97%)	10 (3%)	46	76
1	D	382/391 (98%)	365 (96%)	17 (4%)	27	59
1	E	381/391 (97%)	366 (96%)	15 (4%)	32	64
1	H	381/391 (97%)	371 (97%)	10 (3%)	46	76
All	All	2289/2346 (98%)	2221 (97%)	68 (3%)	41	73

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	93	ARG
1	A	119	LYS
1	A	121	MET
1	A	188	SER
1	A	256	LYS
1	A	287	PHE
1	A	309	CYS
1	A	422	SER
1	A	436	GLU
1	C	52	MET
1	C	73	HIS
1	C	145	LYS
1	C	188	SER
1	C	225	ARG
1	C	256	LYS
1	C	293	PRO
1	C	333	ARG
1	C	379	ARG
1	C	409	LYS
1	D	6	PHE
1	D	13	LYS

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Mol	Chain	Res	Type
1	D	49	ASP
1	D	68	SER
1	D	73	HIS
1	D	93	ARG
1	D	113	ASN
1	D	120	GLU
1	D	256	LYS
1	D	285	ARG
1	D	287	PHE
1	D	318	ARG
1	D	319	SER
1	D	333	ARG
1	D	402	ARG
1	D	428	ASP
1	D	440	ASP
1	E	42	SER
1	E	64	ARG
1	E	173	ASP
1	E	175	VAL
1	E	176	LEU
1	E	234	MET
1	E	242	ASN
1	E	309	CYS
1	E	310	TYR
1	E	316	LYS
1	E	318	ARG
1	E	358	ASP
1	E	365	LYS
1	E	429	TYR
1	E	436	GLU
1	B	49	ASP
1	B	121	MET
1	B	172	ARG
1	B	188	SER
1	B	287	PHE
1	B	365	LYS
1	H	13	LYS
1	H	42	SER
1	H	64	ARG
1	H	66	GLU
1	H	68	SER
1	H	73	HIS

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Mol	Chain	Res	Type
1	H	128	ASP
1	H	147	GLU
1	H	188	SER
1	H	299	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	36	ASN
1	A	196	GLN
1	D	36	ASN
1	E	36	ASN
1	E	196	GLN
1	E	242	ASN
1	E	283	ASN
1	B	264	ASN
1	B	414	HIS
1	H	275	GLN
1	H	378	ASN
1	H	388	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 21 are monoatomic - leaving 13 for Mogul analysis.

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	P3S	H	502	4	11,14,14	2.14	4 (36%)	12,21,21	11.05	6 (50%)
3	P3S	D	502	4	11,14,14	1.88	3 (27%)	12,21,21	10.95	4 (33%)
2	ADP	C	501	4	24,29,29	0.88	0	29,45,45	2.14	11 (37%)
3	P3S	C	502	4	11,14,14	1.78	2 (18%)	12,21,21	12.06	4 (33%)
3	P3S	B	502	4	11,14,14	2.22	3 (27%)	12,21,21	12.01	3 (25%)
3	P3S	E	502	4	11,14,14	2.10	3 (27%)	12,21,21	11.36	3 (25%)
2	ADP	E	501	4	24,29,29	0.84	1 (4%)	29,45,45	1.84	7 (24%)
2	ADP	D	501	4	24,29,29	0.99	2 (8%)	29,45,45	1.63	7 (24%)
3	P3S	A	502	4	11,14,14	1.87	3 (27%)	12,21,21	12.11	4 (33%)
5	SO4	H	505	-	4,4,4	0.15	0	6,6,6	0.11	0
2	ADP	A	501	4	24,29,29	1.06	2 (8%)	29,45,45	1.52	5 (17%)
2	ADP	B	501	4	24,29,29	0.84	1 (4%)	29,45,45	2.06	10 (34%)
2	ADP	H	501	4	24,29,29	1.11	3 (12%)	29,45,45	2.29	8 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P3S	H	502	4	-	6/9/16/16	-
3	P3S	D	502	4	-	5/9/16/16	-
2	ADP	C	501	4	-	4/12/32/32	0/3/3/3
3	P3S	C	502	4	-	5/9/16/16	-
3	P3S	B	502	4	-	8/9/16/16	-
3	P3S	E	502	4	-	3/9/16/16	-
2	ADP	E	501	4	-	4/12/32/32	0/3/3/3
2	ADP	D	501	4	-	2/12/32/32	0/3/3/3
3	P3S	A	502	4	-	5/9/16/16	-
2	ADP	A	501	4	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	501	4	-	7/12/32/32	0/3/3/3
2	ADP	H	501	4	-	2/12/32/32	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	502	P3S	PA-O1A	4.28	1.53	1.46
3	H	502	P3S	PA-NE	4.14	1.74	1.59
3	B	502	P3S	PA-O1A	4.05	1.53	1.46
3	A	502	P3S	PA-O1A	3.81	1.52	1.46
3	C	502	P3S	PA-O1A	3.80	1.52	1.46
3	B	502	P3S	PA-NE	3.78	1.73	1.59
3	E	502	P3S	PA-O1A	3.75	1.52	1.46
3	E	502	P3S	PA-NE	3.74	1.73	1.59
3	D	502	P3S	PA-NE	3.72	1.73	1.59
3	B	502	P3S	CB-CG	3.46	1.56	1.52
3	D	502	P3S	PA-O1A	3.27	1.51	1.46
3	C	502	P3S	PA-NE	3.26	1.71	1.59
3	E	502	P3S	CB-CG	3.15	1.55	1.52
3	A	502	P3S	PA-NE	3.14	1.70	1.59
2	A	501	ADP	O4'-C1'	2.57	1.44	1.41
2	H	501	ADP	O4'-C1'	2.51	1.44	1.41
2	D	501	ADP	O4'-C1'	2.48	1.44	1.41
3	D	502	P3S	CB-CG	2.43	1.55	1.52
2	D	501	ADP	C5-C4	2.38	1.47	1.40
2	H	501	ADP	C5-C4	2.34	1.47	1.40
2	H	501	ADP	C2-N3	2.31	1.35	1.32
2	A	501	ADP	C5-C4	2.29	1.47	1.40
3	H	502	P3S	O-C	2.19	1.28	1.22
3	A	502	P3S	O-C	2.18	1.28	1.22
2	B	501	ADP	C5-C4	2.18	1.46	1.40
2	E	501	ADP	C5-C4	2.07	1.46	1.40
3	H	502	P3S	CB-CG	2.00	1.54	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	P3S	OE-SD-CG	37.90	138.04	108.37
3	A	502	P3S	OE-SD-CG	36.96	137.30	108.37
3	B	502	P3S	OE-SD-CG	36.69	137.09	108.37
3	E	502	P3S	OE-SD-CG	35.57	136.21	108.37
3	D	502	P3S	OE-SD-CG	33.10	134.27	108.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	502	P3S	OE-SD-CG	32.61	133.89	108.37
3	H	502	P3S	OE-SD-CE	-17.44	81.48	109.24
3	B	502	P3S	OE-SD-CE	-16.95	82.26	109.24
3	A	502	P3S	OE-SD-CE	-16.80	82.49	109.24
3	D	502	P3S	OE-SD-CE	-16.16	83.51	109.24
3	C	502	P3S	OE-SD-CE	-15.02	85.32	109.24
3	E	502	P3S	OE-SD-CE	-14.26	86.53	109.24
3	A	502	P3S	CE-SD-NE	9.62	141.10	107.48
3	B	502	P3S	CE-SD-NE	9.19	139.60	107.48
3	C	502	P3S	CE-SD-NE	8.43	136.95	107.48
3	E	502	P3S	CE-SD-NE	8.31	136.51	107.48
3	H	502	P3S	CE-SD-NE	8.22	136.21	107.48
3	D	502	P3S	CE-SD-NE	7.92	135.17	107.48
2	C	501	ADP	C1'-N9-C4	-5.55	116.88	126.64
2	H	501	ADP	C1'-N9-C4	-5.09	117.69	126.64
2	H	501	ADP	C2'-C3'-C4'	4.89	112.14	102.64
2	B	501	ADP	O3'-C3'-C4'	-4.75	97.30	111.05
2	B	501	ADP	C1'-N9-C4	-4.66	118.45	126.64
2	H	501	ADP	O3'-C3'-C4'	-4.64	97.65	111.05
2	C	501	ADP	N3-C2-N1	-4.56	121.55	128.68
2	E	501	ADP	C1'-N9-C4	-4.35	119.01	126.64
2	E	501	ADP	N3-C2-N1	-4.32	121.93	128.68
2	H	501	ADP	O2'-C2'-C1'	4.23	126.48	110.85
2	H	501	ADP	O4'-C1'-C2'	3.99	112.75	106.93
2	D	501	ADP	C2'-C3'-C4'	3.95	110.31	102.64
2	C	501	ADP	O4'-C1'-C2'	3.71	112.34	106.93
2	E	501	ADP	C2'-C3'-C4'	3.71	109.84	102.64
2	B	501	ADP	N3-C2-N1	-3.68	122.92	128.68
3	H	502	P3S	O3A-PA-O1A	-3.67	105.59	113.45
2	D	501	ADP	N3-C2-N1	-3.61	123.04	128.68
2	B	501	ADP	C2'-C3'-C4'	3.47	109.38	102.64
2	A	501	ADP	N3-C2-N1	-3.38	123.40	128.68
2	A	501	ADP	C2'-C3'-C4'	3.09	108.66	102.64
2	A	501	ADP	C4-C5-N7	-3.00	106.28	109.40
3	A	502	P3S	O3A-PA-O1A	-2.98	107.06	113.45
2	H	501	ADP	N3-C2-N1	-2.97	124.04	128.68
2	E	501	ADP	C2-N1-C6	2.95	123.80	118.75
2	A	501	ADP	C1'-N9-C4	-2.94	121.47	126.64
2	C	501	ADP	C5-C6-N6	-2.89	115.95	120.35
2	C	501	ADP	PA-O3A-PB	-2.88	122.93	132.83
2	E	501	ADP	O3'-C3'-C4'	-2.85	102.80	111.05
2	B	501	ADP	C5'-C4'-C3'	2.84	125.81	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	ADP	C1'-N9-C4	-2.79	121.73	126.64
2	A	501	ADP	O3'-C3'-C4'	-2.77	103.05	111.05
2	C	501	ADP	O3'-C3'-C4'	-2.64	103.43	111.05
2	B	501	ADP	O3B-PB-O2B	2.62	117.63	107.64
2	D	501	ADP	O4'-C1'-C2'	2.58	110.69	106.93
3	D	502	P3S	CB-CA-C	2.50	116.26	110.30
2	C	501	ADP	O4'-C4'-C3'	2.49	110.05	105.11
2	B	501	ADP	O4'-C1'-C2'	2.36	110.38	106.93
2	B	501	ADP	PA-O3A-PB	-2.35	124.75	132.83
2	C	501	ADP	C3'-C2'-C1'	-2.32	97.48	100.98
2	D	501	ADP	O3'-C3'-C4'	-2.32	104.34	111.05
2	D	501	ADP	PA-O3A-PB	-2.29	124.95	132.83
3	C	502	P3S	CB-CA-C	-2.27	104.89	110.30
2	B	501	ADP	N6-C6-N1	2.20	123.15	118.57
2	H	501	ADP	PA-O3A-PB	-2.18	125.34	132.83
3	H	502	P3S	OT-C-CA	2.15	120.70	113.38
2	D	501	ADP	C4-C5-N7	-2.13	107.18	109.40
2	H	501	ADP	C3'-C2'-C1'	-2.13	97.77	100.98
2	B	501	ADP	C2-N1-C6	2.11	122.36	118.75
2	E	501	ADP	O4'-C1'-C2'	2.09	109.98	106.93
2	C	501	ADP	O2B-PB-O1B	2.07	118.80	110.68
2	E	501	ADP	PA-O3A-PB	-2.07	125.72	132.83
3	H	502	P3S	OT-C-O	-2.03	119.48	124.09
2	C	501	ADP	O3A-PB-O1B	-2.02	99.99	111.19
2	C	501	ADP	O2A-PA-O1A	2.02	122.21	112.24

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	ADP	O4'-C4'-C5'-O5'
2	C	501	ADP	PA-O3A-PB-O3B
2	D	501	ADP	O4'-C4'-C5'-O5'
2	E	501	ADP	PA-O3A-PB-O2B
2	E	501	ADP	O4'-C4'-C5'-O5'
2	E	501	ADP	C3'-C4'-C5'-O5'
2	B	501	ADP	PA-O3A-PB-O2B
3	A	502	P3S	O-C-CA-N
3	C	502	P3S	CB-CG-SD-CE
3	C	502	P3S	O-C-CA-N
3	D	502	P3S	CB-CG-SD-CE
3	D	502	P3S	O-C-CA-N

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Mol	Chain	Res	Type	Atoms
3	E	502	P3S	CB-CG-SD-OE
3	B	502	P3S	CB-CG-SD-OE
3	B	502	P3S	CB-CG-SD-CE
3	B	502	P3S	N-CA-CB-CG
3	B	502	P3S	O-C-CA-N
3	H	502	P3S	CB-CG-SD-OE
3	H	502	P3S	CB-CG-SD-CE
3	H	502	P3S	N-CA-CB-CG
3	H	502	P3S	C-CA-CB-CG
3	C	502	P3S	OT-C-CA-N
2	C	501	ADP	O4'-C4'-C5'-O5'
2	C	501	ADP	C3'-C4'-C5'-O5'
2	B	501	ADP	O4'-C4'-C5'-O5'
2	H	501	ADP	O4'-C4'-C5'-O5'
3	A	502	P3S	OT-C-CA-N
3	B	502	P3S	OT-C-CA-N
2	A	501	ADP	C3'-C4'-C5'-O5'
2	D	501	ADP	C3'-C4'-C5'-O5'
3	D	502	P3S	OT-C-CA-N
2	H	501	ADP	C3'-C4'-C5'-O5'
3	C	502	P3S	OT-C-CA-CB
3	B	502	P3S	C-CA-CB-CG
2	B	501	ADP	C3'-C4'-C5'-O5'
3	C	502	P3S	O-C-CA-CB
3	B	502	P3S	O-C-CA-CB
3	A	502	P3S	OT-C-CA-CB
3	B	502	P3S	OT-C-CA-CB
3	H	502	P3S	OT-C-CA-CB
3	E	502	P3S	OT-C-CA-CB
2	E	501	ADP	PA-O3A-PB-O3B
2	B	501	ADP	C5'-O5'-PA-O3A
3	H	502	P3S	O-C-CA-CB
2	B	501	ADP	C5'-O5'-PA-O2A
3	A	502	P3S	CB-CG-SD-CE
3	A	502	P3S	O-C-CA-CB
3	E	502	P3S	O-C-CA-CB
3	D	502	P3S	O-C-CA-CB
3	D	502	P3S	OT-C-CA-CB
2	C	501	ADP	PA-O3A-PB-O1B
2	B	501	ADP	PA-O3A-PB-O3B
2	B	501	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	502	P3S	1	0
3	D	502	P3S	1	0
3	B	502	P3S	1	0
3	E	502	P3S	1	0
2	D	501	ADP	4	0
3	A	502	P3S	3	0
5	H	505	SO4	1	0
2	A	501	ADP	3	0
2	B	501	ADP	2	0
2	H	501	ADP	2	0

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

Ligand P3S H 502
Bond lengths
Bond angles
Torsions
Rings

Ligand P3S D 502

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand P3S C 502

Bond lengths

Bond angles

Torsions

Rings

Ligand P3S B 502

Bond lengths

Bond angles

Torsions

Rings

Ligand P3S E 502

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP E 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand P3S A 502

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP H 501

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	442/449 (98%)	0.05	14 (3%)	47	44	47, 68, 96, 106	0
1	B	443/449 (98%)	-0.08	6 (1%)	75	76	41, 62, 92, 111	0
1	C	443/449 (98%)	-0.03	6 (1%)	75	76	42, 59, 87, 105	0
1	D	442/449 (98%)	0.32	28 (6%)	20	17	47, 74, 102, 112	0
1	E	442/449 (98%)	0.41	33 (7%)	14	11	51, 79, 103, 122	1 (0%)
1	H	442/449 (98%)	-0.03	6 (1%)	75	76	40, 61, 88, 102	0
All	All	2654/2694 (98%)	0.11	93 (3%)	44	40	40, 67, 96, 122	1 (0%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	311	ILE	5.4
1	E	267	MET	4.8
1	E	385	VAL	4.8
1	A	385	VAL	4.4
1	E	386	GLY	4.0
1	C	4	ARG	4.0
1	E	364	LEU	3.9
1	E	387	ILE	3.9
1	A	144	GLU	3.6
1	D	387	ILE	3.6
1	A	364	LEU	3.5
1	E	14	PHE	3.3
1	D	12	ARG	3.2
1	E	274	TYR	3.2
1	A	445	GLN	3.2
1	D	87	GLY	3.1
1	E	144	GLU	3.1
1	D	16	GLU	3.0
1	D	145	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	330	LEU	3.0
1	E	13	LYS	3.0
1	D	403	GLU	3.0
1	C	6	PHE	2.9
1	E	312	ALA	2.9
1	A	384	ALA	2.9
1	D	260	PHE	2.9
1	D	383	GLU	2.9
1	D	388	GLN	2.8
1	E	282	LYS	2.8
1	D	269	LEU	2.8
1	E	10	ASP	2.8
1	D	144	GLU	2.8
1	E	269	LEU	2.8
1	E	271	GLU	2.7
1	C	14	PHE	2.7
1	D	86	ALA	2.6
1	D	386	GLY	2.6
1	A	143	ASP	2.6
1	E	260	PHE	2.6
1	A	380	GLU	2.6
1	A	269	LEU	2.5
1	A	446	TYR	2.5
1	E	264	ASN	2.5
1	E	277	THR	2.4
1	H	387	ILE	2.4
1	D	266	GLU	2.4
1	E	257	GLU	2.4
1	D	385	VAL	2.4
1	C	379	ARG	2.4
1	E	366	VAL	2.3
1	D	124	LEU	2.3
1	D	291	CYS	2.3
1	C	9	GLU	2.3
1	D	17	GLU	2.3
1	E	262	ASP	2.3
1	D	313	TRP	2.3
1	E	17	GLU	2.2
1	D	384	ALA	2.2
1	B	86	ALA	2.2
1	E	16	GLU	2.2
1	H	9	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	86	ALA	2.2
1	A	388	GLN	2.2
1	B	87	GLY	2.2
1	B	361	LYS	2.2
1	E	313	TRP	2.1
1	H	144	GLU	2.1
1	E	279	GLY	2.1
1	D	120	GLU	2.1
1	E	380	GLU	2.1
1	E	44	LEU	2.1
1	H	407	ILE	2.1
1	A	362	ASN	2.1
1	E	362	ASN	2.1
1	A	266	GLU	2.1
1	D	88	GLN	2.1
1	E	368	GLU	2.1
1	B	144	GLU	2.1
1	D	104	THR	2.1
1	B	382	ARG	2.1
1	E	20	VAL	2.1
1	D	10	ASP	2.1
1	B	363	LYS	2.1
1	E	280	VAL	2.0
1	D	6	PHE	2.0
1	D	311	ILE	2.0
1	E	278	ALA	2.0
1	A	120	GLU	2.0
1	H	403	GLU	2.0
1	H	411	LEU	2.0
1	A	145	LYS	2.0
1	E	384	ALA	2.0
1	D	332	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
4	MG	C	507	1/1	0.77	0.24	81,81,81,81	0
4	MG	E	505	1/1	0.77	0.61	73,73,73,73	0
5	SO4	H	505	5/5	0.81	0.57	187,187,188,188	0
4	MG	B	505	1/1	0.83	0.12	85,85,85,85	0
4	MG	D	505	1/1	0.84	1.09	104,104,104,104	0
4	MG	B	507	1/1	0.86	0.38	82,82,82,82	0
4	MG	C	506	1/1	0.88	0.09	90,90,90,90	0
4	MG	E	503	1/1	0.88	0.34	63,63,63,63	0
2	ADP	E	501	27/27	0.91	0.24	65,77,96,97	0
4	MG	E	506	1/1	0.92	0.37	89,89,89,89	0
2	ADP	D	501	27/27	0.92	0.21	59,78,96,101	0
4	MG	C	503	1/1	0.93	0.30	48,48,48,48	0
4	MG	D	503	1/1	0.93	0.30	57,57,57,57	0
4	MG	H	503	1/1	0.93	0.36	43,43,43,43	0
2	ADP	A	501	27/27	0.93	0.21	66,75,91,92	0
3	P3S	D	502	15/15	0.94	0.21	62,72,86,86	0
3	P3S	E	502	15/15	0.94	0.22	65,78,93,95	0
3	P3S	H	502	15/15	0.94	0.25	52,64,79,82	0
2	ADP	B	501	27/27	0.94	0.18	49,57,71,73	0
2	ADP	H	501	27/27	0.94	0.21	43,56,71,77	0
4	MG	B	503	1/1	0.95	0.28	48,48,48,48	0
4	MG	B	504	1/1	0.95	0.18	51,51,51,51	0
4	MG	C	504	1/1	0.95	0.29	49,49,49,49	0
2	ADP	C	501	27/27	0.95	0.18	45,49,60,61	0
4	MG	A	503	1/1	0.95	0.40	61,61,61,61	0
3	P3S	A	502	15/15	0.95	0.21	61,67,81,81	0
4	MG	E	504	1/1	0.96	0.16	66,66,66,66	0
3	P3S	C	502	15/15	0.96	0.22	44,48,58,58	0
4	MG	B	506	1/1	0.96	0.15	53,53,53,53	0
3	P3S	B	502	15/15	0.97	0.19	53,67,79,82	0
4	MG	A	504	1/1	0.97	0.19	63,63,63,63	0
4	MG	H	504	1/1	0.97	0.24	53,53,53,53	0
4	MG	C	505	1/1	0.97	0.23	47,47,47,47	0
4	MG	D	504	1/1	0.99	0.12	60,60,60,60	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 ADP E 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
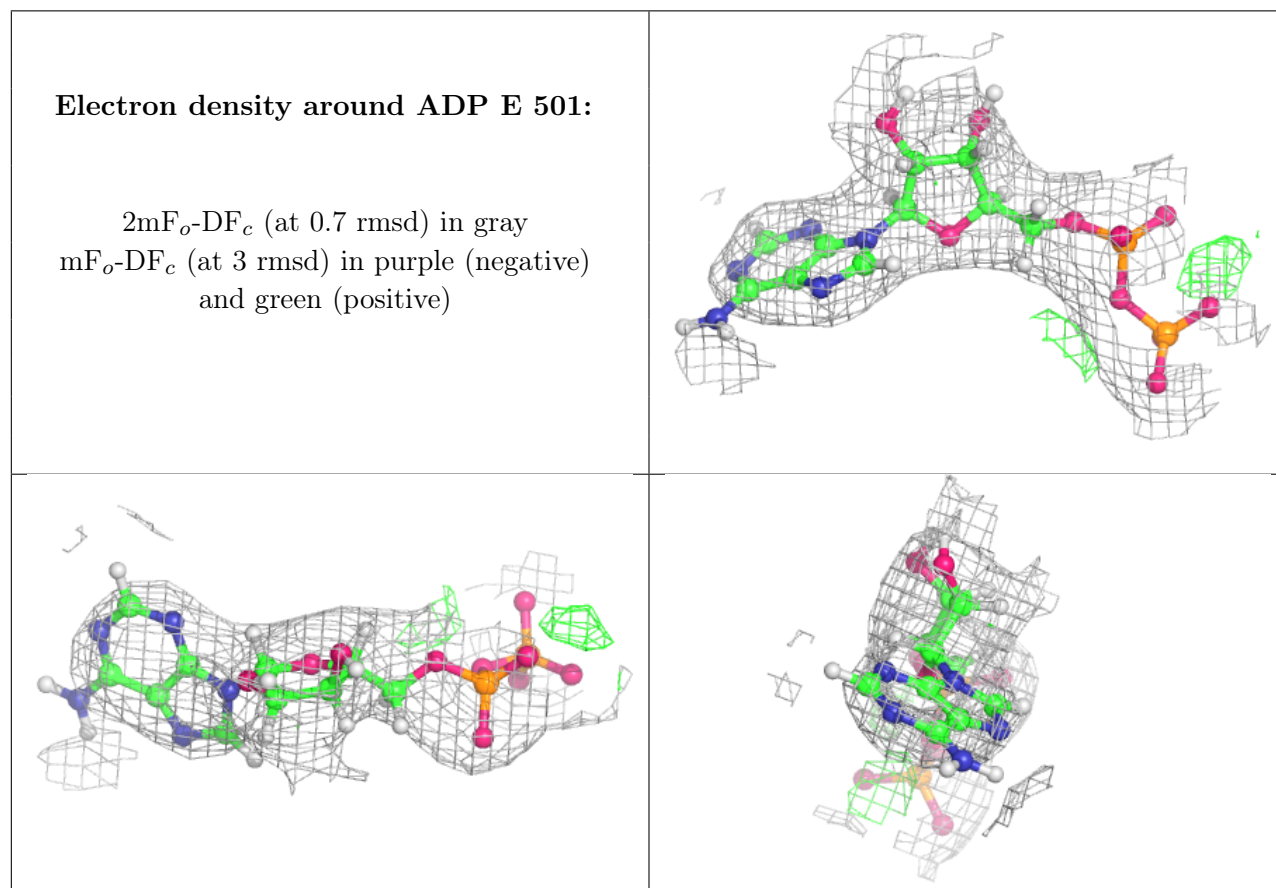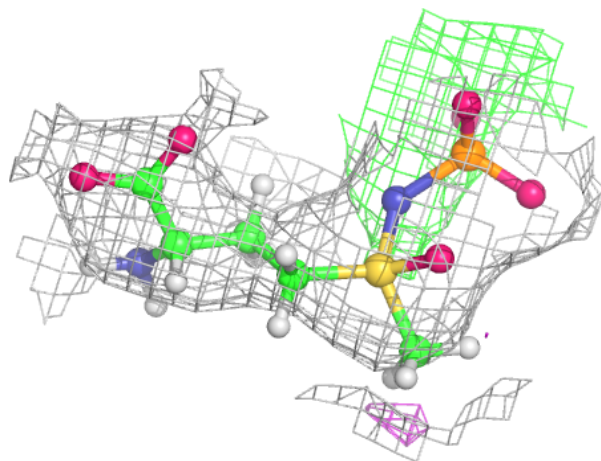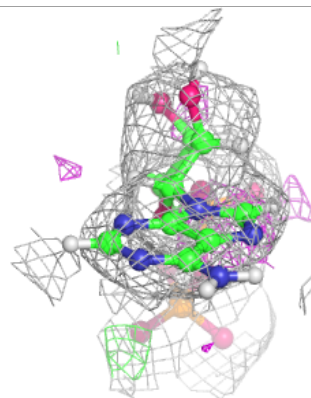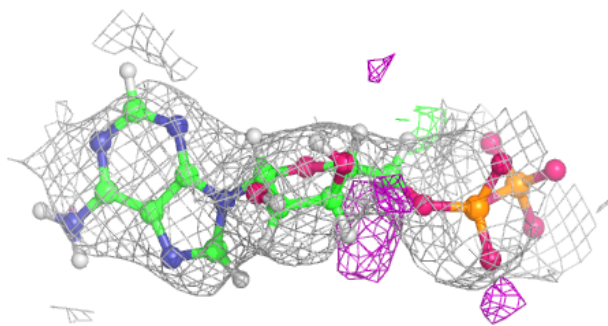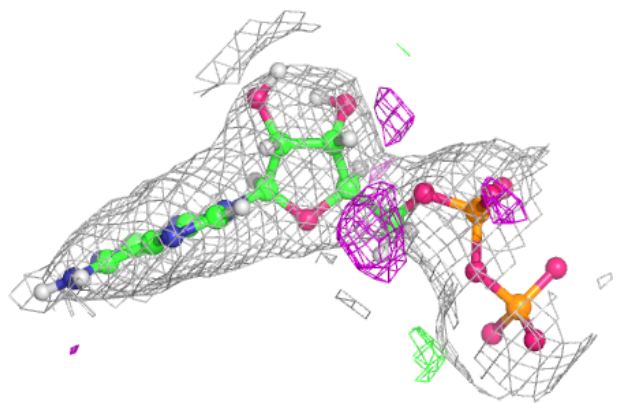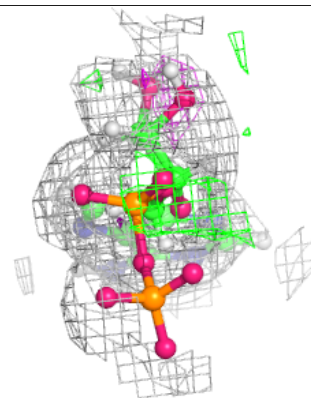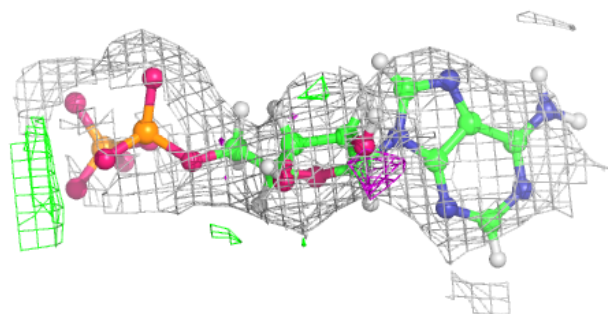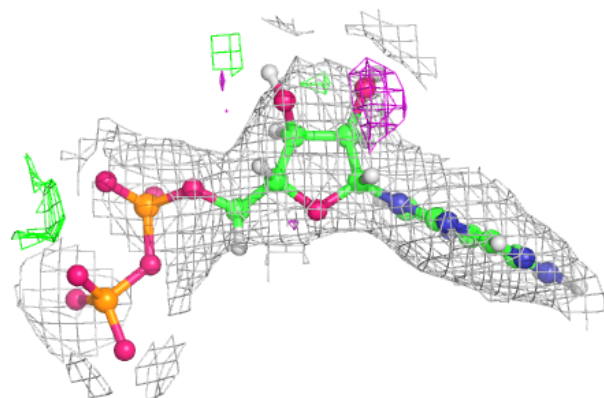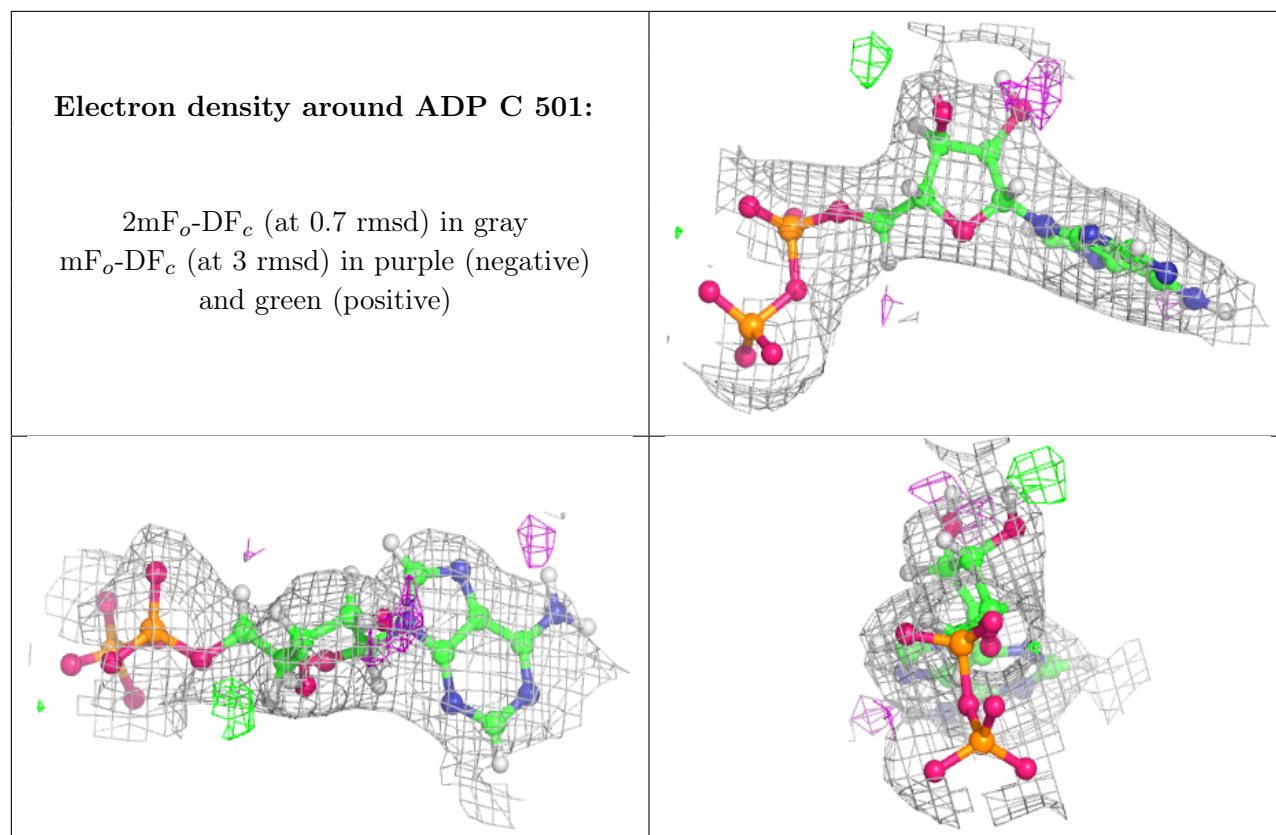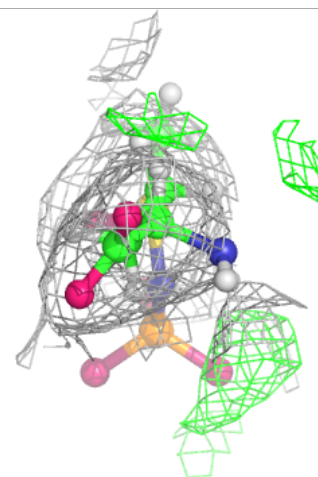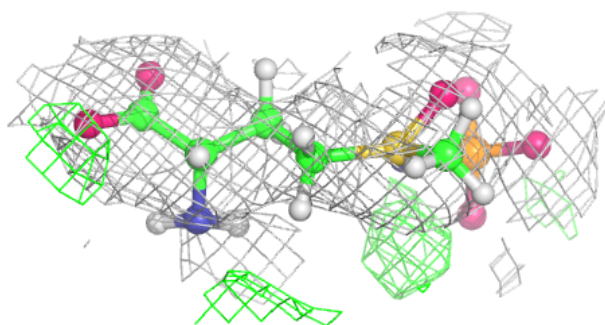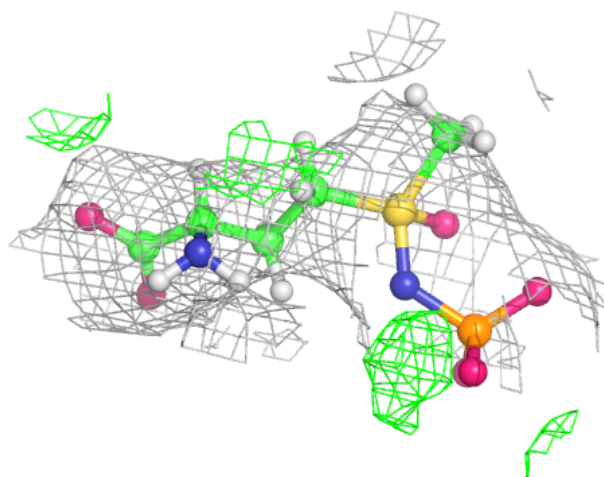
Electron density around ADP D 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
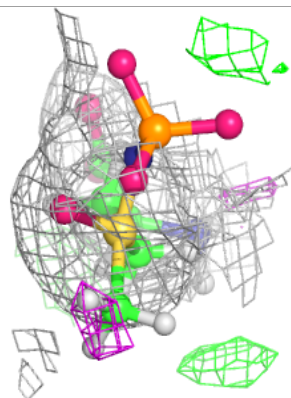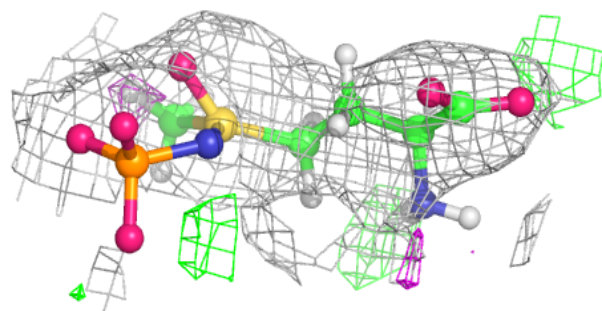and green (positive)
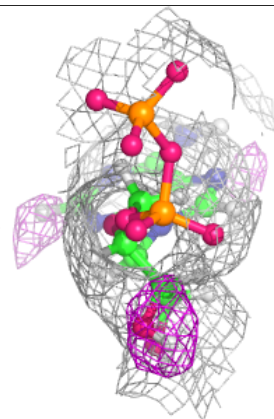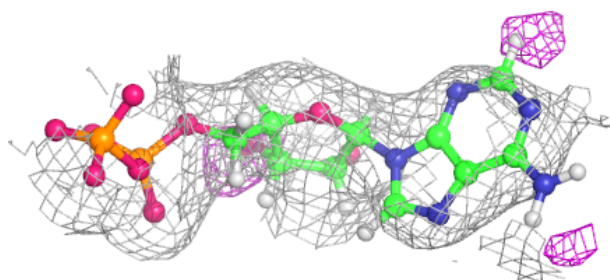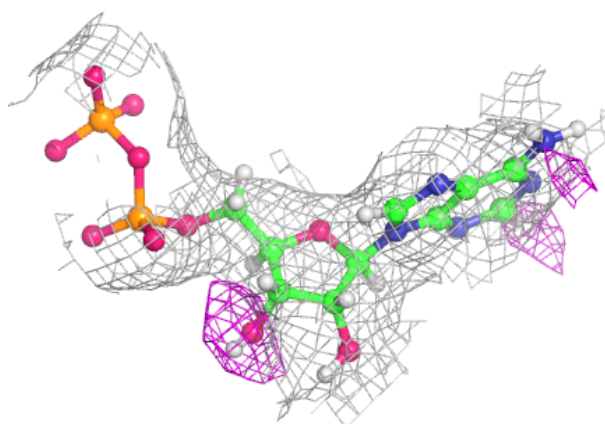
Electron density around ADP A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
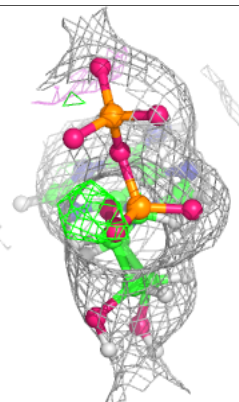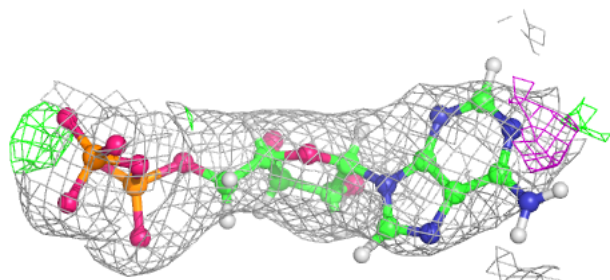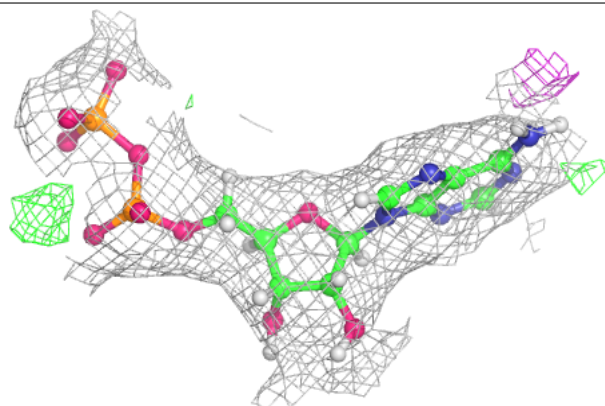
Electron density around P3S D 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
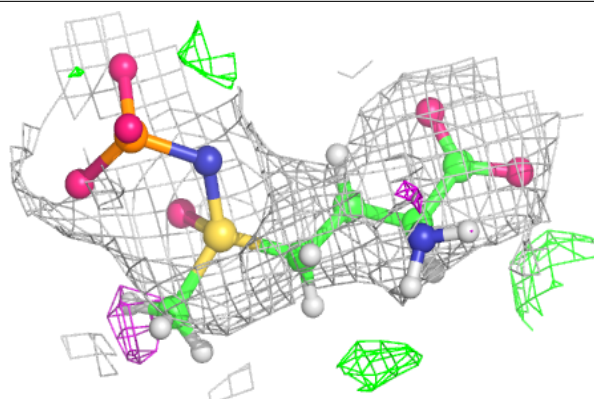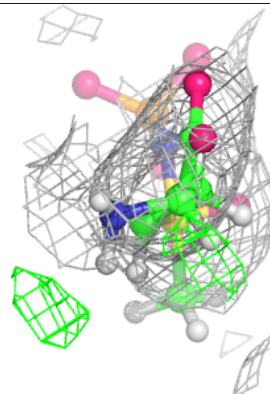and green (positive)
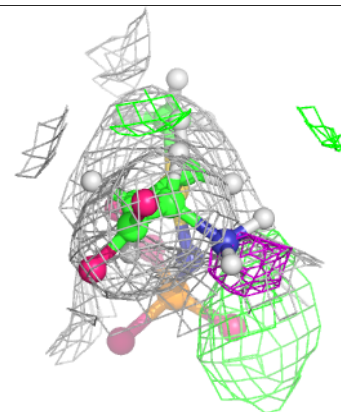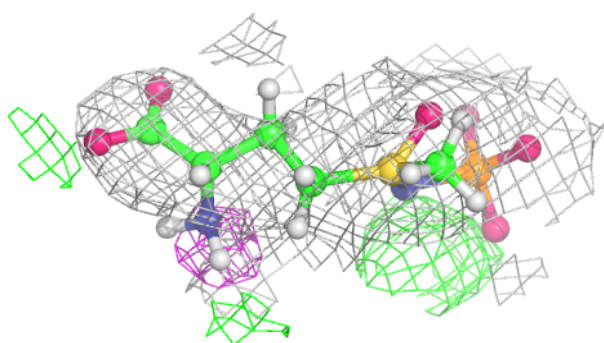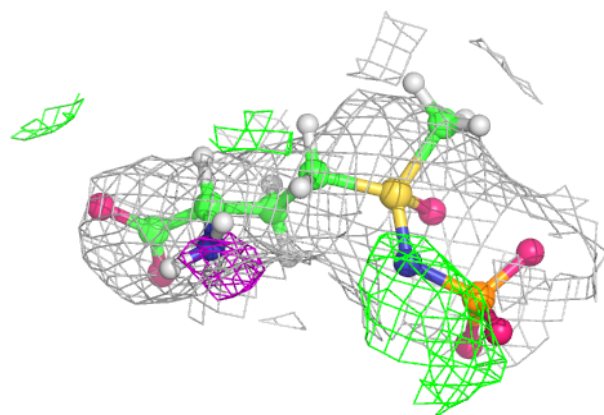
Electron density around P3S E 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
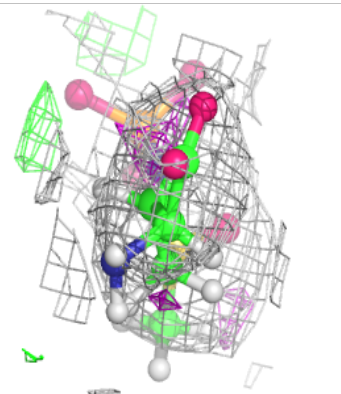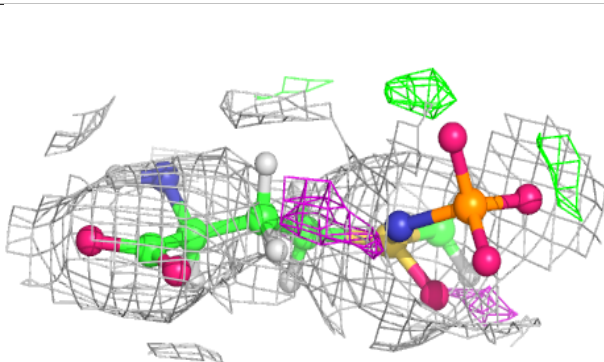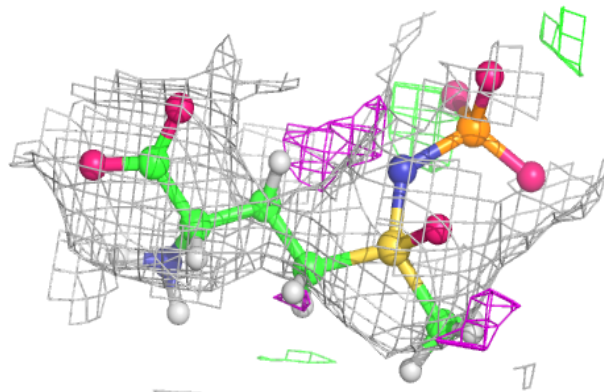
Electron density around P3S H 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
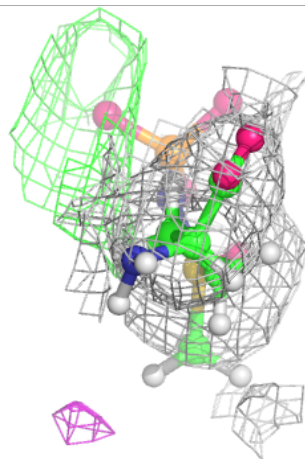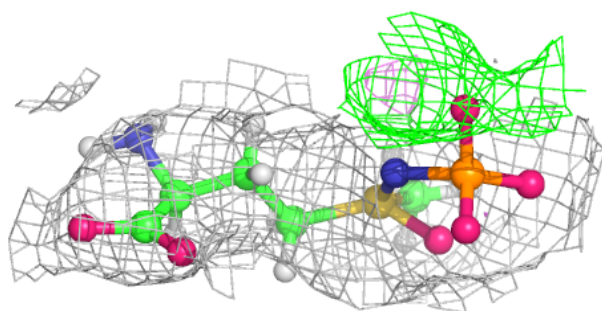
Electron density around ADP B 501:

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

Electron density around ADP H 501:

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

Electron density around ADP C 501:

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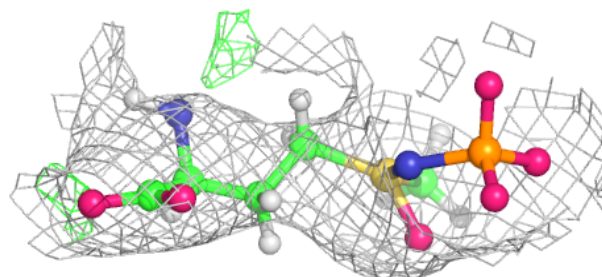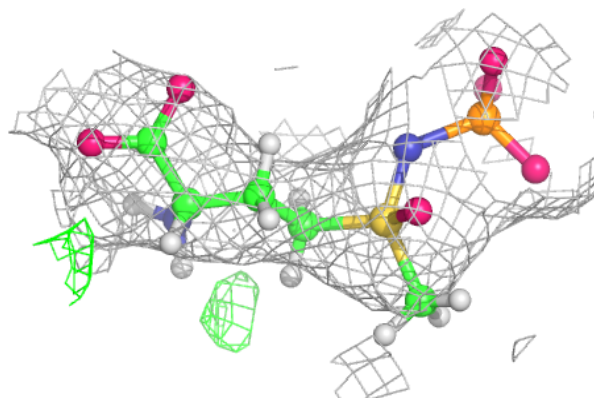and green (positive)

Electron density around P3S A 502:

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

Electron density around P3S C 502:

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

Electron density around P3S B 502:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.