Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 04:08 am BST

PDB ID	:	3TAI
Title	:	Crystal structure of NurA
Authors	:	Chae, J.; Kim, Y.C.; Cho, Y.
Deposited on	:	2011-08-04
Resolution	:	2.82 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 following versions of software and data (see references ⓘ) were used in the production of this report:

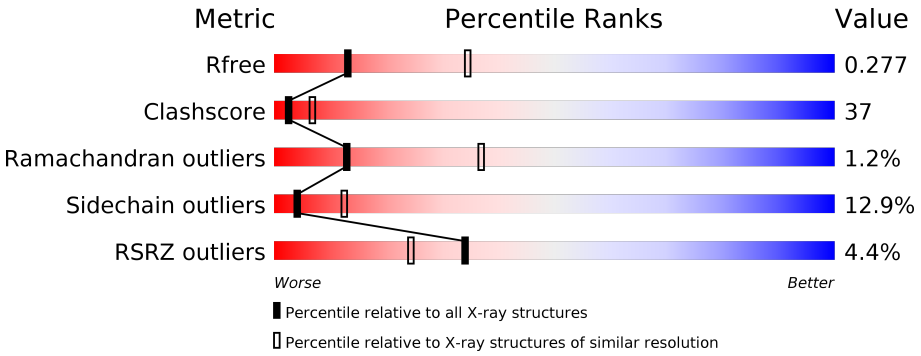
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.82 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	471	2% 43% 41% 7% 9%
1	B	471	6% 38% 46% 8% 9%

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	GOL	A	455	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7002 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 DNA double-strand break repair protein nurA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	Se	0	0	0
			3471	2223	595	646	7			
1	B	430	Total	C	N	O	Se	0	0	0
			3470	2223	594	646	7			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	EXPRESSION TAG	UNP Q8U1N8
A	-18	GLY	-	EXPRESSION TAG	UNP Q8U1N8
A	-17	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	-16	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	-15	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-14	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-13	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-12	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-11	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-10	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-9	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	-8	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	-7	GLY	-	EXPRESSION TAG	UNP Q8U1N8
A	-6	LEU	-	EXPRESSION TAG	UNP Q8U1N8
A	-5	VAL	-	EXPRESSION TAG	UNP Q8U1N8
A	-4	PRO	-	EXPRESSION TAG	UNP Q8U1N8
A	-3	ARG	-	EXPRESSION TAG	UNP Q8U1N8
A	-2	GLY	-	EXPRESSION TAG	UNP Q8U1N8
A	-1	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	0	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-19	MSE	-	EXPRESSION TAG	UNP Q8U1N8
B	-18	GLY	-	EXPRESSION TAG	UNP Q8U1N8
B	-17	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	-16	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	-15	HIS	-	EXPRESSION TAG	UNP Q8U1N8

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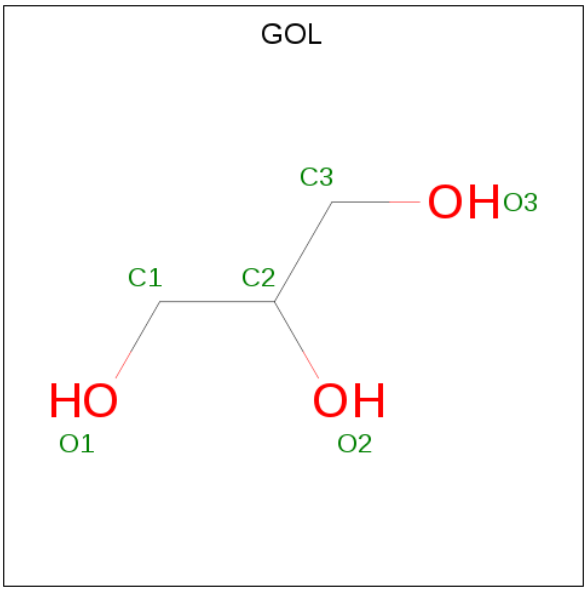
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-13	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-12	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-11	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-10	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-9	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	-8	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	-7	GLY	-	EXPRESSION TAG	UNP Q8U1N8
B	-6	LEU	-	EXPRESSION TAG	UNP Q8U1N8
B	-5	VAL	-	EXPRESSION TAG	UNP Q8U1N8
B	-4	PRO	-	EXPRESSION TAG	UNP Q8U1N8
B	-3	ARG	-	EXPRESSION TAG	UNP Q8U1N8
B	-2	GLY	-	EXPRESSION TAG	UNP Q8U1N8
B	-1	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	0	HIS	-	EXPRESSION TAG	UNP Q8U1N8

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

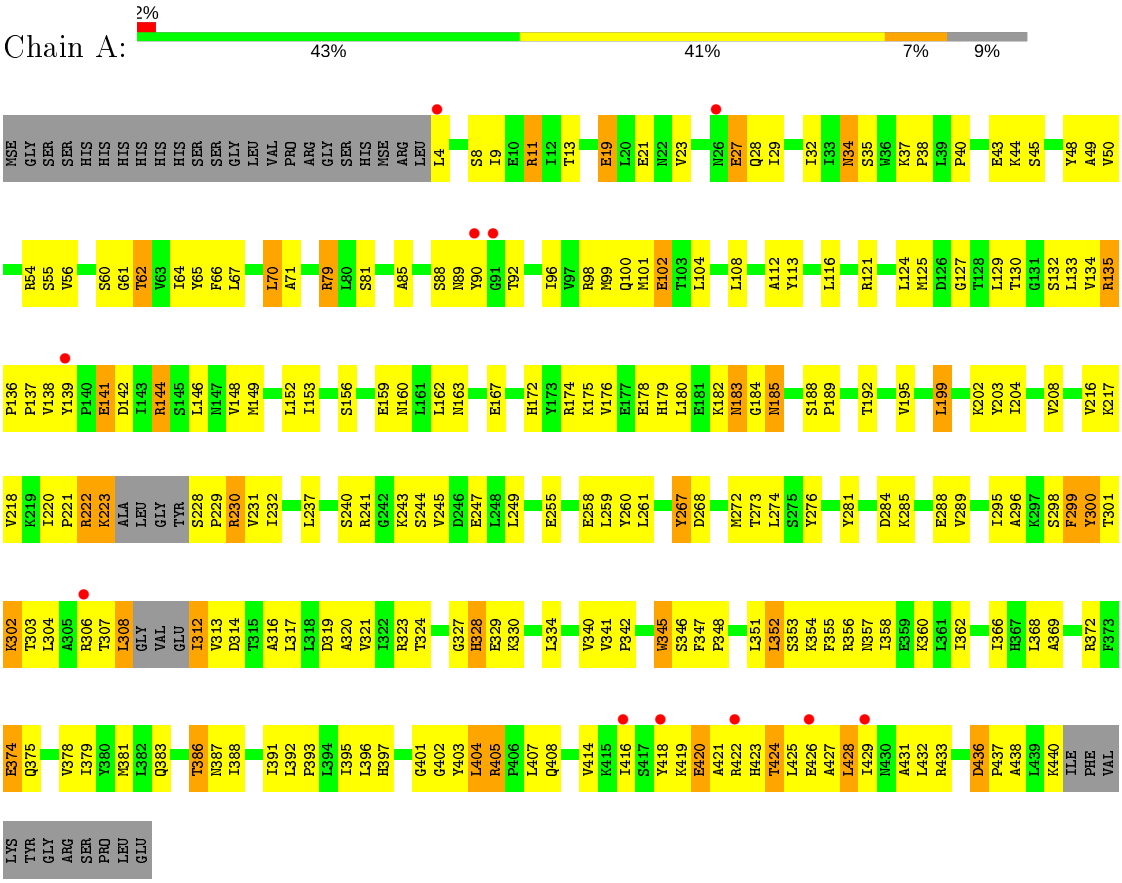
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	15	Total O 15 15	0	0
3	B	4	Total O 4 4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

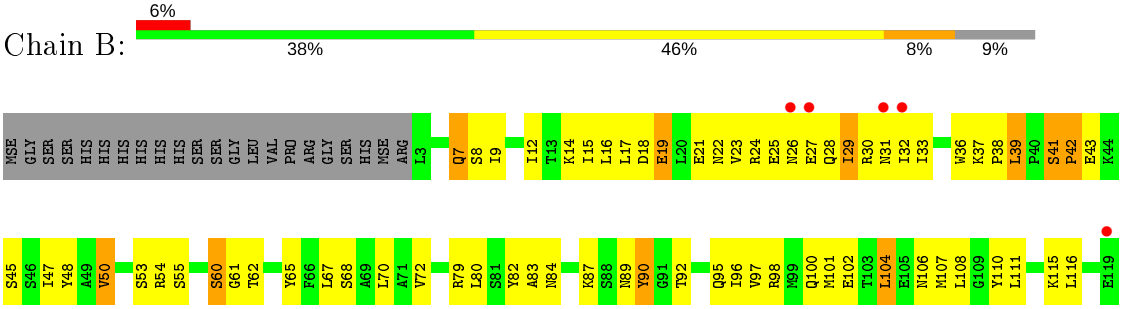
- Molecule 1: DNA double-strand break repair protein nurA

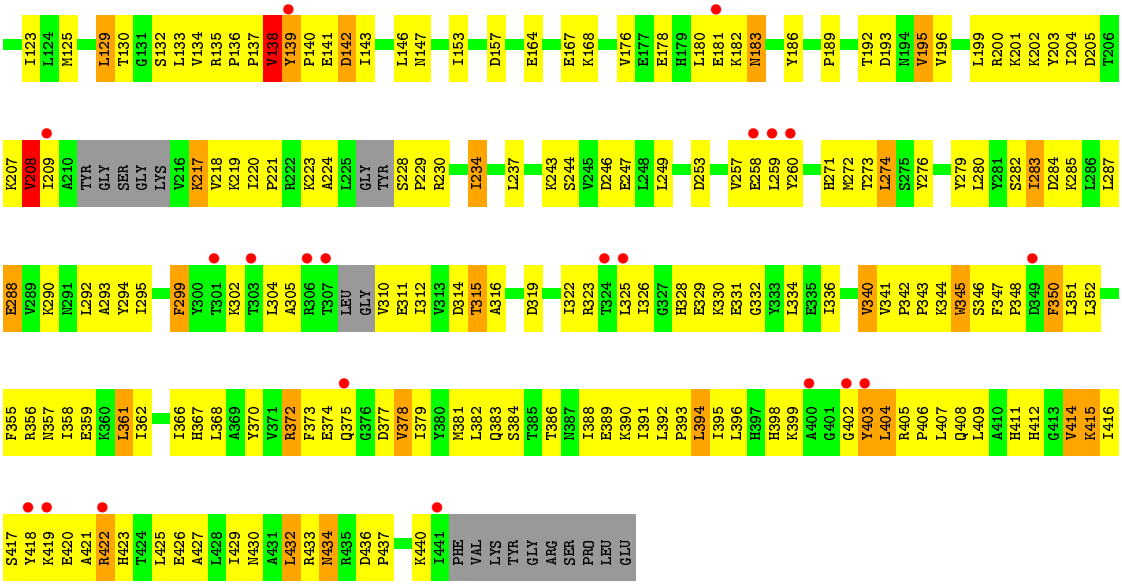
Chain A:



- Molecule 1: DNA double-strand break repair protein nurA

Chain B:




I123 L124 M125 L129 T130 G131 S132 L133 V134 R135 P136 P137 V138 Y139 P140 E141 D142 I143 L146 N147 I153 D157 E164 E167 K168 V176 E177 E178 H179 L180 E181 K182 N183 Y186 P189 T192 D193 N194 V195 V196 L199 R200 K201 K202 Y203 I204 D205 T206
K207 V208 I209 A210 TYR GLY SER GLY LYS V216 K217 V218 K219 I220 P221 R222 K223 A224 L225 GLY TYR S228 P229 R230 I234 L237 K243 S244 V245 D246 E247 L248 L249 D253 V257 E258 L259 Y260 H271 M272 T273 L274 S275 Y276 Y279 L280 Y281 S282 I283 D284 K285 I286 L287
E288 V289 K290 N291 L292 A293 Y294 I295 F299 Y300 T301 K302 T303 L304 A305 R306 T307 LEU GLY V310 E311 I312 V313 D314 T315 A316 D319 I322 R323 T324 L325 I326 G327 H328 E329 K330 E331 G332 Y333 L334 E335 I336 V340 V341 P342 P343 K344 W345 S346 F347 P348 D349 F350 L351 L352
F355 R356 N357 I358 E359 K360 L361 I362 I366 H367 L368 A369 Y370 V371 R372 F373 E374 Q375 G376 D377 V378 I379 Y380 M381 L382 Q383 S384 T385 T386 N387 I388 E389 K390 I391 L392 P393 L394 I395 L396 H397 H398 K399 A400 G401 G402 Y403 L404 R405 P406 L407 Q408 L409 A410 H411 H412 G413 V414 K415 I416
S417 Y418 K419 E420 A421 R422 H423 T424 L425 E426 A427 L428 I429 N430 A431 L432 R433 N434 R435 D436 P437 K440 I441 PHE VAL LYS TYR GLY ARG SER PRO LEU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.00Å 114.21Å 122.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.55 – 2.82 31.73 – 2.49	Depositor EDS
% Data completeness (in resolution range)	95.7 (29.55-2.82) 89.0 (31.73-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.202 , 0.276 0.199 , 0.277	Depositor DCC
R_{free} test set	1141 reflections (3.53%)	wwPDB-VP
Wilson B-factor (Å^2)	64.0	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 71.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7002	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: GOL

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	0.52	0/3523	0.72	1/4741 (0.0%)
1	B	0.46	0/3520	0.66	0/4738
All	All	0.49	0/7043	0.69	1/9479 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	62	THR	N-CA-C	5.19	125.02	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ARG	Sidechain

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	3471	0	3587	271	0
1	B	3470	0	3586	295	0
2	A	36	0	48	9	0
2	B	6	0	8	2	0
3	A	15	0	0	3	0
3	B	4	0	0	0	0
All	All	7002	0	7229	522	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 37.

All (522) 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:54:ARG:HB3	1:A:101:MSE:HE3	1.26	1.11
1:A:138:VAL:HG13	1:A:142:ASP:OD1	1.54	1.07
1:B:347:PHE:HB3	1:B:352:LEU:HD11	1.37	1.05
1:A:135:ARG:NH2	1:B:90:TYR:HB2	1.73	1.04
1:B:67:LEU:HD22	1:B:101:MSE:HE2	1.39	1.03
1:A:54:ARG:HB3	1:A:101:MSE:CE	1.92	0.99
1:B:139:TYR:HB3	1:B:140:PRO:HD3	1.43	0.98
1:B:54:ARG:HB3	1:B:101:MSE:CE	1.94	0.97
1:A:67:LEU:HD22	1:A:101:MSE:HE2	1.43	0.97
1:B:50:VAL:HG13	1:B:125:MSE:HE1	1.48	0.96
1:B:345:TRP:HD1	1:B:346:SER:N	1.63	0.96
1:B:404:LEU:H	1:B:404:LEU:HD12	1.31	0.95
1:A:135:ARG:HH21	1:B:90:TYR:HB2	1.25	0.94
1:B:29:ILE:HG21	1:B:33:ILE:HG13	1.47	0.94
1:B:54:ARG:HB3	1:B:101:MSE:HE3	1.48	0.93
1:A:61:GLY:O	1:A:88:SER:HB2	1.68	0.93
1:A:425:LEU:HD11	1:B:12:ILE:HD13	1.52	0.90
1:A:440:LYS:NZ	1:B:378:VAL:HG22	1.87	0.88
1:A:67:LEU:HD22	1:A:101:MSE:CE	2.03	0.88
1:B:50:VAL:HG13	1:B:125:MSE:CE	2.03	0.88
1:B:50:VAL:CG1	1:B:125:MSE:HE1	2.05	0.87
1:A:139:TYR:OH	1:A:346:SER:HA	1.73	0.86
1:A:135:ARG:HH22	1:B:90:TYR:H	1.24	0.85
1:B:423:HIS:O	1:B:427:ALA:HB2	1.76	0.84
1:B:129:LEU:HG	1:B:294:TYR:CE2	2.12	0.84
1:B:29:ILE:HG13	1:B:33:ILE:HD11	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLY:O	1:A:88:SER:CB	2.26	0.83
1:B:54:ARG:CB	1:B:101:MSE:HE3	2.10	0.81
1:A:141:GLU:O	1:A:144:ARG:HG2	1.79	0.81
1:B:350:PHE:HD2	1:B:350:PHE:H	1.28	0.81
1:B:123:ILE:CG2	1:B:125:MSE:HE3	2.09	0.81
1:A:313:VAL:HG12	1:A:314:ASP:H	1.45	0.81
1:A:301:THR:HG22	1:A:303:THR:H	1.46	0.81
1:B:345:TRP:CD1	1:B:346:SER:N	2.48	0.80
1:A:301:THR:H	1:A:304:LEU:HG	1.44	0.80
1:B:422:ARG:HG3	1:B:423:HIS:N	1.96	0.80
1:A:162:LEU:HD21	1:A:354:LYS:HG3	1.62	0.80
1:B:138:VAL:HG12	1:B:141:GLU:HB2	1.62	0.80
1:B:201:LYS:HA	1:B:205:ASP:HB2	1.64	0.80
1:A:138:VAL:HA	1:A:142:ASP:OD2	1.82	0.80
1:A:223:LYS:H	1:A:223:LYS:HD2	1.46	0.80
1:A:136:PRO:HD2	1:A:139:TYR:CE2	2.18	0.79
1:A:436:ASP:HB2	1:A:437:PRO:HD3	1.64	0.78
1:A:386:THR:OG1	1:A:391:ILE:HD11	1.84	0.78
1:A:418:TYR:HD1	1:A:419:LYS:H	1.32	0.78
1:B:7:GLN:HG3	1:B:8:SER:H	1.47	0.77
1:B:422:ARG:HE	1:B:423:HIS:HD2	1.33	0.77
1:A:419:LYS:C	1:A:421:ALA:H	1.89	0.76
1:A:401:GLY:C	1:A:403:TYR:H	1.86	0.76
1:A:440:LYS:HZ1	1:B:378:VAL:HG22	1.46	0.76
1:B:422:ARG:HG3	1:B:423:HIS:H	1.49	0.75
1:A:11:ARG:NH1	1:B:82:TYR:OH	2.20	0.75
1:B:336:ILE:HD11	1:B:370:TYR:CE2	2.21	0.75
1:A:299:PHE:CZ	1:A:381:MSE:HE3	2.22	0.74
1:B:30:ARG:O	1:B:31:ASN:HB3	1.87	0.74
1:B:107:MSE:HE1	1:B:176:VAL:HG21	1.69	0.74
1:B:404:LEU:N	1:B:404:LEU:HD12	2.01	0.74
1:B:329:GLU:HG2	1:B:329:GLU:O	1.86	0.73
1:B:139:TYR:HB3	1:B:140:PRO:CD	2.18	0.73
1:A:347:PHE:HB3	1:A:352:LEU:HD11	1.70	0.73
1:B:326:ILE:HG22	1:B:328:HIS:NE2	2.03	0.73
1:A:49:ALA:HB1	1:A:407:LEU:HD13	1.70	0.73
1:A:172:HIS:O	1:A:176:VAL:HG23	1.90	0.72
1:A:316:ALA:HB2	1:B:440:LYS:HG3	1.71	0.72
1:B:92:THR:O	1:B:96:ILE:HG12	1.89	0.72
1:B:136:PRO:HG2	1:B:139:TYR:HD1	1.55	0.72
1:A:440:LYS:HE2	1:B:315:THR:CG2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PRO:C	1:A:138:VAL:H	1.93	0.72
1:B:220:ILE:HB	1:B:221:PRO:HD2	1.72	0.71
1:B:67:LEU:CD2	1:B:101:MSE:HE2	2.18	0.71
1:B:130:THR:H	1:B:383:GLN:HE22	1.39	0.70
1:B:419:LYS:NZ	1:B:421:ALA:HB3	2.06	0.70
1:A:222:ARG:HD2	1:A:255:GLU:HG3	1.73	0.70
1:A:299:PHE:H	1:A:299:PHE:HD1	1.41	0.69
1:A:301:THR:N	1:A:304:LEU:HG	2.05	0.69
1:B:422:ARG:O	1:B:426:GLU:HG3	1.90	0.69
1:B:193:ASP:OD1	1:B:271:HIS:HE1	1.74	0.69
1:A:11:ARG:NH2	3:A:469:HOH:O	2.25	0.69
1:B:95:GLN:HB3	1:B:138:VAL:HG22	1.74	0.69
1:B:287:LEU:HD22	1:B:361:LEU:HD13	1.73	0.69
1:B:386:THR:OG1	1:B:391:ILE:HD11	1.92	0.69
1:B:423:HIS:O	1:B:427:ALA:CB	2.41	0.69
1:A:135:ARG:HH12	1:A:301:THR:HG21	1.58	0.68
1:B:305:ALA:HA	1:B:310:VAL:O	1.92	0.68
1:B:123:ILE:HG22	1:B:125:MSE:HE3	1.74	0.68
1:B:146:LEU:CD1	1:B:273:THR:HG23	2.23	0.68
1:A:249:LEU:HD21	1:B:237:LEU:HB3	1.75	0.68
1:A:316:ALA:HA	1:B:440:LYS:HE3	1.74	0.68
1:B:19:GLU:O	1:B:23:VAL:HB	1.94	0.68
1:A:27:GLU:CG	1:A:28:GLN:H	2.07	0.68
1:B:319:ASP:OD2	1:B:372:ARG:NH1	2.26	0.68
1:A:135:ARG:NH1	1:A:301:THR:HG21	2.10	0.67
1:B:299:PHE:CE2	1:B:381:MSE:HG2	2.28	0.67
1:A:175:LYS:O	1:A:179:HIS:HD2	1.77	0.67
1:B:398:HIS:HB3	1:B:406:PRO:HD3	1.76	0.67
1:B:168:LYS:HD3	1:B:195:VAL:HG21	1.77	0.67
1:B:347:PHE:CB	1:B:352:LEU:HD11	2.22	0.66
1:A:419:LYS:O	1:A:421:ALA:N	2.29	0.66
1:B:336:ILE:HD11	1:B:370:TYR:HE2	1.61	0.66
1:A:374:GLU:HB2	1:A:402:GLY:HA2	1.78	0.66
1:A:132:SER:HB2	2:A:455:GOL:O2	1.96	0.66
1:A:136:PRO:HG2	1:A:138:VAL:HB	1.77	0.66
1:B:419:LYS:HB3	1:B:422:ARG:HB3	1.75	0.66
1:B:404:LEU:CD1	1:B:404:LEU:H	2.05	0.66
1:B:244:SER:OG	1:B:247:GLU:HG3	1.94	0.66
1:B:345:TRP:HD1	1:B:346:SER:H	1.41	0.66
1:A:298:SER:HB2	1:B:60:SER:HA	1.78	0.66
1:A:146:LEU:HD21	1:A:351:LEU:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLU:O	1:A:23:VAL:HG23	1.96	0.65
1:B:36:TRP:CZ2	1:B:332:GLY:HA3	2.31	0.65
1:B:374:GLU:OE2	1:B:402:GLY:HA2	1.96	0.65
1:A:138:VAL:CG2	1:A:276:TYR:HE1	2.09	0.65
1:A:420:GLU:O	1:A:424:THR:HG23	1.96	0.65
1:A:420:GLU:HG3	1:A:424:THR:CG2	2.27	0.65
1:B:350:PHE:CD2	1:B:350:PHE:N	2.63	0.65
1:A:102:GLU:OE1	2:A:455:GOL:H31	1.97	0.65
1:A:27:GLU:HG2	1:A:28:GLN:H	1.61	0.65
1:A:419:LYS:C	1:A:421:ALA:N	2.46	0.65
1:A:32:ILE:HG13	1:A:334:LEU:HD11	1.79	0.65
1:A:142:ASP:HB3	1:A:272:MSE:SE	2.48	0.65
1:A:314:ASP:OD1	1:B:60:SER:HB3	1.96	0.65
1:B:129:LEU:O	1:B:133:LEU:HG	1.97	0.64
1:B:395:ILE:HG23	1:B:404:LEU:HD21	1.80	0.64
1:A:208:VAL:HG22	1:A:218:VAL:HG22	1.79	0.64
1:B:54:ARG:CG	1:B:101:MSE:HE3	2.27	0.64
1:A:116:LEU:HD23	1:A:121:ARG:HB3	1.79	0.64
1:A:228:SER:N	1:A:229:PRO:HD3	2.12	0.64
1:B:395:ILE:CG2	1:B:404:LEU:HD21	2.27	0.64
1:A:149:MSE:HE1	1:A:204:ILE:HD11	1.81	0.63
1:A:139:TYR:OH	1:A:346:SER:CA	2.46	0.63
1:B:325:LEU:HD23	1:B:326:ILE:HD11	1.80	0.63
1:A:440:LYS:HE2	1:B:315:THR:HG23	1.80	0.63
1:A:195:VAL:CG1	1:A:199:LEU:HD22	2.28	0.63
1:A:223:LYS:NZ	1:A:230:ARG:HG2	2.13	0.63
1:A:316:ALA:CB	1:B:440:LYS:HG3	2.29	0.62
1:A:425:LEU:HD13	1:B:12:ILE:HG21	1.81	0.62
1:B:342:PRO:HD2	1:B:362:ILE:HA	1.80	0.62
1:B:416:ILE:HG13	1:B:417:SER:O	1.99	0.62
1:B:427:ALA:O	1:B:430:ASN:HB2	2.00	0.62
1:A:138:VAL:HG22	1:A:276:TYR:CE1	2.35	0.62
1:B:178:GLU:O	1:B:181:GLU:HG2	2.00	0.62
1:B:234:ILE:HD13	1:B:234:ILE:O	1.97	0.62
1:A:195:VAL:HG12	1:A:199:LEU:HD22	1.82	0.62
1:A:330:LYS:O	1:A:372:ARG:HD2	2.00	0.62
1:B:367:HIS:O	1:B:368:LEU:HD23	1.99	0.62
1:B:136:PRO:HD2	1:B:139:TYR:CD1	2.35	0.62
1:A:244:SER:OG	1:A:247:GLU:HG3	1.99	0.61
1:A:48:TYR:CD1	1:A:116:LEU:HD13	2.34	0.61
1:A:180:LEU:O	1:A:184:GLY:HA2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LEU:HD12	1:B:273:THR:HG23	1.82	0.61
1:A:27:GLU:OE2	1:A:29:ILE:HG12	2.00	0.61
1:B:217:LYS:HZ2	1:B:260:TYR:HE2	1.47	0.61
1:A:88:SER:O	1:B:302:LYS:HE3	2.01	0.61
1:A:99:MSE:HE2	1:A:137:PRO:HB2	1.82	0.60
1:A:138:VAL:CG2	1:A:276:TYR:CE1	2.84	0.60
1:B:419:LYS:HZ3	1:B:421:ALA:HB3	1.65	0.60
1:A:420:GLU:HG3	1:A:424:THR:HG23	1.83	0.60
1:A:144:ARG:HB2	1:B:230:ARG:HH21	1.67	0.60
1:A:440:LYS:HD3	1:B:316:ALA:HB2	1.84	0.60
1:A:299:PHE:N	1:A:299:PHE:CD1	2.69	0.60
1:B:129:LEU:HB3	1:B:366:ILE:HD13	1.84	0.60
1:B:33:ILE:HD13	1:B:326:ILE:HD11	1.83	0.59
1:B:7:GLN:HG3	1:B:8:SER:N	2.15	0.59
1:A:303:THR:O	1:A:307:THR:HG23	2.03	0.59
1:A:366:ILE:HG22	1:A:368:LEU:HD23	1.84	0.59
1:B:279:TYR:CZ	1:B:283:ILE:HD11	2.38	0.59
1:B:421:ALA:O	1:B:426:GLU:HG2	2.03	0.59
1:A:347:PHE:CB	1:A:352:LEU:HD11	2.33	0.59
1:A:301:THR:H	1:A:304:LEU:CG	2.15	0.59
1:A:354:LYS:O	2:A:452:GOL:H2	2.03	0.58
1:A:37:LYS:HB2	1:A:38:PRO:HD2	1.86	0.58
1:A:241:ARG:O	1:B:246:ASP:OD2	2.22	0.58
1:A:267:TYR:CD2	1:A:268:ASP:OD2	2.56	0.58
1:B:138:VAL:HG11	1:B:272:MSE:HE1	1.85	0.58
1:A:258:GLU:HG3	3:A:459:HOH:O	2.04	0.58
1:A:48:TYR:CD1	1:A:112:ALA:HB1	2.39	0.58
1:A:130:THR:O	1:A:134:VAL:HG12	2.03	0.58
1:B:54:ARG:HH22	1:B:98:ARG:NH2	2.01	0.58
1:B:434:ASN:HB3	1:B:437:PRO:HD2	1.87	0.57
1:B:18:ASP:O	1:B:22:ASN:HB2	2.03	0.57
1:B:425:LEU:O	1:B:429:ILE:HG13	2.03	0.57
1:B:219:LYS:HG3	1:B:258:GLU:HG2	1.84	0.57
1:B:29:ILE:O	1:B:30:ARG:HB2	2.03	0.57
1:A:60:SER:HB2	1:B:314:ASP:OD1	2.04	0.57
1:B:95:GLN:NE2	1:B:138:VAL:HA	2.19	0.57
1:A:240:SER:HB2	1:A:243:LYS:HD2	1.86	0.57
1:A:356:ARG:HD2	2:A:452:GOL:O3	2.05	0.57
1:B:183:ASN:HD22	1:B:183:ASN:N	2.02	0.57
1:B:299:PHE:CZ	1:B:381:MSE:HE3	2.39	0.57
1:B:146:LEU:HD21	1:B:351:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ILE:HG23	1:B:404:LEU:CD2	2.35	0.56
1:B:146:LEU:HD11	1:B:273:THR:HG23	1.88	0.56
1:B:30:ARG:NH2	1:B:311:GLU:HB3	2.20	0.56
1:B:323:ARG:CZ	1:B:329:GLU:HG3	2.36	0.56
1:B:392:LEU:HB3	1:B:393:PRO:HD3	1.88	0.56
1:A:54:ARG:HH22	1:A:98:ARG:NH2	2.03	0.56
1:A:313:VAL:HG12	1:A:314:ASP:N	2.19	0.56
1:A:61:GLY:O	1:A:88:SER:OG	2.24	0.56
1:A:208:VAL:HG13	1:A:216:VAL:HB	1.86	0.56
1:A:425:LEU:O	1:A:429:ILE:HG23	2.06	0.56
1:A:67:LEU:HA	1:A:101:MSE:HE1	1.88	0.56
1:A:130:THR:HG23	1:A:383:GLN:OE1	2.06	0.56
1:A:9:ILE:O	1:A:13:THR:HG23	2.06	0.56
1:A:43:GLU:O	1:A:397:HIS:HB2	2.06	0.55
1:A:426:GLU:HG3	1:A:438:ALA:HB1	1.89	0.55
1:B:65:TYR:OH	1:B:100:GLN:NE2	2.39	0.55
1:A:180:LEU:O	1:A:184:GLY:N	2.40	0.55
1:A:89:ASN:HB2	1:A:92:THR:HB	1.88	0.55
1:B:129:LEU:H	1:B:383:GLN:NE2	2.05	0.55
1:B:288:GLU:OE2	1:B:357:ASN:ND2	2.37	0.55
1:A:299:PHE:CG	1:A:300:TYR:N	2.74	0.55
1:B:348:PRO:O	1:B:352:LEU:HD13	2.06	0.55
1:A:299:PHE:N	1:A:299:PHE:HD1	2.03	0.55
1:A:258:GLU:O	1:A:259:LEU:HD12	2.07	0.55
1:A:340:VAL:HG23	1:A:366:ILE:HB	1.88	0.55
1:A:395:ILE:HG22	1:A:404:LEU:HD22	1.89	0.55
1:B:12:ILE:O	1:B:15:ILE:HG22	2.07	0.55
1:B:36:TRP:HZ2	1:B:331:GLU:O	1.89	0.55
1:A:307:THR:O	1:A:308:LEU:HB2	2.07	0.54
1:B:54:ARG:HG2	1:B:101:MSE:HE3	1.90	0.54
1:B:139:TYR:O	1:B:142:ASP:OD2	2.25	0.54
1:A:425:LEU:O	1:A:429:ILE:N	2.35	0.54
1:B:326:ILE:CG2	1:B:328:HIS:CE1	2.91	0.54
1:A:138:VAL:HG12	1:A:139:TYR:N	2.22	0.54
1:A:178:GLU:O	1:A:182:LYS:HG3	2.07	0.54
1:A:302:LYS:HD3	1:B:87:LYS:HE3	1.88	0.54
1:A:378:VAL:HG13	1:A:379:ILE:N	2.23	0.54
1:B:133:LEU:HD22	1:B:347:PHE:HZ	1.71	0.54
1:A:133:LEU:CD2	1:A:347:PHE:HZ	2.20	0.54
1:B:138:VAL:HG11	1:B:272:MSE:CE	2.38	0.53
1:B:326:ILE:HG22	1:B:328:HIS:CE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:SER:O	1:A:189:PRO:HD3	2.08	0.53
1:B:48:TYR:CD1	1:B:116:LEU:HD13	2.44	0.53
1:A:357:ASN:HA	1:A:360:LYS:HD2	1.90	0.53
1:A:418:TYR:CD1	1:A:419:LYS:N	2.75	0.53
1:B:367:HIS:C	1:B:368:LEU:HD23	2.29	0.53
1:B:45:SER:HB3	1:B:394:LEU:HB3	1.90	0.53
1:A:328:HIS:CD2	1:A:330:LYS:HE2	2.43	0.53
1:B:416:ILE:HD11	1:B:420:GLU:OE1	2.08	0.53
1:A:300:TYR:HA	1:A:304:LEU:HD12	1.91	0.53
1:A:102:GLU:HG2	2:A:455:GOL:O3	2.08	0.53
1:B:136:PRO:CG	1:B:139:TYR:HD1	2.19	0.53
1:B:217:LYS:HA	1:B:259:LEU:O	2.07	0.53
1:B:229:PRO:O	1:B:230:ARG:HB2	2.08	0.53
1:B:95:GLN:CB	1:B:138:VAL:HG22	2.37	0.53
1:A:11:ARG:NH1	1:B:82:TYR:CZ	2.76	0.53
1:A:267:TYR:CD2	1:A:268:ASP:N	2.77	0.53
1:A:27:GLU:CG	1:A:28:GLN:N	2.72	0.52
1:A:422:ARG:O	1:A:426:GLU:HB3	2.09	0.52
1:A:307:THR:O	1:A:308:LEU:CD1	2.58	0.52
1:A:436:ASP:N	1:A:436:ASP:OD1	2.42	0.52
1:A:148:VAL:HG21	1:B:230:ARG:NH1	2.24	0.52
1:A:27:GLU:HG2	1:A:28:GLN:N	2.24	0.52
1:B:96:ILE:HD11	1:B:272:MSE:HE1	1.92	0.52
1:A:440:LYS:CE	1:B:378:VAL:HG22	2.39	0.52
1:A:183:ASN:H	1:A:183:ASN:HD22	1.56	0.52
1:B:433:ARG:C	1:B:433:ARG:HH11	2.13	0.52
1:A:433:ARG:NH1	1:B:17:LEU:HD13	2.24	0.52
1:B:294:TYR:O	1:B:295:ILE:HD13	2.10	0.52
1:A:180:LEU:O	1:A:184:GLY:CA	2.58	0.52
1:A:284:ASP:OD2	1:A:355:PHE:HB3	2.10	0.52
1:A:299:PHE:CD2	1:A:304:LEU:CD1	2.93	0.52
1:B:129:LEU:HG	1:B:294:TYR:CZ	2.45	0.52
1:B:37:LYS:HB3	1:B:38:PRO:HD2	1.92	0.52
1:B:220:ILE:HD12	1:B:224:ALA:HB3	1.91	0.51
1:A:136:PRO:C	1:A:138:VAL:N	2.63	0.51
1:B:217:LYS:HE3	1:B:260:TYR:OH	2.11	0.51
1:A:267:TYR:HD2	1:A:268:ASP:OD2	1.92	0.51
1:A:139:TYR:CZ	1:A:345:TRP:CD1	2.98	0.51
1:B:422:ARG:HE	1:B:423:HIS:CD2	2.19	0.51
1:B:219:LYS:HA	1:B:257:VAL:O	2.11	0.51
1:A:135:ARG:HG2	1:A:135:ARG:HH11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LYS:HE3	1:A:258:GLU:OE2	2.11	0.51
1:A:378:VAL:CG1	1:A:379:ILE:N	2.73	0.51
1:A:60:SER:OG	1:A:61:GLY:N	2.44	0.51
1:A:144:ARG:CB	1:B:230:ARG:HH21	2.22	0.51
1:A:223:LYS:HZ1	1:A:230:ARG:HG2	1.74	0.51
1:A:138:VAL:HG21	1:A:276:TYR:HE1	1.73	0.51
1:B:125:MSE:HE2	1:B:125:MSE:HA	1.92	0.51
1:B:176:VAL:HG22	1:B:186:TYR:CE2	2.46	0.51
1:B:326:ILE:HG22	1:B:328:HIS:CD2	2.45	0.51
1:A:302:LYS:HB2	1:B:87:LYS:HD3	1.93	0.51
1:B:32:ILE:HG22	1:B:334:LEU:HD11	1.92	0.51
1:A:240:SER:CB	1:A:243:LYS:HD2	2.40	0.51
1:B:285:LYS:O	1:B:288:GLU:HB2	2.10	0.51
1:B:30:ARG:O	1:B:31:ASN:CB	2.59	0.51
1:B:342:PRO:HB2	1:B:362:ILE:HD13	1.93	0.51
1:B:29:ILE:O	1:B:30:ARG:CB	2.58	0.51
1:A:54:ARG:CB	1:A:101:MSE:HE3	2.19	0.50
1:A:135:ARG:NH1	1:A:135:ARG:HG2	2.25	0.50
1:A:284:ASP:CG	1:A:355:PHE:HB3	2.31	0.50
1:A:40:PRO:HD2	1:A:396:LEU:HD11	1.93	0.50
1:B:55:SER:OG	1:B:419:LYS:HE2	2.10	0.50
1:B:207:LYS:C	1:B:208:VAL:HG12	2.32	0.50
1:A:222:ARG:HD2	1:A:255:GLU:CG	2.41	0.50
1:A:127:GLY:O	1:A:296:ALA:HB2	2.12	0.50
1:B:137:PRO:C	1:B:138:VAL:HG23	2.32	0.50
1:B:326:ILE:HG22	1:B:326:ILE:O	2.11	0.50
1:A:182:LYS:HB2	1:A:183:ASN:ND2	2.27	0.50
1:B:419:LYS:HG2	1:B:421:ALA:H	1.76	0.50
1:A:319:ASP:OD1	1:A:372:ARG:NH1	2.45	0.50
1:B:374:GLU:HG2	1:B:375:GLN:H	1.77	0.50
1:B:368:LEU:HD22	1:B:383:GLN:HG2	1.93	0.50
1:A:136:PRO:HB2	1:A:138:VAL:HG23	1.92	0.50
1:B:336:ILE:HB	1:B:368:LEU:O	2.12	0.49
1:A:369:ALA:HB2	1:A:388:ILE:HG13	1.93	0.49
1:B:139:TYR:CB	1:B:140:PRO:HD3	2.29	0.49
1:B:326:ILE:CG2	1:B:328:HIS:NE2	2.75	0.49
1:A:146:LEU:CD2	1:A:351:LEU:HD11	2.40	0.49
1:A:139:TYR:CE2	1:A:345:TRP:NE1	2.78	0.49
1:A:267:TYR:C	1:A:267:TYR:CD2	2.85	0.49
1:A:23:VAL:HG21	1:A:317:LEU:HD13	1.94	0.49
1:A:92:THR:HG23	1:A:96:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:SER:N	1:B:229:PRO:CD	2.75	0.49
1:B:9:ILE:H	1:B:9:ILE:HD12	1.76	0.49
1:A:347:PHE:HB3	1:A:352:LEU:CD1	2.40	0.49
1:A:433:ARG:HH11	1:B:17:LEU:HD13	1.78	0.49
1:B:183:ASN:N	1:B:183:ASN:ND2	2.60	0.49
1:B:25:GLU:C	1:B:27:GLU:H	2.16	0.49
1:A:142:ASP:O	1:A:146:LEU:HD13	2.13	0.49
1:B:284:ASP:HB2	1:B:355:PHE:HB3	1.95	0.49
1:A:342:PRO:HG2	1:A:362:ILE:CD1	2.42	0.49
1:B:419:LYS:HZ2	1:B:421:ALA:HB3	1.78	0.49
1:A:368:LEU:HD22	1:A:383:GLN:HG2	1.95	0.49
1:B:280:LEU:HA	1:B:283:ILE:HG13	1.95	0.49
1:B:39:LEU:HD11	1:B:331:GLU:OE2	2.12	0.49
1:B:319:ASP:OD2	1:B:379:ILE:HG13	2.13	0.48
1:B:125:MSE:O	1:B:294:TYR:HA	2.13	0.48
1:B:398:HIS:HB3	1:B:406:PRO:CD	2.44	0.48
1:A:144:ARG:HB2	1:B:230:ARG:NH2	2.29	0.48
1:A:436:ASP:HB2	1:A:437:PRO:CD	2.40	0.48
1:B:414:VAL:O	1:B:414:VAL:HG13	2.13	0.48
1:A:139:TYR:CZ	1:A:346:SER:HA	2.47	0.48
1:A:160:ASN:ND2	2:A:453:GOL:O3	2.38	0.48
1:B:132:SER:OG	2:B:452:GOL:H2	2.14	0.48
1:B:421:ALA:HB1	1:B:425:LEU:HB3	1.96	0.48
1:B:392:LEU:O	1:B:396:LEU:HG	2.14	0.48
1:B:54:ARG:NH2	1:B:98:ARG:NH2	2.62	0.48
1:A:29:ILE:O	1:A:29:ILE:HG22	2.13	0.48
1:A:223:LYS:HZ2	1:A:230:ARG:HD3	1.79	0.48
1:B:143:ILE:O	1:B:147:ASN:ND2	2.46	0.48
1:B:24:ARG:O	1:B:25:GLU:HB2	2.13	0.48
1:B:374:GLU:HB3	1:B:377:ASP:HB2	1.95	0.48
1:B:390:LYS:O	1:B:393:PRO:HD2	2.14	0.48
1:B:196:VAL:HG12	1:B:274:LEU:HD23	1.95	0.48
1:B:67:LEU:HD21	1:B:97:VAL:HG13	1.96	0.48
1:B:70:LEU:HG	1:B:414:VAL:HB	1.96	0.47
1:A:183:ASN:ND2	1:A:183:ASN:N	2.61	0.47
1:B:110:TYR:CD2	1:B:111:LEU:HD23	2.48	0.47
1:B:53:SER:OG	1:B:414:VAL:HG22	2.14	0.47
1:B:41:SER:HA	1:B:42:PRO:HD3	1.63	0.47
1:A:70:LEU:HD22	1:A:71:ALA:N	2.29	0.47
1:A:92:THR:HG23	1:A:96:ILE:CD1	2.44	0.47
1:A:313:VAL:HG12	1:A:317:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:VAL:HG23	1:B:243:LYS:O	2.15	0.47
1:B:388:ILE:HD12	1:B:388:ILE:H	1.80	0.47
1:B:72:VAL:HG11	1:B:409:LEU:HB3	1.96	0.47
1:A:428:LEU:O	1:A:431:ALA:HB3	2.14	0.47
1:B:204:ILE:O	1:B:208:VAL:HG12	2.15	0.47
1:B:358:ILE:O	1:B:362:ILE:HG12	2.15	0.47
1:A:130:THR:HG23	1:A:383:GLN:CD	2.35	0.47
1:B:373:PHE:CE1	1:B:404:LEU:HD11	2.49	0.47
1:A:183:ASN:ND2	1:A:183:ASN:H	2.13	0.46
1:A:366:ILE:HG22	1:A:368:LEU:CD2	2.44	0.46
1:B:102:GLU:OE1	2:B:452:GOL:O3	2.33	0.46
1:B:391:ILE:HA	1:B:394:LEU:HD11	1.97	0.46
1:B:420:GLU:H	1:B:420:GLU:CD	2.17	0.46
1:B:115:LYS:HA	1:B:115:LYS:HD3	1.61	0.46
1:B:274:LEU:HD12	1:B:274:LEU:HA	1.79	0.46
1:A:62:THR:HG21	1:B:16:LEU:HD21	1.96	0.46
1:A:102:GLU:HG2	2:A:455:GOL:C3	2.45	0.46
1:B:218:VAL:O	1:B:258:GLU:HA	2.16	0.46
1:A:134:VAL:C	1:A:135:ARG:HG3	2.35	0.46
1:A:92:THR:O	1:A:96:ILE:HD12	2.16	0.46
1:A:237:LEU:HB3	1:B:249:LEU:HD21	1.97	0.46
1:B:293:ALA:HB2	1:B:395:ILE:HD11	1.98	0.46
1:A:323:ARG:HA	1:A:327:GLY:HA2	1.96	0.46
2:A:455:GOL:H2	2:A:456:GOL:O1	2.16	0.46
1:B:192:THR:HG23	1:B:196:VAL:HG13	1.97	0.46
1:A:401:GLY:C	1:A:403:TYR:N	2.56	0.46
1:A:425:LEU:CD1	1:B:12:ILE:HG21	2.44	0.46
1:B:176:VAL:HG22	1:B:186:TYR:CD2	2.51	0.46
1:A:88:SER:O	1:B:302:LYS:CE	2.64	0.46
1:B:106:ASN:HB2	1:B:282:SER:HB2	1.96	0.45
1:B:295:ILE:HD11	1:B:382:LEU:HD13	1.97	0.45
1:B:356:ARG:HD3	1:B:359:GLU:OE2	2.15	0.45
1:B:405:ARG:N	1:B:406:PRO:HD2	2.31	0.45
1:B:89:ASN:O	1:B:90:TYR:C	2.54	0.45
1:A:134:VAL:HG22	1:A:135:ARG:HG3	1.98	0.45
1:A:260:TYR:CD2	1:A:260:TYR:N	2.83	0.45
1:A:113:TYR:CG	1:A:289:VAL:HG22	2.50	0.45
1:A:81:SER:O	1:A:189:PRO:CD	2.65	0.45
1:A:27:GLU:H	1:A:27:GLU:CD	2.18	0.45
1:A:312:ILE:HD13	1:A:312:ILE:O	2.16	0.45
1:B:15:ILE:CG2	1:B:16:LEU:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LYS:HA	1:B:205:ASP:CB	2.41	0.45
1:A:144:ARG:CG	1:B:230:ARG:HH21	2.30	0.45
1:B:340:VAL:HG11	1:B:368:LEU:HD11	1.98	0.45
1:A:133:LEU:CD2	1:A:347:PHE:CZ	2.99	0.45
1:A:281:TYR:CZ	1:A:285:LYS:CE	3.00	0.45
1:A:152:LEU:HD21	1:A:261:LEU:HD12	1.99	0.45
1:A:29:ILE:HA	1:A:32:ILE:HG22	1.98	0.45
1:B:341:VAL:HA	1:B:342:PRO:HD3	1.76	0.45
1:A:144:ARG:HG3	1:B:230:ARG:HH21	1.81	0.45
1:A:220:ILE:HA	1:A:221:PRO:HD3	1.85	0.45
1:A:159:GLU:HG3	1:A:163:ASN:ND2	2.32	0.44
1:A:405:ARG:O	1:A:408:GLN:HB3	2.17	0.44
1:B:202:LYS:HD3	1:B:203:TYR:CE1	2.52	0.44
1:A:27:GLU:CD	1:A:28:GLN:H	2.20	0.44
1:B:83:ALA:O	1:B:84:ASN:HB2	2.17	0.44
1:A:329:GLU:O	1:A:375:GLN:O	2.35	0.44
1:A:418:TYR:HD1	1:A:419:LYS:N	2.07	0.44
1:B:418:TYR:O	1:B:419:LYS:C	2.56	0.44
1:A:220:ILE:HD11	1:A:259:LEU:HD22	1.98	0.44
1:A:85:ALA:HB3	1:B:15:ILE:HG21	1.99	0.44
1:B:287:LEU:HB3	1:B:357:ASN:HB3	1.99	0.44
1:B:330:LYS:O	1:B:372:ARG:HD2	2.18	0.44
1:B:285:LYS:HD2	1:B:285:LYS:HA	1.85	0.44
1:A:267:TYR:CE2	1:A:268:ASP:OD2	2.71	0.44
1:B:110:TYR:HD2	1:B:111:LEU:HD23	1.83	0.44
1:A:295:ILE:HA	1:A:295:ILE:HD13	1.85	0.44
1:A:423:HIS:O	1:A:427:ALA:HB3	2.18	0.44
1:B:393:PRO:O	1:B:396:LEU:HB2	2.17	0.44
1:B:399:LYS:HA	1:B:404:LEU:HA	1.99	0.44
1:B:129:LEU:HB2	1:B:383:GLN:HE21	1.82	0.44
1:B:433:ARG:O	1:B:433:ARG:NH1	2.47	0.44
1:B:421:ALA:CB	1:B:425:LEU:HB3	2.48	0.44
1:A:44:LYS:HA	1:A:397:HIS:CD2	2.53	0.43
1:B:21:GLU:O	1:B:24:ARG:NE	2.50	0.43
1:B:403:TYR:HD1	1:B:407:LEU:HD23	1.83	0.43
1:A:321:VAL:O	1:A:324:THR:HB	2.18	0.43
1:B:315:THR:HG22	1:B:316:ALA:N	2.34	0.43
1:A:146:LEU:HD11	1:A:273:THR:HG23	2.00	0.43
1:A:386:THR:HG1	1:A:391:ILE:HD11	1.83	0.43
1:B:299:PHE:HZ	1:B:381:MSE:HE3	1.83	0.43
1:B:39:LEU:HD12	1:B:39:LEU:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ASN:N	1:A:34:ASN:OD1	2.50	0.43
1:A:8:SER:OG	3:A:469:HOH:O	2.21	0.43
1:B:104:LEU:HD22	1:B:189:PRO:HB2	2.00	0.43
1:A:64:ILE:HG21	1:A:425:LEU:HD12	2.00	0.43
1:B:284:ASP:O	1:B:287:LEU:HB2	2.18	0.43
1:A:281:TYR:CZ	1:A:285:LYS:HE3	2.53	0.43
1:B:299:PHE:N	1:B:299:PHE:CD1	2.85	0.43
1:B:70:LEU:HB3	1:B:79:ARG:HG2	2.01	0.43
1:B:80:LEU:HG	1:B:108:LEU:HD13	2.01	0.43
1:B:14:LYS:HB3	1:B:14:LYS:HE3	1.79	0.43
1:B:403:TYR:CD1	1:B:407:LEU:HD23	2.54	0.43
1:A:320:ALA:HB2	1:B:436:ASP:HB2	2.01	0.43
1:A:347:PHE:HA	1:A:348:PRO:HD3	1.84	0.43
1:A:60:SER:CB	1:B:314:ASP:OD1	2.66	0.43
1:B:60:SER:HB3	1:B:61:GLY:H	1.66	0.43
1:A:307:THR:O	1:A:308:LEU:CB	2.67	0.42
1:B:136:PRO:HD2	1:B:139:TYR:CE1	2.54	0.42
1:B:221:PRO:HB2	1:B:223:LYS:HE2	2.01	0.42
1:B:325:LEU:HB3	1:B:326:ILE:HD12	2.01	0.42
1:B:326:ILE:HG21	1:B:328:HIS:CE1	2.54	0.42
1:B:329:GLU:O	1:B:375:GLN:O	2.36	0.42
1:A:195:VAL:CG1	1:A:195:VAL:O	2.67	0.42
1:A:223:LYS:H	1:A:223:LYS:CD	2.15	0.42
1:A:300:TYR:HD2	1:B:61:GLY:HA3	1.84	0.42
1:B:15:ILE:HG22	1:B:16:LEU:N	2.34	0.42
1:B:208:VAL:O	1:B:209:ILE:HG12	2.20	0.42
1:B:244:SER:OG	1:B:247:GLU:CG	2.64	0.42
1:A:104:LEU:HD21	1:A:189:PRO:HG2	2.01	0.42
1:A:49:ALA:HA	1:A:124:LEU:O	2.20	0.42
1:B:208:VAL:CG2	1:B:209:ILE:N	2.81	0.42
1:A:420:GLU:C	1:A:424:THR:HG23	2.39	0.42
1:A:135:ARG:NH2	1:B:90:TYR:H	2.04	0.42
1:A:340:VAL:CG2	1:A:366:ILE:HB	2.50	0.42
1:A:65:TYR:OH	1:A:100:GLN:NE2	2.51	0.42
1:A:54:ARG:HB3	1:A:101:MSE:HE1	1.92	0.42
1:B:50:VAL:HG11	1:B:125:MSE:HE1	1.96	0.42
1:A:108:LEU:HA	1:A:108:LEU:HD12	1.82	0.42
1:A:306:ARG:HG3	1:A:307:THR:N	2.33	0.42
1:B:143:ILE:HG23	1:B:147:ASN:HD21	1.85	0.42
1:B:182:LYS:CB	1:B:183:ASN:HD22	2.33	0.42
1:A:392:LEU:N	1:A:393:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:SER:H	1:A:397:HIS:CD2	2.38	0.42
1:B:28:GLN:O	1:B:29:ILE:HB	2.18	0.42
1:A:372:ARG:HB2	1:A:379:ILE:HG12	2.01	0.41
1:A:4:LEU:HD12	1:A:4:LEU:N	2.35	0.41
1:A:249:LEU:HD22	1:B:234:ILE:HD11	2.02	0.41
1:A:153:ILE:HD13	1:A:153:ILE:HG21	1.81	0.41
1:A:307:THR:O	1:A:308:LEU:HD13	2.21	0.41
1:A:416:ILE:O	1:A:416:ILE:CG2	2.67	0.41
1:A:202:LYS:HD2	1:A:203:TYR:CE1	2.56	0.41
1:B:180:LEU:HD23	1:B:180:LEU:HA	1.86	0.41
1:B:395:ILE:HG22	1:B:404:LEU:HD21	2.00	0.41
1:A:130:THR:HG23	1:A:383:GLN:NE2	2.36	0.41
1:B:325:LEU:HD23	1:B:326:ILE:CD1	2.46	0.41
1:A:79:ARG:O	1:A:185:ASN:HA	2.21	0.41
1:A:138:VAL:HG21	1:A:276:TYR:CE1	2.52	0.41
1:A:102:GLU:HG2	2:A:455:GOL:H31	2.01	0.41
1:B:283:ILE:HG22	1:B:287:LEU:HD11	2.02	0.41
1:B:153:ILE:O	1:B:157:ASP:HB2	2.20	0.41
1:B:319:ASP:O	1:B:322:ILE:HB	2.21	0.41
1:A:162:LEU:HD23	1:A:354:LYS:HE2	2.02	0.41
1:A:281:TYR:O	1:A:285:LYS:HG2	2.21	0.41
1:A:70:LEU:HA	1:A:70:LEU:HD23	1.89	0.41
1:B:292:LEU:HD12	1:B:293:ALA:H	1.85	0.41
1:B:134:VAL:HA	1:B:343:PRO:HG2	2.02	0.41
1:B:47:ILE:HG22	1:B:398:HIS:CE1	2.55	0.41
1:B:414:VAL:O	1:B:415:LYS:C	2.59	0.41
1:B:164:GLU:O	1:B:167:GLU:HB2	2.20	0.41
1:B:310:VAL:HG22	1:B:311:GLU:N	2.36	0.41
1:A:138:VAL:HG12	1:A:139:TYR:CD1	2.56	0.41
1:B:276:TYR:CE2	1:B:280:LEU:HD11	2.56	0.41
1:B:323:ARG:NH1	1:B:329:GLU:HG3	2.36	0.41
1:B:419:LYS:HD3	1:B:422:ARG:N	2.35	0.41
1:A:192:THR:HG23	1:A:274:LEU:HB2	2.03	0.41
1:B:106:ASN:CB	1:B:282:SER:HB2	2.51	0.41
1:A:232:ILE:HD13	1:A:232:ILE:HG21	1.83	0.40
1:B:130:THR:HG22	1:B:366:ILE:HD12	2.03	0.40
1:B:342:PRO:HA	1:B:343:PRO:HD3	1.83	0.40
1:B:394:LEU:H	1:B:394:LEU:HG	1.55	0.40
1:A:11:ARG:NH1	1:B:82:TYR:CE1	2.81	0.40
1:A:241:ARG:HD3	1:A:241:ARG:HH11	1.71	0.40
1:A:379:ILE:H	1:B:440:LYS:NZ	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:MSE:HB3	1:A:125:MSE:HE3	2.02	0.40
1:A:358:ILE:O	1:A:362:ILE:HG12	2.21	0.40
1:A:96:ILE:O	1:A:100:GLN:HG3	2.21	0.40
1:B:292:LEU:HD12	1:B:293:ALA:N	2.36	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	424/471 (90%)	390 (92%)	31 (7%)	3 (1%)	22 51
1	B	422/471 (90%)	382 (90%)	33 (8%)	7 (2%)	9 27
All	All	846/942 (90%)	772 (91%)	64 (8%)	10 (1%)	13 37

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	ILE
1	B	43	GLU
1	B	139	TYR
1	A	420	GLU
1	B	42	PRO
1	B	208	VAL
1	A	300	TYR
1	A	424	THR
1	B	432	LEU
1	B	138	VAL

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	385/410 (94%)	337 (88%)	48 (12%)	4	14
1	B	385/410 (94%)	334 (87%)	51 (13%)	4	11
All	All	770/820 (94%)	671 (87%)	99 (13%)	4	12

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	21	GLU
1	A	27	GLU
1	A	34	ASN
1	A	35	SER
1	A	50	VAL
1	A	55	SER
1	A	56	VAL
1	A	66	PHE
1	A	70	LEU
1	A	79	ARG
1	A	90	TYR
1	A	102	GLU
1	A	129	LEU
1	A	135	ARG
1	A	141	GLU
1	A	144	ARG
1	A	156	SER
1	A	167	GLU
1	A	174	ARG
1	A	183	ASN
1	A	185	ASN
1	A	188	SER
1	A	199	LEU
1	A	222	ARG
1	A	223	LYS
1	A	230	ARG

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Mol	Chain	Res	Type
1	A	231	VAL
1	A	267	TYR
1	A	288	GLU
1	A	299	PHE
1	A	302	LYS
1	A	308	LEU
1	A	312	ILE
1	A	328	HIS
1	A	341	VAL
1	A	345	TRP
1	A	352	LEU
1	A	353	SER
1	A	374	GLU
1	A	386	THR
1	A	387	ASN
1	A	404	LEU
1	A	405	ARG
1	A	414	VAL
1	A	428	LEU
1	A	432	LEU
1	A	436	ASP
1	B	7	GLN
1	B	19	GLU
1	B	26	ASN
1	B	39	LEU
1	B	41	SER
1	B	50	VAL
1	B	60	SER
1	B	62	THR
1	B	68	SER
1	B	90	TYR
1	B	104	LEU
1	B	129	LEU
1	B	135	ARG
1	B	138	VAL
1	B	142	ASP
1	B	183	ASN
1	B	195	VAL
1	B	199	LEU
1	B	200	ARG
1	B	208	VAL
1	B	217	LYS

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Mol	Chain	Res	Type
1	B	234	ILE
1	B	253	ASP
1	B	274	LEU
1	B	283	ILE
1	B	288	GLU
1	B	290	LYS
1	B	299	PHE
1	B	304	LEU
1	B	312	ILE
1	B	315	THR
1	B	340	VAL
1	B	344	LYS
1	B	345	TRP
1	B	350	PHE
1	B	361	LEU
1	B	372	ARG
1	B	378	VAL
1	B	384	SER
1	B	389	GLU
1	B	394	LEU
1	B	403	TYR
1	B	404	LEU
1	B	408	GLN
1	B	411	HIS
1	B	412	HIS
1	B	414	VAL
1	B	415	LYS
1	B	422	ARG
1	B	432	LEU
1	B	434	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	106	ASN
1	A	179	HIS
1	A	183	ASN
1	A	271	HIS
1	A	328	HIS
1	A	397	HIS
1	B	95	GLN

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Mol	Chain	Res	Type
1	B	100	GLN
1	B	106	ASN
1	B	147	ASN
1	B	163	ASN
1	B	183	ASN
1	B	185	ASN
1	B	271	HIS
1	B	291	ASN
1	B	383	GLN
1	B	408	GLN
1	B	412	HIS
1	B	423	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

7 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	GOL	A	456	-	5,5,5	0.43	0	5,5,5	0.31	0
2	GOL	A	453	-	5,5,5	0.38	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	A	457	-	5,5,5	0.37	0	5,5,5	0.28	0
2	GOL	B	452	-	5,5,5	0.39	0	5,5,5	0.39	0
2	GOL	A	454	-	5,5,5	0.46	0	5,5,5	0.41	0
2	GOL	A	452	-	5,5,5	0.36	0	5,5,5	0.27	0
2	GOL	A	455	-	5,5,5	0.28	0	5,5,5	0.85	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	GOL	A	456	-	-	2/4/4/4	-
2	GOL	A	453	-	-	4/4/4/4	-
2	GOL	A	457	-	-	3/4/4/4	-
2	GOL	B	452	-	-	2/4/4/4	-
2	GOL	A	454	-	-	4/4/4/4	-
2	GOL	A	452	-	-	4/4/4/4	-
2	GOL	A	455	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	453	GOL	O1-C1-C2-C3
2	A	453	GOL	C1-C2-C3-O3
2	B	452	GOL	O1-C1-C2-C3
2	A	454	GOL	O1-C1-C2-C3
2	A	452	GOL	O1-C1-C2-C3
2	A	452	GOL	C1-C2-C3-O3
2	A	454	GOL	O1-C1-C2-O2
2	A	455	GOL	O1-C1-C2-O2
2	A	456	GOL	O1-C1-C2-C3
2	A	457	GOL	O1-C1-C2-C3
2	A	457	GOL	C1-C2-C3-O3
2	A	454	GOL	C1-C2-C3-O3
2	A	455	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	A	453	GOL	O1-C1-C2-O2
2	A	452	GOL	O1-C1-C2-O2
2	A	452	GOL	O2-C2-C3-O3
2	A	456	GOL	O1-C1-C2-O2
2	A	453	GOL	O2-C2-C3-O3
2	A	457	GOL	O1-C1-C2-O2
2	A	455	GOL	C1-C2-C3-O3
2	B	452	GOL	O1-C1-C2-O2
2	A	454	GOL	O2-C2-C3-O3
2	A	455	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	456	GOL	1	0
2	A	453	GOL	1	0
2	B	452	GOL	2	0
2	A	452	GOL	2	0
2	A	455	GOL	6	0

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, 95^{th} 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	423/471 (89%)	-0.30	11 (2%)	56	46	41, 79, 150, 209	0
1	B	423/471 (89%)	0.02	26 (6%)	21	13	51, 104, 174, 265	0
All	All	846/942 (89%)	-0.14	37 (4%)	34	24	41, 91, 162, 265	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	325	LEU	6.9
1	B	403	TYR	6.8
1	A	139	TYR	4.0
1	B	31	ASN	3.8
1	B	258	GLU	3.6
1	B	26	ASN	3.5
1	B	306	ARG	3.5
1	B	441	ILE	3.5
1	A	306	ARG	3.5
1	B	324	THR	3.5
1	A	418	TYR	3.4
1	B	260	TYR	3.3
1	A	90	TYR	3.2
1	A	429	ILE	3.2
1	B	303	THR	2.9
1	B	402	GLY	2.8
1	B	400	ALA	2.8
1	B	119	GLU	2.7
1	B	301	THR	2.6
1	B	418	TYR	2.6
1	A	426	GLU	2.5
1	B	181	GLU	2.5
1	B	27	GLU	2.5
1	A	26	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	416	ILE	2.3
1	B	32	ILE	2.3
1	B	209	ILE	2.3
1	B	375	GLN	2.3
1	A	91	GLY	2.3
1	B	419	LYS	2.3
1	B	259	LEU	2.2
1	B	422	ARG	2.2
1	B	307	THR	2.2
1	B	139	TYR	2.1
1	B	349	ASP	2.1
1	A	422	ARG	2.1
1	A	4	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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, 95^{th} 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	GOL	A	452	6/6	0.60	0.31	83,118,124,130	0
2	GOL	A	457	6/6	0.84	0.25	93,115,118,121	0
2	GOL	A	453	6/6	0.85	0.14	96,115,118,118	0
2	GOL	A	454	6/6	0.86	0.27	77,104,111,117	0
2	GOL	A	455	6/6	0.87	0.29	68,78,79,91	0
2	GOL	A	456	6/6	0.88	0.46	83,96,100,103	0
2	GOL	B	452	6/6	0.92	0.69	110,131,142,147	0

6.5 Other polymers (i)

There are no such residues in this entry.