Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:38 AM GMT

PDB ID	:	2I07
Title	:	Human Complement Component C3b
Authors	:	Janssen, B.J.C.; Christodoulidou, A.; McCarthy, A.; Lambris, J.D.; Gros, P.
Deposited on	:	2006-08-10
Resolution	:	4.00 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:

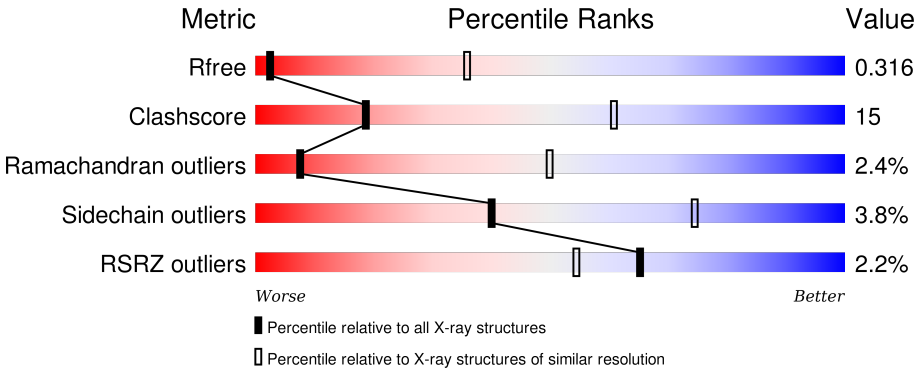
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

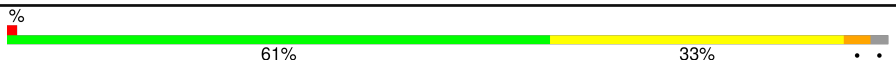
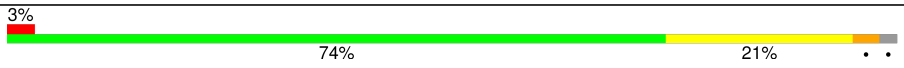
The reported resolution of this entry is 4.00 Å.

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	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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	645	
2	B	915	

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
3	NAG	A	646	X	-	-	-
3	MAN	A	648	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12157 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 Complement C3b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	630	Total	C	N	O	S	0	0	0
			4907	3127	828	937	15			

- Molecule 2 is a protein called Complement C3b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	901	Total	C	N	O	S	0	0	0
			7197	4563	1210	1386	38			

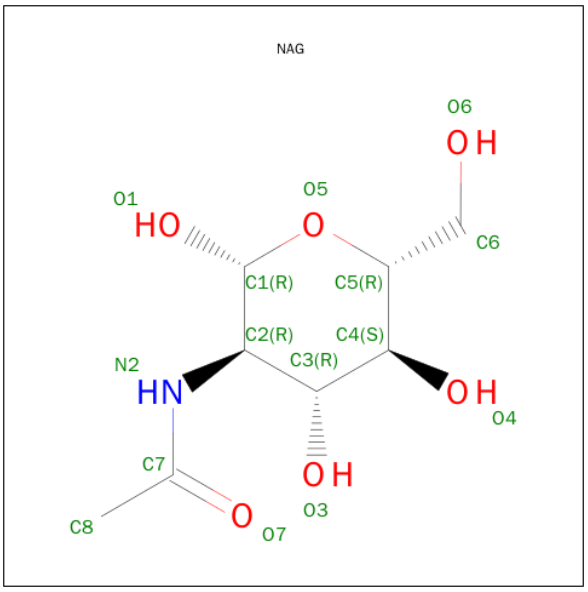
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	991	GLU	GLN	SEE REMARK 999	UNP P01024

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

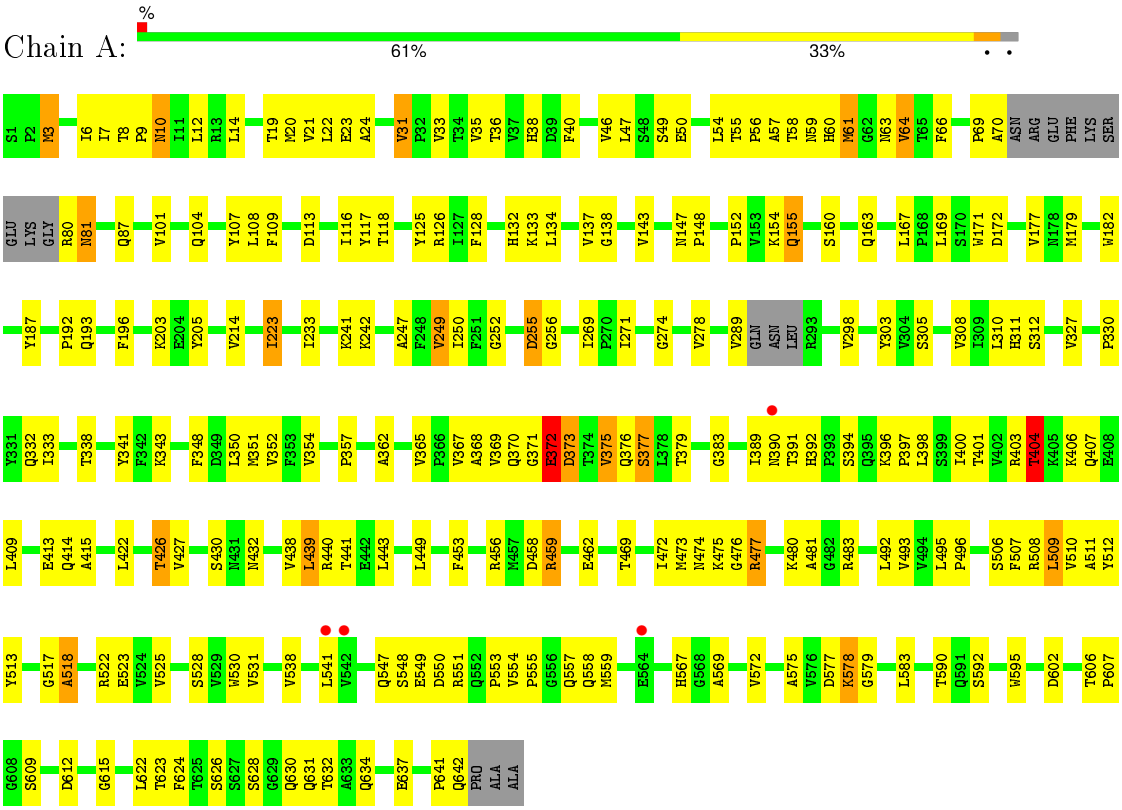


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

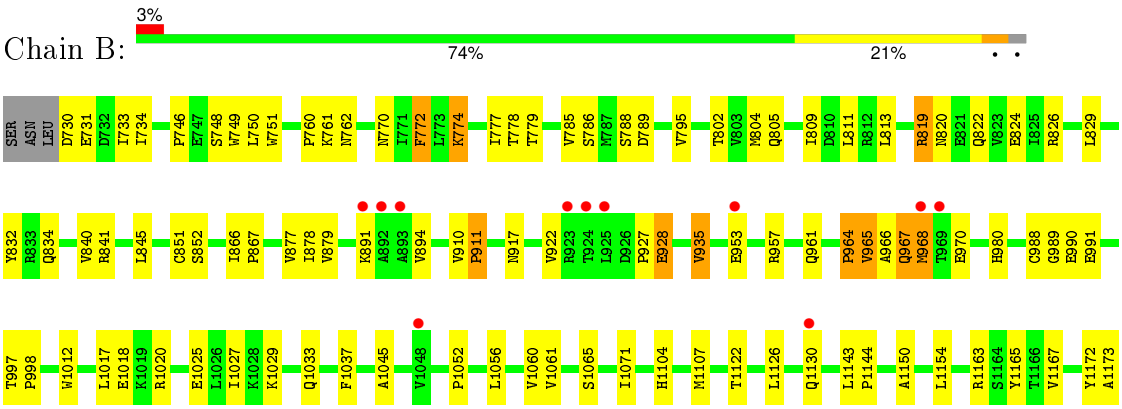
3 Residue-property plots (i)

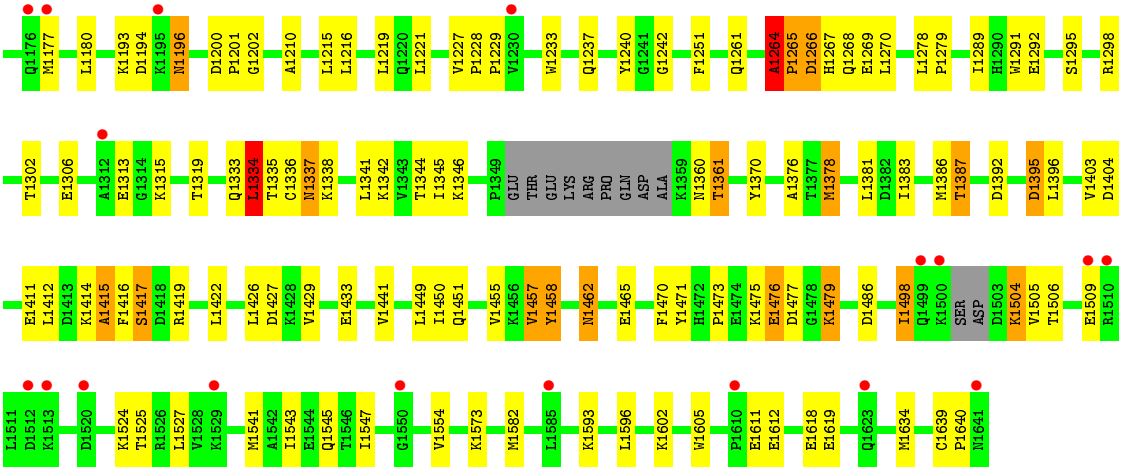
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Complement C3b



- Molecule 2: Complement C3b




Q1176 M1177 L1180 K1193 D1194 K1195 N1196 D1200 P1201 G1202 A1210 L1215 L1216 L1219 Q1220 L1221 V1227 P1228 P1229 V1230 W1233 Q1237 Y1240 G1241 G1242 F1251 Q1261 A1264 P1265 D1266 H1267 Q1268 E1269 L1270 L1278 P1279 I1289 H1290 W1291 E1292 S1295 R1298
T1302 E1306 A1312 E1313 G1314 K1315 T1319 Q1333 L1334 T1335 C1336 N1337 K1338 L1341 K1342 V1343 T1344 I1345 K1346 P1349 GLU THR GLU LYS ARG PRO GLN ASP ALA K1359 N1360 T1361 Y1370 A1376 T1377 M1378 L1381 D1382 I1383 M1386 T1387 D1392 D1395 L1396 V1403 D1404
E1411 L1412 D1413 K1414 A1415 F1416 S1417 D1418 R1419 L1422 L1426 D1427 K1428 V1429 E1433 V1441 L1449 I1450 Q1451 V1455 K1456 V1457 Y1458 N1462 E1465 F1470 Y1471 H1472 P1473 E1474 K1475 E1476 D1477 G1478 K1479 D1486 I1498 Q1499 K1500 SER ASP D1503 K1504 V1505 T1506 E1509 R1510
L1511 D1512 K1513 D1520 K1524 T1525 R1526 L1527 V1528 K1529 M1541 A1542 I1543 E1544 Q1545 T1546 I1547 G1550 V1554 K1573 M1582 L1585 K1593 L1596 K1602 W1605 P1610 E1611 E1612 E1618 E1619 Q1623 M1634 C1639 P1640 N1641

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	123.91Å 128.54Å 147.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 4.00 45.07 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.00-4.00) 99.8 (45.07-4.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.273 , 0.323 0.283 , 0.316	Depositor DCC
R_{free} test set	1044 reflections (5.40%)	DCC
Wilson B-factor (Å^2)	133.2	Xtriage
Anisotropy	0.784	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 114.5	EDS
Estimated twinning fraction	0.054 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 20412 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	12157	wwPDB-VP
Average B, all atoms (Å^2)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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, MAN

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	0.26	0/5004	0.44	0/6799
2	B	0.24	0/7340	0.43	2/9936 (0.0%)
All	All	0.25	0/12344	0.43	2/16735 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	A	2	0
All	All	2	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1264	ALA	C-N-CD	-6.46	106.40	120.60
2	B	1264	ALA	C-N-CA	5.43	144.79	122.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	646	NAG	C1
3	A	648	MAN	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1264	ALA	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	4907	0	4970	219	0
2	B	7197	0	7124	168	0
3	A	39	0	34	1	0
4	B	14	0	13	0	0
All	All	12157	0	12141	375	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 15.

All (375) 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:477:ARG:HG2	1:A:477:ARG:HH11	1.06	1.17
2:B:1264:ALA:HB1	2:B:1265:PRO:O	1.46	1.16
1:A:403:ARG:HB3	1:A:404:THR:HG22	1.24	1.11
1:A:69:PRO:HA	1:A:70:ALA:HB3	1.17	1.09
1:A:69:PRO:HA	1:A:70:ALA:CB	1.77	1.09
1:A:372:GLU:HA	1:A:373:ASP:CB	1.79	1.08
1:A:6:ILE:HD11	1:A:20:MET:HG3	1.34	1.07
1:A:372:GLU:HA	1:A:373:ASP:HB3	1.06	1.05
2:B:819:ARG:HH11	2:B:819:ARG:HG2	1.16	1.04
1:A:404:THR:HG23	1:A:414:GLN:HB3	1.41	1.01
1:A:69:PRO:CA	1:A:70:ALA:HB3	1.90	1.00
2:B:1411:GLU:HG2	2:B:1422:LEU:HD12	1.45	0.98
1:A:6:ILE:HD11	1:A:20:MET:CG	1.98	0.93
1:A:372:GLU:CA	1:A:373:ASP:HB3	1.97	0.92
1:A:477:ARG:HH11	1:A:477:ARG:CG	1.84	0.91
1:A:510:VAL:HG12	1:A:528:SER:HB3	1.51	0.91
2:B:819:ARG:HH11	2:B:819:ARG:CG	1.85	0.90
1:A:404:THR:CG2	1:A:414:GLN:HB3	2.02	0.89
2:B:966:ALA:HB1	2:B:1267:HIS:HA	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:VAL:HG21	1:A:64:VAL:HG21	1.56	0.85
1:A:362:ALA:O	1:A:379:THR:HG21	1.75	0.85
2:B:1387:THR:CG2	2:B:1451:GLN:H	1.89	0.84
2:B:927:PRO:O	2:B:928:GLU:HB2	1.78	0.83
1:A:369:VAL:HG12	1:A:370:GLN:H	1.43	0.83
1:A:7:ILE:HA	1:A:623:THR:O	1.78	0.83
1:A:641:PRO:O	1:A:642:GLN:HB2	1.77	0.82
1:A:477:ARG:NH1	1:A:477:ARG:HG2	1.86	0.81
1:A:372:GLU:CA	1:A:373:ASP:CB	2.56	0.81
1:A:404:THR:HG21	1:A:415:ALA:O	1.82	0.80
1:A:55:THR:HG22	1:A:57:ALA:H	1.46	0.79
2:B:966:ALA:O	2:B:967:GLN:HB2	1.83	0.79
1:A:439:LEU:HD12	1:A:439:LEU:H	1.48	0.77
2:B:804:MET:HG2	2:B:805:GLN:H	1.48	0.77
1:A:369:VAL:HG12	1:A:370:GLN:N	2.00	0.76
1:A:403:ARG:HA	1:A:404:THR:HB	1.66	0.76
1:A:403:ARG:CB	1:A:404:THR:HG22	2.12	0.76
2:B:819:ARG:NH1	2:B:819:ARG:HG2	1.91	0.75
1:A:147:ASN:HB2	1:A:148:PRO:HD2	1.68	0.75
1:A:549:GLU:HG2	1:A:550:ASP:H	1.52	0.74
2:B:1582:MET:HA	2:B:1605:TRP:O	1.87	0.74
2:B:1334:LEU:HG	2:B:1335:THR:O	1.88	0.74
1:A:510:VAL:HG12	1:A:528:SER:CB	2.17	0.74
2:B:1333:GLN:HB3	2:B:1335:THR:HG22	1.69	0.73
1:A:554:VAL:HG13	1:A:555:PRO:HD2	1.70	0.73
2:B:1387:THR:HG22	2:B:1451:GLN:H	1.52	0.73
1:A:31:VAL:HG13	1:A:54:LEU:HB2	1.71	0.73
1:A:370:GLN:HG2	1:A:401:THR:HB	1.72	0.71
2:B:1524:LYS:HB3	2:B:1545:GLN:HG2	1.71	0.71
2:B:1465:GLU:O	2:B:1465:GLU:HG3	1.91	0.71
1:A:3:MET:HE2	1:A:628:SER:HB2	1.72	0.70
2:B:910:VAL:HG13	2:B:911:PRO:HD2	1.73	0.70
1:A:549:GLU:HG2	1:A:550:ASP:N	2.06	0.70
2:B:1334:LEU:N	2:B:1335:THR:HA	2.06	0.70
2:B:1027:ILE:HG22	2:B:1071:ILE:HD13	1.74	0.70
1:A:249:VAL:HG11	1:A:278:VAL:HG11	1.74	0.69
1:A:367:VAL:HA	1:A:404:THR:H	1.58	0.68
1:A:404:THR:CG2	1:A:404:THR:O	2.41	0.68
1:A:40:PHE:CE2	2:B:1017:LEU:HD11	2.28	0.68
1:A:116:ILE:HD11	1:A:203:LYS:HB3	1.75	0.68
2:B:1543:ILE:HD12	2:B:1554:VAL:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:THR:HB	1:A:9:PRO:CD	2.24	0.67
2:B:1414:LYS:O	2:B:1415:ALA:HB3	1.95	0.67
2:B:1386:MET:HG3	2:B:1471:TYR:CE1	2.30	0.66
1:A:474:ASN:C	1:A:476:GLY:H	1.99	0.66
1:A:368:ALA:N	1:A:403:ARG:O	2.20	0.66
2:B:1334:LEU:H	2:B:1335:THR:HA	1.59	0.66
2:B:1338:LYS:HD3	2:B:1465:GLU:HB2	1.77	0.66
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.25	0.65
2:B:1411:GLU:CG	2:B:1422:LEU:HD12	2.24	0.65
2:B:1337:ASN:HB2	2:B:1338:LYS:HD2	1.78	0.65
1:A:506:SER:HB2	1:A:530:TRP:HE1	1.62	0.64
2:B:1267:HIS:CE1	2:B:1291:TRP:CZ2	2.86	0.64
1:A:247:ALA:HB3	1:A:271:ILE:HD11	1.79	0.64
1:A:247:ALA:CB	1:A:271:ILE:HD11	2.28	0.64
1:A:473:MET:HB2	1:A:508:ARG:HB2	1.79	0.64
2:B:1267:HIS:HB3	2:B:1268:GLN:O	1.97	0.64
2:B:970:GLU:HB3	2:B:1261:GLN:HE22	1.63	0.63
1:A:426:THR:HG21	1:A:432:ASN:H	1.63	0.63
1:A:551:ARG:HD2	1:A:551:ARG:H	1.64	0.63
1:A:143:VAL:O	1:A:155:GLN:HA	1.99	0.63
2:B:1336:CYS:O	2:B:1338:LYS:N	2.26	0.63
1:A:23:GLU:HG2	1:A:61:MET:HG2	1.80	0.63
2:B:1611:GLU:HG3	2:B:1612:GLU:H	1.62	0.63
2:B:1414:LYS:O	2:B:1415:ALA:CB	2.47	0.62
1:A:474:ASN:O	1:A:476:GLY:N	2.33	0.62
2:B:1387:THR:HG21	2:B:1451:GLN:H	1.63	0.61
1:A:439:LEU:HD12	1:A:439:LEU:N	2.14	0.61
1:A:177:VAL:HG22	1:A:182:TRP:CZ2	2.35	0.61
2:B:935:VAL:HG11	2:B:1313:GLU:HG3	1.83	0.61
1:A:154:LYS:HD2	1:A:171:TRP:CD1	2.36	0.61
1:A:548:SER:O	1:A:549:GLU:HB2	1.99	0.61
1:A:179:MET:HG3	1:A:203:LYS:HA	1.82	0.60
1:A:22:LEU:HD13	1:A:33:VAL:HG11	1.81	0.60
1:A:369:VAL:CG1	1:A:370:GLN:H	2.15	0.60
1:A:641:PRO:O	1:A:642:GLN:CB	2.48	0.60
1:A:407:GLN:C	1:A:409:LEU:H	2.04	0.60
1:A:177:VAL:HG22	1:A:182:TRP:HZ2	1.66	0.60
2:B:1462:ASN:ND2	2:B:1465:GLU:H	2.00	0.59
2:B:733:ILE:HG12	2:B:734:ILE:N	2.15	0.59
2:B:1419:ARG:HD3	2:B:1422:LEU:HD13	1.84	0.59
2:B:1462:ASN:HB3	2:B:1465:GLU:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:PHE:H	1:A:632:THR:CG2	2.16	0.59
1:A:376:GLN:O	1:A:377:SER:HB3	2.03	0.59
2:B:1404:ASP:HA	2:B:1427:ASP:HB2	1.84	0.59
2:B:852:SER:HB3	2:B:878:ILE:HG22	1.84	0.59
2:B:961:GLN:HB3	2:B:1319:THR:HB	1.85	0.58
2:B:1386:MET:HB3	2:B:1450:ILE:HD13	1.86	0.58
1:A:439:LEU:CD1	1:A:439:LEU:H	2.15	0.58
2:B:1045:ALA:HB2	2:B:1052:PRO:HA	1.85	0.58
2:B:1383:ILE:HG12	2:B:1455:VAL:HG22	1.86	0.58
2:B:1376:ALA:HB3	2:B:1429:VAL:HG22	1.87	0.57
2:B:1126:LEU:HD23	2:B:1173:ALA:HB1	1.87	0.57
1:A:47:LEU:HD13	1:A:66:PHE:HB2	1.86	0.57
2:B:778:THR:OG1	2:B:779:THR:N	2.37	0.57
1:A:507:PHE:CE1	1:A:531:VAL:HB	2.40	0.57
2:B:968:MET:HB2	2:B:1266:ASP:HA	1.87	0.57
2:B:1392:ASP:HB3	2:B:1395:ASP:HB2	1.87	0.57
2:B:1267:HIS:HE1	2:B:1291:TRP:CZ2	2.22	0.56
2:B:927:PRO:O	2:B:928:GLU:CB	2.52	0.56
2:B:811:LEU:HG	2:B:813:LEU:HD13	1.88	0.56
1:A:223:ILE:H	1:A:223:ILE:HD12	1.71	0.56
2:B:819:ARG:O	2:B:820:ASN:HB2	2.06	0.56
2:B:1267:HIS:CE1	2:B:1291:TRP:CE2	2.94	0.56
2:B:1361:THR:HA	2:B:1441:VAL:O	2.05	0.56
1:A:612:ASP:OD1	1:A:615:GLY:N	2.39	0.55
2:B:1386:MET:HG3	2:B:1471:TYR:HE1	1.71	0.55
1:A:250:ILE:HG22	1:A:305:SER:HB3	1.87	0.55
2:B:804:MET:HG2	2:B:805:GLN:N	2.19	0.55
2:B:1370:TYR:CD1	2:B:1376:ALA:HB2	2.42	0.55
2:B:966:ALA:O	2:B:967:GLN:CB	2.55	0.55
2:B:1386:MET:O	2:B:1387:THR:C	2.46	0.54
1:A:332:GLN:HE21	1:A:357:PRO:HA	1.71	0.54
1:A:472:ILE:HD13	1:A:509:LEU:HD22	1.89	0.54
1:A:474:ASN:C	1:A:476:GLY:N	2.60	0.54
1:A:590:THR:HG22	1:A:592:SER:H	1.71	0.54
1:A:458:ASP:N	1:A:458:ASP:OD1	2.40	0.54
2:B:1412:LEU:O	2:B:1419:ARG:NH2	2.40	0.54
2:B:1457:VAL:O	2:B:1458:TYR:HB3	2.08	0.54
1:A:551:ARG:N	1:A:551:ARG:HD2	2.23	0.53
1:A:241:LYS:HG3	2:B:832:TYR:CE2	2.44	0.53
1:A:47:LEU:HD21	1:A:50:GLU:HG2	1.91	0.53
1:A:403:ARG:CA	1:A:404:THR:HB	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:877:VAL:H	2:B:1451:GLN:NE2	2.07	0.53
1:A:541:LEU:HD22	2:B:786:SER:HB3	1.90	0.53
1:A:547:GLN:HE22	1:A:559:MET:HB2	1.74	0.53
1:A:624:PHE:H	1:A:632:THR:HG23	1.74	0.52
1:A:404:THR:O	1:A:404:THR:HG23	2.09	0.52
1:A:341:TYR:HA	1:A:422:LEU:O	2.09	0.52
1:A:362:ALA:O	1:A:379:THR:CG2	2.51	0.52
2:B:966:ALA:HB2	2:B:1267:HIS:ND1	2.25	0.52
2:B:1498:ILE:HD12	2:B:1605:TRP:HE3	1.74	0.52
1:A:391:THR:HG22	1:A:392:HIS:N	2.25	0.52
2:B:910:VAL:CG1	2:B:911:PRO:HD2	2.37	0.52
2:B:964:PRO:HB3	2:B:1291:TRP:HZ3	1.74	0.52
1:A:577:ASP:O	1:A:579:GLY:N	2.43	0.51
2:B:1278:LEU:HD22	2:B:1302:THR:HG21	1.93	0.51
1:A:214:VAL:HG23	1:A:214:VAL:O	2.10	0.51
1:A:376:GLN:O	1:A:377:SER:CB	2.58	0.51
1:A:453:PHE:HB2	1:A:493:VAL:HG23	1.93	0.51
1:A:69:PRO:HA	1:A:70:ALA:HB2	1.82	0.51
1:A:9:PRO:HD2	1:A:12:LEU:HD21	1.93	0.51
1:A:69:PRO:CB	1:A:70:ALA:HB3	2.40	0.50
1:A:22:LEU:HD11	1:A:64:VAL:HG22	1.93	0.50
2:B:819:ARG:NH1	2:B:819:ARG:CG	2.56	0.50
2:B:1193:LYS:O	2:B:1194:ASP:HB2	2.10	0.50
1:A:606:THR:HG23	1:A:607:PRO:HD2	1.93	0.50
1:A:23:GLU:OE2	1:A:512:TYR:OH	2.28	0.50
1:A:249:VAL:CG1	1:A:278:VAL:HG21	2.42	0.50
2:B:851:CYS:HB3	2:B:879:VAL:HB	1.93	0.50
1:A:24:ALA:HB3	1:A:60:HIS:HB3	1.92	0.50
2:B:772:PHE:N	2:B:772:PHE:CD2	2.80	0.50
1:A:6:ILE:HD13	1:A:22:LEU:HD23	1.94	0.50
1:A:558:GLN:HB3	2:B:770:ASN:HD21	1.77	0.50
1:A:55:THR:HB	1:A:58:THR:HG23	1.93	0.50
1:A:628:SER:HB2	1:A:630:GLN:OE1	2.12	0.50
1:A:163:GLN:NE2	1:A:163:GLN:HA	2.27	0.49
2:B:1345:ILE:O	2:B:1345:ILE:HG23	2.11	0.49
1:A:427:VAL:HG21	1:A:523:GLU:HG3	1.94	0.49
2:B:980:HIS:NE2	2:B:1240:TYR:O	2.44	0.49
1:A:558:GLN:NE2	2:B:770:ASN:OD1	2.45	0.49
1:A:370:GLN:CG	1:A:401:THR:HB	2.40	0.49
2:B:777:ILE:HG23	2:B:804:MET:HA	1.94	0.49
2:B:1527:LEU:HD13	2:B:1541:MET:SD	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ILE:HG23	1:A:352:VAL:HG13	1.93	0.49
2:B:1215:LEU:O	2:B:1219:LEU:HG	2.13	0.49
1:A:348:PHE:HD2	1:A:389:ILE:HD11	1.77	0.49
1:A:379:THR:CG2	1:A:383:GLY:HA2	2.43	0.49
2:B:1126:LEU:HG	2:B:1130:GLN:HE21	1.77	0.49
1:A:567:HIS:HB2	2:B:760:PRO:HB3	1.95	0.49
2:B:789:ASP:OD1	2:B:789:ASP:N	2.43	0.49
1:A:338:THR:OG1	1:A:351:MET:N	2.42	0.49
1:A:187:TYR:CD1	1:A:192:PRO:HA	2.48	0.49
1:A:403:ARG:HB3	1:A:404:THR:CG2	2.17	0.49
1:A:569:ALA:HB2	2:B:788:SER:HB2	1.93	0.49
2:B:840:VAL:HG22	2:B:894:VAL:HG12	1.95	0.49
2:B:1291:TRP:O	2:B:1292:GLU:HB2	2.12	0.49
1:A:252:GLY:HA3	1:A:303:TYR:CZ	2.47	0.49
1:A:126:ARG:CZ	1:A:572:VAL:HB	2.43	0.49
2:B:1387:THR:HG22	2:B:1451:GLN:N	2.22	0.49
1:A:108:LEU:HB2	1:A:196:PHE:CD1	2.48	0.49
2:B:1289:ILE:HG12	2:B:1298:ARG:HE	1.78	0.48
1:A:104:GLN:O	1:A:132:HIS:CE1	2.66	0.48
2:B:1061:VAL:O	2:B:1065:SER:OG	2.27	0.48
1:A:104:GLN:O	1:A:132:HIS:HE1	1.97	0.48
1:A:575:ALA:O	2:B:748:SER:HA	2.14	0.48
2:B:1270:LEU:HD12	2:B:1291:TRP:HE3	1.79	0.48
1:A:595:TRP:HA	1:A:595:TRP:CE3	2.48	0.48
2:B:1233:TRP:O	2:B:1237:GLN:HG2	2.14	0.48
2:B:964:PRO:HB3	2:B:1291:TRP:CZ3	2.49	0.48
1:A:8:THR:HB	1:A:9:PRO:HD2	1.95	0.48
2:B:1381:LEU:CD2	2:B:1457:VAL:HG13	2.43	0.48
2:B:1150:ALA:O	2:B:1154:LEU:HG	2.14	0.48
2:B:1165:TYR:HD1	2:B:1210:ALA:HB2	1.79	0.48
1:A:80:ARG:O	1:A:81:ASN:HB2	2.12	0.48
2:B:991:GLU:HG2	2:B:1104:HIS:NE2	2.29	0.48
1:A:3:MET:HE3	1:A:522:ARG:CG	2.43	0.47
1:A:255:ASP:HA	1:A:256:GLY:HA2	1.62	0.47
2:B:1334:LEU:H	2:B:1335:THR:HG22	1.79	0.47
1:A:3:MET:HE3	1:A:522:ARG:HG2	1.96	0.47
2:B:746:PRO:CG	2:B:774:LYS:HG3	2.44	0.47
1:A:118:THR:HG23	1:A:205:TYR:CE2	2.49	0.47
1:A:14:LEU:HD21	1:A:101:VAL:HG11	1.97	0.47
1:A:553:PRO:HD2	2:B:802:THR:O	2.14	0.47
1:A:628:SER:CB	1:A:630:GLN:OE1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:THR:O	1:A:404:THR:HG22	2.14	0.47
2:B:1012:TRP:HB3	2:B:1017:LEU:CD1	2.44	0.47
2:B:1228:PRO:HB2	2:B:1229:PRO:HD3	1.97	0.46
2:B:1200:ASP:O	2:B:1202:GLY:N	2.48	0.46
2:B:761:LYS:O	2:B:762:ASN:HB2	2.16	0.46
1:A:109:PHE:HB2	1:A:128:PHE:HB2	1.98	0.46
2:B:1344:THR:HG21	2:B:1346:LYS:HE2	1.98	0.46
1:A:269:ILE:HD13	1:A:278:VAL:HB	1.97	0.46
2:B:1475:LYS:O	2:B:1476:GLU:C	2.53	0.46
2:B:1172:TYR:CE1	2:B:1216:LEU:HB3	2.49	0.46
1:A:152:PRO:O	2:B:957:ARG:NH2	2.49	0.46
1:A:350:LEU:HD21	1:A:400:ILE:HG21	1.97	0.46
2:B:840:VAL:HG12	2:B:841:ARG:N	2.30	0.46
1:A:113:ASP:OD1	1:A:113:ASP:N	2.47	0.46
2:B:1025:GLU:O	2:B:1029:LYS:HB2	2.15	0.46
2:B:1416:PHE:O	2:B:1417:SER:C	2.54	0.46
1:A:310:LEU:C	1:A:312:SER:H	2.17	0.46
2:B:1180:LEU:HD23	2:B:1221:LEU:HD11	1.98	0.46
1:A:247:ALA:HB2	1:A:308:VAL:HG22	1.98	0.45
2:B:1504:LYS:HD3	2:B:1504:LYS:N	2.30	0.45
2:B:1333:GLN:HG3	2:B:1334:LEU:HD23	1.98	0.45
1:A:6:ILE:HD12	1:A:7:ILE:H	1.81	0.45
2:B:1143:LEU:HB3	2:B:1144:PRO:HD3	1.97	0.45
1:A:438:VAL:HG13	1:A:449:LEU:HD11	1.98	0.45
2:B:988:CYS:O	2:B:990:GLU:N	2.49	0.45
1:A:47:LEU:CD1	1:A:66:PHE:HB2	2.46	0.45
1:A:472:ILE:HG12	1:A:480:LYS:O	2.17	0.45
2:B:730:ASP:HB3	2:B:731:GLU:H	1.62	0.45
2:B:1465:GLU:O	2:B:1465:GLU:CG	2.64	0.45
1:A:310:LEU:O	1:A:312:SER:N	2.49	0.45
1:A:20:MET:HB3	1:A:64:VAL:HG23	1.98	0.45
1:A:6:ILE:HD12	1:A:21:VAL:O	2.16	0.44
2:B:1334:LEU:H	2:B:1335:THR:CA	2.29	0.44
1:A:247:ALA:HB2	1:A:271:ILE:HD11	1.99	0.44
1:A:392:HIS:C	1:A:394:SER:H	2.21	0.44
1:A:481:ALA:H	3:A:646:NAG:H81	1.82	0.44
1:A:50:GLU:HG3	1:A:66:PHE:HB3	1.99	0.44
1:A:403:ARG:HA	1:A:404:THR:CB	2.43	0.44
1:A:177:VAL:CG2	1:A:182:TRP:CZ2	3.00	0.44
1:A:147:ASN:HA	1:A:182:TRP:CE3	2.52	0.44
2:B:1126:LEU:HD21	2:B:1177:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:HD23	1:A:47:LEU:O	2.18	0.44
1:A:133:LYS:O	1:A:134:LEU:HB2	2.17	0.44
1:A:404:THR:CG2	1:A:415:ALA:O	2.61	0.44
2:B:1291:TRP:CD1	2:B:1292:GLU:HG3	2.52	0.44
1:A:469:THR:O	1:A:511:ALA:HA	2.17	0.44
2:B:819:ARG:O	2:B:820:ASN:CB	2.66	0.44
2:B:966:ALA:CB	2:B:1267:HIS:HA	2.38	0.44
2:B:1403:VAL:O	2:B:1404:ASP:HB2	2.18	0.44
1:A:373:ASP:O	1:A:375:VAL:N	2.41	0.44
1:A:624:PHE:O	1:A:631:GLN:HA	2.18	0.44
2:B:1378:MET:HA	2:B:1426:LEU:O	2.18	0.44
2:B:829:LEU:HD12	2:B:829:LEU:N	2.33	0.43
2:B:1196:ASN:HD22	2:B:1196:ASN:N	2.15	0.43
1:A:6:ILE:CD1	1:A:20:MET:HE3	2.49	0.43
2:B:1462:ASN:HD22	2:B:1465:GLU:H	1.65	0.43
2:B:1122:THR:O	2:B:1126:LEU:HB2	2.19	0.43
2:B:1126:LEU:O	2:B:1130:GLN:HG3	2.19	0.43
1:A:365:VAL:H	1:A:379:THR:HB	1.83	0.43
1:A:379:THR:HG23	1:A:383:GLY:HA2	2.01	0.43
1:A:310:LEU:C	1:A:312:SER:N	2.72	0.43
1:A:372:GLU:N	1:A:372:GLU:OE1	2.52	0.43
1:A:453:PHE:O	1:A:492:LEU:HA	2.17	0.43
1:A:606:THR:CG2	1:A:607:PRO:HD2	2.48	0.43
2:B:1506:THR:OG1	2:B:1509:GLU:HG2	2.18	0.43
2:B:1163:ARG:O	2:B:1167:VAL:HG23	2.19	0.43
1:A:443:LEU:HD11	1:A:449:LEU:HD13	2.01	0.43
2:B:1593:LYS:HG2	2:B:1596:LEU:HD11	2.00	0.43
1:A:406:LYS:O	1:A:414:GLN:NE2	2.52	0.43
1:A:517:GLY:O	1:A:518:ALA:C	2.57	0.43
2:B:1618:GLU:O	2:B:1619:GLU:HG3	2.18	0.43
1:A:36:THR:HG21	1:A:38:HIS:CE1	2.54	0.43
2:B:964:PRO:O	2:B:965:VAL:C	2.57	0.42
1:A:249:VAL:HA	1:A:305:SER:O	2.19	0.42
1:A:453:PHE:HB2	1:A:493:VAL:CG2	2.49	0.42
1:A:343:LYS:N	1:A:343:LYS:HD2	2.35	0.42
2:B:785:VAL:HG22	2:B:795:VAL:HG22	2.00	0.42
1:A:409:LEU:HG	1:A:413:GLU:HB2	2.02	0.42
1:A:577:ASP:C	1:A:579:GLY:N	2.72	0.42
2:B:1029:LYS:HG2	2:B:1033:GLN:OE1	2.20	0.42
1:A:407:GLN:C	1:A:409:LEU:N	2.72	0.42
2:B:1404:ASP:CA	2:B:1427:ASP:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:PRO:HG2	1:A:409:LEU:HD11	2.01	0.42
2:B:811:LEU:HG	2:B:813:LEU:CD1	2.49	0.42
1:A:440:ARG:HA	1:A:440:ARG:HD2	1.82	0.42
1:A:19:THR:CG2	1:A:63:ASN:OD1	2.68	0.42
2:B:749:TRP:O	2:B:750:LEU:HB3	2.20	0.42
1:A:495:LEU:HA	1:A:496:PRO:HD3	1.89	0.42
1:A:137:VAL:HG22	1:A:138:GLY:N	2.34	0.42
2:B:1381:LEU:HD23	2:B:1457:VAL:HG13	2.01	0.42
2:B:1396:LEU:HA	2:B:1396:LEU:HD23	1.94	0.42
1:A:6:ILE:HD12	1:A:7:ILE:N	2.35	0.42
2:B:1360:ASN:O	2:B:1361:THR:O	2.37	0.42
2:B:822:GLN:OE1	2:B:1479:LYS:HA	2.19	0.42
1:A:477:ARG:NH1	1:A:477:ARG:CG	2.54	0.41
1:A:108:LEU:HB2	1:A:196:PHE:CG	2.54	0.41
2:B:1227:VAL:HB	2:B:1228:PRO:HD3	2.01	0.41
2:B:988:CYS:HA	2:B:1037:PHE:CZ	2.55	0.41
2:B:1547:ILE:HG22	2:B:1634:MET:HB3	2.02	0.41
1:A:233:ILE:HG13	1:A:269:ILE:HD11	2.02	0.41
1:A:205:TYR:C	1:A:205:TYR:CD1	2.94	0.41
1:A:19:THR:HG22	1:A:63:ASN:OD1	2.21	0.41
1:A:459:ARG:HA	1:A:462:GLU:HG2	2.02	0.41
2:B:1267:HIS:CB	2:B:1268:GLN:CA	2.99	0.41
1:A:247:ALA:HB3	1:A:269:ILE:HG13	2.01	0.41
1:A:59:ASN:HB3	1:A:483:ARG:HH12	1.85	0.41
2:B:1279:PRO:HG2	2:B:1306:GLU:OE1	2.20	0.41
1:A:113:ASP:OD1	1:A:117:TYR:OH	2.35	0.41
2:B:866:ILE:HA	2:B:867:PRO:HD3	1.85	0.41
1:A:403:ARG:CA	1:A:404:THR:CB	2.99	0.41
1:A:7:ILE:HG22	1:A:622:LEU:HD22	2.03	0.41
2:B:1386:MET:SD	2:B:1473:PRO:HD3	2.61	0.41
2:B:824:GLU:OE1	2:B:826:ARG:NH1	2.53	0.41
1:A:369:VAL:CG1	1:A:370:GLN:N	2.70	0.41
1:A:241:LYS:HG3	2:B:832:TYR:CZ	2.55	0.41
1:A:125:TYR:CZ	1:A:169:LEU:HB3	2.56	0.41
1:A:55:THR:HG23	1:A:56:PRO:HD2	2.02	0.41
2:B:1525:THR:HG22	2:B:1543:ILE:HA	2.03	0.41
1:A:59:ASN:O	1:A:60:HIS:HB2	2.21	0.41
1:A:333:ILE:HG12	1:A:354:VAL:HG22	2.02	0.41
1:A:371:GLY:O	1:A:372:GLU:O	2.39	0.41
2:B:964:PRO:O	2:B:965:VAL:O	2.38	0.41
1:A:3:MET:HE1	1:A:626:SER:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1012:TRP:CE2	2:B:1020:ARG:HD2	2.56	0.41
2:B:1341:LEU:HD21	2:B:1455:VAL:HG12	2.02	0.41
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.56	0.41
1:A:578:LYS:HE2	1:A:578:LYS:HB3	1.93	0.41
2:B:1056:LEU:O	2:B:1060:VAL:HG23	2.21	0.41
1:A:249:VAL:HG11	1:A:278:VAL:HG21	2.02	0.41
1:A:12:LEU:O	1:A:101:VAL:HA	2.21	0.41
2:B:1470:PHE:HB2	2:B:1477:ASP:O	2.21	0.41
1:A:513:TYR:CZ	1:A:525:VAL:HB	2.55	0.41
1:A:160:SER:HA	1:A:167:LEU:HD21	2.03	0.41
2:B:997:THR:HG23	2:B:1251:PHE:HB2	2.03	0.41
1:A:163:GLN:HE21	1:A:163:GLN:CA	2.34	0.40
1:A:396:LYS:HG3	1:A:397:PRO:HD2	2.02	0.40
1:A:10:ASN:HA	1:A:10:ASN:HD22	1.57	0.40
1:A:148:PRO:HD3	1:A:182:TRP:CE2	2.57	0.40
1:A:223:ILE:HG12	1:A:298:VAL:HG22	2.02	0.40
1:A:430:SER:OG	1:A:523:GLU:OE1	2.34	0.40
2:B:1639:CYS:HA	2:B:1640:PRO:HD3	1.92	0.40
1:A:87:GLN:HE21	1:A:87:GLN:HB2	1.65	0.40
1:A:554:VAL:O	1:A:557:GLN:HB2	2.22	0.40
2:B:774:LYS:HD3	2:B:774:LYS:HA	1.95	0.40
1:A:242:LYS:HB3	1:A:274:GLY:HA3	2.03	0.40
1:A:528:SER:OG	1:A:609:SER:N	2.55	0.40
1:A:107:TYR:HA	1:A:196:PHE:CZ	2.57	0.40
2:B:1104:HIS:O	2:B:1107:MET:HG2	2.21	0.40
1:A:249:VAL:HG13	1:A:278:VAL:HG21	2.03	0.40
2:B:997:THR:HB	2:B:998:PRO:CD	2.52	0.40
2:B:845:LEU:HD21	2:B:891:LYS:HE3	2.04	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	624/645 (97%)	567 (91%)	45 (7%)	12 (2%)	10 54
2	B	895/915 (98%)	805 (90%)	65 (7%)	25 (3%)	6 47
All	All	1519/1560 (97%)	1372 (90%)	110 (7%)	37 (2%)	7 50

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	SER
1	A	372	GLU
1	A	377	SER
1	A	475	LYS
2	B	928	GLU
2	B	965	VAL
2	B	967	GLN
2	B	1265	PRO
2	B	1361	THR
2	B	1415	ALA
2	B	1476	GLU
2	B	1505	VAL
1	A	373	ASP
1	A	375	VAL
1	A	404	THR
1	A	518	ALA
2	B	935	VAL
2	B	989	GLY
2	B	1266	ASP
2	B	1417	SER
1	A	578	LYS
2	B	911	PRO
2	B	964	PRO
2	B	1334	LEU
2	B	1337	ASN
2	B	1387	THR
2	B	1458	TYR
1	A	311	HIS
2	B	1295	SER
1	A	81	ASN
1	A	255	ASP
2	B	774	LYS
2	B	1201	PRO
2	B	1486	ASP
2	B	1449	LEU

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Mol	Chain	Res	Type
2	B	1498	ILE
2	B	1242	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	555/567 (98%)	526 (95%)	29 (5%)	29 68
2	B	797/810 (98%)	774 (97%)	23 (3%)	50 79
All	All	1352/1377 (98%)	1300 (96%)	52 (4%)	40 74

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	10	ASN
1	A	31	VAL
1	A	46	VAL
1	A	61	MET
1	A	64	VAL
1	A	155	GLN
1	A	172	ASP
1	A	193	GLN
1	A	223	ILE
1	A	249	VAL
1	A	289	VAL
1	A	327	VAL
1	A	372	GLU
1	A	390	ASN
1	A	398	LEU
1	A	404	THR
1	A	426	THR
1	A	439	LEU
1	A	441	THR
1	A	456	ARG

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Mol	Chain	Res	Type
1	A	459	ARG
1	A	477	ARG
1	A	509	LEU
1	A	538	VAL
1	A	583	LEU
1	A	602	ASP
1	A	634	GLN
1	A	637	GLU
2	B	772	PHE
2	B	809	ILE
2	B	819	ARG
2	B	834	GLN
2	B	917	ASN
2	B	922	VAL
2	B	953	GLU
2	B	968	MET
2	B	1018	GLU
2	B	1196	ASN
2	B	1269	GLU
2	B	1315	LYS
2	B	1334	LEU
2	B	1342	LYS
2	B	1378	MET
2	B	1395	ASP
2	B	1433	GLU
2	B	1457	VAL
2	B	1462	ASN
2	B	1479	LYS
2	B	1504	LYS
2	B	1573	LYS
2	B	1602	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	60	HIS
1	A	87	GLN
1	A	104	GLN
1	A	132	HIS
1	A	144	ASN
1	A	155	GLN

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Mol	Chain	Res	Type
1	A	161	GLN
1	A	163	GLN
1	A	332	GLN
1	A	334	HIS
1	A	390	ASN
1	A	490	GLN
1	A	558	GLN
1	A	587	ASN
1	A	634	GLN
2	B	738	ASN
2	B	752	ASN
2	B	762	ASN
2	B	770	ASN
2	B	820	ASN
2	B	834	GLN
2	B	860	HIS
2	B	961	GLN
2	B	967	GLN
2	B	1076	GLN
2	B	1114	ASN
2	B	1141	ASN
2	B	1160	ASN
2	B	1196	ASN
2	B	1204	GLN
2	B	1261	GLN
2	B	1267	HIS
2	B	1277	GLN
2	B	1333	GLN
2	B	1401	ASN
2	B	1451	GLN
2	B	1462	ASN
2	B	1499	GLN
2	B	1620	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 (i)

3 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	$\#\|Z\| > 2$
3	NAG	A	646	1,3	14,14,15	0.56	0	15,19,21	1.05	1 (6%)
3	NAG	A	647	3	14,14,15	0.59	0	15,19,21	0.54	0
3	MAN	A	648	3	11,11,12	0.55	0	14,15,17	1.27	2 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	646	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	647	3	-	0/6/23/26	0/1/1/1
3	MAN	A	648	3	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	648	MAN	C1-O5-C5	2.22	115.07	112.25
3	A	646	NAG	C4-C3-C2	2.34	114.86	111.23
3	A	648	MAN	C1-C2-C3	3.36	113.52	109.54

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	648	MAN	C1
3	A	646	NAG	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	646	NAG	1	0

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
4	NAG	B	1	2	14,14,15	0.52	0	15,19,21	0.61	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
4	NAG	B	1	2	-	0/6/23/26	0/1/1/1

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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	630/645 (97%)	-0.27	4 (0%) 90 86	85, 132, 184, 224	0
2	B	901/915 (98%)	0.06	29 (3%) 51 38	99, 201, 275, 319	0
All	All	1531/1560 (98%)	-0.07	33 (2%) 65 54	85, 164, 262, 319	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1500	LYS	6.1
2	B	1195	LYS	4.0
2	B	968	MET	4.0
2	B	953	GLU	3.5
2	B	1312	ALA	3.4
2	B	1641	ASN	3.3
2	B	1130	GLN	3.2
1	A	564	GLU	3.2
2	B	924	THR	3.1
2	B	1177	MET	3.0
2	B	1499	GLN	3.0
2	B	1509	GLU	2.7
2	B	892	ALA	2.6
2	B	1230	VAL	2.6
2	B	1550	GLY	2.6
2	B	923	ARG	2.6
2	B	1520	ASP	2.5
2	B	893	ALA	2.5
2	B	1512	ASP	2.5
2	B	1610	PRO	2.5
2	B	1585	LEU	2.5
2	B	1176	GLN	2.4
1	A	541	LEU	2.4
2	B	969	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	1529	LYS	2.2
1	A	542	VAL	2.2
2	B	1623	GLN	2.1
2	B	1510	ARG	2.1
2	B	891	LYS	2.1
2	B	925	LEU	2.1
1	A	390	ASN	2.0
2	B	1513	LYS	2.0
2	B	1048	VAL	2.0

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

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

6.3 Carbohydrates (i)

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	NAG	A	646	14/15	0.96	0.18	-1.10	133,148,163,164	0
3	MAN	A	648	11/12	0.73	0.34	-	203,216,241,248	0
3	NAG	A	647	14/15	0.86	0.20	-	171,183,203,204	0

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
4	NAG	B	1	14/15	0.83	0.39	-	203,215,226,226	0

6.5 Other polymers (i)

There are no such residues in this entry.