WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 10:52 AM EST

PDB ID	:	3T0T
Title	:	Crystal structure of S. aureus Pyruvate Kinase
Authors	:	Worrall, L.J.; Vuckovic, M.; Strynadka, N.C.J.
Deposited on	:	2011-07-20
Resolution	:	3.10 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

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 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
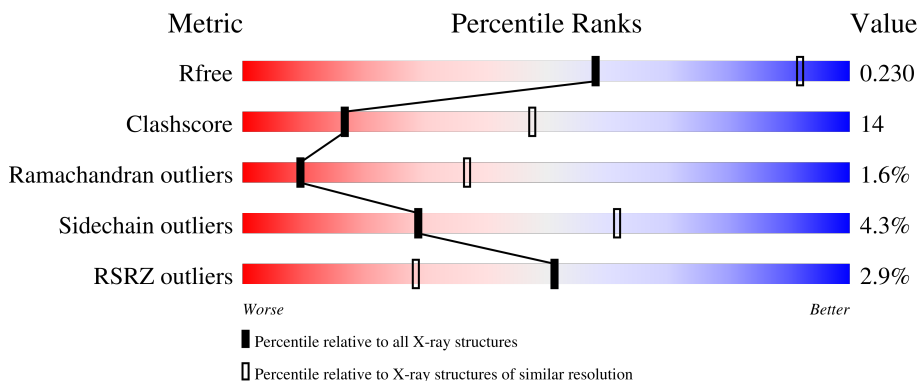
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	606	2% 68% 25% · ·
1	B	606	5% 69% 25% · ·
1	C	606	3% 68% 25% · ·
1	D	606	70% 24% · ·

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
3	PO4	A	587	-	-	X	-
3	PO4	B	586	-	-	X	-
3	PO4	D	587	-	-	X	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 17694 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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	0	0
			4407	2745	764	880	18			
1	B	583	Total	C	N	O	S	0	0	0
			4407	2745	764	880	18			
1	C	583	Total	C	N	O	S	0	0	0
			4407	2745	764	880	18			
1	D	583	Total	C	N	O	S	0	0	0
			4407	2745	764	880	18			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q6GG09
A	-19	GLY	-	expression tag	UNP Q6GG09
A	-18	SER	-	expression tag	UNP Q6GG09
A	-17	SER	-	expression tag	UNP Q6GG09
A	-16	HIS	-	expression tag	UNP Q6GG09
A	-15	HIS	-	expression tag	UNP Q6GG09
A	-14	HIS	-	expression tag	UNP Q6GG09
A	-13	HIS	-	expression tag	UNP Q6GG09
A	-12	HIS	-	expression tag	UNP Q6GG09
A	-11	HIS	-	expression tag	UNP Q6GG09
A	-10	SER	-	expression tag	UNP Q6GG09
A	-9	SER	-	expression tag	UNP Q6GG09
A	-8	GLY	-	expression tag	UNP Q6GG09
A	-7	LEU	-	expression tag	UNP Q6GG09
A	-6	VAL	-	expression tag	UNP Q6GG09
A	-5	PRO	-	expression tag	UNP Q6GG09
A	-4	ARG	-	expression tag	UNP Q6GG09
A	-3	GLY	-	expression tag	UNP Q6GG09
A	-2	SER	-	expression tag	UNP Q6GG09
A	-1	HIS	-	expression tag	UNP Q6GG09
A	0	MET	-	expression tag	UNP Q6GG09

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	expression tag	UNP Q6GG09
B	-19	GLY	-	expression tag	UNP Q6GG09
B	-18	SER	-	expression tag	UNP Q6GG09
B	-17	SER	-	expression tag	UNP Q6GG09
B	-16	HIS	-	expression tag	UNP Q6GG09
B	-15	HIS	-	expression tag	UNP Q6GG09
B	-14	HIS	-	expression tag	UNP Q6GG09
B	-13	HIS	-	expression tag	UNP Q6GG09
B	-12	HIS	-	expression tag	UNP Q6GG09
B	-11	HIS	-	expression tag	UNP Q6GG09
B	-10	SER	-	expression tag	UNP Q6GG09
B	-9	SER	-	expression tag	UNP Q6GG09
B	-8	GLY	-	expression tag	UNP Q6GG09
B	-7	LEU	-	expression tag	UNP Q6GG09
B	-6	VAL	-	expression tag	UNP Q6GG09
B	-5	PRO	-	expression tag	UNP Q6GG09
B	-4	ARG	-	expression tag	UNP Q6GG09
B	-3	GLY	-	expression tag	UNP Q6GG09
B	-2	SER	-	expression tag	UNP Q6GG09
B	-1	HIS	-	expression tag	UNP Q6GG09
B	0	MET	-	expression tag	UNP Q6GG09
C	-20	MET	-	expression tag	UNP Q6GG09
C	-19	GLY	-	expression tag	UNP Q6GG09
C	-18	SER	-	expression tag	UNP Q6GG09
C	-17	SER	-	expression tag	UNP Q6GG09
C	-16	HIS	-	expression tag	UNP Q6GG09
C	-15	HIS	-	expression tag	UNP Q6GG09
C	-14	HIS	-	expression tag	UNP Q6GG09
C	-13	HIS	-	expression tag	UNP Q6GG09
C	-12	HIS	-	expression tag	UNP Q6GG09
C	-11	HIS	-	expression tag	UNP Q6GG09
C	-10	SER	-	expression tag	UNP Q6GG09
C	-9	SER	-	expression tag	UNP Q6GG09
C	-8	GLY	-	expression tag	UNP Q6GG09
C	-7	LEU	-	expression tag	UNP Q6GG09
C	-6	VAL	-	expression tag	UNP Q6GG09
C	-5	PRO	-	expression tag	UNP Q6GG09
C	-4	ARG	-	expression tag	UNP Q6GG09
C	-3	GLY	-	expression tag	UNP Q6GG09
C	-2	SER	-	expression tag	UNP Q6GG09
C	-1	HIS	-	expression tag	UNP Q6GG09
C	0	MET	-	expression tag	UNP Q6GG09

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	expression tag	UNP Q6GG09
D	-19	GLY	-	expression tag	UNP Q6GG09
D	-18	SER	-	expression tag	UNP Q6GG09
D	-17	SER	-	expression tag	UNP Q6GG09
D	-16	HIS	-	expression tag	UNP Q6GG09
D	-15	HIS	-	expression tag	UNP Q6GG09
D	-14	HIS	-	expression tag	UNP Q6GG09
D	-13	HIS	-	expression tag	UNP Q6GG09
D	-12	HIS	-	expression tag	UNP Q6GG09
D	-11	HIS	-	expression tag	UNP Q6GG09
D	-10	SER	-	expression tag	UNP Q6GG09
D	-9	SER	-	expression tag	UNP Q6GG09
D	-8	GLY	-	expression tag	UNP Q6GG09
D	-7	LEU	-	expression tag	UNP Q6GG09
D	-6	VAL	-	expression tag	UNP Q6GG09
D	-5	PRO	-	expression tag	UNP Q6GG09
D	-4	ARG	-	expression tag	UNP Q6GG09
D	-3	GLY	-	expression tag	UNP Q6GG09
D	-2	SER	-	expression tag	UNP Q6GG09
D	-1	HIS	-	expression tag	UNP Q6GG09
D	0	MET	-	expression tag	UNP Q6GG09

- Molecule 2 is N'-[(1E)-1-(1H-benzimidazol-2-yl)ethylidene]-5-bromo-2-hydroxybenzohydrazide (three-letter code: I30) (formula: $C_{16}H_{13}BrN_4O_2$).
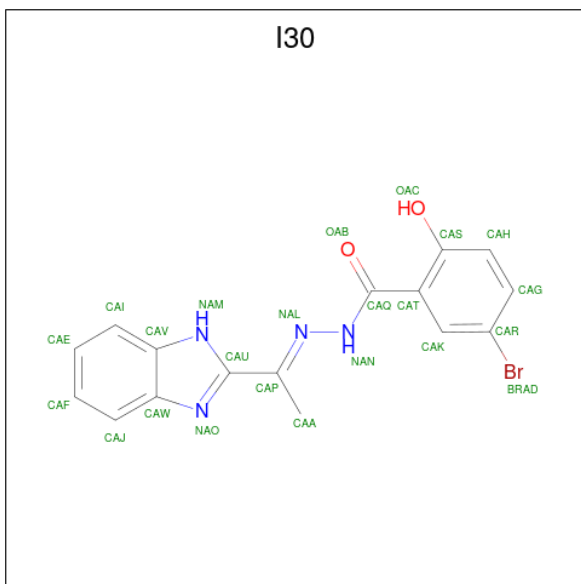
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 23	Br 1	C 16	N 4	O 2	0	0
2	D	1	Total 23	Br 1	C 16	N 4	O 2	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
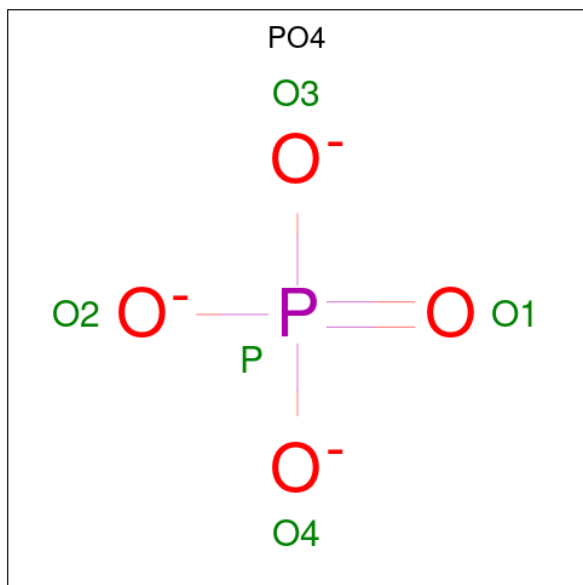
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	P 1	0	0
3	B	1	Total 5	O 4	P 1	0	0
3	C	1	Total 5	O 4	P 1	0	0
3	D	1	Total 5	O 4	P 1	0	0

3 Residue-property plots ⓘ

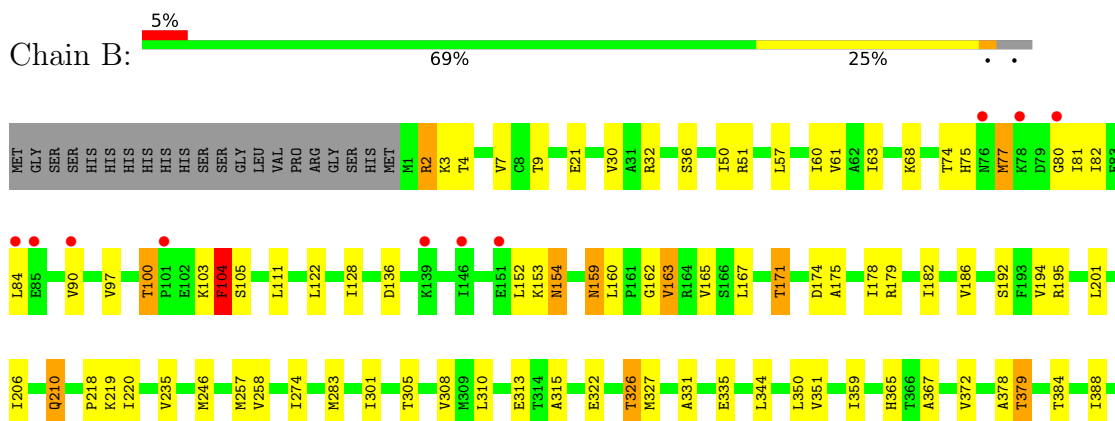These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.
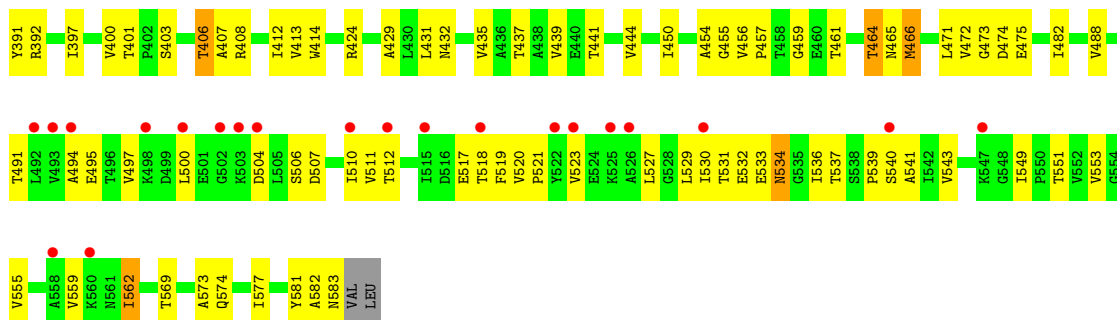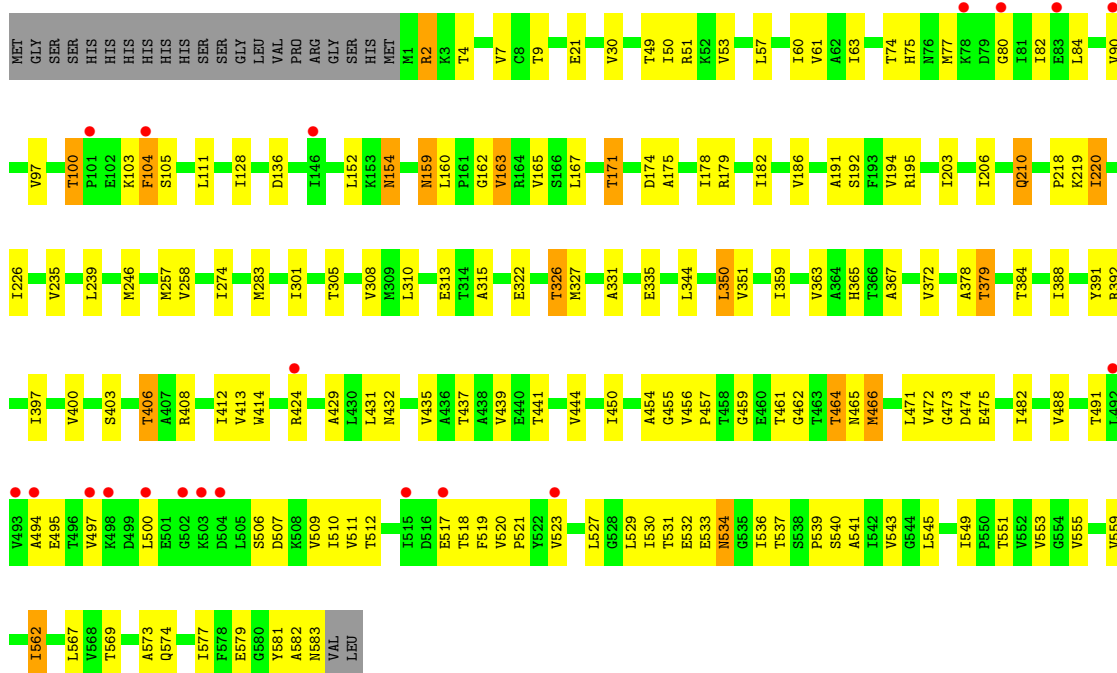
• Molecule 1: Pyruvate kinase
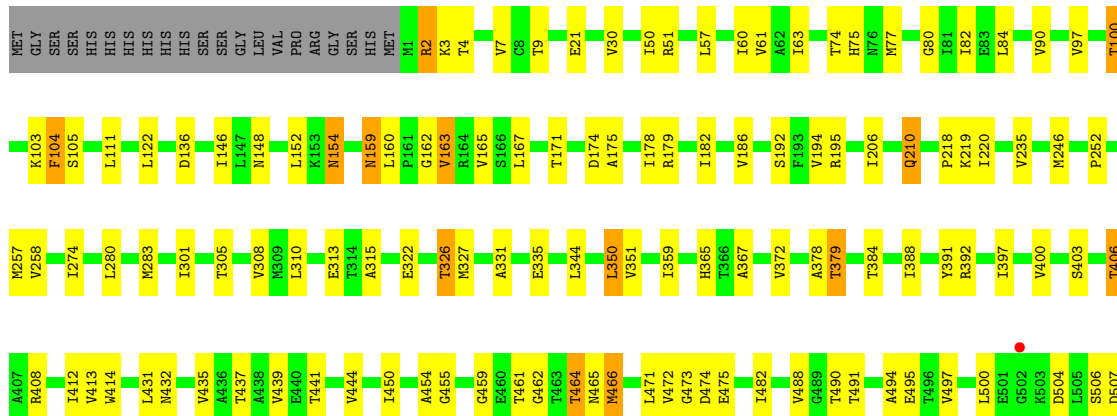
Chain A:

• Molecule 1: Pyruvate kinase

Chain B:

Y391 R392 I397 V400 T401 P402 S403 T406 A407 R408 I412 V413 W414 R424 A429 L430 L431 N432 V435 T437 A438 E440 T441 V444 I450 A454 G455 V456 P457 T458 G459 E460 T461 T464 N465 M466 L471 V472 G473 D474 E475 I482 V488

T491 L492 V493 A494 E495 T496 V497 K498 D499 L500 E501 G502 K503 D504 L505 S506 D507 I510 V511 T512 I515 D516 E517 T518 F519 V520 P521 Y522 V523 E524 K525 A526 L527 G528 L529 T531 E532 E533 N534 G535 I536 T537 S538 P539 S540 A541 I542 V543 K547 G548 I549 P550 T551 V552 G553 G554

V555 A558 V559 K560 N561 I562 T569 A573 Q574 I577 Y581 A582 N583 VAL LEU

• Molecule 1: Pyruvate kinase

Chain C:

3%

68%

25%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET M1 R2 K3 T4 V7 C8 T9 E21 V30 T49 I50 R51 K52 V53 L57 I60 V61 A62 I63 T74 H75 N76 M77 K78 D79 G80 I81 I82 E83 L84 V90

V97 T100 P101 E102 K103 F104 S105 L111 I128 D136 I146 L152 K153 N154 N159 L160 P161 G162 V163 R164 V165 S166 L167 T171 D174 A175 I178 R179 I182 V186 A191 S192 F193 V194 R195 I203 I206 Q210 P218 K219 I220

I226 V235 L239 M246 M257 V258 I274 M283 I301 T305 V308 M309 L310 E313 T314 A315 E322 T326 M327 A331 E335 L344 L350 V351 I359 V363 A364 H365 T366 A367 V372 A378 T379 T384 I388 Y391 R392

I397 V400 S403 T406 A407 R408 I412 V413 W414 R424 A429 L430 L431 N432 V435 A436 T437 A438 V439 E440 T441 V444 I450 A454 G455 V456 P457 T458 G459 E460 T461 G462 T463 T464 N465 M466 L471 V472 G473 D474 E475 I482 V488 T491 L492

V493 A494 E495 T496 V497 K498 D499 L500 E501 G502 K503 D504 L505 S506 D507 K508 V509 I510 V511 T512 I515 D516 E517 T518 F519 V520 P521 Y522 V523 L527 G528 L529 I530 T531 E532 E533 N534 G535 I536 T537 S538 P539 S540 A541 I542 V543 G544 L545 I549 P550 T551 V552 V553 G554 V555 V559

I562 L567 V568 T569 A573 Q574 I577 F578 E579 G580 Y581 A582 N583 VAL LEU

• Molecule 1: Pyruvate kinase

Chain D:

70%

24%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET M1 R2 K3 T4 V7 C8 T9 E21 V30 I50 R51 L57 I60 V61 A62 I63 T74 H75 N76 M77 G80 I81 I82 E83 L84 V90 V97 T100

K103 F104 S105 L111 L122 D136 I146 L147 N148 L152 K153 N154 N159 L160 P161 G162 V163 R164 V165 S166 L167 T171 D174 A175 I178 R179 I182 V186 S192 F193 V194 R195 I206 Q210 P218 K219 I220 V235 M246 P252

M257 V258 I274 L280 M283 I301 T305 V308 M309 L310 E313 T314 A315 E322 T326 M327 A331 E335 L344 L350 V351 I359 H365 T366 A367 V372 A378 T379 T384 I388 Y391 R392 I397 V400 S403 T406

A407 R408 I412 V413 W414 L431 N432 V435 A436 T437 A438 V439 E440 T441 V444 I450 A454 G455 G459 E460 T461 G462 T463 T464 N465 M466 L471 V472 G473 D474 E475 I482 V488 G489 T490 T491 A494 E495 T496 V497 L500 E501 G502 K503 D504 L505 S506 D507

4 Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	113.09Å 113.09Å 315.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.09 – 3.10 53.24 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.4 (113.09-3.10) 90.4 (53.24-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 3.13Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.204 , 0.227 0.207 , 0.230	Depositor DCC
R_{free} test set	3283 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	86.2	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.9	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17694	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: I30, PO4

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	0.47	0/4452	0.61	0/6022
1	B	0.50	0/4452	0.62	0/6022
1	C	0.48	0/4452	0.61	0/6022
1	D	0.51	0/4452	0.62	0/6022
All	All	0.49	0/17808	0.62	0/24088

There are no bond length outliers.

There are no bond angle outliers.

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	4407	0	4533	130	0
1	B	4407	0	4533	131	0
1	C	4407	0	4533	129	0
1	D	4407	0	4533	122	0
2	A	23	0	12	1	0
2	D	23	0	12	1	0
3	A	5	0	0	2	0
3	B	5	0	0	2	0
3	C	5	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	5	0	0	2	0
All	All	17694	0	18156	507	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 14.

All (507) 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:A:569:THR:HG21	1:A:582:ALA:HB3	1.52	0.92
1:D:569:THR:HG21	1:D:582:ALA:HB3	1.54	0.90
1:D:379:THR:HG23	1:D:384:THR:HB	1.56	0.86
1:D:74:THR:HG22	1:D:75:HIS:O	1.75	0.86
1:C:569:THR:HG21	1:C:582:ALA:HB3	1.58	0.86
1:B:531:THR:HG21	1:B:540:SER:HB3	1.58	0.85
1:C:74:THR:HG22	1:C:75:HIS:O	1.76	0.85
1:B:569:THR:HG21	1:B:582:ALA:HB3	1.58	0.85
1:B:74:THR:HG22	1:B:75:HIS:O	1.75	0.85
1:A:531:THR:HG21	1:A:540:SER:HB3	1.58	0.84
1:D:582:ALA:O	1:D:583:ASN:ND2	2.10	0.84
1:C:531:THR:HG21	1:C:540:SER:HB3	1.58	0.83
1:A:379:THR:HG23	1:A:384:THR:HB	1.60	0.83
1:D:84:LEU:HD23	1:D:90:VAL:HG21	1.61	0.83
1:D:494:ALA:HB3	1:D:512:THR:HG22	1.61	0.83
1:C:84:LEU:HD23	1:C:90:VAL:HG21	1.61	0.82
1:A:494:ALA:HB3	1:A:512:THR:HG22	1.59	0.82
1:B:84:LEU:HD23	1:B:90:VAL:HG21	1.60	0.82
1:A:74:THR:HG22	1:A:75:HIS:O	1.79	0.82
1:C:379:THR:HG23	1:C:384:THR:HB	1.62	0.82
1:D:531:THR:HG21	1:D:540:SER:HB3	1.60	0.81
1:B:494:ALA:HB3	1:B:512:THR:HG22	1.61	0.81
1:B:379:THR:HG23	1:B:384:THR:HB	1.60	0.81
1:A:84:LEU:HD23	1:A:90:VAL:HG21	1.62	0.80
1:B:582:ALA:O	1:B:583:ASN:ND2	2.15	0.80
1:A:582:ALA:O	1:A:583:ASN:ND2	2.15	0.79
1:C:494:ALA:HB3	1:C:512:THR:HG22	1.63	0.79
1:B:482:ILE:HD13	1:B:541:ALA:CB	2.14	0.77
1:A:378:ALA:HB3	1:A:454:ALA:HB2	1.65	0.77
1:B:4:THR:HG22	1:B:335:GLU:OE2	1.83	0.77
1:A:482:ILE:HD13	1:A:541:ALA:CB	2.15	0.76
1:C:582:ALA:O	1:C:583:ASN:ND2	2.18	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:THR:HG22	1:D:335:GLU:OE2	1.86	0.74
1:B:510:ILE:HD11	1:B:523:VAL:HG22	1.71	0.73
1:C:482:ILE:HD13	1:C:541:ALA:CB	2.18	0.73
1:B:378:ALA:HB3	1:B:454:ALA:HB2	1.68	0.73
1:D:432:ASN:O	1:D:435:VAL:HG12	1.88	0.73
1:B:344:LEU:HD21	1:B:365:HIS:ND1	2.03	0.73
1:C:510:ILE:HD11	1:C:523:VAL:HG22	1.70	0.72
1:A:344:LEU:HD21	1:A:365:HIS:ND1	2.05	0.72
1:A:510:ILE:HD11	1:A:523:VAL:HG22	1.71	0.71
1:C:4:THR:HG22	1:C:335:GLU:OE2	1.89	0.71
1:A:432:ASN:O	1:A:435:VAL:HG12	1.91	0.71
1:C:378:ALA:HB3	1:C:454:ALA:HB2	1.72	0.71
1:D:235:VAL:HG12	1:D:235:VAL:O	1.90	0.71
1:D:344:LEU:HD21	1:D:365:HIS:ND1	2.06	0.70
1:B:432:ASN:O	1:B:435:VAL:HG12	1.92	0.70
1:C:432:ASN:O	1:C:435:VAL:HG12	1.90	0.70
1:B:178:ILE:HD11	1:B:206:ILE:HD12	1.74	0.69
1:D:482:ILE:HD13	1:D:541:ALA:CB	2.21	0.69
1:B:174:ASP:O	1:B:178:ILE:HG23	1.93	0.69
1:D:529:LEU:HB3	1:D:551:THR:HG22	1.74	0.69
1:A:21:GLU:HG3	1:A:57:LEU:HD11	1.75	0.68
1:B:50:ILE:HG21	1:B:63:ILE:HD11	1.74	0.68
1:D:378:ALA:HB3	1:D:454:ALA:HB2	1.76	0.68
1:D:510:ILE:HD11	1:D:523:VAL:HG22	1.75	0.67
1:B:529:LEU:HB3	1:B:551:THR:HG22	1.76	0.67
1:C:100:THR:HG23	1:C:103:LYS:O	1.95	0.67
1:C:21:GLU:HG3	1:C:57:LEU:HD11	1.77	0.67
1:D:351:VAL:HG21	1:D:391:TYR:CZ	2.29	0.66
1:B:351:VAL:HG21	1:B:391:TYR:CZ	2.31	0.66
1:C:344:LEU:HD21	1:C:365:HIS:ND1	2.10	0.66
1:A:529:LEU:HB3	1:A:551:THR:HG22	1.76	0.66
1:A:4:THR:HG22	1:A:335:GLU:OE2	1.96	0.66
1:A:351:VAL:HG21	1:A:391:TYR:CZ	2.30	0.65
1:A:178:ILE:HD11	1:A:206:ILE:HD12	1.77	0.65
1:C:529:LEU:HB3	1:C:551:THR:HG22	1.77	0.65
1:C:50:ILE:HG21	1:C:63:ILE:HD11	1.78	0.65
1:C:351:VAL:HG21	1:C:391:TYR:CZ	2.33	0.64
1:B:21:GLU:HG3	1:B:57:LEU:HD11	1.79	0.64
1:D:50:ILE:HG21	1:D:63:ILE:HD11	1.78	0.64
1:D:21:GLU:HG3	1:D:57:LEU:HD11	1.78	0.64
1:B:235:VAL:HG12	1:B:235:VAL:O	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:ILE:HD12	1:B:465:ASN:C	2.18	0.64
1:C:488:VAL:HG12	1:C:569:THR:OG1	1.98	0.64
1:D:174:ASP:O	1:D:178:ILE:HG23	1.97	0.64
1:C:246:MET:CE	1:C:258:VAL:HG11	2.28	0.63
1:B:482:ILE:HD13	1:B:541:ALA:HA	1.81	0.63
1:D:400:VAL:HG22	1:D:437:THR:HG21	1.80	0.63
1:D:100:THR:HG23	1:D:103:LYS:O	1.98	0.63
1:A:235:VAL:HG12	1:A:235:VAL:O	1.98	0.63
1:A:437:THR:O	1:A:441:THR:HG23	1.99	0.63
1:A:174:ASP:O	1:A:178:ILE:HG23	1.98	0.63
1:C:400:VAL:HG22	1:C:437:THR:HG21	1.79	0.63
1:A:400:VAL:HG22	1:A:437:THR:HG21	1.79	0.63
1:A:482:ILE:HD13	1:A:541:ALA:HA	1.80	0.62
1:C:178:ILE:HD11	1:C:206:ILE:HD12	1.81	0.62
1:A:50:ILE:HG21	1:A:63:ILE:HD11	1.80	0.62
1:D:178:ILE:HD11	1:D:206:ILE:HD12	1.80	0.62
1:C:482:ILE:HD13	1:C:541:ALA:HA	1.81	0.62
1:B:379:THR:HG22	3:B:586:PO4:O4	1.99	0.62
1:D:235:VAL:O	1:D:235:VAL:CG1	2.47	0.61
1:B:100:THR:HG23	1:B:103:LYS:O	2.00	0.61
1:B:517:GLU:O	1:B:520:VAL:HG22	2.01	0.61
1:D:482:ILE:HD13	1:D:541:ALA:HA	1.82	0.60
1:B:437:THR:O	1:B:441:THR:HG23	2.01	0.60
1:C:235:VAL:O	1:C:235:VAL:HG12	2.02	0.60
1:A:100:THR:HG23	1:A:103:LYS:O	2.01	0.60
1:D:246:MET:CE	1:D:258:VAL:HG11	2.32	0.60
1:B:400:VAL:HG22	1:B:437:THR:HG21	1.83	0.59
1:B:488:VAL:HG12	1:B:569:THR:OG1	2.01	0.59
1:B:246:MET:CE	1:B:258:VAL:HG11	2.32	0.59
1:D:517:GLU:O	1:D:520:VAL:HG22	2.02	0.59
1:B:482:ILE:CD1	1:B:541:ALA:CB	2.81	0.59
1:C:301:ILE:CD1	1:C:331:ALA:HA	2.33	0.59
1:C:517:GLU:O	1:C:520:VAL:HG22	2.03	0.58
1:C:308:VAL:HG11	1:C:327:MET:SD	2.44	0.58
1:A:482:ILE:HD13	1:A:541:ALA:CA	2.33	0.58
1:B:482:ILE:HD13	1:B:541:ALA:CA	2.33	0.58
1:A:545:LEU:HD11	1:B:235:VAL:CG2	2.33	0.58
1:D:9:THR:HG22	1:D:315:ALA:HB2	1.85	0.58
1:B:308:VAL:HG11	1:B:327:MET:SD	2.43	0.58
1:B:532:GLU:O	1:B:555:VAL:N	2.37	0.58
1:A:482:ILE:CD1	1:A:541:ALA:CB	2.82	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:532:GLU:O	1:C:555:VAL:N	2.37	0.57
1:C:437:THR:O	1:C:441:THR:HG23	2.04	0.57
1:A:246:MET:CE	1:A:258:VAL:HG11	2.33	0.57
1:A:359:ILE:HD12	1:A:465:ASN:C	2.24	0.57
1:B:444:VAL:HG21	1:B:450:ILE:HD11	1.86	0.57
1:D:444:VAL:HG21	1:D:450:ILE:HD11	1.86	0.57
1:A:175:ALA:O	1:A:179:ARG:HG3	2.05	0.57
1:A:455:GLY:HA3	1:A:461:THR:HG23	1.87	0.57
1:B:9:THR:HG22	1:B:315:ALA:HB2	1.86	0.56
1:D:532:GLU:O	1:D:555:VAL:N	2.38	0.56
1:A:488:VAL:HG12	1:A:569:THR:OG1	2.04	0.56
1:B:520:VAL:HG12	1:B:543:VAL:HG11	1.88	0.56
1:C:174:ASP:O	1:C:178:ILE:HG23	2.05	0.56
1:C:482:ILE:HD13	1:C:541:ALA:CA	2.35	0.56
1:D:301:ILE:CD1	1:D:331:ALA:HA	2.35	0.56
1:D:437:THR:O	1:D:441:THR:HG23	2.05	0.56
1:B:549:ILE:O	1:B:551:THR:HG23	2.05	0.56
1:A:9:THR:HG22	1:A:315:ALA:HB2	1.88	0.56
1:A:520:VAL:HG12	1:A:543:VAL:HG11	1.88	0.56
1:A:301:ILE:CD1	1:A:331:ALA:HA	2.36	0.56
1:B:455:GLY:HA3	1:B:461:THR:HG23	1.86	0.56
1:D:488:VAL:HG12	1:D:569:THR:OG1	2.06	0.56
1:A:533:GLU:O	1:A:534:ASN:CG	2.44	0.56
1:B:235:VAL:O	1:B:235:VAL:CG1	2.53	0.56
1:A:488:VAL:HG11	1:A:581:TYR:CD2	2.41	0.56
1:C:520:VAL:HG12	1:C:543:VAL:HG11	1.88	0.56
1:D:274:ILE:HD11	1:D:412:ILE:HD11	1.87	0.56
1:D:488:VAL:HG11	1:D:581:TYR:CD2	2.40	0.56
1:C:530:ILE:HG12	1:C:577:ILE:HD13	1.87	0.56
1:D:359:ILE:HD12	1:D:465:ASN:C	2.27	0.55
1:C:533:GLU:O	1:C:534:ASN:CG	2.44	0.55
1:A:531:THR:HG21	1:A:540:SER:CB	2.34	0.55
1:D:455:GLY:HA3	1:D:461:THR:HG23	1.88	0.55
1:A:532:GLU:O	1:A:555:VAL:N	2.40	0.55
1:C:431:LEU:HD21	1:C:466:MET:CE	2.37	0.55
1:D:283:MET:SD	1:D:326:THR:HG21	2.46	0.55
1:D:530:ILE:HG12	1:D:577:ILE:HD13	1.87	0.55
1:B:283:MET:SD	1:B:326:THR:HG21	2.46	0.55
1:C:403:SER:OG	1:C:406:THR:HG23	2.06	0.55
1:C:455:GLY:HA3	1:C:461:THR:HG23	1.87	0.54
1:A:165:VAL:CG1	1:A:167:LEU:HD23	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ALA:O	1:B:179:ARG:HG3	2.07	0.54
1:B:533:GLU:O	1:B:534:ASN:CG	2.45	0.54
1:A:283:MET:SD	1:A:326:THR:HG21	2.47	0.54
1:C:488:VAL:HG11	1:C:581:TYR:CD2	2.42	0.54
1:A:517:GLU:O	1:A:520:VAL:HG22	2.07	0.54
1:C:482:ILE:CD1	1:C:541:ALA:CB	2.86	0.54
1:D:111:LEU:C	1:D:111:LEU:HD23	2.28	0.54
1:A:461:THR:HG21	3:A:587:PO4:O3	2.07	0.54
1:B:488:VAL:HG11	1:B:581:TYR:CD2	2.43	0.54
1:C:359:ILE:HD12	1:C:465:ASN:C	2.27	0.54
1:C:444:VAL:HG21	1:C:450:ILE:HD11	1.90	0.54
1:D:175:ALA:O	1:D:179:ARG:HG3	2.08	0.54
1:B:431:LEU:HD21	1:B:466:MET:CE	2.38	0.54
1:C:283:MET:SD	1:C:326:THR:HG21	2.48	0.54
1:C:549:ILE:O	1:C:551:THR:HG23	2.07	0.54
1:B:530:ILE:HG12	1:B:577:ILE:HD13	1.89	0.54
1:D:4:THR:CG2	1:D:331:ALA:HB1	2.38	0.54
1:A:235:VAL:O	1:A:235:VAL:CG1	2.55	0.53
1:B:301:ILE:CD1	1:B:331:ALA:HA	2.38	0.53
1:D:359:ILE:HD12	1:D:465:ASN:HA	1.90	0.53
1:A:549:ILE:O	1:A:551:THR:HG23	2.08	0.53
1:D:549:ILE:O	1:D:551:THR:HG23	2.08	0.53
1:A:246:MET:HE1	1:A:258:VAL:CG1	2.39	0.53
1:C:444:VAL:HG11	1:C:450:ILE:HD11	1.91	0.53
1:D:308:VAL:HG11	1:D:327:MET:SD	2.49	0.53
1:D:431:LEU:HD21	1:D:466:MET:CE	2.38	0.53
1:A:530:ILE:HG12	1:A:577:ILE:HD13	1.89	0.53
1:C:162:GLY:HA2	1:C:163:VAL:O	2.09	0.53
1:C:274:ILE:HD11	1:C:412:ILE:HD11	1.91	0.53
1:C:235:VAL:O	1:C:235:VAL:CG1	2.57	0.52
1:B:4:THR:HG21	1:B:301:ILE:HD13	1.92	0.52
1:D:431:LEU:HD21	1:D:466:MET:HE2	1.92	0.52
1:D:482:ILE:HD13	1:D:541:ALA:CA	2.37	0.52
1:B:194:VAL:HG21	1:B:218:PRO:HB3	1.91	0.52
1:D:482:ILE:CD1	1:D:541:ALA:CB	2.88	0.52
1:C:194:VAL:HG21	1:C:218:PRO:HB3	1.91	0.52
1:D:403:SER:OG	1:D:406:THR:HG23	2.09	0.52
1:D:520:VAL:HG12	1:D:543:VAL:HG11	1.91	0.52
1:D:533:GLU:O	1:D:534:ASN:CG	2.48	0.52
1:C:9:THR:HG22	1:C:315:ALA:HB2	1.91	0.52
1:D:444:VAL:HG11	1:D:450:ILE:HD11	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:VAL:HG11	1:A:327:MET:SD	2.50	0.52
1:A:473:GLY:HA3	1:A:474:ASP:HB2	1.92	0.52
1:C:165:VAL:CG1	1:C:167:LEU:HD23	2.40	0.52
1:A:359:ILE:HD12	1:A:465:ASN:HA	1.92	0.51
1:A:379:THR:HG22	3:A:587:PO4:O1	2.10	0.51
1:D:165:VAL:CG1	1:D:167:LEU:HD23	2.40	0.51
1:D:182:ILE:HG21	1:D:210:GLN:HG2	1.93	0.51
1:D:435:VAL:O	1:D:439:VAL:HG23	2.10	0.51
2:D:586:I30:OAC	2:D:586:I30:NAN	2.27	0.51
1:B:472:VAL:HG12	1:B:472:VAL:O	2.11	0.51
1:C:175:ALA:O	1:C:179:ARG:HG3	2.10	0.51
1:C:497:VAL:HG11	1:C:518:THR:OG1	2.11	0.51
1:A:246:MET:CE	1:A:258:VAL:CG1	2.89	0.51
1:A:444:VAL:HG11	1:A:450:ILE:HD11	1.93	0.51
1:C:246:MET:CE	1:C:258:VAL:CG1	2.88	0.51
1:D:482:ILE:HD12	1:D:553:VAL:HG13	1.93	0.51
1:A:497:VAL:HG11	1:A:518:THR:HB	1.93	0.51
1:D:194:VAL:HG21	1:D:218:PRO:HB3	1.92	0.51
1:D:159:ASN:C	1:D:160:LEU:HD12	2.31	0.51
1:B:182:ILE:HG21	1:B:210:GLN:HG2	1.92	0.50
1:D:450:ILE:HD12	1:D:472:VAL:CG2	2.41	0.50
1:A:497:VAL:HG11	1:A:518:THR:CB	2.41	0.50
1:C:424:ARG:HB3	1:C:429:ALA:CB	2.42	0.50
1:D:472:VAL:HG12	1:D:472:VAL:O	2.11	0.50
1:A:392:ARG:HD3	1:A:414:TRP:CE3	2.46	0.50
1:A:537:THR:HG22	1:B:201:LEU:HB3	1.93	0.50
1:B:274:ILE:HD11	1:B:412:ILE:HD11	1.93	0.50
1:B:482:ILE:HD13	1:B:541:ALA:HB1	1.94	0.50
1:B:520:VAL:CG2	1:B:521:PRO:HD3	2.41	0.50
1:D:473:GLY:HA3	1:D:474:ASP:HB2	1.93	0.50
1:A:111:LEU:HD23	1:A:111:LEU:C	2.31	0.50
1:C:4:THR:CG2	1:C:331:ALA:HB1	2.42	0.50
1:A:444:VAL:HG21	1:A:450:ILE:HD11	1.94	0.50
1:D:497:VAL:HG11	1:D:518:THR:HB	1.93	0.50
1:A:246:MET:HE1	1:A:258:VAL:HG11	1.92	0.50
1:A:431:LEU:HD21	1:A:466:MET:CE	2.41	0.50
1:A:497:VAL:HG11	1:A:518:THR:OG1	2.11	0.50
1:C:482:ILE:HD12	1:C:553:VAL:HG13	1.94	0.50
1:B:4:THR:HG21	1:B:301:ILE:CD1	2.42	0.50
1:C:178:ILE:O	1:C:182:ILE:HG13	2.11	0.50
1:D:384:THR:HA	1:D:464:THR:HG21	1.94	0.50

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:MET:CE	1:D:258:VAL:CG1	2.90	0.50
1:C:520:VAL:CG2	1:C:521:PRO:HD3	2.42	0.49
1:C:471:LEU:HD23	1:C:472:VAL:N	2.27	0.49
1:A:520:VAL:CG2	1:A:521:PRO:HD3	2.42	0.49
1:D:4:THR:HG21	1:D:301:ILE:CD1	2.42	0.49
1:B:246:MET:CE	1:B:258:VAL:CG1	2.90	0.49
1:C:473:GLY:HA3	1:C:474:ASP:HB2	1.94	0.49
1:B:494:ALA:HB3	1:B:512:THR:CG2	2.40	0.49
1:C:182:ILE:HG21	1:C:210:GLN:HG2	1.94	0.49
1:C:246:MET:HE1	1:C:258:VAL:CG1	2.43	0.49
1:C:533:GLU:O	1:C:534:ASN:CB	2.61	0.49
1:A:520:VAL:HG23	1:A:521:PRO:HD3	1.95	0.49
1:B:511:VAL:HG21	1:B:562:ILE:HD11	1.94	0.49
1:C:384:THR:HA	1:C:464:THR:HG21	1.93	0.49
1:D:497:VAL:HG11	1:D:518:THR:CB	2.43	0.49
1:A:472:VAL:HG12	1:A:472:VAL:O	2.12	0.49
1:D:511:VAL:HG21	1:D:562:ILE:HD11	1.94	0.49
1:A:435:VAL:O	1:A:439:VAL:HG23	2.12	0.49
1:D:359:ILE:HD12	1:D:465:ASN:CA	2.43	0.49
1:D:367:ALA:HA	1:D:372:VAL:HG13	1.93	0.49
2:A:586:I30:OAC	2:A:586:I30:NAN	2.37	0.49
1:B:520:VAL:HG23	1:B:521:PRO:HD3	1.94	0.49
1:C:497:VAL:HG11	1:C:518:THR:CB	2.43	0.49
1:B:507:ASP:HA	1:B:527:LEU:HD12	1.95	0.48
1:C:246:MET:HE1	1:C:258:VAL:HG11	1.94	0.48
1:D:4:THR:HG21	1:D:301:ILE:HD13	1.95	0.48
1:C:301:ILE:HA	1:C:305:THR:HG22	1.94	0.48
1:C:497:VAL:HG11	1:C:518:THR:HB	1.95	0.48
1:D:520:VAL:CG2	1:D:521:PRO:HD3	2.42	0.48
1:B:165:VAL:CG1	1:B:167:LEU:HD23	2.43	0.48
1:C:450:ILE:HD12	1:C:472:VAL:CG2	2.43	0.48
1:D:178:ILE:O	1:D:182:ILE:HG13	2.14	0.48
1:B:4:THR:CG2	1:B:331:ALA:HB1	2.43	0.48
1:B:482:ILE:HD12	1:B:553:VAL:HG13	1.94	0.48
1:C:424:ARG:HB3	1:C:429:ALA:HB1	1.95	0.48
1:D:533:GLU:O	1:D:534:ASN:CB	2.62	0.48
1:B:310:LEU:HD22	1:B:313:GLU:HB2	1.95	0.48
1:B:379:THR:HG22	3:B:586:PO4:P	2.53	0.48
1:B:497:VAL:HG11	1:B:518:THR:HB	1.96	0.48
1:B:246:MET:HE1	1:B:258:VAL:HG11	1.94	0.48
1:B:322:GLU:O	1:B:326:THR:HB	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:ILE:HG22	1:C:397:ILE:HD13	1.94	0.48
1:D:162:GLY:HA2	1:D:163:VAL:O	2.14	0.48
1:B:473:GLY:HA3	1:B:474:ASP:HB2	1.95	0.48
1:B:533:GLU:O	1:B:534:ASN:CB	2.62	0.48
1:C:111:LEU:HD23	1:C:111:LEU:C	2.34	0.48
1:D:7:VAL:HG22	1:D:30:VAL:HB	1.94	0.48
1:A:482:ILE:HD12	1:A:553:VAL:HG13	1.95	0.48
1:C:531:THR:HG21	1:C:540:SER:CB	2.38	0.48
1:A:178:ILE:O	1:A:182:ILE:HG13	2.13	0.48
1:A:274:ILE:HD11	1:A:412:ILE:HD11	1.95	0.48
1:A:494:ALA:HB3	1:A:512:THR:CG2	2.37	0.48
1:B:450:ILE:HD12	1:B:472:VAL:CG2	2.43	0.48
1:C:520:VAL:HG23	1:C:521:PRO:HD3	1.96	0.47
1:D:246:MET:HE1	1:D:258:VAL:HG11	1.96	0.47
1:B:301:ILE:HA	1:B:305:THR:HG22	1.95	0.47
1:A:194:VAL:HG21	1:A:218:PRO:HB3	1.97	0.47
1:A:378:ALA:HB3	1:A:454:ALA:CB	2.42	0.47
1:B:435:VAL:O	1:B:439:VAL:HG23	2.14	0.47
1:C:403:SER:CB	1:C:406:THR:HG23	2.44	0.47
1:C:545:LEU:HD11	1:D:235:VAL:CG2	2.44	0.47
1:A:7:VAL:HG22	1:A:30:VAL:HB	1.97	0.47
1:C:310:LEU:HD22	1:C:313:GLU:HB2	1.97	0.47
1:D:392:ARG:HD3	1:D:414:TRP:CE3	2.50	0.47
1:A:403:SER:OG	1:A:406:THR:HG23	2.14	0.47
1:B:384:THR:HA	1:B:464:THR:HG21	1.97	0.47
1:C:435:VAL:O	1:C:439:VAL:HG23	2.15	0.47
1:B:444:VAL:HG11	1:B:450:ILE:HD11	1.95	0.47
1:D:520:VAL:HG23	1:D:521:PRO:HD3	1.96	0.47
1:A:359:ILE:HD12	1:A:465:ASN:CA	2.45	0.47
1:A:511:VAL:HG21	1:A:562:ILE:HD11	1.97	0.47
1:B:162:GLY:HA2	1:B:163:VAL:O	2.15	0.47
1:B:192:SER:HA	1:B:219:LYS:HD3	1.97	0.47
1:B:367:ALA:HA	1:B:372:VAL:HG13	1.97	0.47
1:D:531:THR:HG21	1:D:540:SER:CB	2.39	0.47
1:A:162:GLY:HA2	1:A:163:VAL:O	2.15	0.47
1:A:573:ALA:O	1:A:574:GLN:HB2	2.15	0.47
1:B:531:THR:HG21	1:B:540:SER:CB	2.37	0.47
1:C:472:VAL:HG12	1:C:472:VAL:O	2.15	0.47
1:B:512:THR:HG21	1:B:519:PHE:CE2	2.49	0.46
1:D:246:MET:HE1	1:D:258:VAL:CG1	2.44	0.46
1:A:159:ASN:C	1:A:160:LEU:HD12	2.35	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ILE:HA	1:A:305:THR:HG22	1.96	0.46
1:B:246:MET:HE1	1:B:258:VAL:CG1	2.44	0.46
1:D:301:ILE:HA	1:D:305:THR:HG22	1.96	0.46
1:A:388:ILE:HG22	1:A:397:ILE:HD13	1.97	0.46
1:C:392:ARG:HD3	1:C:414:TRP:CE3	2.51	0.46
1:B:7:VAL:HG22	1:B:30:VAL:HB	1.98	0.46
1:B:471:LEU:HD23	1:B:472:VAL:N	2.30	0.46
1:B:392:ARG:HD3	1:B:414:TRP:CE3	2.50	0.46
1:B:497:VAL:HG11	1:B:518:THR:CB	2.46	0.46
1:A:182:ILE:HG21	1:A:210:GLN:HG2	1.98	0.46
1:A:384:THR:HA	1:A:464:THR:HG21	1.96	0.46
1:B:482:ILE:CD1	1:B:541:ALA:HB2	2.45	0.46
1:C:536:ILE:HG13	1:C:537:THR:HG23	1.98	0.46
1:A:178:ILE:HD11	1:A:206:ILE:CD1	2.46	0.46
1:A:471:LEU:HD23	1:A:472:VAL:N	2.30	0.46
1:A:482:ILE:CD1	1:A:541:ALA:HB2	2.45	0.46
1:A:507:ASP:HA	1:A:527:LEU:HD12	1.98	0.46
1:C:388:ILE:HG22	1:C:397:ILE:CD1	2.46	0.46
1:D:60:ILE:HG23	1:D:408:ARG:HG2	1.97	0.46
1:D:310:LEU:HD22	1:D:313:GLU:HB2	1.97	0.46
1:A:4:THR:CG2	1:A:331:ALA:HB1	2.45	0.46
1:B:9:THR:OG1	1:B:32:ARG:NH1	2.48	0.46
1:A:450:ILE:HD12	1:A:472:VAL:CG2	2.45	0.46
1:C:512:THR:HG21	1:C:519:PHE:CE2	2.50	0.46
1:B:359:ILE:HD12	1:B:465:ASN:CA	2.45	0.45
1:D:192:SER:HA	1:D:219:LYS:HD3	1.98	0.45
1:A:322:GLU:O	1:A:326:THR:HB	2.17	0.45
1:C:511:VAL:HG21	1:C:562:ILE:HD11	1.97	0.45
1:D:497:VAL:HG11	1:D:518:THR:OG1	2.16	0.45
1:A:533:GLU:O	1:A:534:ASN:CB	2.63	0.45
1:A:495:GLU:OE2	1:A:559:VAL:HG11	2.17	0.45
1:A:482:ILE:HD13	1:A:541:ALA:HB1	1.95	0.45
1:B:378:ALA:HB3	1:B:454:ALA:CB	2.44	0.45
1:C:4:THR:HG21	1:C:301:ILE:CD1	2.47	0.45
1:C:60:ILE:HG23	1:C:408:ARG:HG2	1.98	0.45
1:C:192:SER:HA	1:C:219:LYS:HD3	1.98	0.45
1:B:3:LYS:HD2	1:B:414:TRP:CZ2	2.52	0.45
1:B:77:MET:HE1	1:B:104:PHE:CD2	2.51	0.45
1:B:431:LEU:HD21	1:B:466:MET:HE1	1.97	0.45
1:D:322:GLU:O	1:D:326:THR:HB	2.16	0.45
1:B:384:THR:OG1	1:B:464:THR:HB	2.16	0.45

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:LEU:HD11	1:B:531:THR:HG22	1.99	0.45
1:C:322:GLU:O	1:C:326:THR:HB	2.17	0.45
1:C:574:GLN:OE1	1:D:462:GLY:HA3	2.17	0.45
1:B:573:ALA:O	1:B:574:GLN:HB2	2.17	0.45
1:D:573:ALA:O	1:D:574:GLN:HB2	2.17	0.45
1:A:367:ALA:HA	1:A:372:VAL:HG13	1.98	0.44
1:B:111:LEU:C	1:B:111:LEU:HD23	2.38	0.44
1:B:359:ILE:HD12	1:B:465:ASN:HA	1.98	0.44
1:C:482:ILE:HD13	1:C:541:ALA:HB1	1.97	0.44
1:A:392:ARG:HA	1:A:414:TRP:CZ3	2.52	0.44
1:A:403:SER:CB	1:A:406:THR:HG23	2.47	0.44
1:C:367:ALA:HA	1:C:372:VAL:HG13	1.99	0.44
1:A:350:LEU:HD22	1:A:350:LEU:O	2.17	0.44
1:C:7:VAL:HG22	1:C:30:VAL:HB	1.98	0.44
1:C:350:LEU:O	1:C:350:LEU:HD22	2.17	0.44
1:D:350:LEU:HD22	1:D:350:LEU:O	2.17	0.44
1:D:494:ALA:HB3	1:D:512:THR:CG2	2.39	0.44
1:D:495:GLU:OE2	1:D:559:VAL:HG11	2.18	0.44
1:B:122:LEU:HD12	1:B:122:LEU:N	2.32	0.44
1:C:159:ASN:C	1:C:160:LEU:HD12	2.37	0.44
1:C:359:ILE:O	1:C:363:VAL:HG23	2.18	0.44
1:C:431:LEU:HD21	1:C:466:MET:HE1	1.99	0.44
1:C:495:GLU:OE2	1:C:559:VAL:HG11	2.17	0.44
1:D:491:THR:HG21	1:D:562:ILE:CD1	2.47	0.44
1:A:122:LEU:N	1:A:122:LEU:HD12	2.33	0.44
1:A:310:LEU:HD22	1:A:313:GLU:HB2	1.99	0.43
1:A:512:THR:HG21	1:A:519:PHE:CE2	2.53	0.43
1:B:392:ARG:HA	1:B:414:TRP:CZ3	2.53	0.43
1:D:80:GLY:HA2	1:D:154:ASN:HD21	1.83	0.43
1:A:291:ARG:CB	1:D:252:PRO:HB3	2.48	0.43
1:A:473:GLY:CA	1:A:474:ASP:HB2	2.49	0.43
1:A:491:THR:HG21	1:A:562:ILE:CD1	2.48	0.43
1:B:81:ILE:HD11	1:B:153:LYS:HZ1	1.84	0.43
1:B:456:VAL:HA	1:B:457:PRO:C	2.37	0.43
1:B:497:VAL:HG11	1:B:518:THR:OG1	2.18	0.43
1:C:80:GLY:HA2	1:C:154:ASN:HD21	1.83	0.43
1:D:473:GLY:CA	1:D:474:ASP:HB2	2.48	0.43
1:D:504:ASP:OD2	1:D:504:ASP:N	2.52	0.43
1:A:77:MET:HE1	1:A:104:PHE:CD2	2.53	0.43
1:D:482:ILE:HD13	1:D:541:ALA:HB1	2.00	0.43
1:A:9:THR:OG1	1:A:32:ARG:NH1	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:PRO:O	1:B:543:VAL:HG13	2.19	0.43
1:D:388:ILE:HG22	1:D:397:ILE:HD13	2.01	0.43
1:D:403:SER:CB	1:D:406:THR:HG23	2.49	0.43
1:A:60:ILE:HG23	1:A:408:ARG:HG2	2.00	0.43
1:A:82:ILE:HG22	1:A:152:LEU:HB3	2.01	0.43
1:D:539:PRO:O	1:D:543:VAL:HG13	2.18	0.43
1:A:80:GLY:HA2	1:A:154:ASN:HD21	1.83	0.43
1:B:308:VAL:CG1	1:B:327:MET:SD	3.05	0.43
1:C:507:ASP:HA	1:C:527:LEU:HD12	2.00	0.43
1:D:3:LYS:HD2	1:D:414:TRP:CZ2	2.54	0.43
1:A:388:ILE:HG22	1:A:397:ILE:CD1	2.48	0.43
1:A:431:LEU:HD21	1:A:466:MET:HE1	2.00	0.43
1:B:388:ILE:HG22	1:B:397:ILE:HD13	2.00	0.43
1:C:431:LEU:HD21	1:C:466:MET:HE2	2.00	0.43
1:D:536:ILE:HG13	1:D:537:THR:HG23	2.00	0.43
1:A:456:VAL:HA	1:A:457:PRO:C	2.39	0.43
1:B:536:ILE:HG13	1:B:537:THR:HG23	2.01	0.43
1:C:82:ILE:HG22	1:C:152:LEU:HB3	2.01	0.43
1:D:82:ILE:HG22	1:D:152:LEU:HB3	2.00	0.43
1:D:379:THR:HG22	3:D:587:PO4:O2	2.18	0.43
1:A:424:ARG:HB3	1:A:429:ALA:CB	2.49	0.43
1:B:359:ILE:CD1	1:B:465:ASN:C	2.87	0.43
1:C:379:THR:HG22	3:C:586:PO4:O3	2.19	0.43
1:C:567:LEU:O	1:C:579:GLU:O	2.36	0.43
1:A:49:THR:O	1:A:53:VAL:HG23	2.18	0.42
1:A:97:VAL:HG22	1:A:105:SER:HB3	2.01	0.42
1:A:146:ILE:HD11	1:A:148:ASN:O	2.18	0.42
1:B:159:ASN:C	1:B:160:LEU:HD12	2.39	0.42
1:A:192:SER:HA	1:A:219:LYS:HD3	2.01	0.42
1:A:4:THR:HG21	1:A:301:ILE:CD1	2.49	0.42
1:D:351:VAL:HG21	1:D:391:TYR:OH	2.18	0.42
1:A:3:LYS:HD2	1:A:414:TRP:CZ2	2.54	0.42
1:A:81:ILE:HD11	1:A:153:LYS:HZ1	1.84	0.42
1:B:403:SER:OG	1:B:406:THR:HG23	2.19	0.42
1:B:494:ALA:HB2	1:B:500:LEU:HD23	2.00	0.42
1:D:529:LEU:HB3	1:D:551:THR:CG2	2.46	0.42
1:A:539:PRO:O	1:A:543:VAL:HG13	2.19	0.42
1:A:545:LEU:HD11	1:B:235:VAL:HG22	2.01	0.42
1:D:529:LEU:HD11	1:D:531:THR:HG22	2.01	0.42
1:B:80:GLY:HA2	1:B:154:ASN:HD21	1.84	0.42
1:C:49:THR:O	1:C:53:VAL:HG23	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:LEU:HD13	1:C:128:ILE:HD12	2.01	0.42
1:C:462:GLY:HA3	1:D:574:GLN:OE1	2.19	0.42
1:C:494:ALA:HB2	1:C:500:LEU:HD23	2.01	0.42
1:C:509:VAL:HG23	1:C:509:VAL:O	2.19	0.42
1:A:529:LEU:HB3	1:A:551:THR:CG2	2.46	0.42
1:C:539:PRO:O	1:C:543:VAL:HG13	2.19	0.42
1:B:60:ILE:HG23	1:B:408:ARG:HG2	2.02	0.42
1:B:178:ILE:O	1:B:182:ILE:HG13	2.20	0.42
1:B:491:THR:HG21	1:B:562:ILE:CD1	2.50	0.42
1:C:491:THR:HG21	1:C:562:ILE:CD1	2.50	0.42
1:C:494:ALA:HB3	1:C:512:THR:CG2	2.43	0.42
1:D:122:LEU:HD12	1:D:122:LEU:N	2.35	0.42
1:D:392:ARG:HA	1:D:414:TRP:CZ3	2.55	0.42
1:A:171:THR:HB	1:A:174:ASP:H	1.85	0.42
1:B:81:ILE:HD11	1:B:153:LYS:NZ	2.35	0.42
1:C:529:LEU:HD11	1:C:531:THR:HG22	2.01	0.42
1:C:308:VAL:CG1	1:C:327:MET:SD	3.08	0.42
1:D:471:LEU:HD23	1:D:472:VAL:N	2.35	0.42
1:D:494:ALA:HB2	1:D:500:LEU:HD23	2.02	0.42
1:A:509:VAL:HG23	1:A:509:VAL:O	2.20	0.41
1:B:84:LEU:HD13	1:B:128:ILE:HD12	2.02	0.41
1:C:573:ALA:O	1:C:574:GLN:HB2	2.20	0.41
1:D:146:ILE:HD11	1:D:148:ASN:O	2.20	0.41
1:C:351:VAL:HG21	1:C:391:TYR:OH	2.20	0.41
1:D:512:THR:HG21	1:D:519:PHE:CE2	2.54	0.41
1:A:536:ILE:HG13	1:A:537:THR:HG23	2.02	0.41
1:B:97:VAL:HG22	1:B:105:SER:HB3	2.02	0.41
1:A:165:VAL:HG12	1:A:167:LEU:HD23	2.02	0.41
1:A:351:VAL:HG21	1:A:391:TYR:OH	2.20	0.41
1:A:494:ALA:HB2	1:A:500:LEU:HD23	2.01	0.41
1:B:84:LEU:HD13	1:B:128:ILE:CD1	2.50	0.41
1:B:401:THR:HG21	1:B:407:ALA:HB2	2.02	0.41
1:C:84:LEU:HD13	1:C:128:ILE:CD1	2.50	0.41
1:B:529:LEU:HB3	1:B:551:THR:CG2	2.47	0.41
1:C:171:THR:HB	1:C:174:ASP:H	1.85	0.41
1:C:473:GLY:CA	1:C:474:ASP:HB2	2.50	0.41
1:C:482:ILE:CD1	1:C:541:ALA:HB2	2.50	0.41
1:C:529:LEU:HB3	1:C:551:THR:CG2	2.46	0.41
1:D:160:LEU:HD12	1:D:160:LEU:N	2.35	0.41
1:D:379:THR:HG22	3:D:587:PO4:O1	2.20	0.41
1:B:310:LEU:HD22	1:B:313:GLU:CB	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:SER:CB	1:B:406:THR:HG23	2.50	0.41
1:C:220:ILE:CG2	1:C:226:ILE:HD13	2.50	0.41
1:C:456:VAL:HA	1:C:457:PRO:C	2.42	0.41
1:D:509:VAL:HG23	1:D:509:VAL:O	2.21	0.41
1:B:388:ILE:HG22	1:B:397:ILE:CD1	2.50	0.41
1:B:504:ASP:N	1:B:504:ASP:OD2	2.54	0.41
1:C:220:ILE:HG13	1:C:239:LEU:HD11	2.03	0.41
1:D:97:VAL:HG22	1:D:105:SER:HB3	2.02	0.41
1:B:36:SER:HA	1:B:68:LYS:HB2	2.03	0.41
1:B:495:GLU:OE2	1:B:559:VAL:HG11	2.20	0.41
1:D:490:THR:HA	1:D:567:LEU:HA	2.03	0.41
1:B:82:ILE:HG22	1:B:152:LEU:HB3	2.02	0.40
1:C:310:LEU:HD22	1:C:313:GLU:CB	2.51	0.40
1:D:388:ILE:HG22	1:D:397:ILE:CD1	2.51	0.40
1:B:171:THR:HB	1:B:174:ASP:H	1.86	0.40
1:C:97:VAL:HG22	1:C:105:SER:HB3	2.03	0.40
1:A:504:ASP:N	1:A:504:ASP:OD2	2.54	0.40
1:C:191:ALA:HB2	1:C:203:ILE:CD1	2.51	0.40
1:C:384:THR:OG1	1:C:464:THR:HB	2.22	0.40
1:C:392:ARG:HA	1:C:414:TRP:CZ3	2.55	0.40
1:A:280:LEU:HD13	1:A:326:THR:CG2	2.51	0.40
1:C:178:ILE:HD11	1:C:206:ILE:CD1	2.49	0.40
1:D:280:LEU:HD13	1:D:326:THR:CG2	2.52	0.40
1:B:424:ARG:HB3	1:B:429:ALA:CB	2.52	0.40

There are no symmetry-related clashes.

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	581/606 (96%)	529 (91%)	42 (7%)	10 (2%)	9	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	581/606 (96%)	528 (91%)	44 (8%)	9 (2%)	10	39
1	C	581/606 (96%)	526 (90%)	46 (8%)	9 (2%)	10	39
1	D	581/606 (96%)	529 (91%)	42 (7%)	10 (2%)	9	36
All	All	2324/2424 (96%)	2112 (91%)	174 (8%)	38 (2%)	9	37

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	220	ILE
1	A	475	GLU
1	A	506	SER
1	A	534	ASN
1	B	2	ARG
1	B	154	ASN
1	B	220	ILE
1	B	475	GLU
1	B	506	SER
1	B	534	ASN
1	C	2	ARG
1	C	154	ASN
1	C	220	ILE
1	C	475	GLU
1	C	506	SER
1	C	534	ASN
1	D	2	ARG
1	D	154	ASN
1	D	475	GLU
1	D	506	SER
1	D	534	ASN
1	A	2	ARG
1	D	220	ILE
1	A	104	PHE
1	B	104	PHE
1	C	104	PHE
1	D	104	PHE
1	A	163	VAL
1	A	507	ASP
1	B	163	VAL
1	B	459	GLY
1	C	163	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	163	VAL
1	D	507	ASP
1	A	459	GLY
1	C	459	GLY
1	D	459	GLY

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	490/510 (96%)	469 (96%)	21 (4%)	29	62
1	B	490/510 (96%)	469 (96%)	21 (4%)	29	62
1	C	490/510 (96%)	469 (96%)	21 (4%)	29	62
1	D	490/510 (96%)	469 (96%)	21 (4%)	29	62
All	All	1960/2040 (96%)	1876 (96%)	84 (4%)	29	62

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	51	ARG
1	A	61	VAL
1	A	77	MET
1	A	100	THR
1	A	104	PHE
1	A	136	ASP
1	A	159	ASN
1	A	171	THR
1	A	186	VAL
1	A	195	ARG
1	A	210	GLN
1	A	257	MET
1	A	326	THR
1	A	350	LEU
1	A	379	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	406	THR
1	A	413	VAL
1	A	464	THR
1	A	466	MET
1	A	562	ILE
1	B	2	ARG
1	B	51	ARG
1	B	61	VAL
1	B	77	MET
1	B	100	THR
1	B	104	PHE
1	B	136	ASP
1	B	159	ASN
1	B	171	THR
1	B	186	VAL
1	B	195	ARG
1	B	210	GLN
1	B	257	MET
1	B	326	THR
1	B	350	LEU
1	B	379	THR
1	B	406	THR
1	B	413	VAL
1	B	464	THR
1	B	466	MET
1	B	562	ILE
1	C	2	ARG
1	C	51	ARG
1	C	61	VAL
1	C	77	MET
1	C	100	THR
1	C	104	PHE
1	C	136	ASP
1	C	159	ASN
1	C	171	THR
1	C	186	VAL
1	C	195	ARG
1	C	210	GLN
1	C	257	MET
1	C	326	THR
1	C	350	LEU
1	C	379	THR

Continued from previous page...

Mol	Chain	Res	Type
1	C	406	THR
1	C	413	VAL
1	C	464	THR
1	C	466	MET
1	C	562	ILE
1	D	2	ARG
1	D	51	ARG
1	D	61	VAL
1	D	77	MET
1	D	100	THR
1	D	104	PHE
1	D	136	ASP
1	D	159	ASN
1	D	171	THR
1	D	186	VAL
1	D	195	ARG
1	D	210	GLN
1	D	257	MET
1	D	326	THR
1	D	350	LEU
1	D	379	THR
1	D	406	THR
1	D	413	VAL
1	D	464	THR
1	D	466	MET
1	D	562	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	267	ASN
1	D	267	ASN

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 ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	PO4	D	587	-	4,4,4	0.79	0	6,6,6	0.53	0
3	PO4	B	586	-	4,4,4	0.96	0	6,6,6	0.68	0
2	I30	D	586	-	22,25,25	2.33	3 (13%)	27,35,35	1.80	8 (29%)
2	I30	A	586	-	22,25,25	2.26	3 (13%)	27,35,35	1.66	7 (25%)
3	PO4	A	587	-	4,4,4	0.90	0	6,6,6	0.48	0
3	PO4	C	586	-	4,4,4	0.88	0	6,6,6	0.77	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	I30	D	586	-	-	0/9/13/13	0/3/3/3
2	I30	A	586	-	-	0/9/13/13	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	586	I30	NAN-NAL	-8.64	1.22	1.38
2	A	586	I30	NAN-NAL	-8.47	1.23	1.38
2	D	586	I30	CAP-NAL	3.86	1.33	1.29
2	A	586	I30	CAT-CAQ	3.72	1.57	1.50
2	A	586	I30	CAP-NAL	2.91	1.32	1.29
2	D	586	I30	CAT-CAQ	2.74	1.55	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	586	I30	CAP-NAL-NAN	4.37	125.12	118.31
2	A	586	I30	BRAD-CAR-CAK	4.13	125.00	119.27
2	D	586	I30	CAA-CAP-CAU	3.81	122.15	117.92
2	A	586	I30	CAA-CAP-CAU	3.58	121.88	117.92
2	A	586	I30	BRAD-CAR-CAG	-3.17	114.70	119.30
2	D	586	I30	BRAD-CAR-CAK	2.96	123.38	119.27
2	D	586	I30	BRAD-CAR-CAG	-2.78	115.26	119.30
2	A	586	I30	CAU-NAM-CAV	2.47	108.67	103.78
2	D	586	I30	CAK-CAT-CAQ	2.47	124.68	117.36
2	A	586	I30	CAP-NAL-NAN	2.41	122.06	118.31
2	A	586	I30	CAK-CAT-CAQ	2.35	124.32	117.36
2	D	586	I30	CAU-NAM-CAV	2.27	108.28	103.78
2	A	586	I30	CAU-NAO-CAW	2.27	108.27	103.78
2	D	586	I30	CAU-NAO-CAW	2.03	107.81	103.78
2	D	586	I30	CAF-CAE-CAI	-2.00	117.63	120.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	587	PO4	2	0
3	B	586	PO4	2	0
2	D	586	I30	1	0
2	A	586	I30	1	0
3	A	587	PO4	2	0
3	C	586	PO4	1	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 I30 D 586

Ligand I30 A 586
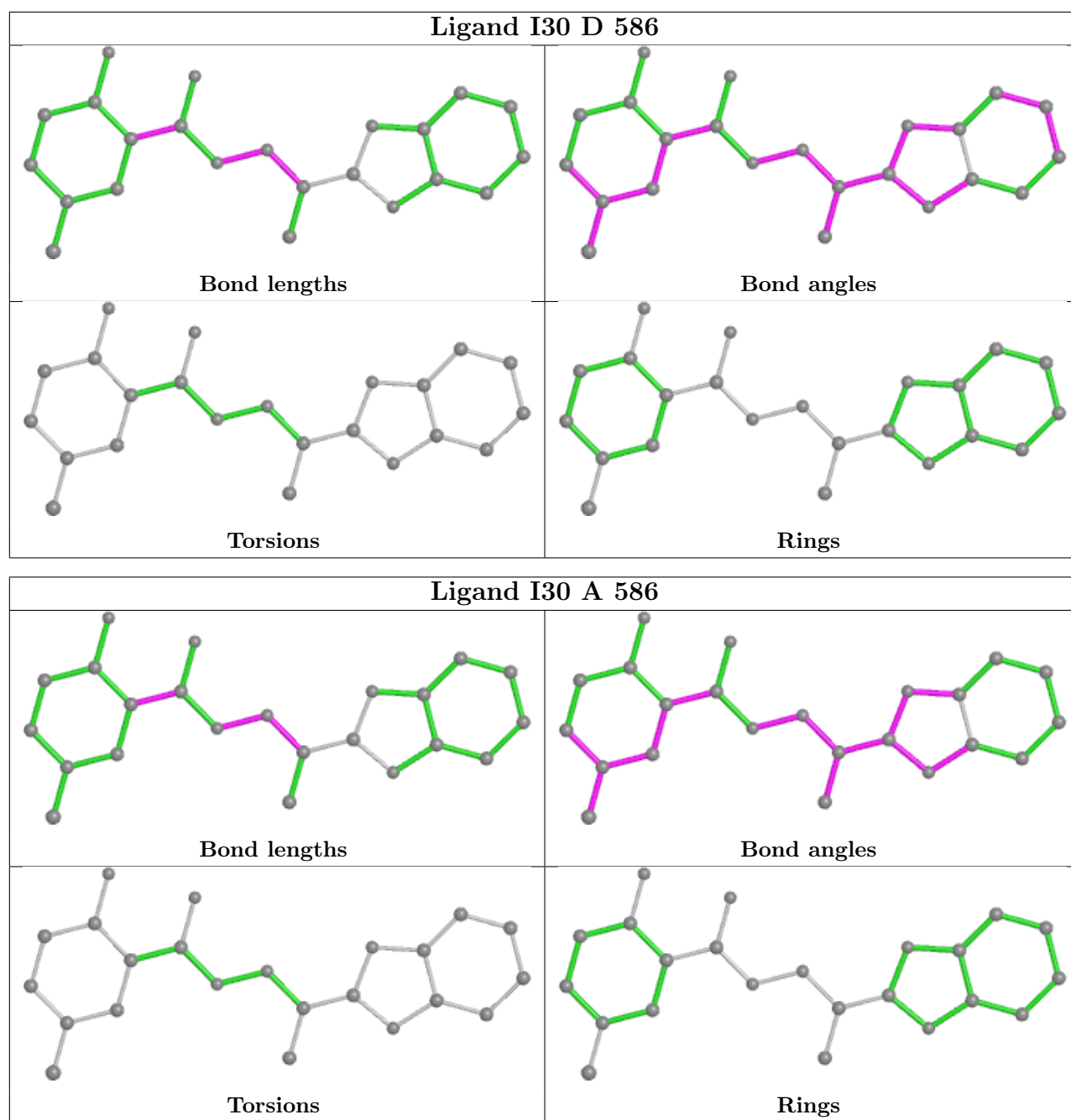
5.7 Other polymers ⓘ

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	583/606 (96%)	0.10	14 (2%)	59	37	56, 91, 133, 168	0
1	B	583/606 (96%)	0.25	31 (5%)	26	12	47, 80, 162, 198	0
1	C	583/606 (96%)	0.16	20 (3%)	45	24	51, 91, 154, 190	0
1	D	583/606 (96%)	-0.01	2 (0%)	94	88	50, 83, 126, 165	0
All	All	2332/2424 (96%)	0.13	67 (2%)	51	28	47, 86, 147, 198	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	502	GLY	4.6
1	C	494	ALA	4.2
1	B	494	ALA	4.1
1	A	497	VAL	4.0
1	B	492	LEU	3.9
1	B	85	GLU	3.6
1	B	503	LYS	3.4
1	C	523	VAL	3.4
1	B	504	ASP	3.4
1	B	522	TYR	3.3
1	C	493	VAL	3.1
1	B	523	VAL	3.0
1	A	494	ALA	3.0
1	A	559	VAL	3.0
1	B	76	ASN	2.9
1	B	515	ILE	2.9
1	C	492	LEU	2.9
1	C	497	VAL	2.8
1	B	540	SER	2.8
1	B	493	VAL	2.8
1	A	504	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	502	GLY	2.7
1	C	515	ILE	2.7
1	C	504	ASP	2.7
1	C	146	ILE	2.7
1	B	530	ILE	2.6
1	B	90	VAL	2.6
1	B	78	LYS	2.6
1	C	498	LYS	2.5
1	C	503	LYS	2.5
1	A	506	SER	2.5
1	B	512	THR	2.5
1	B	101	PRO	2.5
1	A	492	LEU	2.5
1	D	523	VAL	2.5
1	B	518	THR	2.5
1	B	510	ILE	2.4
1	B	547	LYS	2.4
1	B	560	LYS	2.4
1	B	139	LYS	2.4
1	B	500	LEU	2.4
1	A	525	LYS	2.4
1	C	90	VAL	2.3
1	B	558	ALA	2.3
1	B	525	LYS	2.3
1	C	104	PHE	2.3
1	B	80	GLY	2.3
1	B	151	GLU	2.3
1	D	502	GLY	2.3
1	A	510	ILE	2.2
1	A	526	ALA	2.2
1	A	566	VAL	2.2
1	C	500	LEU	2.2
1	C	517	GLU	2.2
1	B	526	ALA	2.1
1	C	424	ARG	2.1
1	A	562	ILE	2.1
1	B	146	ILE	2.1
1	B	498	LYS	2.1
1	C	78	LYS	2.0
1	C	80	GLY	2.0
1	A	574	GLN	2.0
1	A	493	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	83	GLU	2.0
1	A	515	ILE	2.0
1	C	101	PRO	2.0
1	B	84	LEU	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
3	PO4	D	587	5/5	0.89	0.20	94,98,105,111	0
3	PO4	A	587	5/5	0.94	0.12	98,104,106,109	0
3	PO4	C	586	5/5	0.95	0.19	90,99,102,104	0
2	I30	A	586	23/23	0.95	0.23	58,69,78,103	0
2	I30	D	586	23/23	0.96	0.26	50,69,85,103	0
3	PO4	B	586	5/5	0.98	0.11	88,94,96,97	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 I30 A 586:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
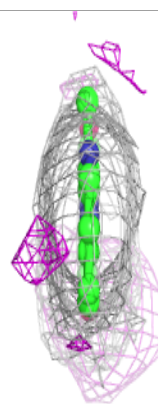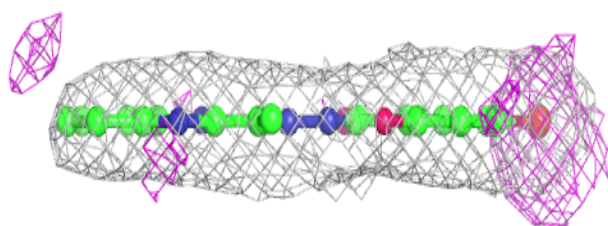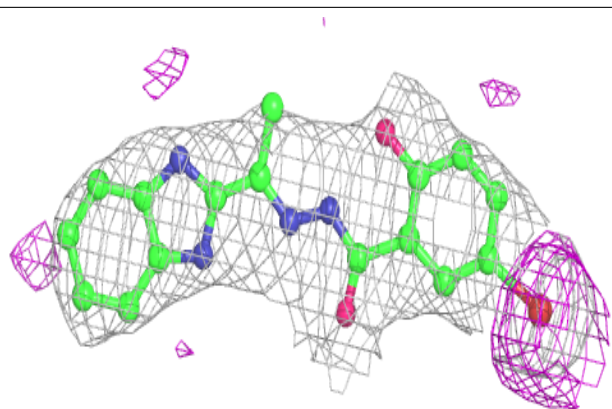
Electron density around I30 D 586:

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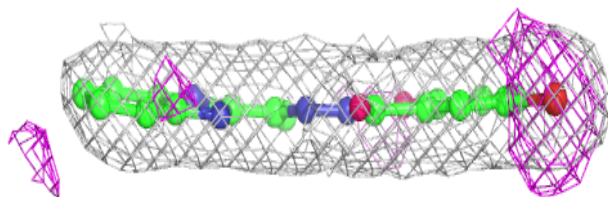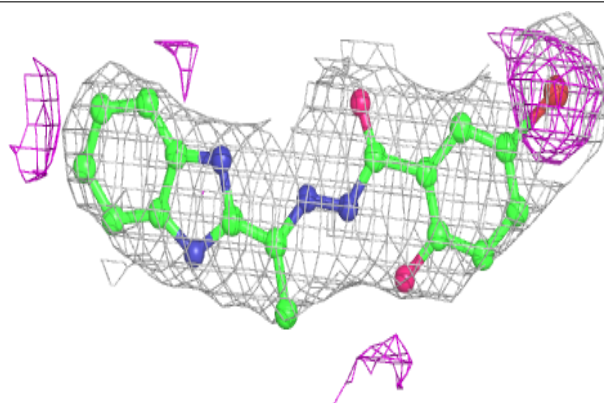
6.5 Other polymers (i)

There are no such residues in this entry.