Full wwPDB X-ray Structure Validation Report (i)

Aug 17, 2022 – 02:25 PM EDT

PDB ID	:	4QG6
Title	:	crystal structure of PKM2-Y105E mutant
Authors	:	Wang, P.; Sun, C.; Zhu, T.; Xu, Y.
Deposited on	:	2014-05-22
Resolution	:	3.21 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

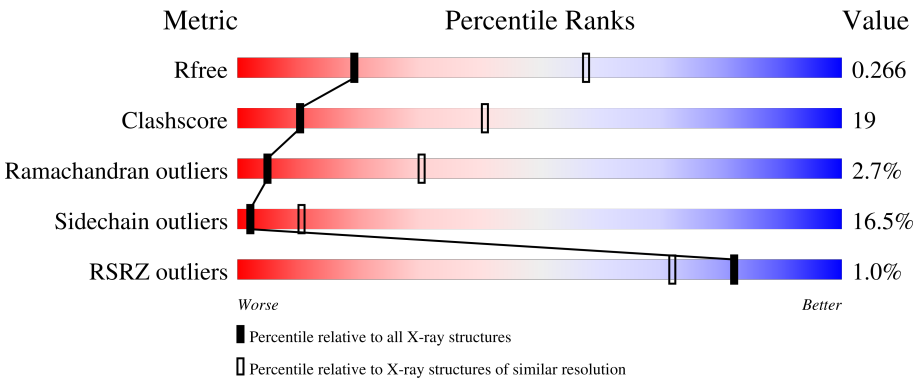
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	535	.% 39% 31% 5% 24%
1	B	535	.% 49% 36% 8% • 6%
1	C	535	.% 43% 29% • 24%
1	D	535	.% 51% 35% 8% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PRO	C	1001	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13991 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.

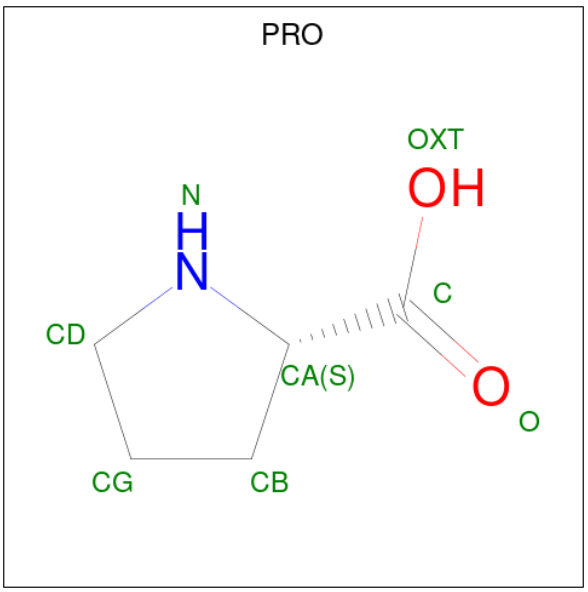
- Molecule 1 is a protein called Pyruvate kinase PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	406	3122	1958	564	579	21	0	0	0
1	B	502	3849	2420	682	723	24	0	0	0
1	C	406	3122	1958	564	579	21	0	0	0
1	D	505	3870	2434	686	726	24	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P14618
A	-2	PRO	-	expression tag	UNP P14618
A	-1	GLY	-	expression tag	UNP P14618
A	0	SER	-	expression tag	UNP P14618
A	105	GLU	TYR	engineered mutation	UNP P14618
B	-3	GLY	-	expression tag	UNP P14618
B	-2	PRO	-	expression tag	UNP P14618
B	-1	GLY	-	expression tag	UNP P14618
B	0	SER	-	expression tag	UNP P14618
B	105	GLU	TYR	engineered mutation	UNP P14618
C	-3	GLY	-	expression tag	UNP P14618
C	-2	PRO	-	expression tag	UNP P14618
C	-1	GLY	-	expression tag	UNP P14618
C	0	SER	-	expression tag	UNP P14618
C	105	GLU	TYR	engineered mutation	UNP P14618
D	-3	GLY	-	expression tag	UNP P14618
D	-2	PRO	-	expression tag	UNP P14618
D	-1	GLY	-	expression tag	UNP P14618
D	0	SER	-	expression tag	UNP P14618
D	105	GLU	TYR	engineered mutation	UNP P14618

- Molecule 2 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



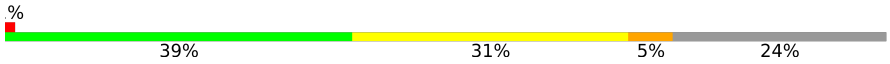
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	7	5	1	1	0	0
2	B	1	7	5	1	1	0	0
2	C	1	7	5	1	1	0	0
2	D	1	7	5	1	1	0	0

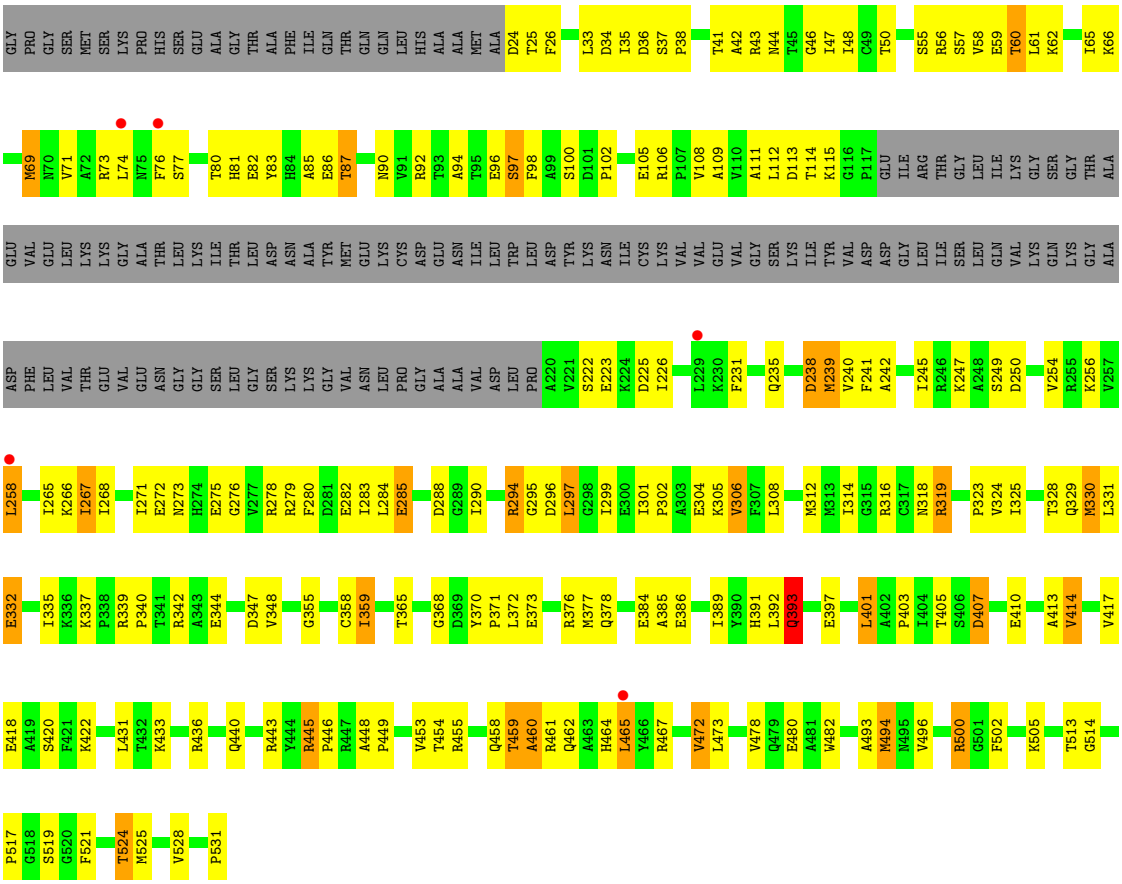
3 Residue-property plots (i)

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

• Molecule 1: Pyruvate kinase PKM

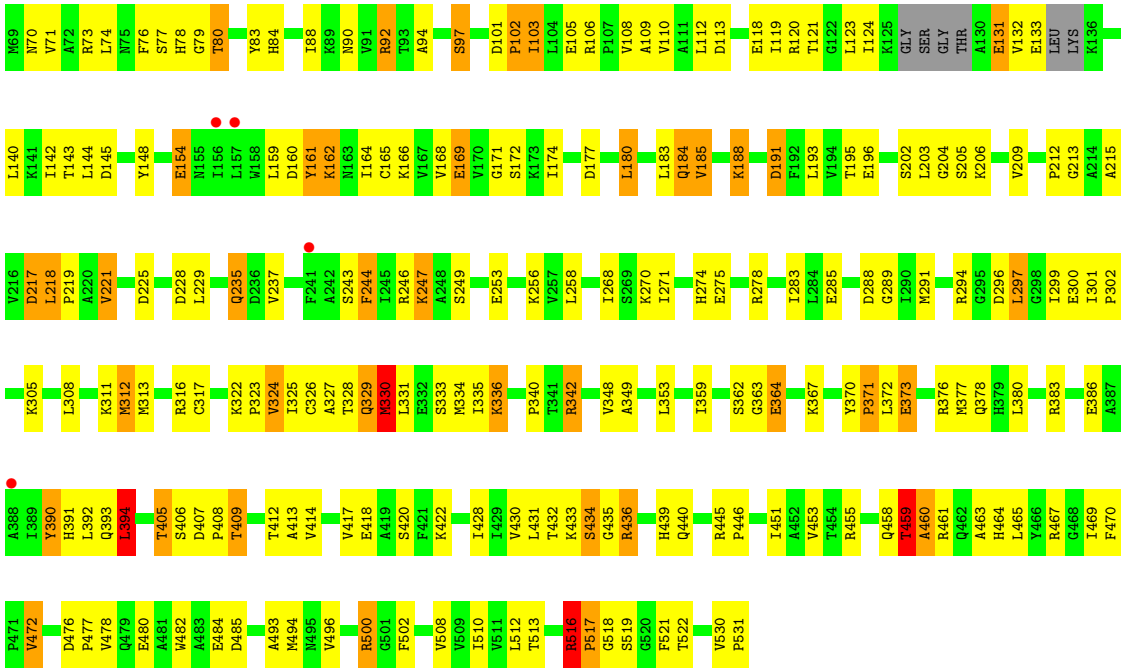
Chain A:





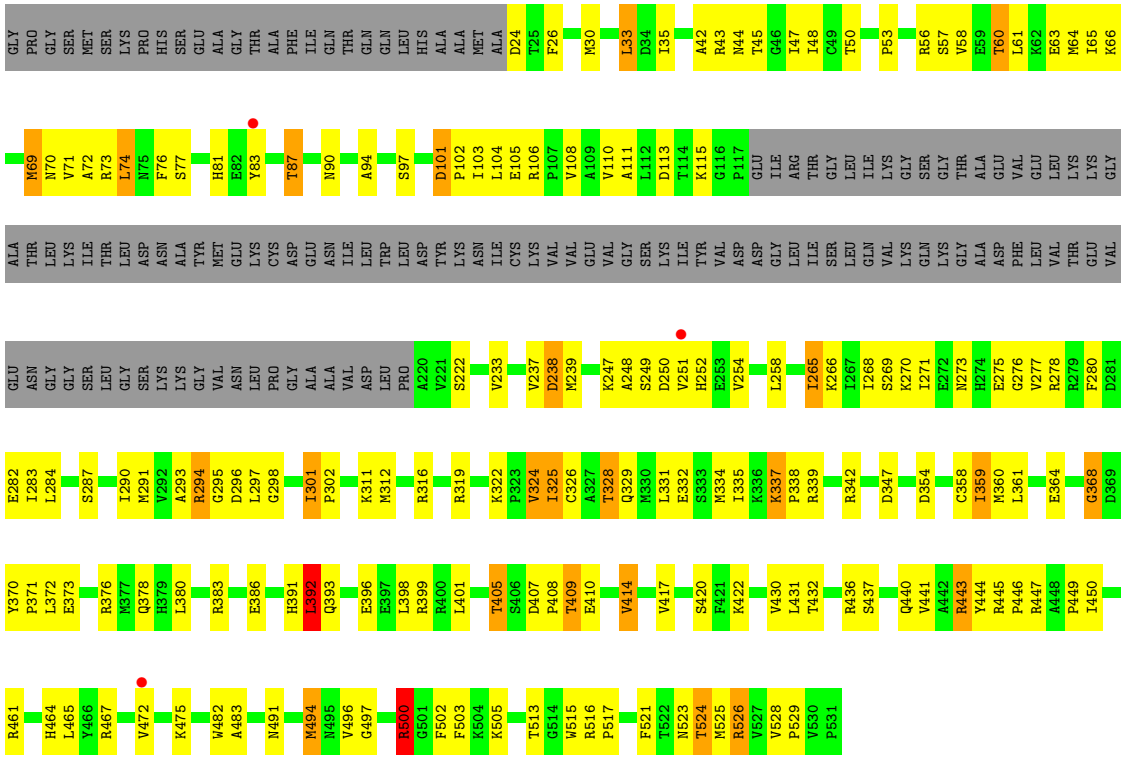
• Molecule 1: Pyruvate kinase PKM

Chain B:



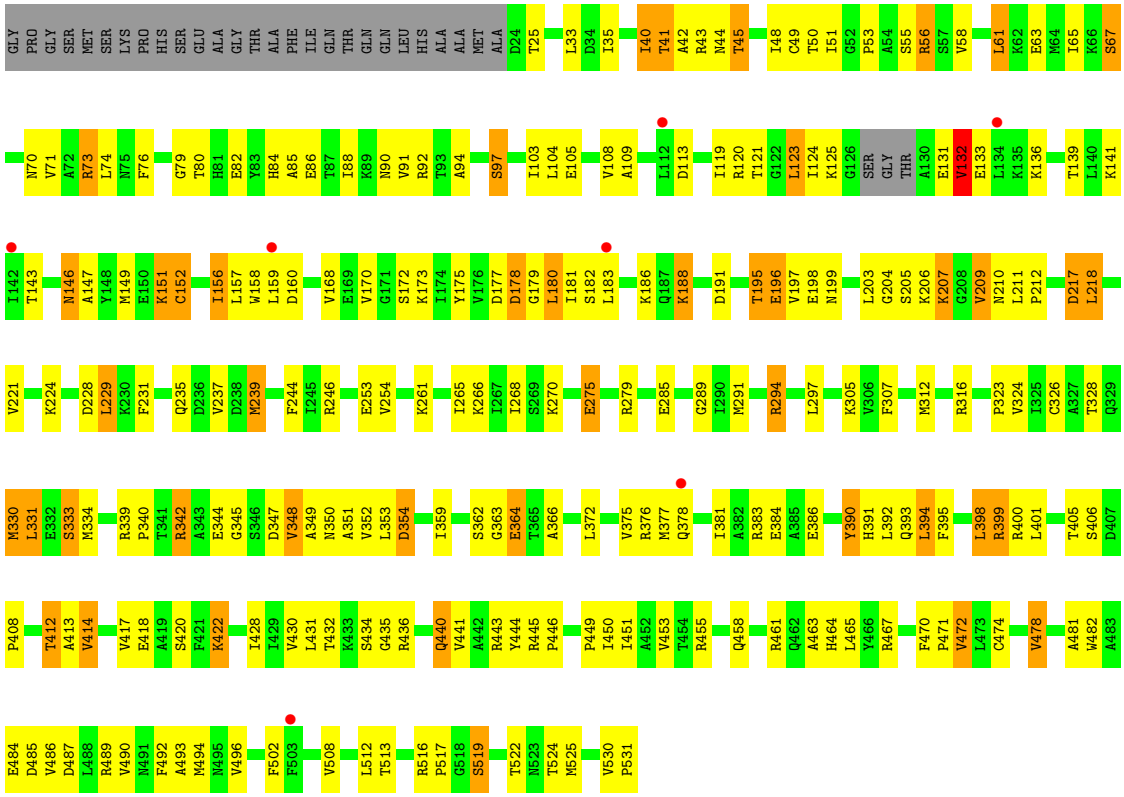
- Molecule 1: Pyruvate kinase PKM

Chain C:



- Molecule 1: Pyruvate kinase PKM

Chain D:


GLY PRO GLY SER MET SER LYS PRO HIS SER GLU ALA GLY THR ALA PHE ILE GLN THR GLN GLN LEU HIS ALA ALA MET ALA D24 T25 L33 D34 I35 I40 T41 A42 R43 N44 T45 I48 C49 T50 I51 G52 P53 A54 S55 R56 S57 V58 L61 K62 E63 M64 I65 K66 S67
N70 V71 A72 R73 L74 N75 F76 G79 T80 H81 E82 Y83 H84 A85 E86 T87 I88 K89 N90 V91 R92 T93 A94 S97 I103 L104 E105 V108 A109 L112 D113 I119 R120 T121 G122 L123 I124 K125 G126 SER GLY THR A130 E131 V132 E133 L134 K135 K136 T139 L140 K141
I142 T143 N146 A147 Y148 M149 E150 K151 C152 I156 L157 W158 L159 D160 V168 E169 V170 G171 S172 K173 I174 Y175 V176 D177 D178 G179 L180 I181 S182 L183 K186 Q187 K188 D191 T195 E196 V197 E198 N199 L203 G204 S205 K206 K207 G208 V209 N210 L211 P212 D217 L218
V221 K224 D228 L229 K230 F231 Q235 D236 V237 D238 M239 F244 I245 R246 E253 V254 K261 I265 K266 I267 I268 S269 K270 E275 R279 E285 G289 I290 M291 R294 L297 K305 V306 F307 M312 R316 P323 V324 I325 C326 A327 T328 Q329
M330 L331 E332 S333 M334 R339 P340 T341 R342 A343 E344 G345 S346 D347 V348 A349 N350 A351 V352 L353 D354 I359 S362 G363 E364 T365 A366 L372 V375 R376 M377 Q378 I381 A382 R383 E384 A385 E386 Y390 H391 L392 Q393 L394 F395 L398 R399 R400 L401 T405 S406 D407
P408 T412 A413 V414 V417 E418 A419 S420 F421 K422 I428 I429 V430 L431 T432 K433 S434 G435 R436 Q440 V441 A442 R443 Y444 R445 P446 P449 I450 I451 A452 V453 T454 R455 Q458 R461 Q462 A463 H464 L465 Y466 R467 F470 P471 V472 L473 C474 V478 A481 W482 A483
E484 D485 V486 D487 L488 R489 V490 N491 F492 A493 M494 N495 V496 F502 F503 V508 L512 T513 R516 P517 G518 S519 T522 N523 T524 M525 V530 P531

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	124.45Å 124.45Å 257.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.62 – 3.21 46.40 – 3.21	Depositor EDS
% Data completeness (in resolution range)	98.2 (45.62-3.21) 98.3 (46.40-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.61 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.220 , 0.265 0.222 , 0.266	Depositor DCC
R_{free} test set	3622 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	95.0	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , -15.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.438 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13991	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.48	0/3175	0.68	0/4287
1	B	0.49	0/3909	0.70	1/5276 (0.0%)
1	C	0.47	0/3175	0.66	0/4287
1	D	0.48	0/3931	0.69	0/5306
All	All	0.48	0/14190	0.68	1/19156 (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	D	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	436	ARG	NE-CZ-NH1	9.39	124.99	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	217	ASP	Peptide
1	D	218	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3122	0	3177	134	0
1	B	3849	0	3929	150	0
1	C	3122	0	3177	120	0
1	D	3870	0	3957	153	0
2	A	7	0	7	2	0
2	B	7	0	7	3	0
2	C	7	0	7	4	0
2	D	7	0	7	0	0
All	All	13991	0	14268	527	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 19.

All (527) 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:B:73:ARG:NH1	1:B:113:ASP:OD2	2.03	0.92
1:D:73:ARG:NH1	1:D:113:ASP:OD2	2.03	0.91
1:C:73:ARG:NH1	1:C:113:ASP:OD2	2.10	0.83
1:D:147:ALA:O	1:D:151:LYS:NZ	2.12	0.83
1:C:422:LYS:HG3	1:D:414:VAL:HG21	1.62	0.82
1:A:445:ARG:HE	1:A:467:ARG:HD3	1.43	0.82
1:C:287:SER:O	1:C:322:LYS:NZ	2.10	0.82
1:C:56:ARG:HG3	1:C:87:THR:HG23	1.62	0.82
1:A:445:ARG:HH11	1:A:445:ARG:HG2	1.44	0.81
1:C:65:ILE:HG23	1:C:69:MET:HE3	1.60	0.80
1:B:417:VAL:HG13	1:B:446:PRO:HB3	1.63	0.80
1:B:312:MET:HE1	1:B:316:ARG:HH21	1.45	0.80
1:D:394:LEU:HD12	1:D:445:ARG:HD3	1.65	0.79
1:D:414:VAL:HG22	1:D:444:TYR:HE2	1.48	0.79
1:C:325:ILE:HG22	1:C:358:CYS:HB2	1.64	0.78
1:B:171:GLY:H	1:B:185:VAL:HG23	1.49	0.77
1:C:516:ARG:NH2	1:D:487:ASP:OD2	2.18	0.77
1:D:92:ARG:NH1	1:D:235:GLN:O	2.17	0.77
1:B:118:GLU:OE1	1:B:120:ARG:NH1	2.18	0.77
1:C:42:ALA:O	1:C:44:ASN:ND2	2.18	0.77
1:B:386:GLU:OE2	1:B:467:ARG:NH2	2.16	0.76
1:D:71:VAL:HG22	1:D:109:ALA:HB3	1.68	0.76
1:A:42:ALA:O	1:A:44:ASN:ND2	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:THR:HG22	1:D:207:LYS:H	1.49	0.75
1:D:451:ILE:HD11	1:D:502:PHE:HD2	1.51	0.75
1:C:386:GLU:OE2	1:C:467:ARG:NH2	2.20	0.75
1:D:70:ASN:HD22	1:D:464:HIS:HD2	1.34	0.74
1:B:58:VAL:HG23	1:B:90:ASN:HD22	1.53	0.74
1:D:70:ASN:HD22	1:D:464:HIS:CD2	2.04	0.74
1:D:354:ASP:OD1	1:D:354:ASP:N	2.18	0.74
1:A:86:GLU:O	1:A:90:ASN:ND2	2.21	0.73
1:A:223:GLU:HA	1:A:226:ILE:HD12	1.69	0.73
1:C:280:PHE:HA	1:C:283:ILE:HD12	1.71	0.73
1:A:328:THR:HG22	1:A:329:GLN:HG3	1.69	0.73
1:C:268:ILE:HG21	1:C:325:ILE:HD11	1.71	0.72
1:D:386:GLU:OE2	1:D:467:ARG:NH2	2.23	0.72
1:D:482:TRP:CD1	1:D:517:PRO:HD3	2.24	0.71
1:A:325:ILE:HG22	1:A:358:CYS:HB2	1.71	0.71
1:D:239:MET:HB3	1:D:266:LYS:HB2	1.73	0.71
1:A:370:TYR:HB3	1:A:373:GLU:HB2	1.73	0.70
1:A:449:PRO:HG3	1:A:502:PHE:HD2	1.56	0.70
1:B:370:TYR:HD1	1:B:373:GLU:HG3	1.55	0.69
1:C:337:LYS:HE2	1:C:338:PRO:HD2	1.73	0.69
1:A:464:HIS:HD2	2:A:1001:PRO:HB2	1.57	0.69
1:C:392:LEU:H	1:C:392:LEU:HD22	1.56	0.69
1:B:328:THR:HG22	1:B:329:GLN:HG2	1.75	0.69
1:C:311:LYS:NZ	1:C:354:ASP:OD1	2.25	0.68
1:B:451:ILE:HD11	1:B:502:PHE:HD2	1.58	0.68
1:B:133:GLU:HG2	1:B:203:LEU:H	1.59	0.68
1:C:370:TYR:HB3	1:C:373:GLU:HB2	1.76	0.68
1:A:73:ARG:NH1	1:A:113:ASP:OD2	2.26	0.68
1:D:270:LYS:HA	1:D:291:MET:HB3	1.76	0.68
1:B:390:TYR:CZ	1:B:394:LEU:HD22	2.29	0.67
1:C:464:HIS:HD2	2:C:1001:PRO:CB	2.08	0.67
1:C:405:THR:HB	1:C:407:ASP:H	1.59	0.67
1:D:170:VAL:HG23	1:D:188:LYS:HE2	1.74	0.67
1:B:92:ARG:NH1	1:B:235:GLN:O	2.28	0.67
1:B:191:ASP:N	1:B:191:ASP:OD1	2.29	0.66
1:A:418:GLU:HG2	1:B:418:GLU:HG3	1.78	0.66
1:D:50:THR:HG22	1:D:366:ALA:HB2	1.77	0.66
1:A:378:GLN:O	1:A:378:GLN:NE2	2.29	0.66
1:B:102:PRO:HA	1:B:105:GLU:HG2	1.77	0.66
1:D:359:ILE:HD11	1:D:378:GLN:OE1	1.95	0.65
1:A:372:LEU:HG	1:A:376:ARG:HD2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:VAL:HG21	1:D:422:LYS:HD3	1.77	0.65
1:D:42:ALA:O	1:D:44:ASN:ND2	2.30	0.65
1:A:417:VAL:O	1:A:420:SER:OG	2.12	0.65
1:B:433:LYS:O	1:B:459:THR:OG1	2.11	0.64
1:A:417:VAL:HG22	1:A:446:PRO:HG3	1.79	0.64
1:D:65:ILE:HD12	1:D:108:VAL:HG21	1.79	0.64
1:C:399:ARG:NH2	1:D:399:ARG:HH12	1.97	0.63
1:B:409:THR:OG1	1:B:440:GLN:NE2	2.27	0.63
1:B:68:GLY:O	1:B:70:ASN:ND2	2.30	0.63
1:A:472:VAL:HG21	1:A:496:VAL:HG11	1.80	0.63
1:B:229:LEU:HD22	1:B:258:LEU:HD21	1.81	0.63
1:B:244:PHE:HD2	1:B:246:ARG:HH11	1.44	0.63
1:C:58:VAL:HG23	1:C:90:ASN:ND2	2.12	0.63
1:D:55:SER:O	1:D:61:LEU:HD23	1.98	0.63
1:D:61:LEU:HD12	1:D:91:VAL:HA	1.81	0.63
1:C:238:ASP:OD2	1:C:461:ARG:NE	2.26	0.62
1:A:464:HIS:HD2	2:A:1001:PRO:CB	2.11	0.62
1:D:229:LEU:HD21	1:D:254:VAL:HG13	1.81	0.62
1:A:238:ASP:OD1	1:A:238:ASP:N	2.32	0.62
1:A:332:GLU:O	1:A:335:ILE:HG13	1.99	0.62
1:D:294:ARG:NH2	1:D:347:ASP:OD2	2.30	0.61
1:B:453:VAL:HG21	1:B:493:ALA:HB2	1.81	0.61
1:C:359:ILE:HD13	1:C:359:ILE:H	1.65	0.61
1:D:61:LEU:HD11	1:D:91:VAL:HG22	1.82	0.61
1:D:88:ILE:HG22	1:D:92:ARG:HE	1.66	0.61
1:A:482:TRP:CD1	1:A:517:PRO:HB3	2.36	0.61
1:B:51:ILE:HD13	1:B:61:LEU:HD21	1.83	0.61
1:B:119:ILE:HB	1:B:209:VAL:HG22	1.82	0.61
1:A:445:ARG:NE	1:A:467:ARG:HD3	2.14	0.60
1:A:403:PRO:O	1:B:422:LYS:NZ	2.33	0.60
1:B:145:ASP:HB3	1:B:148:TYR:HD2	1.67	0.60
1:A:85:ALA:HB2	1:A:231:PHE:HZ	1.66	0.60
1:B:370:TYR:CD1	1:B:373:GLU:HG3	2.36	0.60
1:C:407:ASP:OD2	1:C:409:THR:HG22	2.01	0.60
1:A:403:PRO:HG2	1:A:405:THR:HG23	1.84	0.60
1:A:414:VAL:HG21	1:B:422:LYS:HG2	1.84	0.60
1:A:273:ASN:HD21	1:A:275:GLU:HB3	1.67	0.60
1:B:405:THR:HB	1:B:407:ASP:H	1.67	0.59
1:A:247:LYS:NZ	1:A:275:GLU:OE1	2.35	0.59
1:B:253:GLU:HA	1:B:256:LYS:HE2	1.84	0.59
1:C:391:HIS:O	1:C:393:GLN:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:ARG:NE	1:D:399:ARG:HH22	2.00	0.59
1:D:70:ASN:HB3	1:D:464:HIS:HD2	1.66	0.59
1:A:301:ILE:HG13	1:A:306:VAL:HG23	1.85	0.59
1:D:431:LEU:HD22	1:D:513:THR:HA	1.84	0.59
1:B:458:GLN:O	1:B:460:ALA:N	2.36	0.59
1:C:399:ARG:NH1	1:D:418:GLU:OE2	2.34	0.59
1:A:305:LYS:NZ	1:D:384:GLU:OE1	2.30	0.59
1:B:70:ASN:OD1	1:B:464:HIS:HD2	1.85	0.59
1:D:451:ILE:HD11	1:D:502:PHE:CD2	2.37	0.59
1:A:275:GLU:HA	1:A:278:ARG:HB2	1.85	0.59
1:D:70:ASN:HB3	1:D:464:HIS:CD2	2.37	0.59
1:D:132:VAL:HG23	1:D:203:LEU:HB3	1.85	0.59
1:A:325:ILE:CG2	1:A:358:CYS:HB2	2.33	0.58
1:C:445:ARG:HH11	1:C:467:ARG:HD3	1.68	0.58
1:B:431:LEU:HD22	1:B:513:THR:HA	1.86	0.58
1:A:459:THR:HA	1:A:462:GLN:HB2	1.86	0.58
1:B:406:SER:O	1:B:408:PRO:HD3	2.03	0.58
1:A:35:ILE:O	1:D:305:LYS:NZ	2.31	0.58
1:C:325:ILE:CG2	1:C:358:CYS:HB2	2.31	0.58
1:A:240:VAL:HG21	1:A:258:LEU:HD21	1.86	0.57
1:A:431:LEU:HD22	1:A:513:THR:HG22	1.87	0.57
1:D:191:ASP:N	1:D:191:ASP:OD1	2.37	0.57
1:A:55:SER:HA	1:A:60:THR:HG21	1.87	0.57
1:C:482:TRP:HZ3	1:C:515:TRP:C	2.07	0.57
1:B:312:MET:HE1	1:B:316:ARG:NH2	2.18	0.57
1:B:428:ILE:HG23	1:B:510:ILE:HB	1.87	0.57
1:C:290:ILE:HB	1:C:324:VAL:HG23	1.85	0.57
1:C:399:ARG:CZ	1:D:399:ARG:HH12	2.18	0.57
1:B:30:MET:HE1	1:C:311:LYS:HD3	1.86	0.56
1:A:297:LEU:HD12	1:A:301:ILE:HD11	1.85	0.56
1:A:513:THR:O	1:A:524:THR:HB	2.05	0.56
1:B:142:ILE:HB	1:B:193:LEU:HB2	1.86	0.56
1:C:391:HIS:C	1:C:393:GLN:H	2.08	0.56
1:D:141:LYS:HB3	1:D:156:ILE:HG23	1.87	0.56
1:D:173:LYS:NZ	1:D:198:GLU:OE2	2.29	0.56
1:C:238:ASP:OD1	1:C:238:ASP:N	2.38	0.56
1:B:390:TYR:CE2	1:B:394:LEU:HD22	2.41	0.56
1:D:109:ALA:HA	1:D:461:ARG:HD2	1.87	0.56
1:A:318:ASN:HD21	1:A:355:GLY:HA3	1.70	0.56
1:A:422:LYS:HG3	1:B:414:VAL:HG21	1.88	0.56
1:D:124:ILE:HG12	1:D:132:VAL:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:ILE:HG21	1:D:92:ARG:HH11	1.71	0.56
1:C:399:ARG:CD	1:D:399:ARG:HH22	2.18	0.56
1:B:218:LEU:HD23	1:B:246:ARG:HH21	1.70	0.55
1:C:64:MET:HG2	1:C:372:LEU:HD23	1.88	0.55
1:A:238:ASP:OD2	1:A:461:ARG:NE	2.26	0.55
1:B:48:ILE:HG12	1:B:71:VAL:HB	1.89	0.55
1:D:432:THR:HG21	1:D:435:GLY:HA2	1.89	0.55
1:A:273:ASN:ND2	1:A:275:GLU:HB3	2.21	0.55
1:D:430:VAL:HG22	1:D:512:LEU:HD12	1.87	0.55
1:D:43:ARG:NH1	1:D:45:THR:O	2.40	0.55
1:B:28:GLU:O	1:B:32:ARG:HG2	2.07	0.55
1:C:312:MET:SD	1:C:316:ARG:NH1	2.76	0.55
1:B:61:LEU:O	1:B:65:ILE:HG12	2.07	0.55
1:D:146:ASN:N	1:D:146:ASN:OD1	2.40	0.54
1:A:71:VAL:HG22	1:A:109:ALA:HB3	1.88	0.54
1:C:254:VAL:O	1:C:258:LEU:HD12	2.06	0.54
1:C:417:VAL:HG23	1:C:446:PRO:HG3	1.89	0.54
1:D:395:PHE:O	1:D:398:LEU:HD22	2.07	0.54
1:B:221:VAL:HG12	1:B:225:ASP:HB3	1.89	0.54
1:B:464:HIS:CD2	2:B:1001:PRO:HB2	2.42	0.54
1:B:101:ASP:OD1	1:B:103:ILE:N	2.41	0.54
1:B:472:VAL:HG21	1:B:496:VAL:HG11	1.88	0.54
1:C:83:TYR:O	1:C:87:THR:OG1	2.25	0.54
1:D:481:ALA:HB3	1:D:484:GLU:HG2	1.89	0.54
1:D:494:MET:HG2	1:D:531:PRO:HD2	1.87	0.54
1:B:218:LEU:HB3	1:B:219:PRO:HA	1.90	0.54
1:B:323:PRO:HB3	1:B:465:LEU:O	2.08	0.54
1:B:459:THR:OG1	1:B:459:THR:O	2.22	0.54
1:D:70:ASN:ND2	1:D:464:HIS:HD2	2.05	0.54
1:B:359:ILE:HD11	1:B:378:GLN:CD	2.27	0.54
1:B:106:ARG:NH2	1:B:500:ARG:HD2	2.22	0.54
1:D:221:VAL:HG22	1:D:253:GLU:HG2	1.90	0.54
1:A:295:GLY:HA3	1:A:328:THR:HG21	1.90	0.54
1:B:342:ARG:HD3	1:C:294:ARG:HB3	1.90	0.54
1:C:73:ARG:HA	1:C:111:ALA:HB3	1.88	0.54
1:C:248:ALA:N	1:C:282:GLU:OE2	2.42	0.53
1:A:280:PHE:HA	1:A:283:ILE:HD12	1.89	0.53
1:D:76:PHE:CE1	1:D:84:HIS:CD2	2.96	0.53
1:B:109:ALA:HA	1:B:461:ARG:HD2	1.90	0.53
1:A:271:ILE:HG23	1:A:276:GLY:HA3	1.91	0.53
1:C:361:LEU:HD21	1:C:378:GLN:HE21	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ILE:HG22	1:B:336:LYS:HG2	1.89	0.53
1:A:247:LYS:NZ	1:A:279:ARG:HG3	2.24	0.53
1:B:330:MET:HG3	1:B:348:VAL:HG22	1.89	0.53
1:C:513:THR:O	1:C:524:THR:HB	2.09	0.52
1:D:119:ILE:HB	1:D:209:VAL:HG22	1.91	0.52
1:B:80:THR:HG23	1:B:83:TYR:HB2	1.90	0.52
1:C:417:VAL:O	1:C:420:SER:OG	2.21	0.52
1:A:407:ASP:HB3	1:A:410:GLU:H	1.74	0.52
1:A:294:ARG:NH2	1:A:347:ASP:OD1	2.32	0.52
1:B:268:ILE:HG21	1:B:325:ILE:HD12	1.90	0.52
1:B:275:GLU:HG3	1:B:278:ARG:HH21	1.75	0.52
1:C:431:LEU:HD22	1:C:513:THR:HG22	1.92	0.52
1:C:43:ARG:NH1	1:C:47:ILE:HG13	2.26	0.51
1:C:57:SER:HB3	1:C:60:THR:HB	1.91	0.51
1:C:250:ASP:O	1:C:254:VAL:HG23	2.10	0.51
1:D:48:ILE:HG12	1:D:71:VAL:HB	1.92	0.51
1:C:293:ALA:O	1:C:297:LEU:HB2	2.10	0.51
1:C:464:HIS:HD2	2:C:1001:PRO:HB3	1.75	0.51
1:D:40:ILE:HD13	1:D:40:ILE:H	1.75	0.51
1:A:43:ARG:NH1	1:A:47:ILE:HG13	2.25	0.51
1:B:124:ILE:HG21	1:B:132:VAL:HG13	1.92	0.51
1:B:494:MET:SD	1:B:530:VAL:HG22	2.51	0.51
1:D:103:ILE:HG22	1:D:104:LEU:HD12	1.92	0.51
1:C:482:TRP:CD2	1:C:517:PRO:HG3	2.46	0.51
1:A:50:THR:OG1	1:A:73:ARG:NE	2.41	0.51
1:A:386:GLU:OE2	1:A:467:ARG:NH2	2.40	0.51
1:D:455:ARG:NH2	1:D:485:ASP:OD1	2.40	0.51
1:A:242:ALA:HB1	1:A:245:ILE:HD11	1.93	0.51
1:D:244:PHE:HE1	1:D:246:ARG:HD3	1.75	0.51
1:C:295:GLY:HA3	1:C:328:THR:HG21	1.92	0.51
1:D:482:TRP:CD2	1:D:516:ARG:HG3	2.44	0.51
1:A:372:LEU:HD21	1:A:376:ARG:NH1	2.25	0.50
1:B:29:HIS:CD2	1:B:390:TYR:HA	2.46	0.50
1:B:218:LEU:HD21	1:B:247:LYS:NZ	2.27	0.50
1:B:312:MET:HG3	1:B:313:MET:N	2.26	0.50
1:B:359:ILE:HD11	1:B:378:GLN:NE2	2.26	0.50
1:B:434:SER:HB2	1:B:436:ARG:HG3	1.94	0.50
1:D:218:LEU:HD21	1:D:246:ARG:CZ	2.41	0.50
1:A:494:MET:HG2	1:A:531:PRO:HD2	1.94	0.50
1:C:65:ILE:HD12	1:C:66:LYS:N	2.27	0.50
1:C:372:LEU:HD11	1:C:376:ARG:HH21	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ALA:O	1:C:97:SER:OG	2.25	0.50
1:A:384:GLU:CD	1:D:305:LYS:HD3	2.32	0.50
1:C:331:LEU:HB2	1:C:364:GLU:HG2	1.94	0.50
1:D:175:TYR:CE1	1:D:212:PRO:HG2	2.47	0.50
1:A:57:SER:HB3	1:A:60:THR:HB	1.94	0.50
1:A:365:THR:HA	1:A:371:PRO:HB3	1.94	0.50
1:B:371:PRO:HD2	1:B:372:LEU:H	1.75	0.50
1:D:168:VAL:HG13	1:D:172:SER:HB2	1.93	0.50
1:B:161:TYR:OH	1:B:217:ASP:HB2	2.12	0.50
1:B:195:THR:OG1	1:B:196:GLU:N	2.45	0.50
1:D:244:PHE:CE1	1:D:246:ARG:HD3	2.47	0.50
1:A:319:ARG:HH11	1:A:319:ARG:HB3	1.77	0.50
1:B:76:PHE:CE1	1:B:84:HIS:CD2	2.99	0.50
1:C:335:ILE:HG23	1:C:368:GLY:HA2	1.93	0.50
1:D:41:THR:O	1:D:383:ARG:NE	2.38	0.50
1:D:348:VAL:HG12	1:D:359:ILE:HD12	1.94	0.50
1:D:494:MET:SD	1:D:530:VAL:HG22	2.52	0.50
1:C:65:ILE:HG21	1:C:108:VAL:HG21	1.95	0.49
1:D:453:VAL:HG21	1:D:493:ALA:HB2	1.95	0.49
1:A:71:VAL:HG11	1:A:239:MET:HE1	1.93	0.49
1:B:359:ILE:HD11	1:B:378:GLN:OE1	2.12	0.49
1:B:275:GLU:HG3	1:B:278:ARG:NH2	2.28	0.49
1:B:455:ARG:NH2	1:B:485:ASP:OD1	2.39	0.49
1:C:102:PRO:HA	1:C:105:GLU:OE2	2.11	0.49
1:A:239:MET:SD	1:A:465:LEU:HD21	2.52	0.49
1:D:406:SER:O	1:D:408:PRO:HD3	2.12	0.49
1:B:177:ASP:O	1:B:180:LEU:HB2	2.13	0.49
1:D:270:LYS:HE3	1:D:291:MET:SD	2.52	0.49
1:A:48:ILE:HG12	1:A:71:VAL:HB	1.94	0.49
1:B:131:GLU:HB3	1:B:204:GLY:HA2	1.94	0.49
1:D:333:SER:HB3	1:D:344:GLU:OE1	2.13	0.49
1:A:247:LYS:HZ2	1:A:279:ARG:HG3	1.78	0.49
1:A:65:ILE:HG23	1:A:69:MET:HE3	1.95	0.49
1:D:224:LYS:HG2	1:D:228:ASP:OD2	2.13	0.49
1:B:144:LEU:HD21	1:B:164:ILE:HG22	1.95	0.48
1:D:65:ILE:CD1	1:D:108:VAL:HG21	2.42	0.48
1:A:247:LYS:HE3	1:A:279:ARG:NE	2.27	0.48
1:A:410:GLU:O	1:A:413:ALA:N	2.46	0.48
1:D:61:LEU:O	1:D:65:ILE:HG12	2.12	0.48
1:D:266:LYS:HA	1:D:266:LYS:HD3	1.68	0.48
1:D:268:ILE:HD12	1:D:289:GLY:HA3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ALA:O	1:A:97:SER:OG	2.31	0.48
1:C:44:ASN:N	1:C:44:ASN:HD22	2.11	0.48
1:C:523:ASN:OD1	1:C:523:ASN:N	2.46	0.48
1:D:312:MET:CE	1:D:316:ARG:HH21	2.27	0.48
1:D:472:VAL:HG21	1:D:496:VAL:HG11	1.95	0.48
1:C:464:HIS:HD2	2:C:1001:PRO:HB2	1.78	0.48
1:B:271:ILE:HD11	1:B:283:ILE:HG21	1.95	0.48
1:C:496:VAL:O	1:C:500:ARG:HG2	2.13	0.48
1:C:294:ARG:O	1:C:298:GLY:N	2.47	0.48
1:D:464:HIS:CE1	1:D:471:PRO:HG2	2.49	0.48
1:A:58:VAL:HG23	1:A:90:ASN:OD1	2.14	0.48
1:B:469:ILE:O	2:B:1001:PRO:HB3	2.14	0.48
1:C:239:MET:SD	1:C:465:LEU:HD21	2.54	0.48
1:D:408:PRO:O	1:D:412:THR:OG1	2.30	0.48
1:C:525:MET:HB3	1:D:525:MET:HB3	1.96	0.48
1:D:94:ALA:O	1:D:97:SER:HB3	2.13	0.48
1:C:56:ARG:HH22	1:C:83:TYR:HB3	1.78	0.47
1:D:490:VAL:HG12	1:D:494:MET:HE2	1.96	0.47
1:B:161:TYR:CE1	1:B:217:ASP:HB2	2.48	0.47
1:B:436:ARG:O	1:B:439:HIS:HB2	2.15	0.47
1:C:301:ILE:HB	1:C:302:PRO:HD2	1.95	0.47
1:C:449:PRO:HG3	1:C:502:PHE:CD1	2.49	0.47
1:D:417:VAL:HG13	1:D:446:PRO:HB3	1.97	0.47
1:A:314:ILE:HA	1:A:324:VAL:HG11	1.95	0.47
1:B:244:PHE:CD2	1:B:246:ARG:HD3	2.49	0.47
1:B:123:LEU:HA	1:B:205:SER:HB2	1.96	0.47
1:D:352:VAL:HG12	1:D:353:LEU:HD23	1.95	0.47
1:A:312:MET:HB2	1:D:33:LEU:HB2	1.96	0.47
1:A:458:GLN:O	1:A:460:ALA:N	2.48	0.47
1:B:50:THR:HA	1:B:73:ARG:HB3	1.97	0.47
1:C:104:LEU:O	1:C:106:ARG:NH1	2.48	0.47
1:C:65:ILE:HD12	1:C:66:LYS:H	1.79	0.47
1:C:74:LEU:HD11	1:C:87:THR:HB	1.97	0.47
1:D:331:LEU:HD12	1:D:340:PRO:HB3	1.97	0.47
1:A:519:SER:O	1:A:521:PHE:N	2.44	0.47
1:A:56:ARG:HB2	1:A:87:THR:HG23	1.97	0.46
1:B:174:ILE:N	1:B:183:LEU:O	2.42	0.46
1:B:296:ASP:O	1:B:299:ILE:HG13	2.14	0.46
1:B:413:ALA:O	1:B:417:VAL:HG23	2.15	0.46
1:A:34:ASP:OD1	1:A:36:ASP:N	2.38	0.46
1:A:241:PHE:CE1	1:A:268:ILE:HD13	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:HIS:C	1:A:393:GLN:H	2.19	0.46
1:A:319:ARG:HD3	1:A:401:LEU:HD22	1.97	0.46
1:A:85:ALA:HB2	1:A:231:PHE:CZ	2.49	0.46
1:C:526:ARG:HD3	1:D:524:THR:HG23	1.97	0.46
1:A:65:ILE:HG23	1:A:69:MET:CE	2.45	0.46
1:B:65:ILE:HD12	1:B:108:VAL:HG21	1.97	0.46
1:B:67:SER:OG	1:B:376:ARG:NE	2.42	0.46
1:A:454:THR:HG21	1:A:460:ALA:HB2	1.98	0.46
1:B:57:SER:O	1:B:60:THR:N	2.48	0.46
1:B:464:HIS:HA	2:B:1001:PRO:HG3	1.96	0.46
1:C:103:ILE:HG23	1:C:496:VAL:HA	1.98	0.46
1:C:273:ASN:OD1	1:C:273:ASN:N	2.49	0.46
1:D:349:ALA:C	1:D:351:ALA:H	2.19	0.46
1:B:65:ILE:HD12	1:B:108:VAL:CG2	2.46	0.46
1:B:244:PHE:HD2	1:B:246:ARG:NH1	2.12	0.46
1:B:308:LEU:HD22	1:C:33:LEU:CD2	2.45	0.46
1:B:482:TRP:CD2	1:B:516:ARG:HG2	2.51	0.46
1:D:344:GLU:O	1:D:348:VAL:HG22	2.16	0.46
1:C:61:LEU:O	1:C:65:ILE:HG13	2.16	0.46
1:D:121:THR:O	1:D:206:LYS:HA	2.15	0.46
1:B:268:ILE:HD12	1:B:289:GLY:HA3	1.98	0.46
1:D:177:ASP:OD2	1:D:207:LYS:HD3	2.16	0.46
1:D:195:THR:OG1	1:D:196:GLU:N	2.49	0.46
1:A:302:PRO:HB2	1:A:304:GLU:OE1	2.16	0.45
1:A:329:GLN:OE1	1:D:342:ARG:NE	2.34	0.45
1:B:74:LEU:HD11	1:B:88:ILE:HG12	1.97	0.45
1:D:76:PHE:CD2	1:D:228:ASP:HB3	2.51	0.45
1:D:449:PRO:HB3	1:D:470:PHE:CE1	2.51	0.45
1:A:77:SER:HA	1:A:115:LYS:HB2	1.98	0.45
1:A:391:HIS:O	1:A:393:GLN:N	2.47	0.45
1:D:123:LEU:HD22	1:D:205:SER:HB3	1.97	0.45
1:D:413:ALA:O	1:D:417:VAL:HG23	2.17	0.45
1:A:65:ILE:HD12	1:A:66:LYS:H	1.81	0.45
1:B:430:VAL:HG22	1:B:512:LEU:HD12	1.98	0.45
1:D:149:MET:HG3	1:D:158:TRP:CZ3	2.51	0.45
1:A:96:GLU:C	1:A:98:PHE:H	2.20	0.45
1:A:114:THR:HG22	1:A:242:ALA:HA	1.99	0.45
1:A:340:PRO:HD3	1:A:377:MET:HG2	1.98	0.45
1:B:76:PHE:CD2	1:B:228:ASP:HB3	2.52	0.45
1:C:398:LEU:HD13	1:C:443:ARG:O	2.16	0.45
1:C:505:LYS:HE2	1:C:505:LYS:HB3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:ARG:H	1:D:56:ARG:HG3	1.44	0.45
1:A:453:VAL:HG21	1:A:493:ALA:HB2	1.99	0.45
1:B:342:ARG:HH21	1:C:329:GLN:HB3	1.82	0.45
1:C:48:ILE:HG23	1:C:71:VAL:HB	1.99	0.45
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.51	0.45
1:C:271:ILE:HG23	1:C:276:GLY:HA3	1.97	0.45
1:D:85:ALA:HB2	1:D:231:PHE:CZ	2.52	0.45
1:C:61:LEU:HD23	1:C:64:MET:HE2	1.98	0.45
1:A:267:ILE:HD13	1:A:267:ILE:H	1.82	0.44
1:C:30:MET:HA	1:C:33:LEU:CD1	2.47	0.44
1:D:474:CYS:HA	1:D:492:PHE:CE2	2.53	0.44
1:A:37:SER:HA	1:A:38:PRO:HD3	1.83	0.44
1:B:392:LEU:HD12	1:B:392:LEU:H	1.82	0.44
1:D:70:ASN:CB	1:D:464:HIS:HD2	2.30	0.44
1:A:73:ARG:HA	1:A:111:ALA:HB3	1.99	0.44
1:A:302:PRO:HB3	1:D:339:ARG:HH22	1.81	0.44
1:B:33:LEU:HB2	1:C:312:MET:HB2	1.99	0.44
1:B:291:MET:HE2	1:B:327:ALA:HB2	1.98	0.44
1:C:332:GLU:O	1:C:335:ILE:HG13	2.17	0.44
1:D:85:ALA:HB2	1:D:231:PHE:HZ	1.83	0.44
1:D:340:PRO:HD3	1:D:377:MET:HG3	2.00	0.44
1:D:486:VAL:O	1:D:490:VAL:HG23	2.16	0.44
1:A:482:TRP:CG	1:A:517:PRO:HD3	2.52	0.44
1:B:162:LYS:HD2	1:B:162:LYS:HA	1.76	0.44
1:B:299:ILE:HD12	1:B:300:GLU:HG3	2.00	0.44
1:D:67:SER:OG	1:D:376:ARG:NE	2.43	0.44
1:D:470:PHE:CD1	1:D:470:PHE:N	2.85	0.44
1:A:61:LEU:O	1:A:65:ILE:HG13	2.18	0.44
1:A:272:GLU:HG2	1:A:296:ASP:HB2	2.00	0.44
1:C:63:GLU:O	1:C:372:LEU:HD21	2.18	0.44
1:D:372:LEU:HD12	1:D:372:LEU:HA	1.77	0.44
1:A:266:LYS:HD2	1:A:266:LYS:HA	1.73	0.44
1:A:359:ILE:H	1:A:359:ILE:HG12	1.68	0.44
1:B:517:PRO:HD2	1:B:518:GLY:H	1.82	0.44
1:C:444:TYR:OH	1:D:422:LYS:NZ	2.50	0.44
1:D:160:ASP:N	1:D:160:ASP:OD1	2.51	0.44
1:A:65:ILE:HD12	1:A:66:LYS:N	2.33	0.43
1:C:50:THR:OG1	1:C:73:ARG:NE	2.47	0.43
1:C:410:GLU:HA	1:C:440:GLN:HG2	2.00	0.43
1:C:432:THR:HB	1:C:437:SER:HB2	2.00	0.43
1:D:441:VAL:HG12	1:D:450:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ALA:CB	1:A:245:ILE:HD11	2.48	0.43
1:A:335:ILE:HG23	1:A:368:GLY:HA2	2.00	0.43
1:B:243:SER:HA	1:B:270:LYS:HD3	2.00	0.43
1:B:516:ARG:HB3	1:B:517:PRO:CD	2.48	0.43
1:D:348:VAL:HG11	1:D:378:GLN:HE22	1.83	0.43
1:A:330:MET:O	1:A:344:GLU:HG2	2.18	0.43
1:A:445:ARG:HG2	1:A:445:ARG:NH1	2.21	0.43
1:B:94:ALA:O	1:B:97:SER:HB3	2.18	0.43
1:B:407:ASP:OD2	1:B:409:THR:HG23	2.18	0.43
1:C:408:PRO:HG2	1:C:521:PHE:CD1	2.54	0.43
1:A:76:PHE:HZ	1:A:81:HIS:CE1	2.37	0.43
1:B:312:MET:HG3	1:B:313:MET:HG3	2.00	0.43
1:A:102:PRO:HA	1:A:105:GLU:OE2	2.18	0.43
1:B:322:LYS:HA	1:B:323:PRO:HD3	1.85	0.43
1:B:274:HIS:CD2	1:B:278:ARG:HG3	2.54	0.43
1:B:297:LEU:HD12	1:B:297:LEU:HA	1.87	0.43
1:C:494:MET:HE3	1:C:494:MET:HB2	1.93	0.43
1:A:69:MET:HB3	1:A:69:MET:HE2	1.60	0.43
1:B:432:THR:HG21	1:B:435:GLY:HA2	2.00	0.43
1:B:110:VAL:CG1	1:B:237:VAL:HG12	2.49	0.43
1:D:123:LEU:HA	1:D:205:SER:HB3	2.01	0.43
1:C:449:PRO:HG3	1:C:502:PHE:HD1	1.84	0.43
1:A:58:VAL:HG13	1:A:94:ALA:HB2	2.01	0.43
1:A:92:ARG:NH1	1:A:235:GLN:O	2.45	0.43
1:B:247:LYS:HD2	1:B:249:SER:HB2	2.00	0.43
1:C:482:TRP:CE3	1:C:517:PRO:HG3	2.54	0.43
1:A:288:ASP:O	1:A:323:PRO:HD2	2.19	0.42
1:B:77:SER:C	1:B:78:HIS:HD1	2.23	0.42
1:B:305:LYS:HE3	1:C:35:ILE:O	2.18	0.42
1:A:290:ILE:HB	1:A:324:VAL:HG23	2.01	0.42
1:C:338:PRO:HB3	1:C:370:TYR:CE2	2.54	0.42
1:C:482:TRP:CZ3	1:C:516:ARG:C	2.92	0.42
1:A:241:PHE:HE1	1:A:268:ILE:HD13	1.82	0.42
1:A:505:LYS:HE2	1:A:505:LYS:HB3	1.74	0.42
1:B:362:SER:O	1:B:364:GLU:N	2.51	0.42
1:C:464:HIS:CD2	2:C:1001:PRO:HB2	2.53	0.42
1:D:132:VAL:HB	1:D:133:GLU:H	1.40	0.42
1:B:317:CYS:SG	1:B:324:VAL:HG23	2.60	0.42
1:D:157:LEU:HD21	1:D:203:LEU:HD21	2.02	0.42
1:C:56:ARG:O	1:C:90:ASN:ND2	2.52	0.42
1:D:86:GLU:O	1:D:90:ASN:ND2	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:LEU:HD12	1:D:204:GLY:H	1.84	0.42
1:D:345:GLY:HA2	1:D:381:ILE:HD13	2.02	0.42
1:C:528:VAL:HA	1:C:529:PRO:HD3	1.83	0.42
1:D:331:LEU:HB3	1:D:334:MET:HG3	2.02	0.42
1:B:212:PRO:HA	1:B:213:GLY:HA2	1.56	0.42
1:C:322:LYS:HB3	1:C:322:LYS:HE2	1.87	0.42
1:A:305:LYS:O	1:A:308:LEU:HB2	2.19	0.42
1:B:56:ARG:H	1:B:56:ARG:HG3	1.51	0.42
1:C:472:VAL:HG21	1:C:496:VAL:HG21	2.02	0.42
1:D:186:LYS:HA	1:D:186:LYS:HD3	1.82	0.42
1:B:70:ASN:HB3	1:B:464:HIS:CD2	2.55	0.42
1:B:218:LEU:HB3	1:B:219:PRO:CA	2.50	0.42
1:B:349:ALA:O	1:B:353:LEU:HG	2.20	0.42
1:D:330:MET:HG3	1:D:348:VAL:HG13	2.02	0.42
1:D:178:ASP:C	1:D:180:LEU:H	2.23	0.42
1:B:494:MET:HG2	1:B:531:PRO:HD2	2.01	0.41
1:D:124:ILE:HA	1:D:152:CYS:HB3	2.03	0.41
1:D:348:VAL:HG21	1:D:381:ILE:HG21	2.02	0.41
1:D:362:SER:O	1:D:364:GLU:N	2.53	0.41
1:A:448:ALA:HB1	1:A:449:PRO:HD2	2.02	0.41
1:B:60:THR:HG22	1:B:61:LEU:N	2.36	0.41
1:B:229:LEU:HD23	1:B:229:LEU:HA	1.93	0.41
1:C:69:MET:SD	1:C:72:ALA:HB2	2.59	0.41
1:C:249:SER:O	1:C:252:HIS:HB2	2.20	0.41
1:C:391:HIS:CG	1:C:447:ARG:HG3	2.55	0.41
1:A:431:LEU:HD12	1:A:453:VAL:HB	2.02	0.41
1:A:496:VAL:O	1:A:500:ARG:HB2	2.20	0.41
1:B:342:ARG:HH22	1:C:347:ASP:CG	2.24	0.41
1:B:407:ASP:CG	1:B:409:THR:HG23	2.40	0.41
1:D:482:TRP:NE1	1:D:516:ARG:HA	2.35	0.41
1:A:46:GLY:O	1:A:358:CYS:HB3	2.20	0.41
1:B:331:LEU:HB3	1:B:334:MET:HG3	2.01	0.41
1:A:385:ALA:HA	1:D:307:PHE:HZ	1.85	0.41
1:A:500:ARG:HG2	1:A:502:PHE:HE1	1.86	0.41
1:B:311:LYS:HD3	1:C:30:MET:HE3	2.02	0.41
1:B:340:PRO:HD3	1:B:377:MET:HG3	2.01	0.41
1:C:291:MET:HA	1:C:325:ILE:O	2.19	0.41
1:C:441:VAL:HG12	1:C:450:ILE:HD11	2.02	0.41
1:D:218:LEU:HA	1:D:218:LEU:HD23	1.69	0.41
1:A:71:VAL:CG1	1:A:239:MET:HE1	2.51	0.41
1:A:267:ILE:HD13	1:A:288:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:PHE:H	1:A:502:PHE:HD1	1.66	0.41
1:B:380:LEU:HD23	1:B:380:LEU:HA	1.81	0.41
1:B:476:ASP:HA	1:B:477:PRO:HD3	1.88	0.41
1:C:237:VAL:O	1:C:265:ILE:HD13	2.21	0.41
1:D:51:ILE:HA	1:D:55:SER:OG	2.20	0.41
1:D:182:SER:O	1:D:183:LEU:HD12	2.21	0.41
1:D:182:SER:OG	1:D:199:ASN:HB2	2.20	0.41
1:D:453:VAL:HG22	1:D:472:VAL:HG12	2.03	0.41
1:D:516:ARG:O	1:D:519:SER:HB2	2.21	0.41
1:A:65:ILE:HG21	1:A:108:VAL:CG2	2.51	0.41
1:B:71:VAL:HG22	1:B:109:ALA:HB3	2.03	0.41
1:B:168:VAL:HG12	1:B:169:GLU:O	2.21	0.41
1:B:370:TYR:HB3	1:B:373:GLU:HG3	2.03	0.41
1:A:325:ILE:HD13	1:A:325:ILE:HG21	1.84	0.41
1:A:393:GLN:O	1:A:397:GLU:HG3	2.21	0.41
1:B:58:VAL:CG2	1:B:90:ASN:HD22	2.28	0.41
1:B:288:ASP:O	1:B:323:PRO:HD2	2.21	0.41
1:B:371:PRO:CD	1:B:372:LEU:H	2.33	0.41
1:D:63:GLU:HB3	1:D:372:LEU:HD11	2.03	0.41
1:D:348:VAL:CG2	1:D:381:ILE:HG21	2.51	0.41
1:A:284:LEU:HD13	1:A:290:ILE:HG13	2.03	0.41
1:A:455:ARG:NH2	1:A:478:VAL:HA	2.36	0.41
1:C:284:LEU:O	1:C:322:LYS:NZ	2.49	0.41
1:D:465:LEU:HD23	1:D:465:LEU:HA	1.82	0.41
1:A:295:GLY:HA2	1:A:329:GLN:NE2	2.37	0.40
1:B:188:LYS:HB2	1:B:193:LEU:HD12	2.03	0.40
1:C:70:ASN:HB3	1:C:464:HIS:CG	2.57	0.40
1:D:275:GLU:O	1:D:279:ARG:HG3	2.21	0.40
1:D:434:SER:HB2	1:D:436:ARG:HG3	2.02	0.40
1:A:282:GLU:O	1:A:285:GLU:HB3	2.20	0.40
1:A:473:LEU:HD12	1:A:473:LEU:HA	1.87	0.40
1:D:323:PRO:HB3	1:D:465:LEU:O	2.21	0.40
1:A:222:SER:HB2	1:A:225:ASP:CG	2.42	0.40
1:A:254:VAL:O	1:A:258:LEU:HD12	2.21	0.40
1:A:482:TRP:HH2	1:A:514:GLY:O	2.04	0.40
1:B:184:GLN:HB3	1:B:185:VAL:H	1.77	0.40
1:B:301:ILE:HA	1:B:302:PRO:HD3	1.89	0.40
1:B:470:PHE:N	1:B:470:PHE:CD1	2.89	0.40
1:C:81:HIS:CD2	1:C:81:HIS:H	2.38	0.40
1:C:233:VAL:HG22	1:C:258:LEU:HD23	2.03	0.40
1:C:414:VAL:O	1:C:417:VAL:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:CYS:SG	1:D:375:VAL:HG22	2.61	0.40
1:B:105:GLU:O	1:B:105:GLU:HG3	2.20	0.40
1:C:101:ASP:HA	1:C:102:PRO:HD3	1.91	0.40
1:D:73:ARG:O	1:D:74:LEU:HD23	2.21	0.40
1:D:179:GLY:O	1:D:181:ILE:N	2.53	0.40
1:D:237:VAL:HG23	1:D:265:ILE:HD12	2.03	0.40
1:D:428:ILE:HD13	1:D:428:ILE:HG21	1.91	0.40
1:B:42:ALA:O	1:B:44:ASN:ND2	2.55	0.40
1:B:121:THR:O	1:B:206:LYS:HA	2.20	0.40
1:B:313:MET:HB2	1:B:313:MET:HE3	1.99	0.40
1:D:205:SER:O	1:D:207:LYS:HG2	2.21	0.40
1:D:390:TYR:HD1	1:D:390:TYR:HA	1.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	402/535 (75%)	344 (86%)	49 (12%)	9 (2%)	6	35
1	B	496/535 (93%)	413 (83%)	61 (12%)	22 (4%)	2	19
1	C	402/535 (75%)	344 (86%)	51 (13%)	7 (2%)	9	42
1	D	501/535 (94%)	434 (87%)	57 (11%)	10 (2%)	7	38
All	All	1801/2140 (84%)	1535 (85%)	218 (12%)	48 (3%)	5	30

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	ILE
1	A	299	ILE
1	B	58	VAL

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Mol	Chain	Res	Type
1	B	102	PRO
1	B	371	PRO
1	B	394	LEU
1	B	460	ALA
1	B	516	ARG
1	B	517	PRO
1	C	392	LEU
1	C	500	ARG
1	A	460	ALA
1	B	79	GLY
1	B	215	ALA
1	B	363	GLY
1	B	459	THR
1	B	463	ALA
1	D	58	VAL
1	D	180	LEU
1	D	463	ALA
1	A	97	SER
1	A	330	MET
1	A	436	ARG
1	B	53	PRO
1	B	161	TYR
1	B	330	MET
1	B	390	TYR
1	C	483	ALA
1	A	392	LEU
1	B	202	SER
1	D	53	PRO
1	D	79	GLY
1	D	363	GLY
1	D	440	GLN
1	A	393	GLN
1	B	103	ILE
1	B	154	GLU
1	B	329	GLN
1	B	521	PHE
1	A	459	THR
1	D	125	LYS
1	D	132	VAL
1	B	218	LEU
1	C	414	VAL
1	D	478	VAL

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Mol	Chain	Res	Type
1	C	53	PRO
1	C	371	PRO
1	C	368	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	335/438 (76%)	281 (84%)	54 (16%)	2 11
1	B	415/438 (95%)	350 (84%)	65 (16%)	2 12
1	C	335/438 (76%)	281 (84%)	54 (16%)	2 11
1	D	417/438 (95%)	341 (82%)	76 (18%)	1 8
All	All	1502/1752 (86%)	1253 (83%)	249 (17%)	2 10

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	A	25	THR
1	A	26	PHE
1	A	33	LEU
1	A	41	THR
1	A	59	GLU
1	A	60	THR
1	A	62	LYS
1	A	69	MET
1	A	74	LEU
1	A	80	THR
1	A	82	GLU
1	A	83	TYR
1	A	87	THR
1	A	100	SER
1	A	106	ARG
1	A	112	LEU
1	A	238	ASP

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Mol	Chain	Res	Type
1	A	239	MET
1	A	249	SER
1	A	250	ASP
1	A	256	LYS
1	A	258	LEU
1	A	267	ILE
1	A	285	GLU
1	A	294	ARG
1	A	297	LEU
1	A	306	VAL
1	A	316	ARG
1	A	319	ARG
1	A	331	LEU
1	A	332	GLU
1	A	337	LYS
1	A	339	ARG
1	A	342	ARG
1	A	348	VAL
1	A	359	ILE
1	A	389	ILE
1	A	393	GLN
1	A	401	LEU
1	A	407	ASP
1	A	414	VAL
1	A	433	LYS
1	A	440	GLN
1	A	443	ARG
1	A	445	ARG
1	A	465	LEU
1	A	472	VAL
1	A	480	GLU
1	A	494	MET
1	A	500	ARG
1	A	524	THR
1	A	525	MET
1	A	528	VAL
1	B	24	ASP
1	B	25	THR
1	B	30	MET
1	B	45	THR
1	B	56	ARG
1	B	60	THR

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Mol	Chain	Res	Type
1	B	67	SER
1	B	80	THR
1	B	92	ARG
1	B	97	SER
1	B	112	LEU
1	B	131	GLU
1	B	140	LEU
1	B	143	THR
1	B	154	GLU
1	B	159	LEU
1	B	160	ASP
1	B	162	LYS
1	B	165	CYS
1	B	166	LYS
1	B	169	GLU
1	B	172	SER
1	B	180	LEU
1	B	184	GLN
1	B	185	VAL
1	B	188	LYS
1	B	191	ASP
1	B	217	ASP
1	B	221	VAL
1	B	235	GLN
1	B	244	PHE
1	B	247	LYS
1	B	285	GLU
1	B	294	ARG
1	B	297	LEU
1	B	312	MET
1	B	324	VAL
1	B	326	CYS
1	B	330	MET
1	B	333	SER
1	B	336	LYS
1	B	342	ARG
1	B	364	GLU
1	B	367	LYS
1	B	373	GLU
1	B	383	ARG
1	B	391	HIS
1	B	393	GLN

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Mol	Chain	Res	Type
1	B	394	LEU
1	B	405	THR
1	B	409	THR
1	B	412	THR
1	B	420	SER
1	B	434	SER
1	B	445	ARG
1	B	459	THR
1	B	472	VAL
1	B	478	VAL
1	B	480	GLU
1	B	484	GLU
1	B	500	ARG
1	B	508	VAL
1	B	516	ARG
1	B	519	SER
1	B	522	THR
1	C	24	ASP
1	C	26	PHE
1	C	33	LEU
1	C	45	THR
1	C	60	THR
1	C	69	MET
1	C	74	LEU
1	C	76	PHE
1	C	77	SER
1	C	87	THR
1	C	101	ASP
1	C	110	VAL
1	C	115	LYS
1	C	222	SER
1	C	238	ASP
1	C	247	LYS
1	C	251	VAL
1	C	265	ILE
1	C	266	LYS
1	C	269	SER
1	C	270	LYS
1	C	275	GLU
1	C	277	VAL
1	C	278	ARG
1	C	294	ARG

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Mol	Chain	Res	Type
1	C	296	ASP
1	C	301	ILE
1	C	319	ARG
1	C	324	VAL
1	C	325	ILE
1	C	326	CYS
1	C	328	THR
1	C	334	MET
1	C	337	LYS
1	C	339	ARG
1	C	342	ARG
1	C	359	ILE
1	C	360	MET
1	C	380	LEU
1	C	383	ARG
1	C	392	LEU
1	C	396	GLU
1	C	401	LEU
1	C	405	THR
1	C	409	THR
1	C	430	VAL
1	C	436	ARG
1	C	443	ARG
1	C	475	LYS
1	C	491	ASN
1	C	494	MET
1	C	500	ARG
1	C	524	THR
1	C	526	ARG
1	D	25	THR
1	D	35	ILE
1	D	40	ILE
1	D	41	THR
1	D	45	THR
1	D	56	ARG
1	D	61	LEU
1	D	67	SER
1	D	73	ARG
1	D	80	THR
1	D	82	GLU
1	D	97	SER
1	D	105	GLU

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Mol	Chain	Res	Type
1	D	120	ARG
1	D	123	LEU
1	D	131	GLU
1	D	132	VAL
1	D	136	LYS
1	D	139	THR
1	D	143	THR
1	D	146	ASN
1	D	151	LYS
1	D	152	CYS
1	D	156	ILE
1	D	159	LEU
1	D	178	ASP
1	D	188	LYS
1	D	195	THR
1	D	196	GLU
1	D	197	VAL
1	D	207	LYS
1	D	209	VAL
1	D	210	ASN
1	D	211	LEU
1	D	217	ASP
1	D	229	LEU
1	D	239	MET
1	D	261	LYS
1	D	275	GLU
1	D	285	GLU
1	D	294	ARG
1	D	297	LEU
1	D	324	VAL
1	D	326	CYS
1	D	328	THR
1	D	330	MET
1	D	331	LEU
1	D	333	SER
1	D	342	ARG
1	D	348	VAL
1	D	350	ASN
1	D	354	ASP
1	D	364	GLU
1	D	390	TYR
1	D	391	HIS

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Mol	Chain	Res	Type
1	D	392	LEU
1	D	393	GLN
1	D	394	LEU
1	D	398	LEU
1	D	399	ARG
1	D	400	ARG
1	D	401	LEU
1	D	405	THR
1	D	412	THR
1	D	414	VAL
1	D	420	SER
1	D	422	LYS
1	D	440	GLN
1	D	443	ARG
1	D	458	GLN
1	D	472	VAL
1	D	478	VAL
1	D	489	ARG
1	D	508	VAL
1	D	519	SER
1	D	522	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	318	ASN
1	A	464	HIS
1	B	70	ASN
1	B	84	HIS
1	B	90	ASN
1	B	350	ASN
1	B	464	HIS
1	C	44	ASN
1	C	90	ASN
1	C	378	GLN
1	C	464	HIS
1	D	44	ASN
1	D	84	HIS
1	D	464	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PRO	C	1001	-	5,7,8	0.91	0	7,8,10	1.63	1 (14%)
2	PRO	B	1001	-	5,7,8	0.61	0	7,8,10	2.24	2 (28%)
2	PRO	A	1001	-	5,7,8	0.60	0	7,8,10	1.77	1 (14%)
2	PRO	D	1001	-	5,7,8	0.66	0	7,8,10	1.62	1 (14%)

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	PRO	C	1001	-	-	0/0/9/11	0/1/1/1
2	PRO	B	1001	-	-	0/0/9/11	0/1/1/1
2	PRO	A	1001	-	-	0/0/9/11	0/1/1/1
2	PRO	D	1001	-	-	0/0/9/11	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1001	PRO	O-C-CA	-4.91	111.91	124.78
2	A	1001	PRO	O-C-CA	-3.79	114.86	124.78
2	C	1001	PRO	O-C-CA	-3.69	115.11	124.78
2	D	1001	PRO	O-C-CA	-3.50	115.61	124.78
2	B	1001	PRO	CB-CA-C	-2.54	109.21	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	PRO	4	0
2	B	1001	PRO	3	0
2	A	1001	PRO	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	406/535 (75%)	0.07	5 (1%)	79	67	3, 36, 78, 121	0
1	B	502/535 (93%)	0.11	4 (0%)	86	78	1, 34, 101, 128	0
1	C	406/535 (75%)	0.08	3 (0%)	87	81	2, 35, 80, 134	0
1	D	505/535 (94%)	0.09	7 (1%)	75	63	2, 32, 97, 127	0
All	All	1819/2140 (85%)	0.09	19 (1%)	82	72	1, 35, 91, 134	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	83	TYR	3.3
1	A	74	LEU	3.3
1	A	229	LEU	3.2
1	B	156	ILE	3.1
1	D	134	LEU	3.1
1	D	159	LEU	2.9
1	B	157	LEU	2.9
1	D	142	ILE	2.5
1	A	465	LEU	2.4
1	D	503	PHE	2.3
1	B	388	ALA	2.2
1	D	183	LEU	2.2
1	D	112	LEU	2.2
1	D	378	GLN	2.1
1	B	241	PHE	2.1
1	A	258	LEU	2.1
1	C	472	VAL	2.0
1	A	76	PHE	2.0
1	C	251	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PRO	D	1001	7/8	0.84	0.39	23,23,33,33	0
2	PRO	B	1001	7/8	0.87	0.30	9,9,19,19	0
2	PRO	C	1001	7/8	0.91	0.26	16,16,26,26	0
2	PRO	A	1001	7/8	0.91	0.30	19,19,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.