Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2024 – 12:21 PM EDT

PDB ID	:	6CKB
Title	:	Crystal structure of an extended beta3 integrin P33
Authors	:	Zhou, D.; Zhu, J.
Deposited on	:	2018-02-27
Resolution	:	2.80 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 (1)) were used in the production of this report:

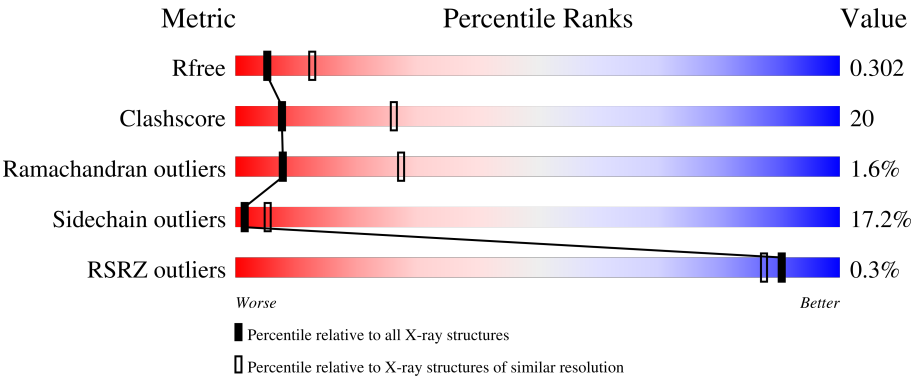
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.80 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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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 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	466	56% 37% 6%
1	B	466	50% 39% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7299 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 Chimera protein of Integrin beta-3 and Integrin alpha-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3606	2247	613	714	32			
1	B	465	Total	C	N	O	S	0	0	0
			3617	2256	614	715	32			

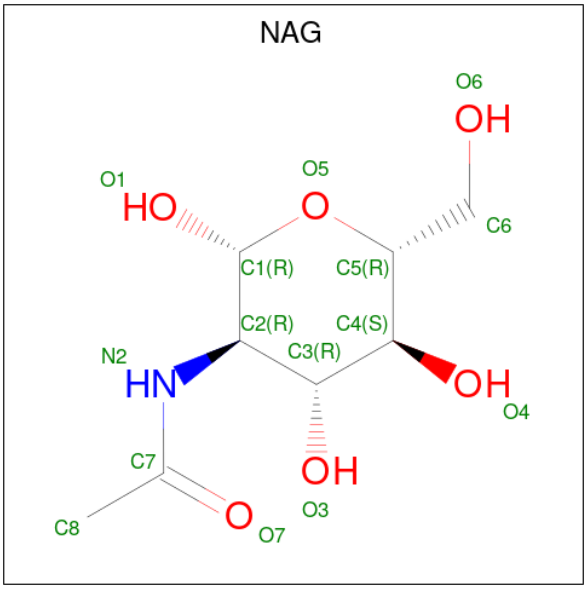
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	PRO	LEU	conflict	UNP P05106
A	171	TRP	ARG	conflict	UNP P20701
A	460	THR	-	expression tag	UNP P05106
A	461	ARG	-	expression tag	UNP P05106
A	462	GLU	-	expression tag	UNP P05106
A	463	LEU	-	expression tag	UNP P05106
A	464	TYR	-	expression tag	UNP P05106
A	465	PHE	-	expression tag	UNP P05106
A	466	GLN	-	expression tag	UNP P05106
B	33	PRO	LEU	conflict	UNP P05106
B	171	TRP	ARG	conflict	UNP P20701
B	460	THR	-	expression tag	UNP P05106
B	461	ARG	-	expression tag	UNP P05106
B	462	GLU	-	expression tag	UNP P05106
B	463	LEU	-	expression tag	UNP P05106
B	464	TYR	-	expression tag	UNP P05106
B	465	PHE	-	expression tag	UNP P05106
B	466	GLN	-	expression tag	UNP P05106

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0

- Molecule 5 is water.

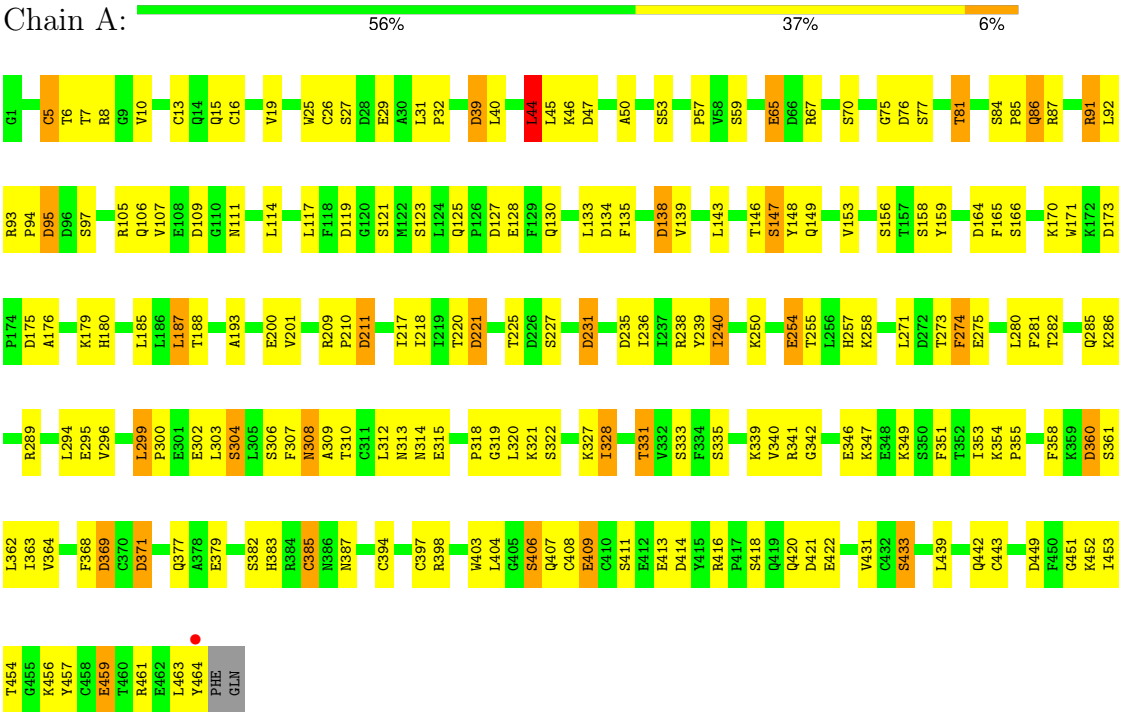
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0

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.

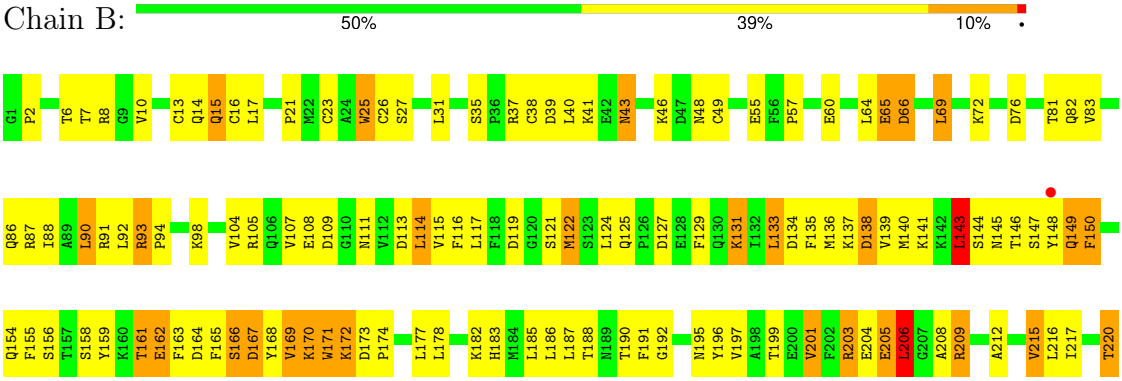
• Molecule 1: Chimera protein of Integrin beta-3 and Integrin alpha-L

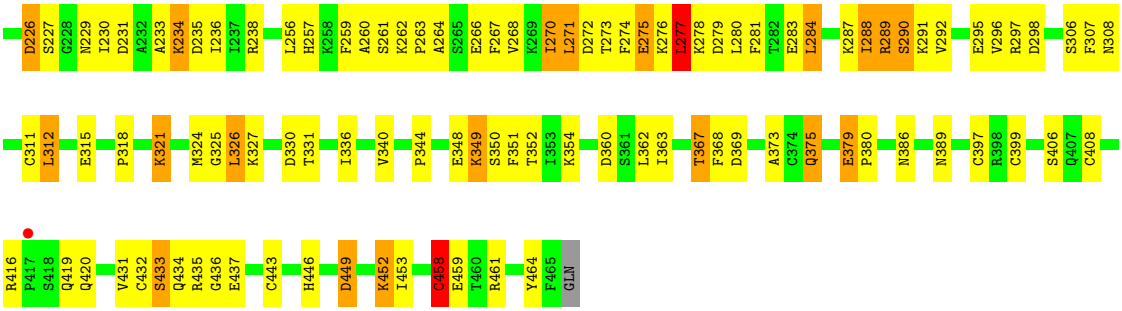
Chain A:



• Molecule 1: Chimera protein of Integrin beta-3 and Integrin alpha-L

Chain B:




D226 S227 G228 N229 I230 D231 A232 A233 K234 D235 I236 I237 R238 L256 H257 K258 F259 A260 S261 K262 P263 A264 S265 E266 F267 V268 K269 I270 L271 D272 T273 F274 E275 K276 L277 K278 D279 L280 F281 T282 E283 L284 K287 I288 R289 S290 K291 V292 E295 V296 R297 D298 S306 F307 N308
C311 L312 E315 P318 K321 M324 G325 L326 K327 D330 T331 I336 V340 P344 E348 K349 S350 F351 T352 I353 K354 D360 S361 L362 I363 T367 F368 D369 A373 C374 Q375 E379 P380 N386 N389 C397 R398 C399 S406 Q407 C408
R416 P417 S418 Q419 Q420 V431 C432 S433 Q434 R435 G436 E437 C443 H446 D449 K452 I453 C458 E459 T460 R461 Y464 F465 GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.08Å 80.91Å 126.72Å 90.00° 96.36° 90.00°	Depositor
Resolution (Å)	58.70 – 2.80 58.70 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.70-2.80) 99.8 (58.70-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.239 , 0.296 0.242 , 0.302	Depositor DCC
R_{free} test set	1484 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	96.1	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 111.1	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	7299	wwPDB-VP
Average B, all atoms (Å^2)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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: MG, CA, NAG

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	0.34	0/3672	0.54	1/4955 (0.0%)
1	B	0.36	1/3684 (0.0%)	0.59	5/4971 (0.1%)
All	All	0.35	1/7356 (0.0%)	0.57	6/9926 (0.1%)

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	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	38	CYS	CB-SG	-5.23	1.73	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	44	LEU	CA-CB-CG	6.02	129.15	115.30
1	B	170	LYS	CA-C-N	-5.83	104.37	117.20
1	B	206	LEU	CA-CB-CG	5.49	127.92	115.30
1	B	143	LEU	CA-CB-CG	5.48	127.91	115.30
1	B	277	LEU	CA-CB-CG	5.36	127.62	115.30
1	B	443	CYS	CA-CB-SG	5.21	123.39	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	206	LEU	Peptide
1	B	279	ASP	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	3606	0	3504	118	1
1	B	3617	0	3511	165	1
2	A	1	0	0	0	0
3	A	28	0	26	1	0
3	B	42	0	39	0	0
4	B	1	0	0	0	0
5	A	4	0	0	1	0
All	All	7299	0	7080	283	1

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 20.

All (283) 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:119:ASP:HB2	1:B:220:THR:HA	1.57	0.86
1:A:67:ARG:HD3	1:A:86:GLN:HE22	1.42	0.84
1:A:306:SER:HB2	3:A:503:NAG:H81	1.64	0.80
1:B:449:ASP:OD1	1:B:449:ASP:N	2.13	0.79
1:A:121:SER:OG	1:A:123:SER:OG	2.03	0.76
1:A:65:GLU:HG3	1:A:87:ARG:HB3	1.68	0.75
1:A:170:LYS:HG3	1:A:171:TRP:CD1	2.23	0.74
1:B:143:LEU:HD11	1:B:150:PHE:HZ	1.52	0.74
1:B:437:GLU:OE2	1:B:446:HIS:NE2	2.20	0.74
1:B:133:LEU:HA	1:B:136:MET:HG2	1.69	0.73
1:B:169:VAL:C	1:B:171:TRP:H	1.91	0.73
1:B:66:ASP:N	1:B:66:ASP:OD1	2.21	0.73
1:B:105:ARG:HB2	1:B:331:THR:HG23	1.72	0.71
1:B:168:TYR:N	1:B:171:TRP:CD1	2.59	0.71
1:A:296:VAL:HG22	1:A:299:LEU:HD22	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ARG:NH1	1:A:369:ASP:OD2	2.25	0.69
1:A:121:SER:CB	1:A:221:ASP:OD2	2.40	0.69
1:A:294:LEU:HB2	1:A:321:LYS:HG2	1.73	0.69
1:A:360:ASP:OD1	1:A:360:ASP:N	2.24	0.69
1:B:65:GLU:OE2	1:B:86:GLN:N	2.26	0.69
1:B:168:TYR:N	1:B:171:TRP:HD1	1.92	0.68
1:A:121:SER:HB3	1:A:221:ASP:OD2	1.94	0.67
1:A:5:CYS:O	1:A:7:THR:N	2.26	0.67
1:B:135:PHE:HB2	1:B:277:LEU:HD13	1.75	0.67
1:A:65:GLU:OE2	1:A:87:ARG:NE	2.20	0.66
1:A:211:ASP:N	1:A:211:ASP:OD1	2.23	0.66
1:A:121:SER:OG	5:A:601:HOH:O	2.12	0.66
1:B:146:THR:OG1	1:B:147:SER:N	2.27	0.66
1:B:10:VAL:HG13	1:B:15:GLN:HB3	1.77	0.66
1:A:231:ASP:OD1	1:A:231:ASP:N	2.26	0.65
1:B:164:ASP:OD1	1:B:166:SER:OG	2.16	0.64
1:A:125:GLN:HB2	1:A:128:GLU:HG3	1.79	0.64
1:B:65:GLU:N	1:B:65:GLU:OE1	2.30	0.64
1:A:403:TRP:HA	1:A:411:SER:HA	1.79	0.64
1:A:57:PRO:O	1:A:93:ARG:NH1	2.26	0.64
1:A:119:ASP:HB2	1:A:220:THR:HA	1.80	0.63
1:A:50:ALA:O	1:A:53:SER:OG	2.16	0.62
1:A:106:GLN:HG3	1:A:328:ILE:HA	1.80	0.62
1:A:327:LYS:HD2	1:A:328:ILE:H	1.63	0.62
1:A:383:HIS:HA	1:A:387:ASN:HA	1.82	0.62
1:B:17:LEU:HA	1:B:93:ARG:NH2	2.15	0.62
1:B:233:ALA:O	1:B:238:ARG:NH1	2.33	0.62
1:B:161:THR:O	1:B:163:PHE:N	2.32	0.62
1:A:75:GLY:O	1:A:77:SER:N	2.33	0.61
1:A:457:TYR:HB2	1:A:459:GLU:HG2	1.82	0.61
1:B:226:ASP:OD1	1:B:226:ASP:N	2.31	0.61
1:B:191:PHE:N	1:B:226:ASP:OD2	2.32	0.61
1:B:204:GLU:OE1	1:B:204:GLU:N	2.31	0.61
1:A:31:LEU:HD12	1:A:32:PRO:HD2	1.81	0.61
1:B:125:GLN:O	1:B:129:PHE:N	2.24	0.60
1:B:281:PHE:HA	1:B:284:LEU:HD11	1.83	0.60
1:A:403:TRP:HB3	1:A:408:CYS:HB3	1.84	0.60
1:B:65:GLU:H	1:B:65:GLU:CD	2.05	0.60
1:B:453:ILE:HG22	1:B:458:CYS:HB2	1.83	0.60
1:A:111:ASN:OD1	1:A:209:ARG:NH1	2.35	0.59
1:B:143:LEU:HD22	1:B:146:THR:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:SER:OG	1:A:385:CYS:HB2	2.03	0.59
1:B:65:GLU:OE2	1:B:87:ARG:N	2.36	0.58
1:A:439:LEU:N	1:A:442:GLN:O	2.27	0.58
1:B:91:ARG:HH11	1:B:369:ASP:HB2	1.69	0.58
1:B:435:ARG:NH1	1:B:461:ARG:HB2	2.19	0.58
1:A:148:TYR:HE1	1:A:289:ARG:HH11	1.52	0.58
1:A:307:PHE:HB2	1:A:319:GLY:HA2	1.85	0.58
1:B:72:LYS:HD3	1:B:107:VAL:HG13	1.86	0.58
1:B:169:VAL:HG13	1:B:170:LYS:H	1.67	0.58
1:A:117:LEU:HD11	1:A:193:ALA:HB1	1.86	0.57
1:A:70:SER:HB2	1:A:107:VAL:HG11	1.85	0.57
1:B:87:ARG:HA	1:B:363:ILE:O	2.04	0.57
1:A:170:LYS:HG3	1:A:171:TRP:HD1	1.68	0.57
1:B:114:LEU:HD11	1:B:217:ILE:HG13	1.87	0.57
1:A:95:ASP:OD1	1:A:342:GLY:N	2.38	0.56
1:B:119:ASP:HB3	1:B:124:LEU:HD11	1.87	0.56
1:A:86:GLN:HA	1:A:362:LEU:HA	1.88	0.56
1:A:217:ILE:HD13	1:A:239:TYR:HB2	1.86	0.56
1:B:291:LYS:HA	1:B:324:MET:HA	1.86	0.56
1:A:27:SER:OG	1:A:394:CYS:SG	2.56	0.56
1:B:46:LYS:O	1:B:48:ASN:ND2	2.39	0.56
1:B:166:SER:N	1:B:206:LEU:O	2.39	0.56
1:A:93:ARG:HB3	1:A:94:PRO:HD2	1.88	0.56
1:B:146:THR:HG21	1:B:148:TYR:HB2	1.89	0.55
1:A:121:SER:OG	1:A:221:ASP:OD2	2.24	0.55
1:B:348:GLU:HG2	1:B:367:THR:HG23	1.89	0.55
1:B:31:LEU:HB3	1:B:35:SER:HB3	1.89	0.55
1:B:170:LYS:HE3	1:B:171:TRP:CZ3	2.42	0.55
1:B:154:GLN:H	1:B:162:GLU:HG2	1.71	0.55
1:B:155:PHE:HZ	1:B:190:THR:HG22	1.72	0.55
1:B:192:GLY:HA2	1:B:195:ASN:ND2	2.22	0.55
1:B:308:ASN:OD1	1:B:318:PRO:HA	2.06	0.54
1:B:205:GLU:OE1	1:B:206:LEU:N	2.40	0.54
1:B:291:LYS:HE2	1:B:324:MET:HE2	1.88	0.54
1:B:14:GLN:OE1	1:B:375:GLN:NE2	2.39	0.54
1:B:238:ARG:HB2	1:B:260:ALA:HA	1.89	0.54
1:B:349:LYS:HD3	1:B:350:SER:H	1.73	0.54
1:B:43:ASN:N	1:B:43:ASN:OD1	2.40	0.54
1:A:187:LEU:HB2	1:A:225:THR:HG21	1.90	0.53
1:B:209:ARG:N	1:B:209:ARG:HD3	2.23	0.53
1:A:59:SER:HB2	1:A:93:ARG:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ARG:HH21	1:A:418:SER:HA	1.73	0.53
1:B:65:GLU:OE1	1:B:87:ARG:HB3	2.08	0.53
1:B:271:LEU:HD22	1:B:280:LEU:HD22	1.89	0.53
1:B:459:GLU:CD	1:B:459:GLU:H	2.12	0.53
1:B:435:ARG:HH12	1:B:461:ARG:HB2	1.73	0.53
1:B:69:LEU:HD12	1:B:81:THR:HG22	1.90	0.52
1:B:149:GLN:HG2	1:B:209:ARG:NH2	2.24	0.52
1:A:67:ARG:HD3	1:A:86:GLN:NE2	2.20	0.52
1:A:304:SER:N	1:A:339:LYS:O	2.40	0.52
1:A:8:ARG:HB2	1:A:10:VAL:HG13	1.90	0.52
1:B:297:ARG:HH22	1:B:354:LYS:HE2	1.73	0.52
1:A:105:ARG:HE	1:A:331:THR:HG23	1.74	0.52
1:B:119:ASP:OD1	1:B:121:SER:OG	2.27	0.52
1:B:307:PHE:HD1	1:B:336:ILE:HG12	1.75	0.52
1:A:93:ARG:HE	1:A:94:PRO:HD2	1.74	0.52
1:A:353:ILE:O	1:A:362:LEU:N	2.41	0.52
1:B:163:PHE:CG	1:B:177:LEU:HD21	2.44	0.52
1:B:165:PHE:HD1	1:B:206:LEU:HD12	1.75	0.52
1:B:60:GLU:HA	1:B:98:LYS:HE3	1.92	0.52
1:B:144:SER:OG	1:B:145:ASN:N	2.43	0.52
1:B:432:CYS:O	1:B:434:GLN:N	2.42	0.52
1:A:304:SER:HB2	1:A:339:LYS:HB3	1.92	0.52
1:A:254:GLU:HA	1:A:257:HIS:CE1	2.45	0.51
1:B:297:ARG:O	1:B:351:PHE:HB2	2.11	0.51
1:A:87:ARG:HA	1:A:363:ILE:O	2.10	0.51
1:B:168:TYR:O	1:B:172:LYS:HA	2.11	0.51
1:B:295:GLU:N	1:B:354:LYS:O	2.32	0.51
1:B:170:LYS:HB3	1:B:171:TRP:CE3	2.46	0.51
1:A:130:GLN:HA	1:A:133:LEU:HD12	1.93	0.51
1:A:451:GLY:HA2	1:A:463:LEU:HA	1.93	0.50
1:B:203:ARG:O	1:B:206:LEU:HB2	2.12	0.50
1:A:16:CYS:O	1:A:19:VAL:HG22	2.11	0.50
1:A:295:GLU:N	1:A:354:LYS:O	2.24	0.50
1:B:325:GLY:O	1:B:326:LEU:HD12	2.12	0.50
1:A:320:LEU:HG	1:A:322:SER:H	1.75	0.50
1:B:92:LEU:HD13	1:B:340:VAL:HB	1.94	0.50
1:B:139:VAL:O	1:B:143:LEU:HB3	2.12	0.49
1:A:250:LYS:O	1:A:254:GLU:HG2	2.13	0.49
1:B:55:GLU:CD	1:B:373:ALA:H	2.15	0.49
1:A:354:LYS:HG3	1:A:361:SER:HB3	1.93	0.49
1:A:416:ARG:NH2	1:A:418:SER:HA	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ASN:OD1	1:B:196:TYR:N	2.45	0.49
1:B:229:ASN:OD1	1:B:231:ASP:N	2.42	0.49
1:B:270:ILE:O	1:B:270:ILE:HG13	2.12	0.49
1:A:109:ASP:OD2	1:A:147:SER:N	2.44	0.49
1:B:14:GLN:HB2	1:B:375:GLN:HE22	1.77	0.49
1:A:281:PHE:HE2	1:A:285:GLN:HE21	1.60	0.49
1:B:65:GLU:HG2	1:B:86:GLN:OE1	2.12	0.49
1:B:326:LEU:HB2	1:B:330:ASP:OD2	2.12	0.49
1:B:287:LYS:HA	1:B:290:SER:HB2	1.94	0.49
1:B:82:GLN:HG3	1:B:360:ASP:HB2	1.94	0.49
1:A:135:PHE:CE1	1:A:281:PHE:HB2	2.48	0.48
1:A:299:LEU:H	1:A:299:LEU:HD23	1.78	0.48
1:A:347:LYS:HA	1:A:368:PHE:HD1	1.78	0.48
1:B:109:ASP:OD1	1:B:289:ARG:NH2	2.46	0.48
1:B:197:VAL:O	1:B:201:VAL:HG12	2.13	0.48
1:A:70:SER:OG	1:A:81:THR:N	2.46	0.48
1:A:92:LEU:HD13	1:A:340:VAL:HG21	1.96	0.48
1:B:116:PHE:CE2	1:B:136:MET:HB2	2.49	0.48
1:A:67:ARG:O	1:A:84:SER:OG	2.19	0.48
1:B:191:PHE:HE2	1:B:227:SER:HA	1.79	0.48
1:A:236:ILE:O	1:A:238:ARG:HG3	2.14	0.47
1:B:264:ALA:O	1:B:268:VAL:HB	2.14	0.47
1:A:166:SER:O	1:A:170:LYS:HG2	2.14	0.47
1:B:433:SER:O	1:B:435:ARG:HG3	2.14	0.47
1:B:284:LEU:H	1:B:284:LEU:HD13	1.77	0.47
1:B:260:ALA:HB1	1:B:267:PHE:HB3	1.96	0.47
1:B:154:GLN:NE2	1:B:182:LYS:O	2.47	0.47
1:B:169:VAL:N	1:B:171:TRP:CD1	2.83	0.47
1:B:90:LEU:O	1:B:367:THR:N	2.46	0.47
1:B:115:VAL:HG23	1:B:216:LEU:HB2	1.95	0.47
1:A:308:ASN:HB3	1:A:335:SER:HB3	1.95	0.47
1:B:161:THR:HG23	1:B:196:TYR:OH	2.14	0.47
1:B:167:ASP:O	1:B:177:LEU:HD11	2.14	0.47
1:A:114:LEU:HD11	1:A:217:ILE:HG12	1.97	0.46
1:A:134:ASP:O	1:A:138:ASP:HB2	2.16	0.46
1:B:397:CYS:HB2	1:B:406:SER:O	2.14	0.46
1:A:383:HIS:C	1:A:385:CYS:H	2.19	0.46
1:B:290:SER:C	1:B:325:GLY:H	2.19	0.46
1:A:15:GLN:O	1:A:19:VAL:HG13	2.15	0.46
1:A:26:CYS:SG	1:A:27:SER:N	2.89	0.46
1:B:93:ARG:HG2	1:B:94:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:SER:HA	1:B:325:GLY:O	2.16	0.46
1:A:309:ALA:HB3	1:A:320:LEU:HB3	1.97	0.46
1:B:57:PRO:HB2	1:B:93:ARG:HG3	1.98	0.46
1:B:183:HIS:CG	1:B:185:LEU:HD12	2.51	0.46
1:B:137:LYS:HA	1:B:140:MET:HG3	1.98	0.45
1:B:275:GLU:OE1	1:B:275:GLU:N	2.28	0.45
1:A:397:CYS:HB2	1:A:406:SER:O	2.15	0.45
1:A:308:ASN:HA	1:A:318:PRO:HA	1.99	0.45
1:B:174:PRO:HA	1:B:177:LEU:HB2	1.99	0.45
1:A:188:THR:O	1:A:225:THR:HG22	2.16	0.45
1:A:282:THR:O	1:A:286:LYS:HE2	2.16	0.45
1:A:109:ASP:HB3	1:A:147:SER:HB2	1.99	0.45
1:A:139:VAL:HG13	1:A:281:PHE:CE2	2.52	0.45
1:A:452:LYS:HD2	1:A:452:LYS:N	2.32	0.45
1:B:236:ILE:HD12	1:B:236:ILE:H	1.82	0.45
1:B:284:LEU:O	1:B:288:ILE:HG12	2.17	0.45
1:A:143:LEU:O	1:A:146:THR:OG1	2.30	0.45
1:B:196:TYR:HA	1:B:199:THR:HG22	1.99	0.45
1:A:86:GLN:HB2	1:A:361:SER:O	2.18	0.44
1:A:218:ILE:HB	1:A:240:ILE:HG12	1.99	0.44
1:A:271:LEU:HD21	1:A:280:LEU:HD22	1.98	0.44
1:B:26:CYS:SG	1:B:27:SER:N	2.90	0.44
1:B:91:ARG:HA	1:B:367:THR:O	2.17	0.44
1:B:143:LEU:HD13	1:B:144:SER:N	2.32	0.44
1:A:39:ASP:H	1:A:44:LEU:HD23	1.82	0.44
1:B:420:GLN:N	1:B:420:GLN:OE1	2.51	0.44
1:A:433:SER:OG	1:A:457:TYR:O	2.35	0.44
1:B:2:PRO:HB3	1:B:6:THR:HG21	1.99	0.44
1:B:113:ASP:OD1	1:B:149:GLN:NE2	2.51	0.44
1:A:371:ASP:OD1	1:A:371:ASP:N	2.49	0.43
1:B:154:GLN:HE22	1:B:183:HIS:HA	1.83	0.43
1:A:40:LEU:HD12	1:A:40:LEU:HA	1.76	0.43
1:A:273:THR:O	1:A:274:PHE:HB2	2.18	0.43
1:B:115:VAL:HG11	1:B:201:VAL:HG11	1.99	0.43
1:B:7:THR:HG22	1:B:452:LYS:HD2	2.00	0.43
1:B:167:ASP:HA	1:B:171:TRP:CD1	2.54	0.43
1:A:300:PRO:HB3	1:A:349:LYS:HD3	2.00	0.43
1:B:41:LYS:HE2	1:B:41:LYS:HB3	1.80	0.43
1:B:65:GLU:CD	1:B:87:ARG:HB3	2.39	0.43
1:B:206:LEU:HB2	1:B:208:ALA:HB2	2.01	0.43
1:B:321:LYS:H	1:B:321:LYS:HG3	1.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:PHE:HE2	1:A:353:ILE:HD11	1.83	0.43
1:B:135:PHE:O	1:B:139:VAL:HG22	2.19	0.43
1:B:169:VAL:C	1:B:171:TRP:N	2.66	0.43
1:B:352:THR:HA	1:B:363:ILE:HA	2.01	0.43
1:B:436:GLY:HA2	1:B:446:HIS:CD2	2.54	0.43
1:A:173:ASP:OD1	1:A:176:ALA:N	2.52	0.42
1:B:13:CYS:SG	1:B:25:TRP:CD1	3.12	0.42
1:B:137:LYS:HZ3	1:B:174:PRO:HB2	1.84	0.42
1:A:105:ARG:HB2	1:A:331:THR:HG23	2.01	0.42
1:A:407:GLN:O	1:A:409:GLU:N	2.51	0.42
1:B:273:THR:O	1:B:276:LYS:HB2	2.19	0.42
1:A:84:SER:HA	1:A:85:PRO:HA	1.89	0.42
1:B:263:PRO:HD2	1:B:266:GLU:HB2	2.01	0.42
1:A:271:LEU:HD11	1:A:280:LEU:HD22	2.00	0.42
1:B:172:LYS:HG3	1:B:173:ASP:N	2.31	0.42
1:B:288:ILE:HG12	1:B:288:ILE:H	1.42	0.42
1:B:122:MET:H	1:B:122:MET:HG3	1.60	0.42
1:B:256:LEU:HA	1:B:259:PHE:HD2	1.84	0.42
1:B:164:ASP:CG	1:B:206:LEU:HD13	2.40	0.42
1:B:195:ASN:O	1:B:199:THR:N	2.53	0.42
1:A:175:ASP:O	1:A:179:LYS:HB3	2.19	0.42
1:A:275:GLU:N	1:A:275:GLU:OE1	2.53	0.42
1:A:313:ASN:O	1:A:315:GLU:N	2.52	0.42
1:B:164:ASP:O	1:B:167:ASP:N	2.46	0.42
1:B:344:PRO:HG2	1:B:368:PHE:CZ	2.54	0.42
1:B:17:LEU:HA	1:B:93:ARG:HH22	1.83	0.42
1:B:65:GLU:N	1:B:65:GLU:CD	2.71	0.42
1:A:47:ASP:OD1	1:A:47:ASP:N	2.53	0.41
1:A:456:LYS:NZ	1:A:457:TYR:CZ	2.87	0.41
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.85	0.41
1:B:326:LEU:HB2	1:B:327:LYS:H	1.75	0.41
1:A:148:TYR:HE1	1:A:289:ARG:HD3	1.85	0.41
1:B:140:MET:O	1:B:143:LEU:HD12	2.20	0.41
1:B:23:CYS:O	1:B:93:ARG:NH2	2.48	0.41
1:B:379:GLU:N	1:B:380:PRO:HD3	2.35	0.41
1:A:453:ILE:HG12	1:A:461:ARG:HG3	2.01	0.41
1:B:21:PRO:HA	1:B:93:ARG:NH1	2.35	0.41
1:A:302:GLU:OE2	1:A:302:GLU:N	2.53	0.41
1:A:355:PRO:HG2	1:A:358:PHE:CG	2.55	0.41
1:B:131:LYS:HA	1:B:134:ASP:HB2	2.03	0.41
1:A:13:CYS:HB2	1:A:25:TRP:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:PRO:HG2	1:A:303:LEU:HG	2.02	0.41
1:A:153:VAL:HG21	1:A:201:VAL:HG21	2.02	0.41
1:B:114:LEU:HD22	1:B:215:VAL:HG13	2.02	0.41
1:B:7:THR:HG21	1:B:464:TYR:CE2	2.56	0.41
1:B:8:ARG:CZ	1:B:449:ASP:HB3	2.51	0.41
1:B:83:VAL:HG22	1:B:104:VAL:HG22	2.02	0.41
1:B:274:PHE:O	1:B:276:LYS:N	2.54	0.41
1:B:280:LEU:HB3	1:B:281:PHE:HD1	1.85	0.41
1:B:297:ARG:HB2	1:B:352:THR:OG1	2.21	0.41
1:B:134:ASP:O	1:B:138:ASP:HB2	2.21	0.41
1:B:298:ASP:HB2	1:B:351:PHE:HA	2.02	0.41
1:A:149:GLN:NE2	1:A:165:PHE:HB3	2.36	0.40
1:B:64:LEU:HB2	1:B:65:GLU:OE1	2.21	0.40
1:B:143:LEU:CD1	1:B:150:PHE:HZ	2.28	0.40
1:A:25:TRP:NE1	1:A:26:CYS:O	2.54	0.40
1:A:185:LEU:HD23	1:A:185:LEU:HA	1.87	0.40
1:B:139:VAL:HG23	1:B:140:MET:CE	2.51	0.40
1:A:420:GLN:O	1:A:422:GLU:N	2.54	0.40
1:B:116:PHE:CD2	1:B:136:MET:HB2	2.56	0.40
1:B:234:LYS:HD3	1:B:235:ASP:H	1.87	0.40
1:B:312:LEU:HG	1:B:326:LEU:HD23	2.03	0.40
1:B:386:ASN:HB2	1:B:408:CYS:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LYS:NZ	1:B:386:ASN:OD1[2_458]	2.19	0.01

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	462/466 (99%)	407 (88%)	47 (10%)	8 (2%)	7 26
1	B	463/466 (99%)	403 (87%)	53 (11%)	7 (2%)	8 29
All	All	925/932 (99%)	810 (88%)	100 (11%)	15 (2%)	8 27

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	314	ASN
1	A	406	SER
1	B	433	SER
1	B	458	CYS
1	A	76	ASP
1	A	274	PHE
1	B	156	SER
1	B	162	GLU
1	A	308	ASN
1	B	212	ALA
1	B	275	GLU
1	A	5	CYS
1	A	6	THR
1	A	210	PRO
1	B	169	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	412/414 (100%)	353 (86%)	59 (14%)	2 9
1	B	413/414 (100%)	330 (80%)	83 (20%)	1 3
All	All	825/828 (100%)	683 (83%)	142 (17%)	1 5

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU

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Mol	Chain	Res	Type
1	A	39	ASP
1	A	44	LEU
1	A	45	LEU
1	A	46	LYS
1	A	65	GLU
1	A	81	THR
1	A	86	GLN
1	A	91	ARG
1	A	95	ASP
1	A	97	SER
1	A	127	ASP
1	A	138	ASP
1	A	147	SER
1	A	156	SER
1	A	158	SER
1	A	159	TYR
1	A	164	ASP
1	A	180	HIS
1	A	187	LEU
1	A	200	GLU
1	A	211	ASP
1	A	221	ASP
1	A	227	SER
1	A	231	ASP
1	A	235	ASP
1	A	240	ILE
1	A	254	GLU
1	A	255	THR
1	A	258	LYS
1	A	299	LEU
1	A	304	SER
1	A	310	THR
1	A	312	LEU
1	A	328	ILE
1	A	331	THR
1	A	333	SER
1	A	341	ARG
1	A	346	GLU
1	A	360	ASP
1	A	364	VAL
1	A	369	ASP
1	A	371	ASP

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Mol	Chain	Res	Type
1	A	377	GLN
1	A	379	GLU
1	A	385	CYS
1	A	398	ARG
1	A	404	LEU
1	A	409	GLU
1	A	413	GLU
1	A	414	ASP
1	A	421	ASP
1	A	431	VAL
1	A	433	SER
1	A	443	CYS
1	A	449	ASP
1	A	454	THR
1	A	459	GLU
1	A	464	TYR
1	B	15	GLN
1	B	16	CYS
1	B	25	TRP
1	B	37	ARG
1	B	39	ASP
1	B	40	LEU
1	B	43	ASN
1	B	49	CYS
1	B	65	GLU
1	B	66	ASP
1	B	69	LEU
1	B	76	ASP
1	B	88	ILE
1	B	90	LEU
1	B	93	ARG
1	B	108	GLU
1	B	111	ASN
1	B	114	LEU
1	B	117	LEU
1	B	122	MET
1	B	127	ASP
1	B	131	LYS
1	B	133	LEU
1	B	138	ASP
1	B	141	LYS
1	B	143	LEU

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Mol	Chain	Res	Type
1	B	149	GLN
1	B	150	PHE
1	B	158	SER
1	B	159	TYR
1	B	161	THR
1	B	166	SER
1	B	167	ASP
1	B	171	TRP
1	B	172	LYS
1	B	178	LEU
1	B	186	LEU
1	B	187	LEU
1	B	188	THR
1	B	201	VAL
1	B	203	ARG
1	B	205	GLU
1	B	206	LEU
1	B	209	ARG
1	B	215	VAL
1	B	220	THR
1	B	226	ASP
1	B	230	ILE
1	B	234	LYS
1	B	257	HIS
1	B	261	SER
1	B	262	LYS
1	B	270	ILE
1	B	271	LEU
1	B	272	ASP
1	B	277	LEU
1	B	278	LYS
1	B	283	GLU
1	B	284	LEU
1	B	288	ILE
1	B	289	ARG
1	B	290	SER
1	B	292	VAL
1	B	296	VAL
1	B	306	SER
1	B	311	CYS
1	B	312	LEU
1	B	315	GLU

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Mol	Chain	Res	Type
1	B	321	LYS
1	B	326	LEU
1	B	349	LYS
1	B	362	LEU
1	B	367	THR
1	B	375	GLN
1	B	379	GLU
1	B	389	ASN
1	B	399	CYS
1	B	416	ARG
1	B	419	GLN
1	B	431	VAL
1	B	449	ASP
1	B	452	LYS
1	B	458	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	B	501	1	14,14,15	1.10	2 (14%)	17,19,21	0.84	1 (5%)
3	NAG	B	502	1	14,14,15	0.30	0	17,19,21	0.57	0
3	NAG	B	503	1	14,14,15	0.42	0	17,19,21	0.42	0
3	NAG	A	502	1	14,14,15	0.48	0	17,19,21	0.52	0
3	NAG	A	503	1	14,14,15	0.72	0	17,19,21	0.79	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
3	NAG	B	501	1	-	2/6/23/26	0/1/1/1
3	NAG	B	502	1	-	0/6/23/26	0/1/1/1
3	NAG	B	503	1	-	1/6/23/26	0/1/1/1
3	NAG	A	502	1	-	2/6/23/26	0/1/1/1
3	NAG	A	503	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	NAG	O5-C1	-3.35	1.38	1.43
3	B	501	NAG	C1-C2	-2.04	1.49	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	503	NAG	C1-O5-C5	2.54	115.59	112.19
3	B	501	NAG	C1-O5-C5	-2.30	109.11	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	NAG	C4-C5-C6-O6
3	B	501	NAG	O5-C5-C6-O6
3	A	502	NAG	O5-C5-C6-O6
3	A	502	NAG	C4-C5-C6-O6
3	A	503	NAG	O5-C5-C6-O6
3	B	503	NAG	O5-C5-C6-O6
3	A	503	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	NAG	1	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	464/466 (99%)	-0.38	1 (0%)	92	89	63, 137, 212, 290	0
1	B	465/466 (99%)	-0.30	2 (0%)	89	85	87, 144, 224, 301	0
All	All	929/932 (99%)	-0.34	3 (0%)	90	87	63, 142, 220, 301	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	417	PRO	2.8
1	A	464	TYR	2.5
1	B	148	TYR	2.2

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	NAG	A	502	14/15	0.71	0.13	142,193,258,263	0
3	NAG	A	503	14/15	0.72	0.14	164,244,289,303	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	B	503	14/15	0.80	0.15	122,143,175,179	0
3	NAG	B	502	14/15	0.81	0.16	180,212,238,256	0
3	NAG	B	501	14/15	0.92	0.09	62,90,112,126	0
2	MG	A	501	1/1	0.96	0.06	130,130,130,130	0
4	CA	B	504	1/1	0.96	0.08	191,191,191,191	0

6.5 Other polymers (i)

There are no such residues in this entry.