Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:16 AM GMT

PDB ID	:	3LII
Title	:	Recombinant human acetylcholinesterase
Authors	:	Dvir, H.; Rosenberry, T.; Harel, M.; Silman, I.; Sussman, J.
Deposited on	:	2010-01-25
Resolution	:	3.20 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:

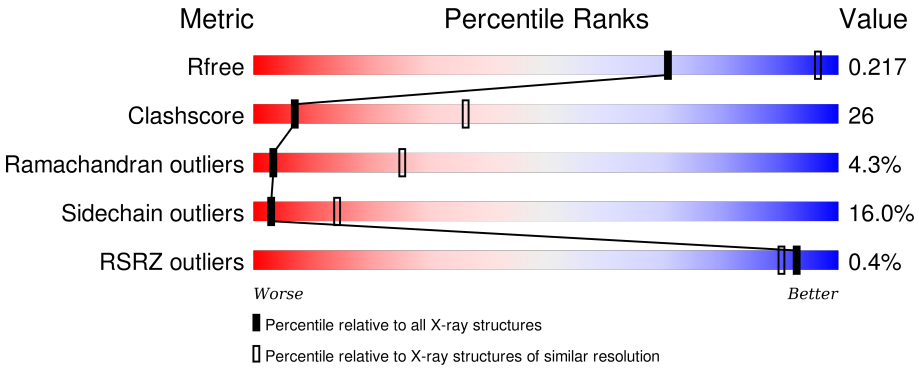
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	540	54% 37% 8%
1	B	540	% 43% 43% 11%

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	NAG	A	1001	X	-	-	-
2	NAG	B	1003	X	-	-	-
3	SO4	B	1014	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8448 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.

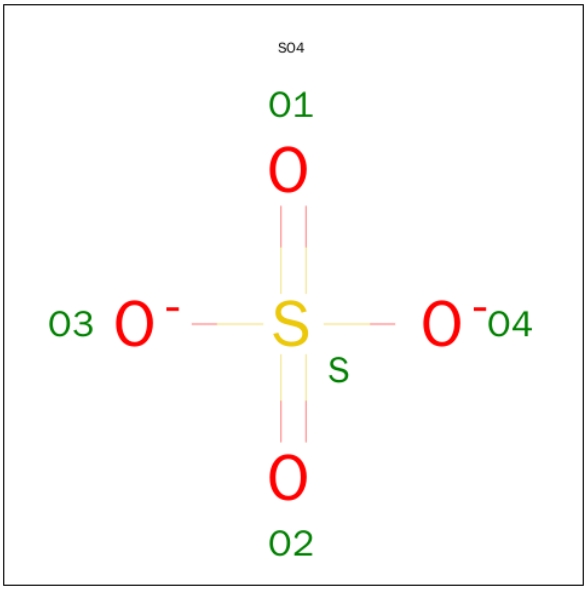
- Molecule 1 is a protein called Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4154	2666	726	749	13			
1	B	532	Total	C	N	O	S	0	0	0
			4139	2658	721	747	13			

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

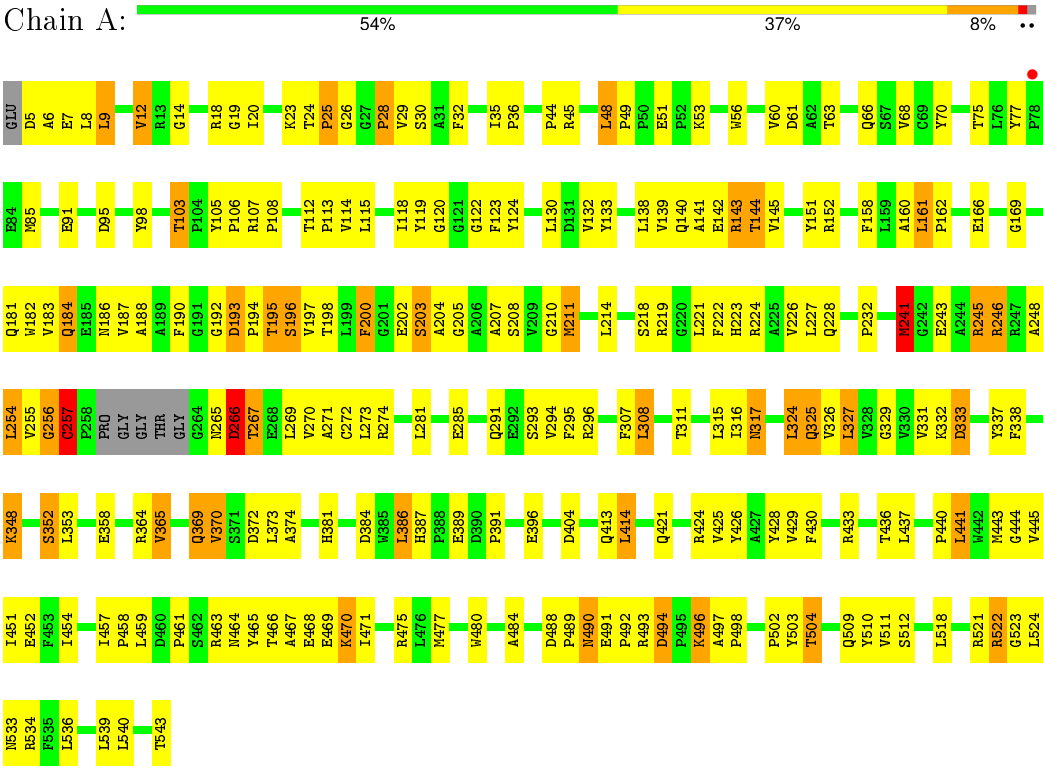
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	34	Total O 34 34	0	0
4	B	20	Total O 20 20	0	0

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.

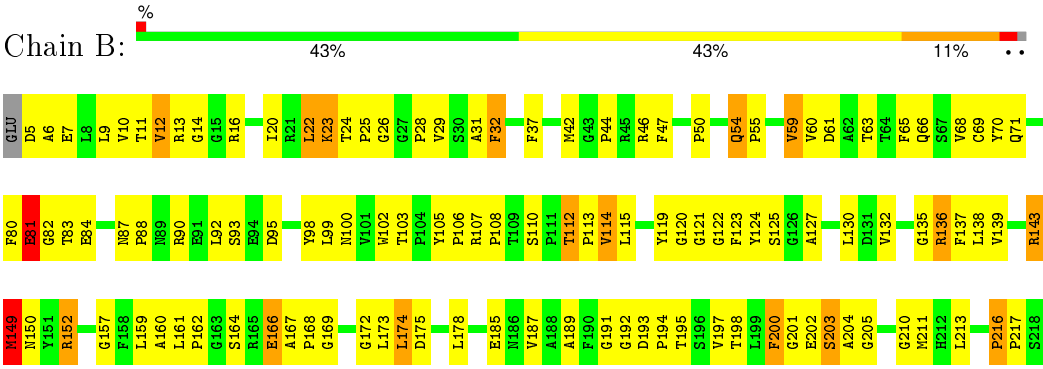
- Molecule 1: Acetylcholinesterase

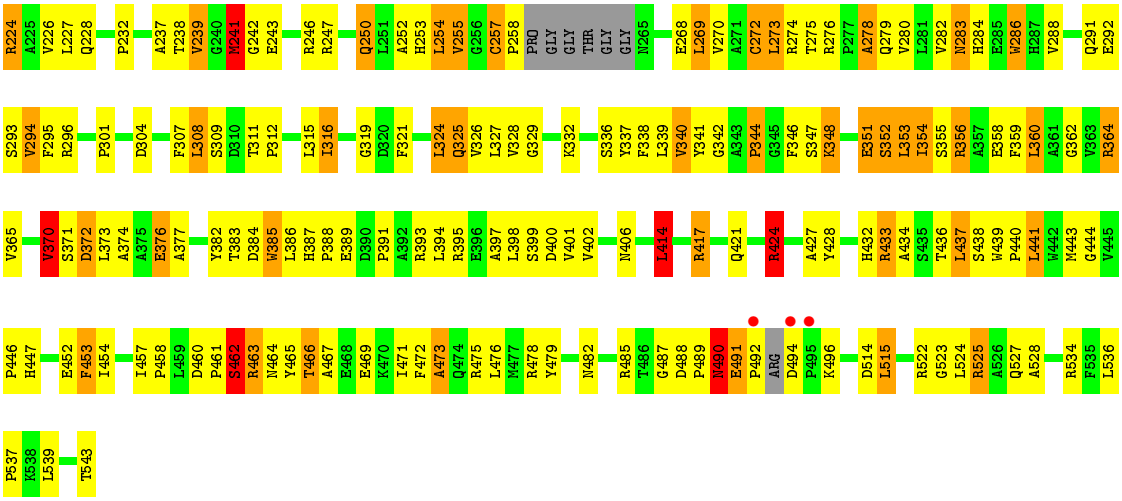
Chain A:



- Molecule 1: Acetylcholinesterase

Chain B:




R224 A225 V226 L227 Q228 P232 A237 T238 V239 G240 M241 G242 E243 R246 R247 Q250 L251 A252 H253 L254 V255 G256 C257 P258 PRO GLY GLY THR GLY GLY N265 E268 L269 V270 A271 C272 L273 R274 T275 R276 P277 A278 Q279 V280 L281 V282 N283 H284 E285 W286 H287 Y288 Q291 E292
S293 V294 F295 R296 P301 D304 F307 L308 S309 D310 T311 P312 L315 I316 G319 D320 F321 L324 Q325 V326 L327 V328 G329 K332 S336 Y337 F338 L339 V340 Y341 G342 A343 P344 G345 F346 S347 K348 E351 S352 L353 I354 S355 R356 A357 E358 F359 L360 A361 G362 V363 R364
V365 V370 S371 D372 L373 A374 A375 E376 A377 Y382 T383 D384 W385 L386 H387 P388 E389 D390 P391 A392 R393 L394 R395 E396 A397 L398 S399 D400 V401 V402 N406 L414 R417 Q421 R424 A427 Y428 H432 R433 A434 S435 T436 L437 S438 W439 P440 L441 W442 M443 G444 V445
P446 H447 E452 F453 I454 I457 P458 L459 D460 P461 S462 R463 N464 Y465 T466 A467 E468 E469 K470 I471 F472 A473 Q474 R475 L476 N477 R478 Y479 N482 R485 T486 G487 D488 P489 N490 E491 P492 ARG D494 P495 K496 D514 L515 R522 G523 L524 R525 A526 Q527 A528 R534 F535 L536
P537 K538 L539 T543

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	210.90Å 210.90Å 115.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.05 – 3.20 31.05 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (31.05-3.20) 99.7 (31.05-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.176 , 0.220 0.176 , 0.217	Depositor DCC
R_{free} test set	2470 reflections (5.43%)	DCC
Wilson B-factor (Å^2)	78.7	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.6	EDS
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 47977 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8448	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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: NAG, SO4

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	1.17	4/4281 (0.1%)	1.12	11/5851 (0.2%)
1	B	1.15	8/4265 (0.2%)	1.16	19/5829 (0.3%)
All	All	1.16	12/8546 (0.1%)	1.14	30/11680 (0.3%)

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
1	B	0	3
2	A	1	0
2	B	1	0
All	All	2	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	376	GLU	CG-CD	11.26	1.68	1.51
1	A	529	CYS	CB-SG	10.33	1.99	1.82
1	B	376	GLU	CB-CG	10.09	1.71	1.52
1	A	51	GLU	CG-CD	6.38	1.61	1.51
1	B	81	GLU	CG-CD	6.16	1.61	1.51
1	B	286	TRP	CB-CG	-6.04	1.39	1.50
1	B	385	TRP	CB-CG	-5.80	1.39	1.50
1	B	166	GLU	CG-CD	5.59	1.60	1.51
1	B	364	ARG	CB-CG	5.42	1.67	1.52
1	B	424	ARG	CB-CG	5.25	1.66	1.52
1	A	68	VAL	CB-CG2	-5.12	1.42	1.52
1	A	331	VAL	CB-CG2	-5.00	1.42	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	475	ARG	NE-CZ-NH1	-8.34	116.13	120.30
1	A	152	ARG	NE-CZ-NH1	-8.25	116.17	120.30
1	B	417	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	B	152	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	B	130	LEU	CB-CG-CD1	-6.95	99.19	111.00
1	A	386	LEU	CA-CB-CG	-6.78	99.71	115.30
1	A	193	ASP	CB-CG-OD1	6.70	124.33	118.30
1	B	92	LEU	CB-CG-CD1	-6.54	99.88	111.00
1	B	149	MET	CG-SD-CE	6.36	110.37	100.20
1	B	370	VAL	N-CA-C	-6.36	93.83	111.00
1	A	470	LYS	CD-CE-NZ	-6.09	97.69	111.70
1	A	95	ASP	CB-CG-OD1	5.88	123.59	118.30
1	B	360	LEU	CA-CB-CG	5.88	128.83	115.30
1	B	376	GLU	OE1-CD-OE2	-5.87	116.26	123.30
1	B	174	LEU	CA-CB-CG	-5.73	102.11	115.30
1	A	327	LEU	CB-CG-CD1	-5.72	101.28	111.00
1	B	224	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	273	LEU	CA-CB-CG	5.52	128.00	115.30
1	B	376	GLU	CB-CA-C	5.46	121.32	110.40
1	B	304	ASP	CB-CG-OD2	5.32	123.08	118.30
1	B	360	LEU	CB-CG-CD1	-5.29	102.00	111.00
1	B	417	ARG	CG-CD-NE	5.18	122.67	111.80
1	B	120	GLY	N-CA-C	5.13	125.92	113.10
1	A	257	CYS	CA-CB-SG	5.10	123.19	114.00
1	B	273	LEU	CA-CB-CG	5.10	127.02	115.30
1	B	146	LEU	CA-CB-CG	5.06	126.94	115.30
1	A	296	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	9	LEU	CB-CG-CD2	5.03	119.55	111.00
1	B	414	LEU	CB-CG-CD2	-5.02	102.47	111.00
1	B	174	LEU	CB-CG-CD1	5.02	119.53	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1001	NAG	C1
2	B	1003	NAG	C1

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	503	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	B	22	LEU	Peptide
1	B	490	ASN	Peptide
1	B	491	GLU	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	4154	0	4039	183	0
1	B	4139	0	4022	257	0
2	A	28	0	25	0	0
2	B	28	0	25	1	0
3	A	30	0	0	1	0
3	B	15	0	0	1	0
4	A	34	0	0	1	0
4	B	20	0	0	4	0
All	All	8448	0	8111	435	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 26.

All (435) 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:351:GLU:HA	1:B:351:GLU:OE1	1.43	1.17
1:B:50:PRO:HG3	1:B:175:ASP:OD1	1.53	1.09
1:B:54:GLN:HA	1:B:54:GLN:HE21	1.08	1.08
1:A:426:TYR:CE1	1:A:489:PRO:HD2	1.95	1.00
1:B:417:ARG:NH2	4:B:649:HOH:O	1.91	0.96
1:B:354:ILE:O	1:B:391:PRO:HB3	1.66	0.96
1:B:54:GLN:HA	1:B:54:GLN:NE2	1.80	0.95
1:B:54:GLN:CA	1:B:54:GLN:HE21	1.82	0.93
1:A:24:THR:HG22	1:A:26:GLY:H	1.33	0.92
1:B:54:GLN:NE2	1:B:55:PRO:HD3	1.83	0.92
1:B:69:CYS:O	1:B:71:GLN:HG2	1.68	0.92
1:B:417:ARG:NH1	4:B:649:HOH:O	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LEU:HD23	1:B:77:TYR:CE2	2.08	0.89
1:B:458:PRO:HA	1:B:465:TYR:CD1	2.09	0.87
1:A:184:GLN:HA	1:A:184:GLN:HE21	1.40	0.86
1:B:463:ARG:HH11	1:B:463:ARG:HG3	1.40	0.86
1:A:224:ARG:NH1	1:A:484:ALA:O	2.09	0.86
1:B:433:ARG:CG	1:B:433:ARG:HH11	1.90	0.85
1:A:5:ASP:OD1	1:A:7:GLU:HB2	1.77	0.84
1:A:386:LEU:HD11	1:B:523:GLY:HA3	1.59	0.84
1:A:373:LEU:HD23	1:A:539:LEU:HD21	1.61	0.82
1:B:54:GLN:HE21	1:B:55:PRO:HD3	1.43	0.82
1:A:426:TYR:CD1	1:A:489:PRO:HD2	2.18	0.79
1:A:490:ASN:H	1:A:490:ASN:HD22	1.28	0.79
1:A:114:VAL:HG12	1:A:197:VAL:HG22	1.62	0.79
1:B:46:ARG:O	1:B:274:ARG:NH1	2.17	0.78
1:B:203:SER:HB2	1:B:447:HIS:NE2	2.00	0.77
1:B:433:ARG:HH21	1:B:441:LEU:HA	1.48	0.77
1:B:362:GLY:O	1:B:365:VAL:HG12	1.84	0.77
1:A:19:GLY:HA3	1:A:32:PHE:CE1	2.21	0.75
1:B:76:LEU:HD23	1:B:77:TYR:HE2	1.49	0.75
1:A:7:GLU:O	1:A:107:ARG:NH2	2.20	0.74
1:B:114:VAL:HG13	1:B:145:VAL:HB	1.69	0.74
1:A:324:LEU:HD22	1:A:326:VAL:HG12	1.70	0.74
1:A:195:THR:HA	1:A:223:HIS:NE2	2.02	0.73
1:B:108:PRO:HG2	1:B:112:THR:HG21	1.71	0.73
1:B:463:ARG:HG3	1:B:463:ARG:NH1	2.03	0.72
1:A:426:TYR:CD1	1:A:489:PRO:CD	2.73	0.72
1:B:293:SER:HA	1:B:365:VAL:HG22	1.73	0.71
1:A:108:PRO:HG3	1:A:112:THR:HG21	1.72	0.71
1:A:214:LEU:HB3	1:A:315:LEU:HD23	1.70	0.71
1:A:257:CYS:HB2	1:A:272:CYS:SG	2.29	0.71
1:B:348:LYS:O	1:B:440:PRO:HG3	1.91	0.70
1:B:340:VAL:O	1:B:340:VAL:HG23	1.91	0.70
1:A:490:ASN:H	1:A:490:ASN:ND2	1.88	0.70
1:A:270:VAL:HG12	1:A:274:ARG:HE	1.56	0.70
1:A:26:GLY:O	1:A:140:GLN:NE2	2.25	0.70
1:B:458:PRO:HG2	1:B:473:ALA:HB2	1.74	0.70
1:A:218:SER:HA	1:A:221:LEU:HD12	1.75	0.69
1:B:346:PHE:HA	1:B:352:SER:OG	1.92	0.69
1:B:433:ARG:HH11	1:B:433:ARG:HG2	1.56	0.69
1:A:494:ASP:OD2	1:A:496:LYS:HB3	1.92	0.69
1:A:265:ASN:CG	1:A:266:ASP:H	1.96	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ALA:HB2	1:A:169:GLY:CA	2.22	0.69
1:B:77:TYR:CE1	1:B:348:LYS:HG3	2.28	0.69
1:B:316:ILE:HD11	1:B:414:LEU:HD12	1.73	0.69
1:B:444:GLY:O	1:B:446:PRO:HD3	1.93	0.68
1:A:327:LEU:HD12	1:A:426:TYR:O	1.92	0.68
1:B:42:MET:O	1:B:44:PRO:HD2	1.93	0.68
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.75	0.68
1:A:504:THR:HB	3:A:1011:SO4:O4	1.94	0.68
1:B:115:LEU:HD23	1:B:198:THR:HB	1.75	0.68
1:B:77:TYR:CE1	1:B:348:LYS:CD	2.77	0.68
1:A:224:ARG:HD3	1:A:325:GLN:HE21	1.59	0.68
1:B:370:VAL:HG13	1:B:374:ALA:HB3	1.76	0.67
1:A:160:ALA:HB2	1:A:169:GLY:HA2	1.75	0.67
1:B:351:GLU:CA	1:B:351:GLU:OE1	2.31	0.67
1:B:50:PRO:CG	1:B:175:ASP:OD1	2.36	0.67
1:B:77:TYR:CE1	1:B:348:LYS:CG	2.77	0.67
1:B:434:ALA:O	1:B:437:LEU:HB2	1.95	0.66
1:B:433:ARG:NH2	1:B:439:TRP:O	2.27	0.66
1:A:457:ILE:N	1:A:458:PRO:CD	2.59	0.66
1:A:224:ARG:HD3	1:A:325:GLN:NE2	2.11	0.66
1:A:183:VAL:O	1:A:187:VAL:HG12	1.96	0.66
1:A:329:GLY:HA3	1:A:428:TYR:CE2	2.31	0.65
1:A:114:VAL:CG2	1:A:145:VAL:HB	2.26	0.65
1:A:197:VAL:HG12	1:A:222:PHE:HA	1.76	0.65
1:B:32:PHE:CD2	1:B:32:PHE:N	2.64	0.65
1:B:488:ASP:OD1	1:B:490:ASN:ND2	2.30	0.64
1:B:195:THR:HA	1:B:223:HIS:CE1	2.32	0.64
1:A:425:VAL:C	1:A:426:TYR:HD2	2.02	0.63
1:B:112:THR:HG23	1:B:191:GLY:O	1.99	0.63
1:A:370:VAL:HG13	1:A:374:ALA:HB3	1.80	0.63
1:B:76:LEU:HD23	1:B:77:TYR:CD2	2.33	0.63
1:B:453:PHE:CD1	1:B:453:PHE:N	2.64	0.63
1:A:294:VAL:HG21	1:A:338:PHE:O	1.98	0.62
1:B:354:ILE:HG22	1:B:358:GLU:OE1	1.99	0.62
1:B:137:PHE:CZ	1:B:460:ASP:HB2	2.34	0.62
1:A:381:HIS:HB3	4:A:607:HOH:O	1.99	0.62
1:B:219:ARG:HH11	1:B:219:ARG:HG2	1.65	0.62
1:A:373:LEU:CD2	1:A:539:LEU:HD21	2.29	0.61
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.34	0.61
1:A:468:GLU:HA	1:A:471:ILE:HD12	1.81	0.61
1:B:22:LEU:HD13	1:B:136:ARG:HH21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ILE:CD1	1:B:414:LEU:HD12	2.31	0.61
1:B:255:VAL:HG23	1:B:284:HIS:ND1	2.16	0.61
1:B:253:HIS:O	1:B:255:VAL:N	2.33	0.60
1:B:461:PRO:C	1:B:463:ARG:H	2.04	0.60
1:B:216:PRO:HB2	1:B:217:PRO:HD3	1.83	0.60
1:B:87:ASN:HB3	1:B:88:PRO:HD2	1.84	0.60
1:B:12:VAL:HG12	1:B:14:GLY:H	1.65	0.60
1:B:80:PHE:HZ	1:B:438:SER:O	1.84	0.60
1:A:207:ALA:O	1:A:211:MET:HG2	2.01	0.60
1:A:184:GLN:HA	1:A:184:GLN:NE2	2.14	0.60
1:B:433:ARG:HH11	1:B:433:ARG:HG3	1.67	0.60
1:A:19:GLY:CA	1:A:32:PHE:CE1	2.85	0.60
1:A:56:TRP:NE1	1:A:60:VAL:HG23	2.16	0.59
1:B:32:PHE:HD2	1:B:32:PHE:N	2.00	0.59
1:B:224:ARG:HG3	1:B:224:ARG:HH11	1.66	0.59
1:B:203:SER:HB2	1:B:447:HIS:CE1	2.37	0.59
1:A:522:ARG:HH22	1:B:387:HIS:CE1	2.20	0.59
1:B:321:PHE:O	1:B:324:LEU:HB2	2.01	0.59
1:B:432:HIS:ND1	1:B:515:LEU:HD11	2.18	0.59
1:A:183:VAL:HG13	1:A:187:VAL:HB	1.84	0.59
1:B:200:PHE:CB	1:B:226:VAL:HB	2.32	0.59
1:B:54:GLN:HE21	1:B:55:PRO:CD	2.15	0.59
1:A:466:THR:O	1:A:469:GLU:HB2	2.03	0.59
1:B:342:GLY:O	1:B:344:PRO:HD3	2.02	0.59
1:A:344:PRO:HB2	1:A:358:GLU:HG2	1.86	0.58
1:B:84:GLU:HA	1:B:87:ASN:HD22	1.68	0.58
1:A:413:GLN:HE21	1:A:533:ASN:HB3	1.68	0.58
1:B:172:GLY:O	1:B:175:ASP:HB2	2.03	0.57
1:A:114:VAL:HG21	1:A:187:VAL:HG21	1.86	0.57
1:A:115:LEU:HD23	1:A:198:THR:HB	1.86	0.57
1:B:270:VAL:O	1:B:273:LEU:HB3	2.04	0.57
1:B:65:PHE:HB2	1:B:90:ARG:NH1	2.18	0.57
1:A:192:GLY:O	1:A:194:PRO:HD3	2.05	0.57
1:B:77:TYR:CE1	1:B:348:LYS:HD2	2.39	0.57
1:B:77:TYR:CD1	1:B:348:LYS:CE	2.88	0.57
1:B:453:PHE:H	1:B:453:PHE:HD1	1.51	0.57
1:A:200:PHE:CB	1:A:226:VAL:HB	2.35	0.57
1:B:210:GLY:HA3	1:B:232:PRO:HG3	1.87	0.57
1:A:203:SER:HB2	1:A:447:HIS:NE2	2.20	0.57
1:B:102:TRP:HB3	1:B:139:VAL:HG21	1.87	0.56
1:B:31:ALA:C	1:B:32:PHE:CD2	2.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:TYR:CE1	1:A:151:TYR:CE2	2.94	0.56
1:B:68:VAL:HG22	1:B:127:ALA:CB	2.36	0.56
1:A:227:LEU:HD12	1:A:227:LEU:N	2.20	0.56
1:B:491:GLU:OE1	1:B:492:PRO:HD3	2.06	0.56
1:A:256:GLY:O	1:A:257:CYS:CB	2.53	0.56
1:A:106:PRO:O	1:A:107:ARG:C	2.43	0.55
1:B:37:PHE:HD1	1:B:178:LEU:HD23	1.71	0.55
1:B:340:VAL:HG11	1:B:443:MET:CE	2.36	0.55
1:A:193:ASP:OD1	1:A:195:THR:N	2.36	0.55
1:A:490:ASN:N	1:A:490:ASN:ND2	2.53	0.55
1:A:106:PRO:HG2	1:A:143:ARG:NH1	2.21	0.55
1:B:77:TYR:CD1	1:B:348:LYS:NZ	2.75	0.55
1:B:20:ILE:CG2	1:B:63:THR:HA	2.37	0.55
1:B:278:ALA:O	1:B:280:VAL:N	2.40	0.55
1:A:114:VAL:HG22	1:A:145:VAL:HB	1.89	0.55
1:B:213:LEU:HD23	1:B:222:PHE:HZ	1.72	0.55
1:A:80:PHE:CD1	1:A:348:LYS:HE2	2.42	0.55
1:B:202:GLU:HA	1:B:228:GLN:O	2.07	0.55
1:A:162:PRO:HD2	1:A:245:ARG:NH1	2.22	0.54
1:B:453:PHE:HD1	1:B:453:PHE:N	2.05	0.54
1:B:102:TRP:CB	1:B:139:VAL:HG21	2.38	0.54
1:B:213:LEU:HD23	1:B:222:PHE:CZ	2.42	0.54
1:A:120:GLY:HA2	1:A:205:GLY:H	1.73	0.54
1:A:257:CYS:CB	1:A:272:CYS:SG	2.95	0.54
1:B:200:PHE:HB2	1:B:226:VAL:HB	1.90	0.54
1:B:54:GLN:NE2	1:B:55:PRO:CD	2.65	0.54
1:A:5:ASP:O	1:A:7:GLU:N	2.40	0.54
1:B:389:GLU:OE1	1:B:389:GLU:HA	2.08	0.53
1:A:387:HIS:CE1	1:B:522:ARG:HH22	2.26	0.53
1:A:210:GLY:HA3	1:A:232:PRO:HD3	1.90	0.53
1:B:312:PRO:O	1:B:316:ILE:HB	2.08	0.53
1:B:113:PRO:HG2	1:B:144:THR:HG22	1.91	0.53
1:A:496:LYS:HD2	1:A:496:LYS:C	2.28	0.53
1:A:114:VAL:CG1	1:A:197:VAL:HG22	2.35	0.53
1:A:291:GLN:OE1	1:A:369:GLN:HB3	2.09	0.53
1:B:539:LEU:HD23	1:B:539:LEU:C	2.30	0.53
1:A:450:GLU:HG2	1:A:451:ILE:N	2.24	0.53
1:A:265:ASN:CG	1:A:266:ASP:N	2.62	0.52
1:A:246:ARG:HH21	1:A:250:GLN:HG2	1.73	0.52
1:B:339:LEU:C	1:B:341:TYR:H	2.13	0.52
1:A:24:THR:HG22	1:A:26:GLY:N	2.15	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:LEU:O	1:B:341:TYR:N	2.42	0.52
1:A:36:PRO:HB2	1:A:53:LYS:HG2	1.91	0.52
1:A:203:SER:HB2	1:A:447:HIS:CE1	2.45	0.52
1:B:160:ALA:HB2	1:B:169:GLY:HA2	1.91	0.52
1:A:457:ILE:N	1:A:458:PRO:HD2	2.23	0.52
1:A:426:TYR:HE1	1:A:489:PRO:HD2	1.65	0.52
1:B:13:ARG:NH2	1:B:185:GLU:HG2	2.24	0.52
1:B:113:PRO:HG3	1:B:485:ARG:HG2	1.91	0.52
1:B:528:ALA:N	3:B:1016:SO4:O3	2.43	0.52
1:B:37:PHE:CD2	1:B:99:LEU:HD23	2.45	0.51
1:B:439:TRP:HB3	1:B:440:PRO:HD2	1.92	0.51
1:B:137:PHE:HZ	1:B:460:ASP:HB2	1.75	0.51
1:A:227:LEU:CD1	1:A:227:LEU:N	2.73	0.51
1:B:66:GLN:HG3	1:B:98:TYR:CD1	2.46	0.51
1:B:24:THR:HG22	1:B:26:GLY:H	1.76	0.51
1:A:29:VAL:HG22	1:A:140:GLN:HB2	1.93	0.51
1:A:543:THR:HG22	1:B:543:THR:HG22	1.91	0.51
1:B:250:GLN:HE21	1:B:288:VAL:HA	1.74	0.51
1:A:488:ASP:OD1	1:A:490:ASN:ND2	2.44	0.51
1:A:12:VAL:HG12	1:A:14:GLY:H	1.75	0.51
1:B:382:TYR:CG	1:B:401:VAL:HG22	2.45	0.51
1:B:472:PHE:CE1	1:B:514:ASP:O	2.64	0.51
1:B:307:PHE:HD1	1:B:308:LEU:HD13	1.74	0.51
1:B:138:LEU:HD23	1:B:146:LEU:HD23	1.91	0.51
1:B:325:GLN:HE21	1:B:487:GLY:HA3	1.74	0.51
1:A:266:ASP:O	1:A:269:LEU:N	2.44	0.51
1:B:250:GLN:HG3	1:B:288:VAL:HG12	1.93	0.51
1:B:124:TYR:CD1	1:B:125:SER:HB3	2.45	0.51
1:A:195:THR:O	1:A:196:SER:C	2.50	0.50
1:B:482:ASN:ND2	1:B:492:PRO:HG3	2.26	0.50
1:B:417:ARG:CZ	4:B:649:HOH:O	2.30	0.50
1:A:202:GLU:HG3	1:A:451:ILE:HD11	1.94	0.50
1:B:257:CYS:HB2	1:B:258:PRO:HA	1.93	0.50
1:B:110:SER:O	1:B:112:THR:HG22	2.11	0.50
1:A:162:PRO:HG2	1:A:241:MET:HB3	1.93	0.50
1:B:355:SER:O	1:B:356:ARG:C	2.48	0.50
1:A:226:VAL:C	1:A:227:LEU:HD12	2.31	0.50
1:A:138:LEU:HD12	1:A:477:MET:HB3	1.92	0.50
1:B:84:GLU:HA	1:B:87:ASN:ND2	2.26	0.50
1:A:333:ASP:OD2	1:A:444:GLY:HA3	2.12	0.50
1:A:44:PRO:O	1:A:274:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ARG:NH1	1:B:185:GLU:HG2	2.27	0.49
1:A:122:GLY:O	1:A:123:PHE:HB2	2.12	0.49
1:A:200:PHE:HB2	1:A:226:VAL:HB	1.95	0.49
1:B:328:VAL:O	1:B:427:ALA:HA	2.13	0.49
1:A:161:LEU:HD13	1:A:248:ALA:HB3	1.95	0.49
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.47	0.49
2:B:1003:NAG:O3	2:B:1004:NAG:O5	2.29	0.49
1:A:141:ALA:O	1:A:142:GLU:HG2	2.13	0.49
1:B:383:THR:HG22	1:B:384:ASP:N	2.28	0.49
1:B:433:ARG:HH21	1:B:441:LEU:CA	2.23	0.48
1:B:316:ILE:HD11	1:B:414:LEU:CD1	2.43	0.48
1:B:66:GLN:HG3	1:B:98:TYR:CG	2.48	0.48
1:B:77:TYR:CE1	1:B:348:LYS:CE	2.96	0.48
1:B:292:GLU:O	1:B:365:VAL:HG23	2.14	0.48
1:A:256:GLY:O	1:A:257:CYS:HB3	2.12	0.48
1:B:5:ASP:O	1:B:7:GLU:N	2.46	0.48
1:B:10:VAL:CG1	1:B:11:THR:N	2.76	0.48
1:A:426:TYR:N	1:A:426:TYR:HD2	2.11	0.48
1:B:255:VAL:O	1:B:255:VAL:HG13	2.13	0.48
1:B:61:ASP:OD2	1:B:63:THR:HG23	2.14	0.48
1:B:467:ALA:O	1:B:471:ILE:HD12	2.13	0.48
1:A:197:VAL:H	1:A:223:HIS:HD2	1.61	0.48
1:B:472:PHE:O	1:B:475:ARG:N	2.47	0.48
1:B:195:THR:HA	1:B:223:HIS:HE1	1.77	0.48
1:A:510:TYR:CZ	1:A:521:ARG:HB2	2.49	0.48
1:B:237:ALA:O	1:B:301:PRO:HD2	2.14	0.48
1:A:202:GLU:HA	1:A:228:GLN:O	2.13	0.48
1:B:382:TYR:CD2	1:B:401:VAL:HG22	2.48	0.48
1:B:400:ASP:O	1:B:401:VAL:C	2.49	0.48
1:B:201:GLY:O	1:B:228:GLN:HB2	2.14	0.48
1:A:66:GLN:HG3	1:A:98:TYR:CG	2.49	0.48
1:B:162:PRO:HG2	1:B:241:MET:HB3	1.96	0.48
1:B:81:GLU:HB2	1:B:438:SER:HB3	1.95	0.48
1:B:46:ARG:O	1:B:47:PHE:HB2	2.13	0.48
1:B:374:ALA:O	1:B:377:ALA:HB3	2.14	0.48
1:B:193:ASP:O	1:B:195:THR:N	2.47	0.48
1:B:80:PHE:CZ	1:B:438:SER:O	2.67	0.47
1:B:68:VAL:HG11	1:B:88:PRO:HB3	1.95	0.47
1:B:42:MET:O	1:B:44:PRO:CD	2.62	0.47
1:A:317:ASN:O	1:A:421:GLN:NE2	2.46	0.47
1:B:351:GLU:HB3	1:B:353:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:THR:OG1	1:A:113:PRO:HD2	2.14	0.47
1:A:426:TYR:N	1:A:426:TYR:CD2	2.82	0.47
1:B:24:THR:O	1:B:26:GLY:N	2.48	0.47
1:B:402:VAL:O	1:B:406:ASN:HB2	2.14	0.47
1:B:354:ILE:HD11	1:B:395:ARG:HA	1.96	0.47
1:B:79:GLY:HA2	1:B:84:GLU:HG3	1.97	0.47
1:B:336:SER:O	1:B:337:TYR:C	2.51	0.47
1:A:246:ARG:NH2	1:A:250:GLN:HG2	2.28	0.47
1:A:384:ASP:C	1:A:384:ASP:OD1	2.53	0.47
1:B:373:LEU:HD23	1:B:543:THR:HG21	1.97	0.47
1:A:197:VAL:H	1:A:223:HIS:CD2	2.33	0.47
1:B:135:GLY:O	1:B:136:ARG:C	2.53	0.47
1:A:118:ILE:HG22	1:A:205:GLY:HA2	1.96	0.47
1:A:29:VAL:HG12	1:A:103:THR:O	2.15	0.46
1:B:294:VAL:HG21	1:B:338:PHE:O	2.14	0.46
1:A:106:PRO:HG2	1:A:143:ARG:HH12	1.80	0.46
1:A:522:ARG:NH2	1:B:387:HIS:CE1	2.84	0.46
1:B:491:GLU:HB3	1:B:494:ASP:OD1	2.15	0.46
1:B:276:ARG:HH11	1:B:276:ARG:HG2	1.79	0.46
1:B:13:ARG:CZ	1:B:185:GLU:HG2	2.45	0.46
1:B:536:LEU:N	1:B:537:PRO:CD	2.78	0.46
1:A:440:PRO:HG2	1:A:443:MET:HG3	1.95	0.46
1:B:54:GLN:CA	1:B:54:GLN:NE2	2.55	0.46
1:A:8:LEU:HD23	1:A:8:LEU:N	2.31	0.46
1:B:433:ARG:HG2	1:B:433:ARG:NH1	2.27	0.46
1:A:457:ILE:H	1:A:458:PRO:CD	2.28	0.46
1:B:68:VAL:HG22	1:B:127:ALA:HB1	1.97	0.46
1:A:429:VAL:O	1:A:429:VAL:HG12	2.15	0.46
1:A:467:ALA:HA	1:A:470:LYS:HG3	1.96	0.46
1:B:463:ARG:NH1	1:B:463:ARG:CG	2.77	0.46
1:B:340:VAL:CG1	1:B:443:MET:CE	2.93	0.46
1:B:197:VAL:HB	1:B:222:PHE:HA	1.98	0.46
1:B:149:MET:HG2	1:B:150:ASN:N	2.25	0.46
1:A:337:TYR:HA	1:A:443:MET:CE	2.46	0.46
1:A:77:TYR:CE1	1:A:348:LYS:HG2	2.50	0.46
1:A:66:GLN:HG3	1:A:98:TYR:CD1	2.51	0.46
1:B:202:GLU:O	1:B:205:GLY:N	2.49	0.45
1:B:228:GLN:HG2	1:B:428:TYR:OH	2.16	0.45
1:B:149:MET:H	1:B:149:MET:HE3	1.81	0.45
1:B:398:LEU:O	1:B:398:LEU:HG	2.16	0.45
1:A:28:PRO:HG2	1:A:105:TYR:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LEU:HD22	1:A:391:PRO:HB2	1.97	0.45
1:A:251:LEU:HA	1:A:254:LEU:HD12	1.99	0.45
1:A:433:ARG:NH2	1:A:441:LEU:HA	2.32	0.45
1:B:80:PHE:CD2	1:B:348:LYS:NZ	2.82	0.45
1:A:113:PRO:HG2	1:A:144:THR:HG22	1.98	0.45
1:A:511:VAL:HG11	1:A:518:LEU:HD13	1.96	0.45
1:B:253:HIS:C	1:B:255:VAL:H	2.19	0.45
1:B:224:ARG:HG3	1:B:224:ARG:NH1	2.31	0.45
1:B:29:VAL:HG13	1:B:103:THR:O	2.17	0.45
1:A:32:PHE:CD2	1:A:190:PHE:HE1	2.35	0.45
1:B:164:SER:C	1:B:166:GLU:H	2.20	0.45
1:B:77:TYR:CE1	1:B:348:LYS:HE3	2.51	0.45
1:B:274:ARG:CG	1:B:274:ARG:HH11	2.30	0.45
1:A:193:ASP:O	1:A:195:THR:O	2.34	0.45
1:B:44:PRO:HA	1:B:274:ARG:HD3	1.99	0.45
1:B:536:LEU:HB3	1:B:537:PRO:HD3	1.99	0.45
1:A:497:ALA:HB1	1:A:498:PRO:HD2	1.98	0.44
1:B:276:ARG:HG2	1:B:276:ARG:NH1	2.31	0.44
1:A:524:LEU:HD12	1:A:524:LEU:HA	1.60	0.44
1:A:430:PHE:CD1	1:A:430:PHE:C	2.91	0.44
1:B:93:SER:OG	1:B:95:ASP:N	2.49	0.44
1:B:370:VAL:HG13	1:B:374:ALA:CB	2.45	0.44
1:B:187:VAL:HG22	1:B:192:GLY:HA3	2.00	0.44
1:B:219:ARG:HG2	1:B:219:ARG:NH1	2.33	0.44
1:B:336:SER:HA	1:B:339:LEU:HD12	1.99	0.44
1:A:178:LEU:HA	1:A:181:GLN:HG3	1.99	0.44
1:B:458:PRO:HG2	1:B:473:ALA:CB	2.44	0.44
1:A:386:LEU:HA	1:A:386:LEU:HD23	1.42	0.44
1:A:333:ASP:OD2	1:A:445:VAL:N	2.48	0.44
1:A:166:GLU:HB3	1:A:270:VAL:HG11	1.99	0.44
1:B:316:ILE:HD13	1:B:316:ILE:HG21	1.60	0.44
1:B:115:LEU:HA	1:B:115:LEU:HD23	1.77	0.44
1:B:238:THR:HG22	1:B:301:PRO:HB2	1.99	0.44
1:B:454:ILE:HD13	1:B:476:LEU:HB3	2.00	0.44
1:A:316:ILE:CD1	1:A:414:LEU:HD12	2.48	0.44
1:B:106:PRO:O	1:B:107:ARG:C	2.57	0.44
1:A:24:THR:O	1:A:25:PRO:C	2.57	0.43
1:A:492:PRO:HD2	1:A:493:ARG:H	1.82	0.43
1:B:359:PHE:CG	1:B:394:LEU:HD22	2.53	0.43
1:A:19:GLY:N	1:A:32:PHE:HE1	2.16	0.43
1:B:336:SER:OG	1:B:337:TYR:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.67	0.43
1:B:37:PHE:CD1	1:B:178:LEU:HD23	2.52	0.43
1:B:275:THR:O	1:B:276:ARG:C	2.54	0.43
1:B:465:TYR:HD2	1:B:469:GLU:OE1	2.01	0.43
1:B:173:LEU:HA	1:B:173:LEU:HD23	1.81	0.43
1:A:195:THR:CA	1:A:223:HIS:NE2	2.78	0.43
1:B:274:ARG:HG2	1:B:274:ARG:HH11	1.84	0.43
1:B:387:HIS:N	1:B:388:PRO:HD3	2.34	0.43
1:A:118:ILE:O	1:A:118:ILE:HG22	2.18	0.43
1:A:35:ILE:HA	1:A:36:PRO:HD2	1.89	0.43
1:A:459:LEU:N	1:A:459:LEU:HD23	2.33	0.43
1:A:203:SER:OG	1:A:204:ALA:N	2.51	0.43
1:A:139:VAL:HG22	1:A:144:THR:O	2.19	0.43
1:A:454:ILE:HD12	1:A:480:TRP:CE2	2.54	0.43
1:A:45:ARG:O	1:A:48:LEU:HB2	2.19	0.43
1:B:372:ASP:OD1	1:B:372:ASP:N	2.52	0.43
1:A:187:VAL:HG22	1:A:192:GLY:HA3	2.00	0.43
1:B:226:VAL:HA	1:B:327:LEU:O	2.19	0.43
1:A:281:LEU:HD23	1:A:281:LEU:HA	1.79	0.43
1:B:167:ALA:HA	1:B:168:PRO:HD3	1.80	0.43
1:B:82:GLY:N	1:B:438:SER:OG	2.48	0.43
1:A:107:ARG:O	1:A:108:PRO:C	2.57	0.43
1:A:265:ASN:O	1:A:267:THR:N	2.52	0.43
1:B:371:SER:O	1:B:374:ALA:HB3	2.19	0.43
1:B:80:PHE:CG	1:B:348:LYS:NZ	2.78	0.42
1:A:5:ASP:C	1:A:7:GLU:H	2.22	0.42
1:A:195:THR:C	1:A:223:HIS:CD2	2.92	0.42
1:B:336:SER:O	1:B:338:PHE:N	2.52	0.42
1:B:286:TRP:CD1	1:B:286:TRP:N	2.87	0.42
1:B:457:ILE:O	1:B:458:PRO:C	2.56	0.42
1:B:527:GLN:HE21	1:B:527:GLN:HB3	1.53	0.42
1:A:364:ARG:HD2	1:A:364:ARG:HA	1.69	0.42
1:A:426:TYR:HD1	1:A:489:PRO:CG	2.32	0.42
1:B:200:PHE:HB3	1:B:226:VAL:HB	2.00	0.42
1:B:268:GLU:O	1:B:272:CYS:HB2	2.19	0.42
1:B:243:GLU:OE2	1:B:247:ARG:NE	2.40	0.42
1:B:525:ARG:NH1	4:B:620:HOH:O	2.51	0.42
1:B:354:ILE:HG13	1:B:354:ILE:H	1.60	0.42
1:B:193:ASP:C	1:B:195:THR:N	2.73	0.42
1:A:293:SER:HA	1:A:365:VAL:HG23	2.01	0.42
1:A:140:GLN:C	1:A:140:GLN:CD	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:TYR:HE1	1:B:348:LYS:HG3	1.82	0.42
1:A:493:ARG:O	1:A:494:ASP:HB2	2.19	0.42
1:B:460:ASP:OD1	1:B:462:SER:HB3	2.20	0.42
1:A:510:TYR:HE1	1:A:523:GLY:O	2.02	0.42
1:B:319:GLY:H	1:B:421:GLN:HE22	1.67	0.42
1:B:294:VAL:CG2	1:B:338:PHE:O	2.67	0.42
1:B:123:PHE:CZ	1:B:204:ALA:HB1	2.54	0.42
1:A:130:LEU:HD12	1:A:133:TYR:CE2	2.54	0.42
1:A:124:TYR:CD1	1:A:124:TYR:C	2.93	0.42
1:B:115:LEU:CD2	1:B:198:THR:HB	2.46	0.42
1:B:432:HIS:CE1	1:B:515:LEU:HD11	2.55	0.42
1:B:424:ARG:HB2	1:B:424:ARG:HE	1.49	0.42
1:B:87:ASN:CB	1:B:88:PRO:HD2	2.45	0.42
1:A:243:GLU:OE1	1:A:246:ARG:HD3	2.20	0.42
1:A:158:PHE:CZ	1:A:172:GLY:HA3	2.54	0.42
1:A:307:PHE:HD1	1:A:308:LEU:HD13	1.85	0.42
1:A:425:VAL:C	1:A:426:TYR:CD2	2.88	0.41
1:B:77:TYR:CZ	1:B:348:LYS:HG3	2.54	0.41
1:A:522:ARG:NH2	1:B:387:HIS:HE1	2.18	0.41
1:A:452:GLU:O	1:A:457:ILE:HG12	2.20	0.41
1:A:182:TRP:O	1:A:186:ASN:HB2	2.20	0.41
1:B:31:ALA:C	1:B:32:PHE:HD2	2.20	0.41
1:B:22:LEU:HD22	1:B:23:LYS:HE3	2.02	0.41
1:A:271:ALA:HA	1:A:274:ARG:HD2	2.02	0.41
1:A:337:TYR:HA	1:A:443:MET:HE2	2.03	0.41
1:B:16:ARG:HD2	1:B:59:VAL:HG12	2.02	0.41
1:B:280:VAL:O	1:B:283:ASN:HB2	2.20	0.41
1:B:252:ALA:CB	1:B:269:LEU:HD21	2.50	0.41
1:B:479:TYR:HA	1:B:489:PRO:O	2.20	0.41
1:A:32:PHE:CD2	1:A:190:PHE:CE1	3.09	0.41
1:B:339:LEU:HA	1:B:339:LEU:HD23	1.68	0.41
1:B:315:LEU:HA	1:B:315:LEU:HD12	1.66	0.41
1:A:458:PRO:HG3	1:A:465:TYR:CD2	2.56	0.41
1:B:329:GLY:HA3	1:B:428:TYR:CE1	2.56	0.41
1:A:251:LEU:HD21	1:A:281:LEU:HD22	2.03	0.41
1:B:393:ARG:O	1:B:395:ARG:N	2.54	0.41
1:B:276:ARG:HB3	1:B:280:VAL:HG21	2.03	0.41
1:B:20:ILE:HG22	1:B:63:THR:HA	2.03	0.41
1:B:119:TYR:HE2	1:B:150:ASN:HA	1.86	0.41
1:A:200:PHE:HB3	1:A:226:VAL:HB	2.02	0.41
1:B:494:ASP:C	1:B:496:LYS:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:LEU:HD11	1:B:399:SER:HA	2.02	0.41
1:A:370:VAL:HG22	1:A:540:LEU:HD21	2.03	0.40
1:B:193:ASP:C	1:B:195:THR:H	2.24	0.40
1:A:12:VAL:HG13	1:A:186:ASN:OD1	2.21	0.40
1:B:174:LEU:HA	1:B:174:LEU:HD23	1.43	0.40
1:A:426:TYR:CD1	1:A:489:PRO:CG	3.05	0.40
1:A:24:THR:HA	1:A:25:PRO:HD2	1.94	0.40
1:B:77:TYR:CZ	1:B:348:LYS:CG	3.04	0.40
1:B:152:ARG:O	1:B:157:GLY:HA3	2.20	0.40
1:A:346:PHE:CD2	1:A:352:SER:HB3	2.56	0.40
1:A:316:ILE:HD11	1:A:414:LEU:HD12	2.03	0.40
1:B:123:PHE:CE2	1:B:204:ALA:HB1	2.56	0.40
1:B:282:VAL:H	1:B:282:VAL:HG23	1.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	530/540 (98%)	456 (86%)	56 (11%)	18 (3%)	5 31
1	B	526/540 (97%)	422 (80%)	77 (15%)	27 (5%)	2 20
All	All	1056/1080 (98%)	878 (83%)	133 (13%)	45 (4%)	3 25

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ALA
1	A	28	PRO
1	A	257	CYS
1	B	6	ALA
1	B	189	ALA

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Mol	Chain	Res	Type
1	B	241	MET
1	B	254	LEU
1	B	257	CYS
1	B	340	VAL
1	B	385	TRP
1	B	462	SER
1	A	196	SER
1	A	267	THR
1	A	352	SER
1	B	25	PRO
1	B	122	GLY
1	B	143	ARG
1	B	242	GLY
1	B	356	ARG
1	B	397	ALA
1	B	452	GLU
1	B	473	ALA
1	A	61	ASP
1	A	188	ALA
1	A	256	GLY
1	A	266	ASP
1	A	494	ASP
1	B	28	PRO
1	B	81	GLU
1	B	136	ARG
1	B	278	ALA
1	A	241	MET
1	A	317	ASN
1	A	369	GLN
1	A	464	ASN
1	B	279	GLN
1	B	524	LEU
1	B	272	CYS
1	B	466	THR
1	A	404	ASP
1	B	121	GLY
1	B	194	PRO
1	B	239	VAL
1	A	461	PRO
1	A	25	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	433/436 (99%)	369 (85%)	64 (15%)	4 18
1	B	432/436 (99%)	358 (83%)	74 (17%)	2 12
All	All	865/872 (99%)	727 (84%)	138 (16%)	3 14

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	12	VAL
1	A	18	ARG
1	A	20	ILE
1	A	23	LYS
1	A	30	SER
1	A	48	LEU
1	A	49	PRO
1	A	63	THR
1	A	70	TYR
1	A	75	THR
1	A	83	THR
1	A	85	MET
1	A	91	GLU
1	A	103	THR
1	A	132	VAL
1	A	143	ARG
1	A	144	THR
1	A	161	LEU
1	A	184	GLN
1	A	195	THR
1	A	200	PHE
1	A	203	SER
1	A	208	SER
1	A	211	MET
1	A	219	ARG
1	A	241	MET

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Mol	Chain	Res	Type
1	A	245	ARG
1	A	246	ARG
1	A	254	LEU
1	A	255	VAL
1	A	266	ASP
1	A	285	GLU
1	A	295	PHE
1	A	308	LEU
1	A	311	THR
1	A	324	LEU
1	A	325	GLN
1	A	332	LYS
1	A	333	ASP
1	A	348	LYS
1	A	365	VAL
1	A	370	VAL
1	A	372	ASP
1	A	389	GLU
1	A	396	GLU
1	A	414	LEU
1	A	424	ARG
1	A	436	THR
1	A	437	LEU
1	A	441	LEU
1	A	450	GLU
1	A	463	ARG
1	A	490	ASN
1	A	491	GLU
1	A	496	LYS
1	A	502	PRO
1	A	504	THR
1	A	509	GLN
1	A	512	SER
1	A	522	ARG
1	A	525	ARG
1	A	534	ARG
1	A	536	LEU
1	B	9	LEU
1	B	12	VAL
1	B	23	LYS
1	B	32	PHE
1	B	54	GLN

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Mol	Chain	Res	Type
1	B	59	VAL
1	B	60	VAL
1	B	70	TYR
1	B	83	THR
1	B	100	ASN
1	B	105	TYR
1	B	112	THR
1	B	114	VAL
1	B	132	VAL
1	B	143	ARG
1	B	144	THR
1	B	146	LEU
1	B	149	MET
1	B	159	LEU
1	B	161	LEU
1	B	200	PHE
1	B	203	SER
1	B	211	MET
1	B	216	PRO
1	B	219	ARG
1	B	239	VAL
1	B	241	MET
1	B	246	ARG
1	B	250	GLN
1	B	254	LEU
1	B	255	VAL
1	B	269	LEU
1	B	283	ASN
1	B	291	GLN
1	B	294	VAL
1	B	295	PHE
1	B	296	ARG
1	B	308	LEU
1	B	309	SER
1	B	311	THR
1	B	316	ILE
1	B	324	LEU
1	B	325	GLN
1	B	326	VAL
1	B	332	LYS
1	B	344	PRO
1	B	347	SER

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Mol	Chain	Res	Type
1	B	348	LYS
1	B	351	GLU
1	B	352	SER
1	B	353	LEU
1	B	354	ILE
1	B	360	LEU
1	B	364	ARG
1	B	370	VAL
1	B	372	ASP
1	B	376	GLU
1	B	386	LEU
1	B	414	LEU
1	B	424	ARG
1	B	433	ARG
1	B	436	THR
1	B	437	LEU
1	B	441	LEU
1	B	453	PHE
1	B	462	SER
1	B	463	ARG
1	B	464	ASN
1	B	466	THR
1	B	478	ARG
1	B	490	ASN
1	B	515	LEU
1	B	525	ARG
1	B	534	ARG

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	184	GLN
1	A	228	GLN
1	A	322	HIS
1	A	325	GLN
1	A	369	GLN
1	A	387	HIS
1	A	474	GLN
1	A	490	ASN
1	A	509	GLN
1	B	54	GLN
1	B	184	GLN

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Mol	Chain	Res	Type
1	B	250	GLN
1	B	265	ASN
1	B	283	ASN
1	B	291	GLN
1	B	325	GLN
1	B	369	GLN
1	B	387	HIS
1	B	421	GLN
1	B	482	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

4 carbohydrates 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	NAG	A	1001	1,2	14,14,15	1.93	3 (21%)	15,19,21	3.37	5 (33%)
2	NAG	A	1002	2	14,14,15	1.75	2 (14%)	15,19,21	2.73	6 (40%)
2	NAG	B	1003	1,2	14,14,15	1.92	3 (21%)	15,19,21	4.02	5 (33%)
2	NAG	B	1004	2	14,14,15	1.43	2 (14%)	15,19,21	2.20	7 (46%)

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	NAG	A	1001	1,2	1/1/5/7	1/6/23/26	0/1/1/1
2	NAG	A	1002	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1003	1,2	1/1/5/7	1/6/23/26	0/1/1/1
2	NAG	B	1004	2	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	NAG	O5-C1	-2.32	1.39	1.43
2	B	1003	NAG	O7-C7	2.05	1.28	1.23
2	B	1004	NAG	C3-C2	2.29	1.57	1.52
2	A	1002	NAG	C2-N2	3.08	1.51	1.46
2	B	1003	NAG	C1-C2	3.23	1.56	1.52
2	A	1001	NAG	C1-C2	3.65	1.57	1.52
2	B	1004	NAG	C1-C2	3.70	1.57	1.52
2	A	1002	NAG	C1-C2	4.47	1.58	1.52
2	A	1001	NAG	C2-N2	4.66	1.54	1.46
2	B	1003	NAG	C2-N2	4.92	1.55	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1004	NAG	O6-C6-C5	-2.76	102.20	111.33
2	B	1003	NAG	C3-C4-C5	-2.62	105.63	110.20
2	B	1004	NAG	O3-C3-C4	-2.61	104.45	110.34
2	A	1001	NAG	O3-C3-C2	-2.40	104.37	109.11
2	A	1002	NAG	O7-C7-C8	-2.18	118.06	122.06
2	B	1004	NAG	O7-C7-C8	-2.10	118.21	122.06
2	A	1002	NAG	O6-C6-C5	-2.09	104.43	111.33
2	B	1004	NAG	O4-C4-C3	-2.03	105.77	110.34
2	B	1004	NAG	O4-C4-C5	2.17	115.00	109.24
2	A	1002	NAG	C3-C4-C5	2.25	114.12	110.20
2	A	1001	NAG	C6-C5-C4	2.54	119.27	113.02
2	A	1001	NAG	C8-C7-N2	2.65	121.17	116.11
2	B	1003	NAG	O4-C4-C3	3.05	117.21	110.34
2	B	1004	NAG	C2-N2-C7	3.32	127.31	123.04
2	A	1002	NAG	C4-C3-C2	3.58	116.80	111.23
2	A	1001	NAG	C4-C3-C2	3.63	116.86	111.23
2	B	1003	NAG	C4-C3-C2	4.13	117.66	111.23
2	B	1004	NAG	O3-C3-C2	4.90	118.83	109.11
2	A	1002	NAG	C2-N2-C7	5.87	130.59	123.04
2	A	1002	NAG	C1-O5-C5	6.51	120.51	112.25
2	B	1003	NAG	C1-O5-C5	8.82	123.44	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1003	NAG	C2-N2-C7	10.99	137.16	123.04
2	A	1001	NAG	C2-N2-C7	11.13	137.34	123.04

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1003	NAG	C1
2	A	1001	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1003	NAG	O7-C7-N2-C2
2	A	1001	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1003	NAG	1	0
2	B	1004	NAG	1	0

5.6 Ligand geometry (i)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	1005	-	4,4,4	0.28	0	6,6,6	0.42	0
3	SO4	A	1010	-	4,4,4	0.40	0	6,6,6	0.77	0
3	SO4	A	1011	-	4,4,4	0.28	0	6,6,6	0.28	0
3	SO4	A	1012	-	4,4,4	0.34	0	6,6,6	0.48	0
3	SO4	A	1013	-	4,4,4	0.56	0	6,6,6	0.36	0
3	SO4	A	1017	-	4,4,4	0.18	0	6,6,6	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	B	1014	-	4,4,4	0.44	0	6,6,6	0.70	0
3	SO4	B	1015	-	4,4,4	0.15	0	6,6,6	0.21	0
3	SO4	B	1016	-	4,4,4	0.23	0	6,6,6	0.26	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
3	SO4	A	1005	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1010	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1011	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1012	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1013	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1017	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1014	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1015	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1016	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1011	SO4	1	0
3	B	1016	SO4	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	534/540 (98%)	-0.36	1 (0%)	95	94	47, 69, 97, 114	0
1	B	532/540 (98%)	-0.33	3 (0%)	90	84	49, 79, 112, 137	0
All	All	1066/1080 (98%)	-0.35	4 (0%)	93	90	47, 73, 107, 137	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	495	PRO	2.8
1	B	492	PRO	2.2
1	A	78	PRO	2.1
1	B	494	ASP	2.0

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

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

6.3 Carbohydrates

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	NAG	B	1003	14/15	0.90	0.20	-	79,85,89,98	0
2	NAG	A	1002	14/15	0.84	0.33	-	92,109,119,120	0
2	NAG	B	1004	14/15	0.77	0.38	-	107,112,125,125	0
2	NAG	A	1001	14/15	0.90	0.16	-	80,85,89,98	0

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. 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
3	SO4	B	1014	5/5	0.84	0.23	2.75	119,120,122,123	0
3	SO4	A	1012	5/5	0.86	0.37	1.22	128,130,130,131	0
3	SO4	B	1016	5/5	0.93	0.14	0.05	130,131,131,132	0
3	SO4	A	1005	5/5	0.88	0.21	-	131,131,132,133	0
3	SO4	A	1011	5/5	0.93	0.16	-	115,115,117,117	0
3	SO4	B	1015	5/5	0.95	0.21	-	107,107,108,108	0
3	SO4	A	1013	5/5	0.91	0.20	-	130,130,132,132	0
3	SO4	A	1017	5/5	0.91	0.21	-	112,112,113,114	0
3	SO4	A	1010	5/5	0.92	0.15	-	112,112,113,115	0

6.5 Other polymers

There are no such residues in this entry.