Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:53 PM GMT

PDB ID	:	1HSJ
Title	:	SARR MBP FUSION STRUCTURE
Authors	:	Zhang, G.
Deposited on	:	2000-12-26
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

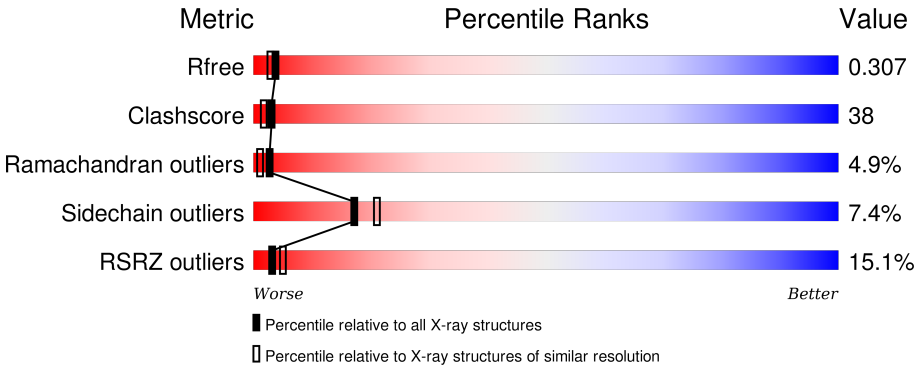
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	487	16% 46% 46% 7% •
1	B	487	14% 47% 45% 7% •

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	GLC	A	671	-	-	X	-
2	GLC	A	672	-	-	X	-
2	GLC	B	674	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7730 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.

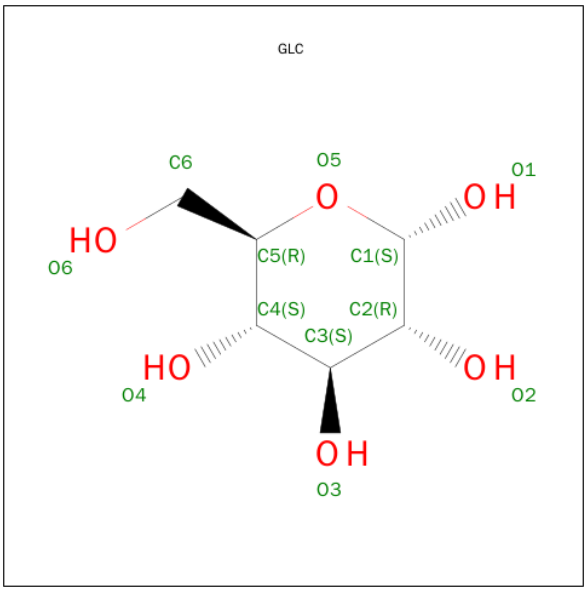
- Molecule 1 is a protein called FUSION PROTEIN CONSISTING OF STAPHYLOCOCCUS ACCESSORY REGULATOR PROTEIN R AND MALTOSE BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3841	2471	628	734	8			
1	B	487	Total	C	N	O	S	0	0	0
			3841	2471	628	734	8			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	ALA	LYS	ENGINEERED	UNP P02928
A	363	ALA	ASP	ENGINEERED	UNP P02928
A	368	ALA	SER	ENGINEERED	UNP P02928
A	369	ALA	SER	ENGINEERED	UNP P02928
A	370	ALA	SER	ENGINEERED	UNP P02928
A	371	GLU	-	CLONING ARTIFACT	UNP P02928
A	372	PHE	-	CLONING ARTIFACT	UNP P02928
B	362	ALA	LYS	ENGINEERED	UNP P02928
B	363	ALA	ASP	ENGINEERED	UNP P02928
B	368	ALA	SER	ENGINEERED	UNP P02928
B	369	ALA	SER	ENGINEERED	UNP P02928
B	370	ALA	SER	ENGINEERED	UNP P02928
B	371	GLU	-	CLONING ARTIFACT	UNP P02928
B	372	PHE	-	CLONING ARTIFACT	UNP P02928

- Molecule 2 is SUGAR (GLUCOSE) (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



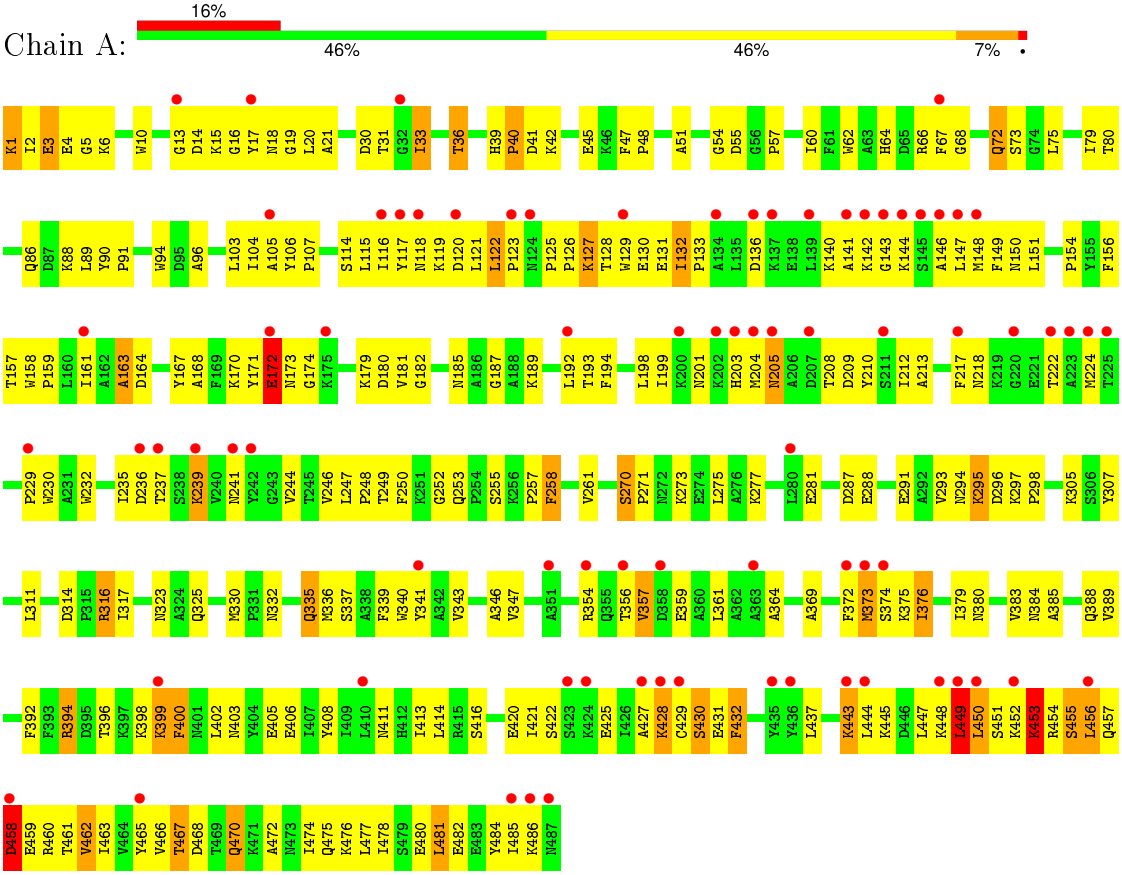
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 6 6	0	0
2	A	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0

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 errors 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.

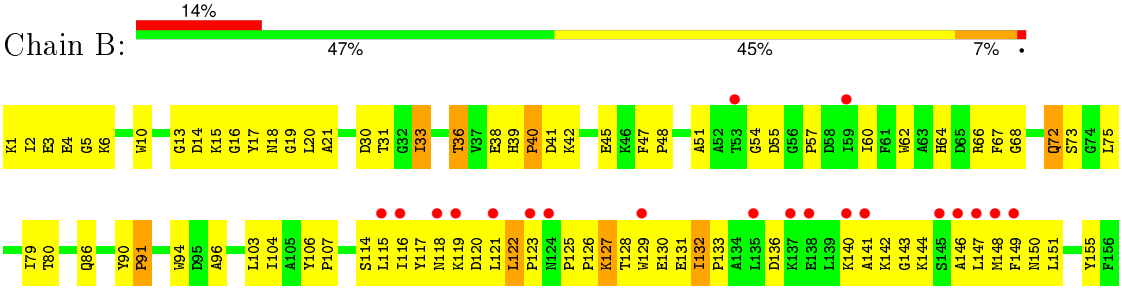
• Molecule 1: FUSION PROTEIN CONSISTING OF STAPHYLOCOCCUS ACCESSORY REGULATOR PROTEIN R AND MALTOSE BINDING PROTEIN

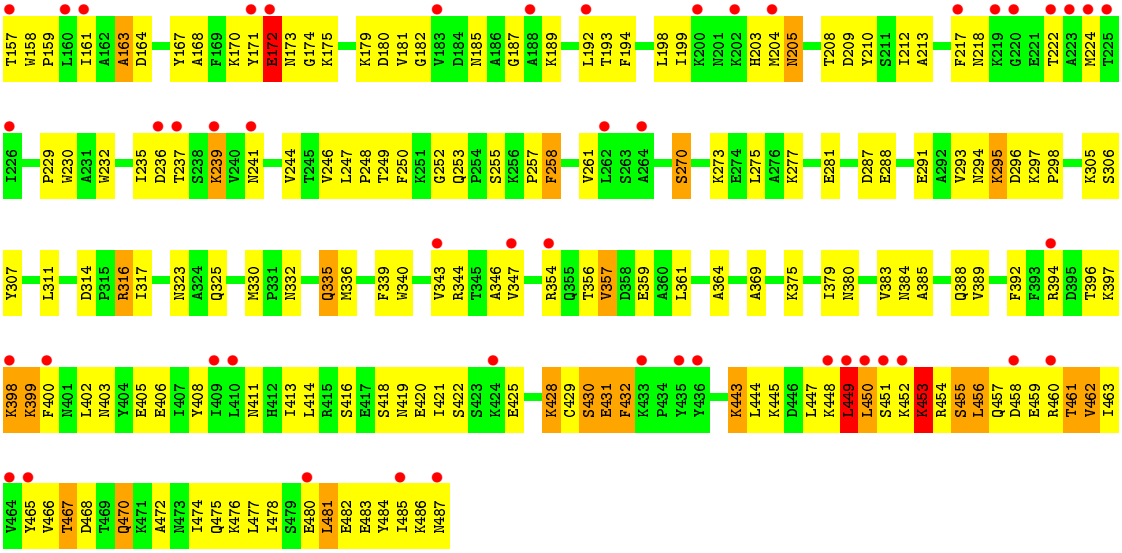
Chain A:



• Molecule 1: FUSION PROTEIN CONSISTING OF STAPHYLOCOCCUS ACCESSORY REGULATOR PROTEIN R AND MALTOSE BINDING PROTEIN

Chain B:




T157 W158 P159 L160 I161 A162 A163 D164
Y167 A168 F169 K170 Y171 E172 N173 G174 K175
K179 D180 V181 G182 Y183 D184 N185 A186 G187 A188 K189
L192 T193 F194
L198 I199 K200 N201 K202 H203 M204 N205
T208 D209 Y210 S211 I212 A213
F217 N218 K219 G220 E221 T222 A223 M224 T225
I226 P229 W230 A231 W232 I235 D236 T237 S238 K239 V240 N241
V244 T245 V246 L247 P248 T249 F250 K251 G252 Q253 P254 S255 K256 P257 F258
V261 L262 S263 A264 S270 K273 E274 L275 A276 K277 E281 D287 E288 E291 A292 V293 N294 K295 D296 K297 P298 K305 S306
Y307 L311 D314 P315 R316 I317 N323 A324 Q325 M330 P331 N332 Q335 M336 F339 W340 V343 R344 T345 A346 V347 R354 Q355 T356 V357 D358 E359 A360 L361 A364 A369 K375 I379 N380 V383 N384 A385 Q388 V389 F392 F393 R394 D395 T396 K397
K398 K399 F400 N401 L402 N403 Y404 E405 E406 I407 Y408 I409 L410 N411 H412 I413 L414 R415 S416 E417 S418 N419 E420 I421 S422 S423 K424 E425 K428 C429 S430 E431 F432 K433 P434 Y435 Y436 K443 L444 K445 D446 L447 K448 L449 L450 S451 K452 R453 R454 S455 L456 Q457 D458 E459 R460 T461 V462 I463
V464 Y465 V466 T467 D468 T469 Q470 K471 A472 N473 I474 Q475 K476 L477 I478 S479 E480 L481 E482 E483 Y484 I485 K486 N487

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	64.74Å 70.64Å 75.47Å 65.72° 67.18° 69.58°	Depositor
Resolution (Å)	19.95 – 2.30 19.94 – 2.21	Depositor EDS
% Data completeness (in resolution range)	80.6 (19.95-2.30) 78.9 (19.94-2.21)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.21Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.263 , 0.304 0.273 , 0.307	Depositor DCC
R_{free} test set	2202 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	49.0	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 67.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 46308 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7730	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GLC

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	0.46	0/3924	0.66	1/5310 (0.0%)
1	B	0.46	0/3924	0.66	1/5310 (0.0%)
All	All	0.46	0/7848	0.66	2/10620 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	453	LYS	N-CA-C	-6.02	94.75	111.00
1	A	453	LYS	N-CA-C	-5.95	94.94	111.00

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	3841	0	3851	301	0
1	B	3841	0	3851	303	0
2	A	24	0	24	8	0
2	B	24	0	24	6	0
All	All	7730	0	7750	594	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 38.

All (594) 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:1:LYS:HE2	1:B:354:ARG:HB3	1.25	1.16
1:A:451:SER:HB2	1:A:470:GLN:HG2	1.29	1.12
1:B:451:SER:HB2	1:B:470:GLN:HG2	1.28	1.12
1:A:414:LEU:HD12	1:A:478:ILE:HD12	1.33	1.10
1:B:456:LEU:HD13	1:B:457:GLN:H	1.14	1.06
1:B:414:LEU:HD12	1:B:478:ILE:HD12	1.28	1.06
1:A:456:LEU:CD1	1:A:457:GLN:H	1.69	1.04
1:A:456:LEU:HD13	1:A:457:GLN:H	1.21	1.01
2:B:673:GLC:O1	2:B:674:GLC:H62	1.65	0.96
1:A:33:ILE:HD13	1:A:275:LEU:HD13	1.47	0.95
1:B:335:GLN:H	1:B:335:GLN:NE2	1.65	0.95
1:A:335:GLN:NE2	1:A:335:GLN:H	1.63	0.95
1:A:456:LEU:HD12	1:A:458:ASP:H	1.29	0.95
1:B:467:THR:HG22	1:B:468:ASP:H	1.31	0.95
1:A:192:LEU:HD23	1:A:357:VAL:HG13	1.49	0.93
1:B:456:LEU:CD1	1:B:457:GLN:H	1.80	0.93
1:B:192:LEU:HD23	1:B:357:VAL:HG13	1.49	0.93
1:B:33:ILE:HD13	1:B:275:LEU:HD13	1.48	0.92
1:A:467:THR:HG22	1:A:468:ASP:H	1.32	0.92
2:A:671:GLC:O1	2:A:672:GLC:H62	1.73	0.89
1:A:373:MET:HB2	1:B:384:ASN:HD21	1.36	0.88
1:A:456:LEU:HD12	1:A:458:ASP:N	1.91	0.86
1:A:411:ASN:HD21	1:B:380:ASN:HD22	1.23	0.86
1:A:31:THR:HG22	1:A:33:ILE:HG23	1.57	0.86
1:A:414:LEU:HD11	1:A:475:GLN:HA	1.57	0.85
1:B:398:LYS:HG3	1:B:399:LYS:H	1.39	0.84
1:A:380:ASN:HD22	1:B:411:ASN:HD21	1.25	0.83
1:B:31:THR:HG22	1:B:33:ILE:HG23	1.59	0.82
1:B:80:THR:HG22	1:B:80:THR:O	1.81	0.81
1:A:316:ARG:CG	1:A:316:ARG:HH11	1.94	0.81
1:A:467:THR:CB	1:A:470:GLN:HB2	2.11	0.80
1:B:467:THR:CB	1:B:470:GLN:HB2	2.11	0.80
1:B:316:ARG:HH11	1:B:316:ARG:CG	1.95	0.80
1:A:1:LYS:HE2	1:B:354:ARG:CB	2.09	0.80
1:A:80:THR:O	1:A:80:THR:HG22	1.81	0.80
1:B:68:GLY:HA3	1:B:332:ASN:O	1.82	0.79
1:A:405:GLU:HA	1:A:432:PHE:CZ	2.18	0.79
1:A:68:GLY:HA3	1:A:332:ASN:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:THR:CG2	1:B:33:ILE:HG23	2.13	0.79
1:A:354:ARG:HG3	1:A:354:ARG:HH11	1.48	0.79
1:B:384:ASN:O	1:B:388:GLN:HG2	1.84	0.78
1:A:486:LYS:O	1:A:486:LYS:HD3	1.83	0.78
1:A:31:THR:CG2	1:A:33:ILE:HG23	2.13	0.78
1:B:335:GLN:H	1:B:335:GLN:HE21	1.31	0.78
1:B:451:SER:HB2	1:B:470:GLN:CG	2.12	0.78
1:A:10:TRP:CD1	1:A:57:PRO:HB3	2.19	0.77
1:B:405:GLU:HA	1:B:432:PHE:CZ	2.20	0.77
1:B:218:ASN:HD21	1:B:235:ILE:HG12	1.49	0.77
1:B:354:ARG:HH11	1:B:354:ARG:HG3	1.50	0.77
1:A:467:THR:HB	1:A:470:GLN:HB2	1.66	0.77
1:B:10:TRP:CD1	1:B:57:PRO:HB3	2.20	0.77
1:A:218:ASN:HD21	1:A:235:ILE:HG12	1.48	0.76
1:A:316:ARG:HH11	1:A:316:ARG:HG3	1.48	0.76
1:B:467:THR:HB	1:B:470:GLN:HB2	1.66	0.76
1:A:335:GLN:HE21	1:A:335:GLN:H	1.30	0.76
1:B:447:LEU:HD22	1:B:449:LEU:HD12	1.68	0.76
1:B:181:VAL:HG21	1:B:369:ALA:HB2	1.66	0.75
1:A:384:ASN:O	1:A:388:GLN:HG2	1.85	0.75
1:B:316:ARG:HG3	1:B:316:ARG:HH11	1.50	0.75
1:A:447:LEU:HD22	1:A:449:LEU:HD12	1.68	0.74
1:A:444:LEU:HB3	1:A:450:LEU:HB2	1.69	0.74
1:A:128:THR:OG1	1:A:131:GLU:HG2	1.88	0.74
1:B:128:THR:OG1	1:B:131:GLU:HG2	1.87	0.74
1:A:456:LEU:HD13	1:A:457:GLN:N	2.01	0.74
1:B:129:TRP:HA	1:B:132:ILE:HD12	1.70	0.74
1:B:244:VAL:HG21	1:B:316:ARG:HA	1.68	0.73
1:B:483:GLU:HA	1:B:486:LYS:HG2	1.71	0.73
1:A:244:VAL:HG21	1:A:316:ARG:HA	1.69	0.73
1:A:115:LEU:HD22	1:A:248:PRO:HD3	1.71	0.73
1:B:115:LEU:HD22	1:B:248:PRO:HD3	1.70	0.73
1:B:444:LEU:HB3	1:B:450:LEU:HB2	1.70	0.73
1:A:451:SER:HB2	1:A:470:GLN:CG	2.14	0.73
1:A:209:ASP:OD1	1:A:212:ILE:HD13	1.89	0.72
1:B:136:ASP:O	1:B:140:LYS:HB2	1.89	0.72
1:A:181:VAL:HG21	1:A:369:ALA:HB2	1.71	0.72
1:A:136:ASP:O	1:A:140:LYS:HB2	1.90	0.71
1:B:456:LEU:HD13	1:B:457:GLN:N	1.99	0.71
1:B:414:LEU:HD11	1:B:475:GLN:HA	1.73	0.71
1:A:129:TRP:HA	1:A:132:ILE:HD12	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:TYR:CZ	1:A:430:SER:HB3	2.25	0.71
1:A:456:LEU:CD1	1:A:458:ASP:H	2.04	0.70
1:B:209:ASP:OD1	1:B:212:ILE:HD13	1.92	0.70
1:A:136:ASP:HA	1:A:146:ALA:HB2	1.73	0.70
1:A:451:SER:HB3	1:A:465:TYR:O	1.92	0.70
2:B:673:GLC:C1	2:B:674:GLC:HO4	2.03	0.70
1:B:136:ASP:HA	1:B:146:ALA:HB2	1.73	0.69
1:A:18:ASN:HB2	1:A:296:ASP:OD2	1.93	0.69
1:B:18:ASN:HB2	1:B:296:ASP:OD2	1.91	0.69
1:A:460:ARG:NE	1:A:460:ARG:HA	2.06	0.68
1:A:150:ASN:HD22	1:A:210:TYR:HB2	1.58	0.68
1:A:172:GLU:CD	1:A:173:ASN:H	1.97	0.68
1:B:4:GLU:HG2	1:B:5:GLY:N	2.10	0.67
1:B:482:GLU:C	1:B:486:LYS:HE3	2.15	0.67
1:A:453:LYS:HD2	1:A:462:VAL:HG11	1.75	0.67
1:B:449:LEU:HD13	1:B:450:LEU:N	2.10	0.67
1:A:466:VAL:HG12	1:A:470:GLN:HB3	1.76	0.67
1:A:316:ARG:HH11	1:A:316:ARG:HB2	1.60	0.67
1:A:140:LYS:HD2	1:A:144:LYS:O	1.94	0.67
1:A:72:GLN:HE21	1:A:72:GLN:HA	1.59	0.67
1:B:159:PRO:HG3	1:B:257:PRO:HA	1.77	0.67
1:A:4:GLU:HG2	1:A:5:GLY:N	2.10	0.67
1:B:408:TYR:CZ	1:B:430:SER:HB3	2.30	0.67
1:B:244:VAL:CG2	1:B:316:ARG:HA	2.25	0.66
1:A:244:VAL:CG2	1:A:316:ARG:HA	2.26	0.66
1:B:316:ARG:HH11	1:B:316:ARG:HB2	1.60	0.66
1:A:467:THR:HG22	1:A:468:ASP:N	2.09	0.66
1:A:316:ARG:CB	1:A:316:ARG:HH11	2.09	0.66
1:B:72:GLN:HE21	1:B:72:GLN:HA	1.61	0.66
2:B:673:GLC:HO1	2:B:674:GLC:C4	2.08	0.66
1:B:150:ASN:HD22	1:B:210:TYR:HB2	1.61	0.66
1:B:217:PHE:HA	1:B:222:THR:HG22	1.76	0.66
1:A:449:LEU:HD13	1:A:450:LEU:N	2.09	0.66
1:B:307:TYR:O	1:B:311:LEU:HD13	1.96	0.66
1:A:217:PHE:HA	1:A:222:THR:HG22	1.76	0.66
1:B:140:LYS:HD2	1:B:144:LYS:O	1.95	0.66
1:A:356:THR:OG1	1:A:359:GLU:HG3	1.96	0.65
1:B:451:SER:HB3	1:B:465:TYR:O	1.97	0.65
1:A:346:ALA:HB2	1:A:364:ALA:HB2	1.78	0.65
1:A:307:TYR:O	1:A:311:LEU:HD13	1.96	0.65
1:B:316:ARG:HH11	1:B:316:ARG:CB	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LEU:HD22	1:A:463:ILE:HD13	1.78	0.65
1:B:482:GLU:O	1:B:486:LYS:HE3	1.97	0.65
1:A:354:ARG:HG3	1:A:354:ARG:NH1	2.12	0.65
1:A:467:THR:HB	1:A:470:GLN:H	1.62	0.65
1:B:129:TRP:HA	1:B:132:ILE:CD1	2.27	0.65
1:B:354:ARG:HG3	1:B:354:ARG:NH1	2.12	0.65
1:A:411:ASN:ND2	1:B:380:ASN:HD22	1.95	0.65
1:B:164:ASP:O	1:B:187:GLY:HA3	1.97	0.65
1:B:172:GLU:CD	1:B:173:ASN:H	1.99	0.65
1:B:430:SER:C	1:B:432:PHE:H	2.00	0.65
1:B:466:VAL:HG12	1:B:470:GLN:HB3	1.80	0.64
1:A:159:PRO:HG3	1:A:257:PRO:HA	1.79	0.64
1:A:164:ASP:O	1:A:187:GLY:HA3	1.98	0.64
1:A:461:THR:O	1:A:461:THR:HG22	1.98	0.64
1:B:307:TYR:CE2	1:B:311:LEU:HD11	2.33	0.64
1:A:456:LEU:CD2	1:A:463:ILE:HD13	2.27	0.64
2:A:671:GLC:HO1	2:A:672:GLC:C4	2.10	0.64
1:B:467:THR:HB	1:B:470:GLN:H	1.62	0.64
1:B:467:THR:HG22	1:B:468:ASP:N	2.09	0.63
1:A:316:ARG:HG3	1:A:316:ARG:NH1	2.10	0.63
1:B:403:ASN:ND2	1:B:406:GLU:HG3	2.12	0.63
1:B:119:LYS:O	1:B:123:PRO:HG3	1.98	0.63
1:A:119:LYS:O	1:A:123:PRO:HG3	1.98	0.63
1:B:406:GLU:HB3	1:B:444:LEU:HD11	1.79	0.63
1:B:316:ARG:HG3	1:B:316:ARG:NH1	2.12	0.63
1:A:402:LEU:HD11	1:A:477:LEU:HD21	1.81	0.63
1:B:346:ALA:HB2	1:B:364:ALA:HB2	1.81	0.62
1:A:379:ILE:HG23	1:B:482:GLU:OE2	1.98	0.62
1:B:414:LEU:CD1	1:B:478:ILE:HD12	2.19	0.62
1:B:356:THR:OG1	1:B:359:GLU:HG3	1.98	0.62
1:B:453:LYS:HD2	1:B:462:VAL:HG11	1.82	0.62
1:A:430:SER:C	1:A:432:PHE:H	2.03	0.62
1:B:129:TRP:CD1	1:B:248:PRO:HB2	2.35	0.62
1:B:90:TYR:CE1	1:B:305:LYS:HG2	2.35	0.62
1:B:456:LEU:CD2	1:B:463:ILE:HD13	2.30	0.62
1:A:129:TRP:HA	1:A:132:ILE:CD1	2.29	0.62
1:A:237:THR:C	1:A:239:LYS:H	2.03	0.62
1:A:405:GLU:HA	1:A:432:PHE:HZ	1.65	0.61
1:A:375:LYS:O	1:A:376:ILE:HB	1.99	0.61
1:B:130:GLU:O	1:B:133:PRO:HD2	2.00	0.61
1:A:31:THR:HG21	1:A:33:ILE:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:TYR:CE1	1:A:305:LYS:HG2	2.36	0.61
1:A:466:VAL:CG1	1:A:470:GLN:HB3	2.31	0.61
1:B:461:THR:O	1:B:461:THR:HG22	1.99	0.61
1:A:130:GLU:O	1:A:133:PRO:HD2	2.01	0.61
1:A:450:LEU:HD22	1:A:450:LEU:O	2.01	0.60
1:A:307:TYR:CE2	1:A:311:LEU:HD11	2.35	0.60
1:A:403:ASN:ND2	1:A:406:GLU:HG3	2.16	0.60
1:B:449:LEU:HD23	1:B:474:ILE:HG12	1.81	0.60
1:B:237:THR:C	1:B:239:LYS:H	2.04	0.60
1:A:449:LEU:HD23	1:A:474:ILE:HG12	1.83	0.60
1:A:129:TRP:CD1	1:A:248:PRO:HB2	2.37	0.60
1:A:294:ASN:OD1	1:A:298:PRO:HA	2.02	0.60
1:A:64:HIS:HE1	1:A:330:MET:O	1.84	0.60
1:A:478:ILE:O	1:A:482:GLU:HB2	2.02	0.60
1:B:456:LEU:HD12	1:B:458:ASP:N	2.16	0.59
1:B:459:GLU:CD	1:B:460:ARG:H	2.03	0.59
2:A:671:GLC:O1	2:A:672:GLC:C6	2.47	0.59
1:B:80:THR:CG2	1:B:80:THR:O	2.50	0.59
1:B:171:TYR:OH	1:B:174:GLY:HA2	2.02	0.59
1:B:478:ILE:O	1:B:482:GLU:HB2	2.02	0.59
1:B:163:ALA:HB2	1:B:255:SER:HA	1.84	0.59
1:B:199:ILE:HG23	1:B:204:MET:O	2.03	0.59
1:A:163:ALA:HB2	1:A:255:SER:HA	1.85	0.59
1:B:450:LEU:O	1:B:450:LEU:HD22	2.02	0.59
1:B:430:SER:O	1:B:432:PHE:N	2.35	0.59
1:A:406:GLU:HB3	1:A:444:LEU:HD11	1.83	0.59
2:B:673:GLC:O1	2:B:674:GLC:C6	2.48	0.59
1:A:198:LEU:O	1:A:203:HIS:HB2	2.02	0.59
1:B:47:PHE:CG	1:B:60:ILE:HD12	2.38	0.58
1:B:132:ILE:H	1:B:133:PRO:CD	2.17	0.58
1:B:294:ASN:OD1	1:B:298:PRO:HA	2.04	0.58
1:B:198:LEU:O	1:B:203:HIS:HB2	2.03	0.58
1:B:31:THR:HG21	1:B:33:ILE:HG12	1.84	0.58
1:B:194:PHE:CZ	1:B:198:LEU:HD21	2.38	0.58
1:A:171:TYR:OH	1:A:174:GLY:HA2	2.04	0.58
1:A:450:LEU:HD13	1:A:451:SER:O	2.04	0.58
1:B:447:LEU:HD23	1:B:448:LYS:N	2.18	0.58
1:A:64:HIS:CE1	1:A:330:MET:O	2.56	0.58
1:A:449:LEU:O	1:A:470:GLN:HG3	2.03	0.58
1:B:466:VAL:CG1	1:B:470:GLN:HB3	2.34	0.58
1:B:15:LYS:O	1:B:17:TYR:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:HIS:HE1	1:B:330:MET:O	1.86	0.57
1:A:447:LEU:HD23	1:A:448:LYS:N	2.19	0.57
1:B:450:LEU:HD13	1:B:451:SER:O	2.04	0.57
1:A:428:LYS:HG3	1:A:429:CYS:N	2.19	0.57
1:A:217:PHE:CE1	1:A:224:MET:HA	2.39	0.57
1:B:64:HIS:CE1	1:B:330:MET:O	2.58	0.57
1:B:175:LYS:NZ	1:B:418:SER:HA	2.20	0.57
1:A:132:ILE:H	1:A:133:PRO:CD	2.17	0.57
1:A:194:PHE:CZ	1:A:198:LEU:HD21	2.39	0.57
1:B:205:ASN:H	1:B:205:ASN:ND2	2.03	0.57
1:A:47:PHE:CG	1:A:60:ILE:HD12	2.40	0.57
1:A:2:ILE:N	1:A:2:ILE:HD12	2.20	0.56
1:A:205:ASN:ND2	1:A:205:ASN:H	2.03	0.56
1:B:149:PHE:O	1:B:151:LEU:CD1	2.54	0.56
1:B:314:ASP:OD1	1:B:316:ARG:HB2	2.05	0.56
1:B:428:LYS:HG3	1:B:429:CYS:N	2.19	0.56
1:A:449:LEU:CD2	1:A:474:ILE:HG12	2.35	0.56
1:B:14:ASP:OD1	1:B:15:LYS:HG3	2.06	0.56
1:A:199:ILE:HG23	1:A:204:MET:O	2.05	0.56
1:A:117:TYR:CE2	1:A:125:PRO:HD3	2.40	0.56
1:A:452:LYS:HG2	1:A:465:TYR:HB3	1.87	0.56
1:A:14:ASP:OD1	1:A:15:LYS:HG3	2.05	0.56
1:B:217:PHE:CE1	1:B:224:MET:HA	2.40	0.56
1:B:117:TYR:CE2	1:B:125:PRO:HD3	2.41	0.56
1:A:430:SER:O	1:A:432:PHE:N	2.39	0.56
1:A:336:MET:O	1:A:339:PHE:HB3	2.05	0.56
1:B:405:GLU:HA	1:B:432:PHE:HZ	1.67	0.56
1:A:126:PRO:HD2	1:A:224:MET:HE1	1.88	0.56
1:A:149:PHE:O	1:A:151:LEU:CD1	2.53	0.56
1:B:336:MET:O	1:B:339:PHE:HB3	2.06	0.55
1:A:33:ILE:O	1:A:33:ILE:HG13	2.07	0.55
1:B:127:LYS:HB2	1:B:127:LYS:HZ3	1.71	0.55
1:A:314:ASP:OD2	1:A:316:ARG:NH1	2.39	0.55
1:B:147:LEU:O	1:B:148:MET:HG2	2.07	0.55
1:A:399:LYS:O	1:A:400:PHE:CD2	2.60	0.55
1:A:167:TYR:CE2	1:A:182:GLY:HA3	2.42	0.55
1:A:459:GLU:HG3	1:A:461:THR:OG1	2.06	0.55
1:A:31:THR:HG22	1:A:33:ILE:H	1.70	0.55
1:A:67:PHE:HB3	1:A:104:ILE:HD12	1.88	0.55
1:B:343:VAL:O	1:B:347:VAL:HG23	2.07	0.55
1:B:457:GLN:HA	1:B:457:GLN:NE2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:GLU:HA	1:B:459:GLU:OE2	2.06	0.55
1:A:80:THR:O	1:A:80:THR:CG2	2.51	0.55
1:A:64:HIS:CD2	1:A:261:VAL:H	2.24	0.55
2:A:671:GLC:O1	2:A:672:GLC:O4	2.10	0.55
1:B:31:THR:HG22	1:B:33:ILE:H	1.72	0.55
1:A:15:LYS:O	1:A:17:TYR:N	2.38	0.55
1:B:447:LEU:HB3	1:B:449:LEU:HD12	1.88	0.54
1:B:456:LEU:HD22	1:B:463:ILE:HD13	1.88	0.54
1:A:185:ASN:O	1:A:189:LYS:HG3	2.06	0.54
1:B:67:PHE:HB3	1:B:104:ILE:HD12	1.90	0.54
1:A:140:LYS:HA	1:A:144:LYS:O	2.08	0.54
1:B:126:PRO:HD2	1:B:224:MET:HE1	1.87	0.54
1:B:167:TYR:CE2	1:B:182:GLY:HA3	2.42	0.54
1:A:447:LEU:HB3	1:A:449:LEU:HD12	1.89	0.54
1:B:467:THR:CG2	1:B:468:ASP:H	2.04	0.54
1:A:127:LYS:HB2	1:A:127:LYS:HZ3	1.73	0.54
1:B:449:LEU:CD2	1:B:474:ILE:HG12	2.37	0.54
1:B:121:LEU:O	1:B:122:LEU:HB2	2.07	0.54
1:A:456:LEU:CD1	1:A:457:GLN:N	2.55	0.54
1:A:121:LEU:O	1:A:122:LEU:HB2	2.08	0.54
1:A:456:LEU:HD12	1:A:457:GLN:H	1.67	0.54
1:B:79:ILE:HG12	1:B:103:LEU:O	2.08	0.54
1:A:3:GLU:HB2	1:B:354:ARG:NE	2.23	0.53
1:B:456:LEU:CD1	1:B:457:GLN:N	2.61	0.53
1:B:64:HIS:CD2	1:B:261:VAL:H	2.25	0.53
1:A:205:ASN:N	1:A:205:ASN:HD22	2.06	0.53
2:B:673:GLC:C1	2:B:674:GLC:O4	2.51	0.53
1:B:205:ASN:HD22	1:B:205:ASN:N	2.06	0.53
1:B:33:ILE:HG13	1:B:33:ILE:O	2.09	0.53
1:B:2:ILE:N	1:B:2:ILE:HD12	2.24	0.53
1:A:405:GLU:HG3	1:A:432:PHE:CE2	2.43	0.53
1:A:79:ILE:HG12	1:A:103:LEU:O	2.08	0.53
1:B:185:ASN:O	1:B:189:LYS:HG3	2.07	0.53
1:A:467:THR:OG1	1:A:470:GLN:NE2	2.42	0.53
1:B:41:ASP:O	1:B:42:LYS:HB2	2.08	0.53
1:B:335:GLN:NE2	1:B:335:GLN:N	2.47	0.53
1:A:205:ASN:H	1:A:205:ASN:HD22	1.57	0.53
1:A:3:GLU:HB2	1:B:354:ARG:HE	1.72	0.52
1:A:314:ASP:OD1	1:A:316:ARG:HB2	2.08	0.52
1:A:41:ASP:O	1:A:42:LYS:HB2	2.09	0.52
1:A:147:LEU:O	1:A:148:MET:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ILE:HD11	1:B:54:GLY:O	2.09	0.52
1:B:212:ILE:HG22	1:B:213:ALA:N	2.24	0.52
1:B:232:TRP:HB2	1:B:298:PRO:HG2	1.90	0.52
1:B:205:ASN:HD22	1:B:205:ASN:H	1.57	0.52
1:A:396:THR:HG22	1:A:484:TYR:CD2	2.44	0.52
1:B:456:LEU:HD12	1:B:458:ASP:H	1.74	0.52
1:A:340:TRP:CD1	2:A:671:GLC:H4	2.45	0.52
1:B:379:ILE:O	1:B:383:VAL:HG23	2.10	0.52
1:B:429:CYS:O	1:B:430:SER:CB	2.57	0.52
1:B:13:GLY:O	1:B:17:TYR:HE2	1.93	0.52
1:B:445:LYS:HD2	1:B:453:LYS:HG2	1.92	0.51
1:A:232:TRP:HB2	1:A:298:PRO:HG2	1.92	0.51
1:A:311:LEU:O	1:A:317:ILE:HG13	2.10	0.51
1:B:288:GLU:O	1:B:291:GLU:HG2	2.09	0.51
1:A:385:ALA:O	1:A:389:VAL:HG23	2.10	0.51
1:B:314:ASP:OD2	1:B:316:ARG:NH1	2.39	0.51
1:A:335:GLN:NE2	1:A:335:GLN:N	2.45	0.51
1:A:15:LYS:NZ	2:A:672:GLC:O2	2.32	0.51
1:A:115:LEU:HB2	1:A:247:LEU:HD12	1.92	0.51
1:B:140:LYS:HA	1:B:144:LYS:O	2.09	0.51
1:B:467:THR:OG1	1:B:470:GLN:NE2	2.44	0.51
1:A:411:ASN:HD21	1:B:380:ASN:ND2	2.00	0.51
1:A:130:GLU:CD	1:A:130:GLU:H	2.14	0.51
1:B:64:HIS:ND1	1:B:96:ALA:HB1	2.26	0.51
1:A:451:SER:HB3	1:A:466:VAL:HA	1.93	0.51
1:A:13:GLY:O	1:A:17:TYR:HE2	1.94	0.51
1:B:14:ASP:O	1:B:230:TRP:HB2	2.11	0.51
1:A:2:ILE:HD11	1:A:54:GLY:O	2.11	0.51
1:A:451:SER:CB	1:A:466:VAL:HA	2.41	0.51
1:A:114:SER:C	1:A:247:LEU:HD11	2.31	0.51
1:B:120:ASP:C	1:B:121:LEU:HD12	2.31	0.51
1:A:3:GLU:HB3	1:B:354:ARG:HH21	1.76	0.51
1:A:86:GLN:HA	1:A:94:TRP:CZ2	2.46	0.51
1:A:172:GLU:OE1	1:A:173:ASN:N	2.44	0.50
1:B:151:LEU:HD13	1:B:208:THR:HB	1.93	0.50
1:A:343:VAL:O	1:A:347:VAL:HG23	2.10	0.50
1:B:115:LEU:HD12	1:B:116:ILE:N	2.26	0.50
1:A:14:ASP:O	1:A:230:TRP:HB2	2.12	0.50
1:A:429:CYS:O	1:A:430:SER:CB	2.59	0.50
1:B:217:PHE:CA	1:B:222:THR:HG22	2.42	0.50
1:A:217:PHE:CA	1:A:222:THR:HG22	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:GLU:HG3	1:B:432:PHE:CE2	2.47	0.50
1:A:64:HIS:HD2	1:A:261:VAL:H	1.58	0.50
1:B:175:LYS:HZ3	1:B:418:SER:HA	1.76	0.50
1:B:237:THR:C	1:B:239:LYS:N	2.65	0.50
1:B:115:LEU:HB2	1:B:247:LEU:HD12	1.94	0.50
1:A:131:GLU:O	1:A:131:GLU:HG3	2.12	0.50
1:B:255:SER:O	1:B:257:PRO:HD3	2.12	0.50
1:A:379:ILE:O	1:A:383:VAL:HG23	2.11	0.50
1:B:86:GLN:HA	1:B:94:TRP:CZ2	2.47	0.49
1:A:1:LYS:CE	1:B:354:ARG:HB3	2.18	0.49
1:A:456:LEU:CD1	1:A:458:ASP:OD1	2.60	0.49
1:B:130:GLU:H	1:B:130:GLU:CD	2.16	0.49
1:A:295:LYS:HE2	1:A:295:LYS:N	2.27	0.49
1:B:295:LYS:N	1:B:295:LYS:HE2	2.27	0.49
1:A:237:THR:C	1:A:239:LYS:N	2.65	0.49
1:A:379:ILE:HG13	1:A:380:ASN:N	2.27	0.49
1:B:47:PHE:N	1:B:48:PRO:HD2	2.27	0.49
1:A:47:PHE:N	1:A:48:PRO:HD2	2.27	0.49
1:A:288:GLU:O	1:A:291:GLU:HG2	2.13	0.49
1:A:414:LEU:HD11	1:A:475:GLN:CA	2.38	0.49
1:A:449:LEU:HD13	1:A:450:LEU:H	1.77	0.49
1:B:419:ASN:ND2	1:B:467:THR:O	2.46	0.49
1:B:460:ARG:O	1:B:461:THR:OG1	2.26	0.49
1:B:114:SER:C	1:B:247:LEU:HD11	2.33	0.49
1:A:151:LEU:HD13	1:A:208:THR:HB	1.94	0.49
1:B:118:ASN:HB3	1:B:121:LEU:HB2	1.94	0.49
1:B:385:ALA:O	1:B:389:VAL:HG23	2.11	0.49
1:A:244:VAL:HG21	1:A:316:ARG:CA	2.41	0.49
1:B:181:VAL:CG2	1:B:369:ALA:HB2	2.38	0.49
1:B:64:HIS:HD2	1:B:261:VAL:H	1.61	0.49
1:B:467:THR:CG2	1:B:468:ASP:N	2.73	0.49
1:A:192:LEU:CD2	1:A:357:VAL:HG13	2.33	0.49
1:A:445:LYS:HD2	1:A:453:LYS:HG2	1.95	0.48
1:B:172:GLU:OE1	1:B:173:ASN:N	2.46	0.48
1:A:452:LYS:CG	1:A:465:TYR:HB3	2.42	0.48
1:A:115:LEU:HD12	1:A:116:ILE:N	2.28	0.48
1:A:212:ILE:HG22	1:A:213:ALA:N	2.27	0.48
1:B:402:LEU:HD11	1:B:477:LEU:HD21	1.94	0.48
1:B:244:VAL:HG21	1:B:316:ARG:CA	2.40	0.48
1:A:147:LEU:HD12	1:A:224:MET:O	2.13	0.48
1:A:486:LYS:C	1:A:486:LYS:HD3	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:SER:O	1:A:257:PRO:HD3	2.14	0.48
1:B:361:LEU:HA	1:B:364:ALA:HB3	1.95	0.48
1:A:6:LYS:NZ	1:A:36:THR:HG21	2.28	0.48
1:B:129:TRP:HB3	1:B:194:PHE:CE2	2.49	0.48
1:B:430:SER:C	1:B:432:PHE:N	2.67	0.48
1:A:64:HIS:ND1	1:A:96:ALA:HB1	2.28	0.48
1:A:106:TYR:CE2	1:A:281:GLU:HG3	2.49	0.48
1:B:379:ILE:HG13	1:B:380:ASN:N	2.26	0.48
1:A:62:TRP:CD1	1:A:66:ARG:HG3	2.48	0.48
1:B:73:SER:HB2	1:B:75:LEU:HG	1.96	0.48
1:B:311:LEU:O	1:B:317:ILE:HG13	2.13	0.48
1:B:408:TYR:C	1:B:408:TYR:CD2	2.86	0.48
1:A:118:ASN:HB3	1:A:121:LEU:HB2	1.94	0.48
1:B:170:LYS:HB3	1:B:180:ASP:HB3	1.96	0.48
1:B:131:GLU:HG3	1:B:131:GLU:O	2.13	0.47
1:B:121:LEU:N	1:B:121:LEU:HD12	2.29	0.47
1:A:448:LYS:N	1:A:448:LYS:HD2	2.30	0.47
1:A:361:LEU:HA	1:A:364:ALA:HB3	1.95	0.47
1:A:450:LEU:HD13	1:A:450:LEU:O	2.14	0.47
1:A:453:LYS:O	1:A:453:LYS:HG3	2.14	0.47
1:B:449:LEU:HD13	1:B:450:LEU:H	1.77	0.47
1:A:130:GLU:N	1:A:130:GLU:CD	2.68	0.47
1:A:45:GLU:O	1:A:48:PRO:HG2	2.14	0.47
1:A:120:ASP:C	1:A:121:LEU:HD12	2.35	0.47
1:A:406:GLU:OE1	1:A:443:LYS:HD2	2.15	0.47
1:B:6:LYS:NZ	1:B:36:THR:HG21	2.29	0.47
1:B:453:LYS:O	1:B:453:LYS:HG3	2.15	0.47
1:B:398:LYS:HG3	1:B:399:LYS:N	2.19	0.47
1:A:408:TYR:C	1:A:408:TYR:CD2	2.87	0.47
1:A:116:ILE:HG12	1:A:244:VAL:HG12	1.97	0.47
1:B:217:PHE:HE1	1:B:224:MET:HA	1.80	0.47
1:B:149:PHE:O	1:B:151:LEU:HD12	2.15	0.47
1:A:295:LYS:NZ	1:A:295:LYS:HA	2.30	0.47
1:A:454:ARG:NH1	1:A:454:ARG:HB3	2.29	0.47
1:B:454:ARG:NH1	1:B:454:ARG:HB3	2.30	0.46
1:A:154:PRO:HG2	2:A:671:GLC:O6	2.15	0.46
1:A:129:TRP:HB3	1:A:194:PHE:CE2	2.49	0.46
1:B:116:ILE:HG12	1:B:244:VAL:HG12	1.97	0.46
1:B:340:TRP:HA	1:B:340:TRP:CE3	2.50	0.46
1:B:456:LEU:HB3	1:B:459:GLU:H	1.81	0.46
1:B:483:GLU:HA	1:B:486:LYS:CG	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:GLU:O	1:B:48:PRO:HG2	2.15	0.46
1:B:20:LEU:N	1:B:293:VAL:HG22	2.30	0.46
1:B:62:TRP:CD1	1:B:66:ARG:HG3	2.50	0.46
1:B:147:LEU:HD12	1:B:224:MET:O	2.15	0.46
1:B:398:LYS:CG	1:B:399:LYS:H	2.16	0.46
1:A:249:THR:HB	1:A:253:GLN:O	2.16	0.46
1:B:482:GLU:O	1:B:486:LYS:HG2	2.16	0.46
1:A:430:SER:C	1:A:432:PHE:N	2.69	0.46
1:A:73:SER:HB2	1:A:75:LEU:HG	1.97	0.46
1:A:2:ILE:HD12	1:A:2:ILE:H	1.81	0.46
1:B:4:GLU:HG2	1:B:5:GLY:H	1.81	0.46
1:B:205:ASN:N	1:B:205:ASN:ND2	2.62	0.46
1:A:149:PHE:O	1:A:151:LEU:HD12	2.14	0.46
1:B:396:THR:O	1:B:400:PHE:O	2.33	0.46
1:A:452:LYS:HZ3	1:A:465:TYR:HD2	1.63	0.45
1:A:217:PHE:HE1	1:A:224:MET:HA	1.79	0.45
1:B:413:ILE:O	1:B:416:SER:HB3	2.16	0.45
1:A:244:VAL:CG2	1:A:316:ARG:HG2	2.46	0.45
1:A:149:PHE:CD1	1:A:204:MET:HE1	2.52	0.45
1:A:394:ARG:NH2	1:B:431:GLU:HB2	2.30	0.45
1:B:421:ILE:HG22	1:B:422:SER:N	2.32	0.45
1:B:484:TYR:CD1	1:B:484:TYR:N	2.85	0.45
1:A:394:ARG:NH1	1:B:431:GLU:HG3	2.31	0.45
1:B:277:LYS:O	1:B:281:GLU:HB2	2.17	0.45
1:A:421:ILE:HG22	1:A:422:SER:N	2.32	0.45
1:B:244:VAL:CG2	1:B:316:ARG:HG2	2.47	0.45
1:B:255:SER:O	1:B:257:PRO:CD	2.65	0.45
1:A:255:SER:O	1:A:257:PRO:CD	2.65	0.45
1:B:106:TYR:CE2	1:B:281:GLU:HG3	2.52	0.45
1:B:472:ALA:O	1:B:476:LYS:HG3	2.17	0.45
1:A:205:ASN:N	1:A:205:ASN:ND2	2.63	0.45
1:A:157:THR:O	1:A:161:ILE:HG13	2.17	0.45
1:A:467:THR:CG2	1:A:468:ASP:H	2.05	0.45
1:B:448:LYS:HD2	1:B:448:LYS:N	2.31	0.45
1:B:467:THR:OG1	1:B:470:GLN:HB2	2.16	0.45
1:A:405:GLU:HG3	1:A:432:PHE:CZ	2.51	0.45
1:A:413:ILE:O	1:A:416:SER:HB3	2.16	0.45
1:A:121:LEU:HD12	1:A:121:LEU:N	2.32	0.45
1:B:445:LYS:C	1:B:447:LEU:N	2.70	0.45
1:B:452:LYS:HG2	1:B:465:TYR:HB3	1.98	0.45
1:A:472:ALA:O	1:A:476:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:LEU:O	1:B:450:LEU:HD13	2.17	0.44
1:A:340:TRP:CE3	1:A:340:TRP:HA	2.51	0.44
1:B:249:THR:HB	1:B:253:GLN:O	2.18	0.44
1:A:244:VAL:HG21	1:A:316:ARG:CG	2.48	0.44
1:B:314:ASP:HB3	1:B:317:ILE:HG12	1.99	0.44
1:A:484:TYR:CD1	1:A:484:TYR:N	2.85	0.44
1:B:295:LYS:HA	1:B:295:LYS:NZ	2.32	0.44
1:A:117:TYR:CD1	1:A:117:TYR:N	2.86	0.44
1:A:454:ARG:HH11	1:A:454:ARG:HB3	1.83	0.44
1:B:406:GLU:OE1	1:B:443:LYS:HD2	2.17	0.44
1:B:454:ARG:HH11	1:B:454:ARG:HB3	1.83	0.44
1:B:130:GLU:N	1:B:130:GLU:CD	2.70	0.44
1:B:4:GLU:CG	1:B:5:GLY:N	2.80	0.44
1:A:445:LYS:C	1:A:447:LEU:N	2.71	0.44
1:B:356:THR:O	1:B:357:VAL:C	2.55	0.44
1:A:287:ASP:OD1	1:A:307:TYR:HB2	2.18	0.44
1:A:380:ASN:ND2	1:B:411:ASN:HD21	2.05	0.44
1:B:428:LYS:HB3	1:B:428:LYS:NZ	2.33	0.44
1:B:18:ASN:O	1:B:21:ALA:HB3	2.17	0.44
1:A:20:LEU:N	1:A:293:VAL:HG22	2.32	0.44
1:B:478:ILE:O	1:B:481:LEU:HD12	2.18	0.44
1:B:287:ASP:OD1	1:B:307:TYR:HB2	2.18	0.44
1:A:10:TRP:CG	1:A:57:PRO:HB3	2.52	0.44
1:B:449:LEU:O	1:B:470:GLN:HG3	2.18	0.43
1:B:244:VAL:HG21	1:B:316:ARG:CG	2.48	0.43
1:B:158:TRP:HB3	1:B:159:PRO:HD3	2.00	0.43
1:B:149:PHE:CD1	1:B:204:MET:HE1	2.53	0.43
1:A:482:GLU:OE2	1:B:379:ILE:HG23	2.18	0.43
1:A:277:LYS:O	1:A:281:GLU:HB2	2.17	0.43
1:B:476:LYS:O	1:B:480:GLU:HB2	2.19	0.43
1:A:170:LYS:HB3	1:A:180:ASP:HB3	1.99	0.43
2:A:671:GLC:O1	2:A:672:GLC:C4	2.63	0.43
1:A:18:ASN:O	1:A:21:ALA:HB3	2.19	0.43
1:B:67:PHE:CD1	1:B:67:PHE:N	2.87	0.43
1:A:394:ARG:HH12	1:B:431:GLU:HG3	1.83	0.43
1:B:447:LEU:HD23	1:B:448:LYS:H	1.81	0.43
1:A:193:THR:HA	1:A:357:VAL:HG21	2.00	0.43
1:B:405:GLU:HG3	1:B:432:PHE:CZ	2.54	0.43
1:A:375:LYS:NZ	1:B:487:ASN:OD1	2.40	0.43
1:B:117:TYR:CD1	1:B:117:TYR:N	2.87	0.43
1:A:67:PHE:N	1:A:67:PHE:CD1	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:PHE:C	1:A:252:GLY:N	2.72	0.43
1:A:467:THR:OG1	1:A:470:GLN:HB2	2.17	0.43
1:A:356:THR:O	1:A:357:VAL:C	2.56	0.43
1:B:306:SER:OG	1:B:307:TYR:N	2.52	0.43
1:A:48:PRO:HA	1:A:75:LEU:CD1	2.47	0.43
1:B:484:TYR:HD1	1:B:484:TYR:N	2.17	0.43
1:A:392:PHE:HD1	1:A:485:ILE:HG23	1.83	0.43
1:A:179:LYS:HA	1:A:179:LYS:HE2	2.01	0.43
1:A:156:PHE:O	1:A:159:PRO:HD2	2.18	0.43
1:B:307:TYR:CZ	1:B:311:LEU:HD11	2.52	0.43
1:A:411:ASN:HB2	1:B:379:ILE:HD11	2.01	0.43
1:B:10:TRP:CG	1:B:57:PRO:HB3	2.53	0.43
1:A:239:LYS:HA	1:A:239:LYS:HD2	1.86	0.43
1:B:250:PHE:C	1:B:252:GLY:N	2.71	0.43
1:A:453:LYS:HA	1:A:463:ILE:O	2.19	0.42
1:B:461:THR:O	1:B:462:VAL:C	2.58	0.42
1:A:454:ARG:O	1:A:455:SER:C	2.57	0.42
1:A:88:LYS:C	1:A:89:LEU:HD12	2.39	0.42
1:B:459:GLU:CG	1:B:460:ARG:N	2.83	0.42
1:A:258:PHE:CG	1:A:330:MET:HG2	2.54	0.42
1:A:154:PRO:HB3	1:A:343:VAL:HG12	2.01	0.42
1:A:428:LYS:NZ	1:A:428:LYS:HB3	2.33	0.42
1:A:4:GLU:CG	1:A:5:GLY:N	2.79	0.42
1:B:258:PHE:CG	1:B:330:MET:HG2	2.55	0.42
1:B:451:SER:CB	1:B:466:VAL:HA	2.49	0.42
1:B:454:ARG:O	1:B:455:SER:C	2.57	0.42
1:A:307:TYR:CZ	1:A:311:LEU:HD11	2.54	0.42
1:A:314:ASP:HB3	1:A:317:ILE:HG12	2.01	0.42
1:B:296:ASP:OD1	1:B:297:LYS:HG2	2.20	0.42
1:B:172:GLU:CD	1:B:173:ASN:N	2.71	0.42
1:A:86:GLN:HA	1:A:94:TRP:HZ2	1.84	0.42
1:B:392:PHE:HD1	1:B:485:ILE:HG23	1.84	0.42
1:B:157:THR:O	1:B:161:ILE:HG13	2.19	0.42
1:A:456:LEU:HD11	1:A:458:ASP:OD1	2.19	0.42
1:A:172:GLU:CD	1:A:173:ASN:N	2.70	0.42
1:B:150:ASN:ND2	1:B:210:TYR:HB2	2.32	0.42
1:A:67:PHE:H	1:A:67:PHE:HD1	1.67	0.42
1:A:141:ALA:C	1:A:143:GLY:H	2.23	0.42
1:A:296:ASP:OD1	1:A:297:LYS:HG2	2.20	0.42
1:A:258:PHE:HB3	1:A:330:MET:CG	2.50	0.42
1:A:476:LYS:O	1:A:480:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:SER:O	1:A:341:TYR:HD2	2.02	0.42
1:A:427:ALA:HB2	1:A:437:LEU:HD11	2.02	0.42
1:A:484:TYR:HD1	1:A:484:TYR:N	2.17	0.42
1:B:2:ILE:H	1:B:2:ILE:HD12	1.84	0.42
1:A:372:PHE:O	1:A:373:MET:HB3	2.19	0.42
1:A:396:THR:O	1:A:400:PHE:O	2.38	0.42
1:B:179:LYS:HA	1:B:179:LYS:HE2	2.01	0.42
1:B:258:PHE:HB3	1:B:330:MET:CG	2.49	0.42
1:A:270:SER:O	1:A:273:LYS:NZ	2.45	0.42
1:B:402:LEU:HD12	1:B:481:LEU:HD23	2.00	0.42
1:B:19:GLY:HA3	1:B:293:VAL:HA	2.02	0.42
1:B:244:VAL:HG21	1:B:316:ARG:CB	2.50	0.41
1:B:167:TYR:O	1:B:182:GLY:O	2.38	0.41
1:B:39:HIS:O	1:B:40:PRO:C	2.58	0.41
1:B:396:THR:HG22	1:B:484:TYR:CD2	2.55	0.41
1:A:51:ALA:HA	1:A:55:ASP:O	2.20	0.41
1:B:141:ALA:C	1:B:143:GLY:H	2.24	0.41
1:A:460:ARG:HE	1:A:460:ARG:HA	1.81	0.41
1:A:4:GLU:HG2	1:A:5:GLY:H	1.83	0.41
1:A:167:TYR:O	1:A:182:GLY:O	2.38	0.41
1:A:467:THR:HB	1:A:470:GLN:N	2.32	0.41
1:B:193:THR:HA	1:B:357:VAL:HG21	2.03	0.41
1:B:132:ILE:N	1:B:133:PRO:CD	2.82	0.41
1:B:67:PHE:HD1	1:B:67:PHE:H	1.68	0.41
1:A:19:GLY:HA3	1:A:293:VAL:HA	2.02	0.41
1:B:451:SER:HB3	1:B:466:VAL:HA	2.02	0.41
1:A:414:LEU:CD1	1:A:478:ILE:HD12	2.25	0.41
1:A:478:ILE:O	1:A:481:LEU:HD12	2.20	0.41
1:A:244:VAL:HG21	1:A:316:ARG:CB	2.51	0.41
1:A:232:TRP:CH2	1:A:316:ARG:HB3	2.54	0.41
1:A:48:PRO:HA	1:A:75:LEU:HD13	2.02	0.41
1:B:94:TRP:CZ3	1:B:107:PRO:HD3	2.55	0.41
1:A:201:ASN:HB2	1:A:203:HIS:CD2	2.56	0.41
1:B:172:GLU:N	1:B:172:GLU:OE1	2.53	0.41
1:A:158:TRP:N	1:A:159:PRO:CD	2.84	0.41
1:B:38:GLU:C	1:B:40:PRO:HD3	2.41	0.41
1:B:192:LEU:CD2	1:B:357:VAL:HG13	2.34	0.41
1:A:172:GLU:OE1	1:A:172:GLU:N	2.53	0.41
1:B:487:ASN:HD22	1:B:487:ASN:N	2.19	0.41
1:A:246:VAL:HA	1:A:323:ASN:HD21	1.86	0.41
1:B:155:TYR:CD2	2:B:674:GLC:H61	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:TRP:CZ3	1:A:107:PRO:HD3	2.56	0.41
1:B:51:ALA:HA	1:B:55:ASP:O	2.20	0.41
1:A:39:HIS:O	1:A:40:PRO:C	2.58	0.41
1:B:270:SER:O	1:B:273:LYS:NZ	2.46	0.41
1:B:380:ASN:O	1:B:384:ASN:HB2	2.21	0.41
1:B:164:ASP:O	1:B:187:GLY:CA	2.68	0.41
1:B:86:GLN:HA	1:B:94:TRP:HZ2	1.86	0.41
1:A:1:LYS:HZ3	1:A:1:LYS:HB3	1.86	0.41
1:B:344:ARG:HB2	1:B:344:ARG:HE	1.77	0.41
1:A:3:GLU:CB	1:B:354:ARG:HH21	2.34	0.40
1:B:447:LEU:HB3	1:B:449:LEU:CD1	2.51	0.40
1:B:457:GLN:C	1:B:459:GLU:N	2.75	0.40
1:B:6:LYS:HZ1	1:B:36:THR:HG21	1.86	0.40
1:A:461:THR:O	1:A:462:VAL:C	2.59	0.40
1:B:455:SER:C	1:B:456:LEU:O	2.59	0.40
1:B:429:CYS:O	1:B:430:SER:HB3	2.20	0.40
1:A:429:CYS:O	1:A:430:SER:HB3	2.21	0.40
1:A:132:ILE:O	1:A:133:PRO:C	2.59	0.40
1:B:246:VAL:HA	1:B:323:ASN:HD21	1.86	0.40
1:B:397:LYS:O	1:B:398:LYS:O	2.40	0.40
1:A:148:MET:HB2	1:A:222:THR:HG21	2.03	0.40
1:B:487:ASN:N	1:B:487:ASN:ND2	2.70	0.40
1:A:79:ILE:HD13	1:A:105:ALA:C	2.42	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	485/487 (100%)	403 (83%)	57 (12%)	25 (5%)	2 1
1	B	485/487 (100%)	409 (84%)	53 (11%)	23 (5%)	3 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	970/974 (100%)	812 (84%)	110 (11%)	48 (5%)	3 1

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	ALA
1	A	398	LYS
1	A	400	PHE
1	A	462	VAL
1	A	467	THR
1	B	168	ALA
1	B	398	LYS
1	B	399	LYS
1	B	462	VAL
1	B	467	THR
1	A	16	GLY
1	A	122	LEU
1	A	373	MET
1	A	430	SER
1	A	431	GLU
1	A	432	PHE
1	A	455	SER
1	A	456	LEU
1	B	16	GLY
1	B	122	LEU
1	B	430	SER
1	B	431	GLU
1	B	432	PHE
1	B	455	SER
1	B	456	LEU
1	A	357	VAL
1	A	3	GLU
1	A	132	ILE
1	A	163	ALA
1	A	239	LYS
1	A	374	SER
1	A	376	ILE
1	B	3	GLU
1	B	132	ILE
1	B	163	ALA
1	B	239	LYS
1	B	357	VAL

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Mol	Chain	Res	Type
1	A	172	GLU
1	A	458	ASP
1	B	172	GLU
1	B	461	THR
1	A	449	LEU
1	B	449	LEU
1	B	270	SER
1	B	40	PRO
1	A	40	PRO
1	A	270	SER
1	B	91	PRO

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	405/405 (100%)	374 (92%)	31 (8%)	16 20
1	B	405/405 (100%)	376 (93%)	29 (7%)	18 22
All	All	810/810 (100%)	750 (93%)	60 (7%)	17 21

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LYS
1	A	30	ASP
1	A	33	ILE
1	A	36	THR
1	A	72	GLN
1	A	91	PRO
1	A	127	LYS
1	A	142	LYS
1	A	172	GLU
1	A	205	ASN
1	A	229	PRO
1	A	236	ASP

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Mol	Chain	Res	Type
1	A	241	ASN
1	A	258	PHE
1	A	271	PRO
1	A	295	LYS
1	A	316	ARG
1	A	325	GLN
1	A	335	GLN
1	A	394	ARG
1	A	399	LYS
1	A	420	GLU
1	A	425	GLU
1	A	428	LYS
1	A	443	LYS
1	A	449	LEU
1	A	450	LEU
1	A	453	LYS
1	A	458	ASP
1	A	470	GLN
1	A	481	LEU
1	B	1	LYS
1	B	30	ASP
1	B	33	ILE
1	B	36	THR
1	B	72	GLN
1	B	91	PRO
1	B	127	LYS
1	B	142	LYS
1	B	172	GLU
1	B	205	ASN
1	B	229	PRO
1	B	236	ASP
1	B	241	ASN
1	B	258	PHE
1	B	295	LYS
1	B	316	ARG
1	B	325	GLN
1	B	335	GLN
1	B	375	LYS
1	B	394	ARG
1	B	420	GLU
1	B	425	GLU
1	B	428	LYS

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Mol	Chain	Res	Type
1	B	443	LYS
1	B	449	LEU
1	B	450	LEU
1	B	453	LYS
1	B	470	GLN
1	B	481	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	64	HIS
1	A	72	GLN
1	A	205	ASN
1	A	218	ASN
1	A	323	ASN
1	A	325	GLN
1	A	335	GLN
1	A	380	ASN
1	A	411	ASN
1	A	419	ASN
1	A	457	GLN
1	A	470	GLN
1	B	39	HIS
1	B	64	HIS
1	B	72	GLN
1	B	205	ASN
1	B	218	ASN
1	B	323	ASN
1	B	325	GLN
1	B	335	GLN
1	B	349	ASN
1	B	384	ASN
1	B	388	GLN
1	B	419	ASN
1	B	457	GLN
1	B	470	GLN

5.3.3 RNA

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 carbohydrates 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	GLC	A	671	-	12,12,12	0.39	0	17,17,17	0.64	0
2	GLC	A	672	-	12,12,12	0.37	0	17,17,17	0.60	0
2	GLC	B	673	2	12,12,12	0.38	0	17,17,17	0.61	0
2	GLC	B	674	2	12,12,12	0.63	0	17,17,17	0.82	1 (5%)

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	GLC	A	671	-	-	0/2/22/22	0/1/1/1
2	GLC	A	672	-	-	0/2/22/22	0/1/1/1
2	GLC	B	673	2	-	0/2/22/22	0/1/1/1
2	GLC	B	674	2	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	674	GLC	O4-C4-C3	-2.37	105.00	110.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	671	GLC	7	0
2	A	672	GLC	6	0
2	B	673	GLC	5	0
2	B	674	GLC	6	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

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	487/487 (100%)	0.94	78 (16%)	3 4	21, 72, 109, 127	0
1	B	487/487 (100%)	0.81	69 (14%)	4 6	27, 69, 108, 127	0
All	All	974/974 (100%)	0.87	147 (15%)	3 5	21, 71, 109, 127	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	LEU	9.3
1	A	143	GLY	8.8
1	A	429	CYS	8.3
1	A	435	TYR	6.1
1	B	224	MET	5.9
1	A	239	LYS	5.8
1	A	139	LEU	5.8
1	B	225	THR	5.4
1	B	223	ALA	5.4
1	B	217	PHE	5.2
1	A	147	LEU	4.9
1	B	241	ASN	4.8
1	B	398	LYS	4.7
1	A	372	PHE	4.7
1	B	116	ILE	4.7
1	A	428	LYS	4.5
1	B	222	THR	4.5
1	B	183	VAL	4.5
1	B	435	TYR	4.2
1	A	161	ILE	4.1
1	B	141	ALA	4.1
1	A	450	LEU	4.0
1	A	424	LYS	4.0
1	A	436	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	237	THR	3.9
1	B	161	ILE	3.9
1	B	448	LYS	3.9
1	B	137	LYS	3.9
1	B	140	LYS	3.7
1	B	148	MET	3.7
1	A	124	ASN	3.6
1	A	202	LYS	3.6
1	B	160	LEU	3.6
1	A	452	LYS	3.6
1	A	200	LYS	3.5
1	B	146	ALA	3.5
1	A	123	PRO	3.5
1	A	207	ASP	3.4
1	A	465	TYR	3.4
1	A	354	ARG	3.4
1	B	436	TYR	3.4
1	B	400	PHE	3.3
1	A	399	LYS	3.3
1	B	145	SER	3.2
1	A	351	ALA	3.2
1	A	341	TYR	3.2
1	A	224	MET	3.2
1	B	123	PRO	3.1
1	A	449	LEU	3.1
1	A	116	ILE	3.1
1	A	448	LYS	3.1
1	A	356	THR	3.1
1	B	204	MET	3.1
1	A	136	ASP	3.1
1	B	129	TRP	3.1
1	A	134	ALA	3.0
1	B	433	LYS	3.0
1	A	241	ASN	3.0
1	A	144	LYS	3.0
1	A	225	THR	3.0
1	A	237	THR	3.0
1	B	452	LYS	2.9
1	A	137	LYS	2.9
1	B	262	LEU	2.9
1	A	141	ALA	2.9
1	B	460	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	146	ALA	2.9
1	B	465	TYR	2.9
1	A	443	LYS	2.8
1	A	487	ASN	2.8
1	A	203	HIS	2.8
1	A	217	PHE	2.8
1	A	17	TYR	2.8
1	A	456	LEU	2.8
1	B	409	ILE	2.8
1	B	171	TYR	2.8
1	A	363	ALA	2.8
1	A	223	ALA	2.7
1	B	424	LYS	2.7
1	B	53	THR	2.7
1	A	211	SER	2.7
1	A	204	MET	2.7
1	B	149	PHE	2.7
1	B	480	GLU	2.7
1	B	115	LEU	2.7
1	A	444	LEU	2.6
1	A	280	LEU	2.6
1	B	135	LEU	2.6
1	A	172	GLU	2.6
1	A	192	LEU	2.6
1	A	410	LEU	2.6
1	A	129	TRP	2.6
1	A	117	TYR	2.6
1	B	124	ASN	2.6
1	B	192	LEU	2.6
1	B	343	VAL	2.6
1	A	145	SER	2.5
1	A	373	MET	2.5
1	A	358	ASP	2.5
1	B	200	LYS	2.5
1	B	239	LYS	2.5
1	B	485	ILE	2.5
1	A	120	ASP	2.5
1	B	119	LYS	2.5
1	B	121	LEU	2.5
1	B	157	THR	2.5
1	A	175	LYS	2.5
1	A	205	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	394	ARG	2.5
1	A	236	ASP	2.4
1	B	172	GLU	2.4
1	B	59	ILE	2.4
1	A	220	GLY	2.4
1	A	374	SER	2.4
1	A	427	ALA	2.4
1	A	486	LYS	2.4
1	A	485	ILE	2.4
1	A	13	GLY	2.4
1	A	67	PHE	2.4
1	A	242	TYR	2.4
1	B	264	ALA	2.4
1	A	32	GLY	2.3
1	B	449	LEU	2.3
1	B	410	LEU	2.3
1	B	451	SER	2.3
1	A	148	MET	2.2
1	A	142	LYS	2.2
1	A	458	ASP	2.2
1	B	458	ASP	2.2
1	B	138	GLU	2.2
1	A	222	THR	2.2
1	B	450	LEU	2.1
1	B	487	ASN	2.1
1	A	423	SER	2.1
1	B	226	ILE	2.1
1	A	229	PRO	2.1
1	B	219	LYS	2.1
1	B	236	ASP	2.1
1	B	464	VAL	2.1
1	B	202	LYS	2.1
1	B	347	VAL	2.1
1	A	118	ASN	2.0
1	A	105	ALA	2.0
1	B	220	GLY	2.0
1	B	354	ARG	2.0
1	B	188	ALA	2.0
1	B	118	ASN	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	GLC	A	672	12/12	0.89	0.19	1.31	71,77,84,84	0
2	GLC	A	671	12/12	0.89	0.16	0.19	53,64,76,78	0
2	GLC	B	674	12/12	0.92	0.13	-1.35	31,50,58,64	0
2	GLC	B	673	12/12	0.94	0.12	-1.38	30,35,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.