Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:57 am BST

PDB ID	:	5C6O
Title	:	protein B
Authors	:	Lu, M.
Deposited on	:	2015-06-23
Resolution	:	3.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

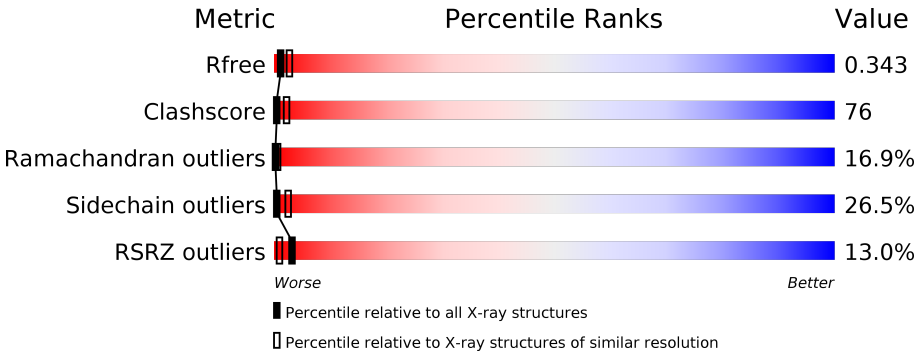
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	464	13% 17% 50% 25% 5%

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	4YH	A	501	-	-	-	X

2 Entry composition

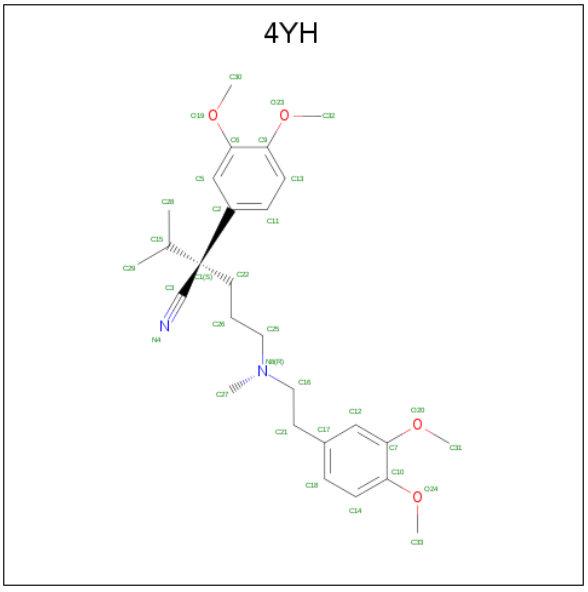
There are 2 unique types of molecules in this entry. The entry contains 3446 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BH2163 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3413	2263	548	574	28	0	0	0

- Molecule 2 is (2S)-2-(3,4-dimethoxyphenyl)-5-{[2-(3,4-dimethoxyphenyl)ethyl](methyl)amino}-2-(propan-2-yl)pentanenitrile (three-letter code: 4YH) (formula: $C_{27}H_{38}N_2O_4$).



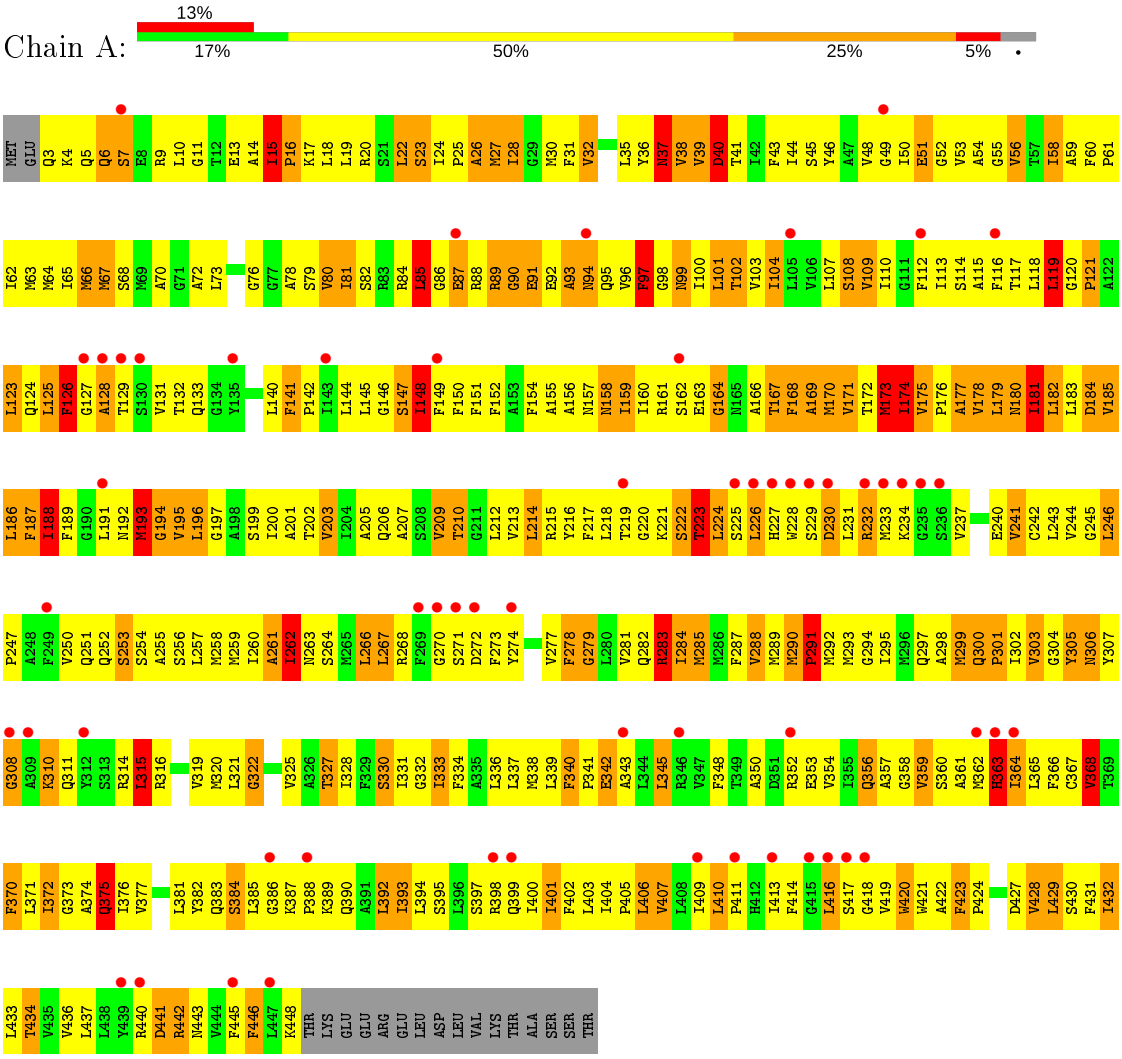
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	33	27	2	4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: BH2163 protein

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.06Å 94.15Å 102.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 14.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (15.00-3.00) 91.8 (14.98-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.270 , 0.290 0.353 , 0.343	Depositor DCC
R_{free} test set	837 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	101.8	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.09 , 37.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.32$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	0.168 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3446	wwPDB-VP
Average B, all atoms (Å^2)	243.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.94% 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: 4YH

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	0.61	2/3481 (0.1%)	0.91	5/4714 (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	A	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	VAL	C-N	5.95	1.47	1.34
1	A	40	ASP	CA-CB	5.43	1.66	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	308	GLY	N-CA-C	-7.83	93.53	113.10
1	A	85	LEU	N-CA-C	-6.32	93.93	111.00
1	A	40	ASP	CA-CB-CG	6.26	127.16	113.40
1	A	315	LEU	CB-CG-CD1	5.39	120.16	111.00
1	A	416	LEU	CA-CB-CG	5.24	127.34	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	LEU	Peptide
1	A	14	ALA	Peptide
1	A	15	ILE	Peptide
1	A	306	ASN	Peptide
1	A	87	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	3413	0	3608	534	0
2	A	33	0	38	18	0
All	All	3446	0	3646	542	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 76.

All (542) 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:156:ALA:O	1:A:160:ILE:HG23	1.44	1.16
1:A:404:ILE:HG13	1:A:405:PRO:HD3	1.30	1.14
1:A:364:ILE:HG23	1:A:367:CYS:SG	1.87	1.13
1:A:224:LEU:O	1:A:226:LEU:HG	1.48	1.13
1:A:406:LEU:HD22	1:A:422:ALA:HA	1.30	1.12
1:A:240:GLU:HA	1:A:243:LEU:HD12	1.23	1.12
1:A:148:ILE:HG13	1:A:149:PHE:N	1.62	1.10
1:A:254:SER:HB3	1:A:399:GLN:HG2	1.11	1.09
1:A:78:ALA:HA	1:A:162:SER:HB2	1.36	1.07
1:A:148:ILE:HG13	1:A:149:PHE:H	1.09	1.07
1:A:66:MET:HE3	1:A:67:MET:N	1.68	1.06
1:A:254:SER:CB	1:A:399:GLN:HG2	1.84	1.05
1:A:402:PHE:CD1	1:A:429:LEU:HD21	1.93	1.02
1:A:299:MET:CE	1:A:322:GLY:HA2	1.90	1.00
1:A:66:MET:HE3	1:A:67:MET:H	1.27	0.99
1:A:173:MET:O	1:A:175:VAL:N	1.94	0.98
1:A:357:ALA:HA	1:A:360:SER:HB2	1.39	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:PHE:O	1:A:101:LEU:HD23	1.64	0.97
1:A:87:GLU:HB2	1:A:308:GLY:HA2	1.44	0.96
1:A:170:MET:O	1:A:174:ILE:HG23	1.65	0.96
1:A:96:VAL:HA	1:A:99:ASN:OD1	1.65	0.95
1:A:407:VAL:O	1:A:411:PRO:HD2	1.66	0.94
1:A:7:SER:HB2	1:A:223:THR:O	1.66	0.94
1:A:247:PRO:HG3	1:A:388:PRO:HB2	1.48	0.93
1:A:173:MET:O	1:A:176:PRO:HD2	1.69	0.92
1:A:373:GLY:O	1:A:377:VAL:HG23	1.69	0.92
1:A:78:ALA:HA	1:A:162:SER:CB	1.99	0.91
1:A:404:ILE:CG1	1:A:405:PRO:HD3	2.01	0.90
1:A:149:PHE:HD2	1:A:207:ALA:HA	1.37	0.90
1:A:149:PHE:CD2	1:A:207:ALA:HA	2.07	0.90
1:A:304:GLY:O	1:A:307:TYR:O	1.91	0.89
1:A:299:MET:HE3	1:A:322:GLY:HA2	1.54	0.89
1:A:354:VAL:O	1:A:358:GLY:HA3	1.73	0.89
1:A:353:GLU:HA	1:A:356:GLN:HB2	1.54	0.88
1:A:128:ALA:HB1	1:A:133:GLN:OE1	1.74	0.87
1:A:157:ASN:ND2	1:A:172:THR:OG1	2.09	0.86
1:A:87:GLU:HB2	1:A:308:GLY:CA	2.04	0.86
1:A:66:MET:CE	1:A:150:PHE:CE2	2.59	0.85
1:A:404:ILE:HG13	1:A:405:PRO:CD	2.05	0.85
1:A:19:LEU:HD12	1:A:321:LEU:HD23	1.59	0.85
1:A:411:PRO:HD3	1:A:418:GLY:HA3	1.56	0.85
1:A:62:ILE:O	1:A:65:ILE:HG12	1.76	0.85
1:A:244:VAL:O	1:A:247:PRO:HD2	1.75	0.84
1:A:334:PHE:HE1	1:A:367:CYS:HA	1.42	0.84
1:A:237:VAL:HA	1:A:240:GLU:HG3	1.59	0.82
1:A:35:LEU:O	1:A:38:VAL:HB	1.79	0.82
1:A:202:THR:O	1:A:202:THR:HG22	1.79	0.82
1:A:145:LEU:N	1:A:146:GLY:HA3	1.94	0.82
1:A:345:LEU:HG	1:A:359:VAL:HG23	1.62	0.81
1:A:299:MET:HE1	1:A:322:GLY:HA2	1.60	0.80
1:A:385:LEU:O	1:A:387:LYS:N	2.12	0.80
1:A:179:LEU:HD22	1:A:183:LEU:HG	1.62	0.80
1:A:442:ARG:O	1:A:446:PHE:HB3	1.82	0.80
1:A:188:ILE:HG23	1:A:189:PHE:H	1.45	0.80
1:A:96:VAL:HG22	1:A:237:VAL:HG11	1.63	0.79
1:A:224:LEU:O	1:A:226:LEU:CG	2.30	0.79
1:A:66:MET:HE2	1:A:150:PHE:CE2	2.17	0.79
1:A:420:TRP:O	1:A:424:PRO:HD2	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:MET:HE1	1:A:150:PHE:CD2	2.18	0.78
1:A:179:LEU:CD1	1:A:205:ALA:HA	2.13	0.78
1:A:227:HIS:CD2	1:A:231:LEU:HB2	2.17	0.78
1:A:254:SER:HB3	1:A:399:GLN:CG	2.05	0.78
1:A:365:LEU:HD23	1:A:366:PHE:CE1	2.18	0.78
1:A:37:ASN:OD1	1:A:283:ARG:HG2	1.84	0.78
1:A:101:LEU:HA	1:A:104:ILE:HD12	1.64	0.77
1:A:289:MET:HA	1:A:289:MET:CE	2.14	0.77
1:A:410:LEU:HD21	1:A:421:TRP:HB2	1.66	0.77
1:A:315:LEU:HD12	1:A:316:ARG:N	2.00	0.76
1:A:419:VAL:O	1:A:423:PHE:CD1	2.37	0.76
1:A:37:ASN:HB2	2:A:501:4YH:H34	1.66	0.76
1:A:161:ARG:HD3	1:A:300:GLN:HE22	1.49	0.75
1:A:67:MET:SD	2:A:501:4YH:H9	2.26	0.75
1:A:159:ILE:HD11	1:A:217:PHE:CZ	2.21	0.75
1:A:31:PHE:HA	1:A:290:MET:HE1	1.67	0.75
1:A:70:ALA:O	1:A:73:LEU:HB2	1.87	0.75
1:A:59:ALA:HB1	1:A:140:LEU:HD13	1.67	0.75
1:A:24:ILE:HG13	1:A:25:PRO:HD3	1.69	0.75
1:A:334:PHE:CE1	1:A:367:CYS:HA	2.23	0.74
1:A:283:ARG:O	1:A:287:PHE:HB2	1.87	0.74
1:A:9:ARG:NH2	1:A:305:TYR:HB2	2.02	0.74
1:A:218:LEU:O	1:A:221:LYS:HG2	1.88	0.74
1:A:209:VAL:O	1:A:212:LEU:N	2.22	0.73
1:A:364:ILE:CG2	1:A:367:CYS:SG	2.74	0.73
1:A:88:ARG:O	1:A:90:GLY:N	2.18	0.73
1:A:222:SER:O	1:A:226:LEU:HD11	1.87	0.73
1:A:233:MET:HG2	1:A:234:LYS:HG2	1.69	0.73
1:A:259:MET:HA	1:A:262:ILE:HG13	1.70	0.72
1:A:108:SER:OG	1:A:148:ILE:HA	1.89	0.72
1:A:72:ALA:HB1	1:A:245:GLY:HA3	1.71	0.72
1:A:382:TYR:OH	1:A:437:LEU:O	2.07	0.72
1:A:419:VAL:O	1:A:423:PHE:HD1	1.70	0.72
1:A:40:ASP:O	1:A:43:PHE:HB2	1.88	0.72
1:A:300:GLN:CB	1:A:301:PRO:HD3	2.20	0.71
1:A:357:ALA:HA	1:A:360:SER:CB	2.19	0.71
1:A:15:ILE:HA	1:A:18:LEU:HB2	1.72	0.71
1:A:66:MET:HE1	1:A:150:PHE:CE2	2.24	0.71
1:A:247:PRO:O	1:A:251:GLN:HG3	1.91	0.71
1:A:410:LEU:O	1:A:414:PHE:HB2	1.91	0.71
1:A:67:MET:SD	2:A:501:4YH:H19	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:PHE:HB3	1:A:61:PRO:HD3	1.72	0.71
1:A:66:MET:HB2	1:A:151:PHE:HE2	1.55	0.71
1:A:13:GLU:HG2	1:A:314:ARG:HD2	1.73	0.70
1:A:24:ILE:O	1:A:27:MET:HB2	1.91	0.70
1:A:290:MET:HG2	1:A:291:PRO:HD3	1.74	0.70
1:A:156:ALA:CB	1:A:213:VAL:HG11	2.21	0.69
1:A:149:PHE:HB3	1:A:206:GLN:O	1.93	0.69
1:A:13:GLU:OE2	1:A:306:ASN:ND2	2.26	0.69
1:A:170:MET:O	1:A:174:ILE:N	2.26	0.69
1:A:257:LEU:HD12	1:A:260:ILE:HD11	1.74	0.69
1:A:299:MET:CE	1:A:322:GLY:CA	2.69	0.69
1:A:9:ARG:HH22	1:A:86:GLY:N	1.91	0.69
1:A:227:HIS:HB3	1:A:231:LEU:HD22	1.75	0.69
1:A:289:MET:HA	1:A:289:MET:HE2	1.73	0.68
1:A:290:MET:O	1:A:291:PRO:C	2.31	0.68
1:A:320:MET:HB2	1:A:445:PHE:HE1	1.57	0.68
1:A:36:TYR:O	1:A:40:ASP:HB3	1.94	0.68
1:A:46:TYR:HB3	1:A:189:PHE:CZ	2.28	0.68
1:A:342:GLU:O	1:A:345:LEU:N	2.27	0.68
1:A:66:MET:CE	1:A:67:MET:H	2.04	0.68
1:A:302:ILE:C	1:A:304:GLY:H	1.96	0.68
1:A:78:ALA:CA	1:A:162:SER:HB2	2.18	0.68
1:A:188:ILE:HG23	1:A:189:PHE:N	2.08	0.68
1:A:179:LEU:HD12	1:A:205:ALA:HA	1.75	0.68
1:A:402:PHE:CG	1:A:429:LEU:HD21	2.27	0.68
1:A:66:MET:HE2	1:A:67:MET:HB2	1.74	0.68
1:A:76:GLY:C	1:A:241:VAL:HG22	2.14	0.68
1:A:147:SER:O	1:A:150:PHE:HB3	1.94	0.68
1:A:281:VAL:O	1:A:281:VAL:HG12	1.93	0.67
1:A:166:ALA:O	1:A:169:ALA:HB3	1.94	0.67
1:A:129:THR:HB	1:A:132:THR:HG22	1.77	0.67
1:A:407:VAL:O	1:A:411:PRO:CD	2.39	0.67
2:A:501:4YH:C11	2:A:501:4YH:H16	2.25	0.67
1:A:79:SER:OG	1:A:244:VAL:HG11	1.95	0.67
1:A:410:LEU:HB3	1:A:418:GLY:HA2	1.75	0.66
1:A:63:MET:O	1:A:66:MET:HG3	1.96	0.66
1:A:192:ASN:H	1:A:193:MET:HE3	1.60	0.66
1:A:290:MET:HG2	1:A:291:PRO:CD	2.25	0.66
1:A:142:PRO:CG	1:A:199:SER:HB2	2.26	0.66
1:A:370:PHE:HD2	1:A:370:PHE:N	1.94	0.66
1:A:115:ALA:HB2	1:A:144:LEU:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:SER:HA	1:A:401:ILE:HG12	1.78	0.66
1:A:188:ILE:CG2	1:A:189:PHE:H	2.09	0.65
1:A:301:PRO:HD2	1:A:302:ILE:H	1.62	0.65
1:A:187:PHE:HA	1:A:191:LEU:HD12	1.78	0.65
1:A:410:LEU:HD23	1:A:418:GLY:HA2	1.78	0.65
1:A:142:PRO:HG3	1:A:199:SER:OG	1.97	0.64
1:A:169:ALA:O	1:A:171:VAL:N	2.30	0.64
1:A:67:MET:SD	2:A:501:4YH:C11	2.86	0.64
1:A:92:GLU:O	1:A:95:GLN:HB3	1.97	0.64
1:A:152:PHE:HE2	1:A:213:VAL:HB	1.62	0.64
1:A:420:TRP:HZ3	1:A:421:TRP:CE3	2.14	0.64
1:A:54:ALA:O	1:A:58:ILE:HG13	1.97	0.64
1:A:247:PRO:HG2	1:A:383:GLN:NE2	2.14	0.63
1:A:428:VAL:HG12	1:A:429:LEU:N	2.13	0.63
1:A:67:MET:SD	2:A:501:4YH:C26	2.87	0.63
1:A:247:PRO:HG3	1:A:388:PRO:CB	2.26	0.63
1:A:167:THR:O	1:A:171:VAL:HG23	1.97	0.63
1:A:394:LEU:O	1:A:397:SER:OG	2.16	0.63
1:A:339:LEU:C	1:A:341:PRO:HD3	2.20	0.63
1:A:66:MET:HB2	1:A:151:PHE:CE2	2.33	0.63
1:A:93:ALA:O	1:A:94:ASN:C	2.36	0.63
1:A:24:ILE:HD12	1:A:25:PRO:N	2.14	0.62
1:A:148:ILE:CG1	1:A:149:PHE:N	2.48	0.62
1:A:222:SER:O	1:A:224:LEU:N	2.32	0.62
1:A:18:LEU:O	1:A:22:LEU:HB2	1.99	0.62
1:A:370:PHE:N	1:A:370:PHE:CD2	2.65	0.62
1:A:64:MET:HG2	1:A:256:SER:HB3	1.81	0.62
1:A:9:ARG:NH2	1:A:85:LEU:HB3	2.14	0.62
1:A:145:LEU:H	1:A:146:GLY:HA3	1.64	0.62
2:A:501:4YH:C28	2:A:501:4YH:H9	2.30	0.62
1:A:160:ILE:HG22	1:A:217:PHE:HZ	1.65	0.61
1:A:160:ILE:HD11	1:A:169:ALA:HA	1.83	0.61
1:A:184:ASP:O	1:A:185:VAL:C	2.39	0.61
1:A:253:SER:HA	1:A:256:SER:OG	2.00	0.61
1:A:394:LEU:HD13	1:A:437:LEU:HD12	1.83	0.61
2:A:501:4YH:C11	2:A:501:4YH:C28	2.79	0.61
1:A:6:GLN:O	1:A:6:GLN:HG3	2.00	0.61
1:A:300:GLN:HB2	1:A:301:PRO:HD3	1.82	0.61
1:A:66:MET:CE	1:A:67:MET:HB2	2.30	0.61
1:A:339:LEU:N	1:A:341:PRO:HD3	2.16	0.61
1:A:37:ASN:O	1:A:38:VAL:C	2.37	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PRO:O	1:A:65:ILE:HG23	2.01	0.61
1:A:27:MET:SD	1:A:294:GLY:HA3	2.40	0.60
1:A:363:HIS:O	1:A:365:LEU:N	2.33	0.60
1:A:247:PRO:CG	1:A:388:PRO:HB2	2.29	0.60
1:A:407:VAL:HG12	1:A:411:PRO:HG2	1.84	0.60
1:A:66:MET:HE2	1:A:150:PHE:HE2	1.66	0.60
1:A:169:ALA:O	1:A:172:THR:N	2.35	0.60
1:A:281:VAL:HA	1:A:284:ILE:HD11	1.84	0.60
1:A:80:VAL:HG12	1:A:81:ILE:N	2.15	0.60
1:A:174:ILE:O	1:A:178:VAL:HG22	2.02	0.60
1:A:283:ARG:H	1:A:283:ARG:HD2	1.66	0.60
1:A:46:TYR:HB3	1:A:189:PHE:HZ	1.66	0.60
1:A:361:ALA:O	1:A:365:LEU:HB2	2.02	0.59
1:A:36:TYR:HA	1:A:181:ILE:HD11	1.84	0.59
1:A:41:THR:HA	1:A:44:ILE:HD12	1.84	0.59
1:A:102:THR:HG21	1:A:233:MET:O	2.02	0.59
1:A:202:THR:O	1:A:202:THR:CG2	2.49	0.59
1:A:24:ILE:HD12	1:A:24:ILE:C	2.22	0.59
1:A:410:LEU:HB3	1:A:418:GLY:CA	2.32	0.59
1:A:89:ARG:O	1:A:91:GLU:N	2.36	0.59
1:A:15:ILE:HD13	1:A:15:ILE:O	2.02	0.59
1:A:26:ALA:O	1:A:27:MET:C	2.38	0.59
1:A:250:VAL:HG12	1:A:251:GLN:N	2.18	0.59
1:A:142:PRO:HG3	1:A:199:SER:CB	2.33	0.58
1:A:46:TYR:CB	1:A:189:PHE:HZ	2.16	0.58
2:A:501:4YH:H13	2:A:501:4YH:C26	2.33	0.58
1:A:237:VAL:HG13	1:A:240:GLU:HB2	1.84	0.58
1:A:251:GLN:HG2	1:A:395:SER:OG	2.04	0.58
1:A:420:TRP:CZ3	1:A:421:TRP:CD2	2.92	0.58
2:A:501:4YH:H13	2:A:501:4YH:H20	1.86	0.57
1:A:274:TYR:O	1:A:277:VAL:HG22	2.04	0.57
1:A:160:ILE:HG22	1:A:217:PHE:CZ	2.39	0.57
1:A:141:PHE:N	1:A:142:PRO:HD2	2.20	0.57
1:A:332:GLY:O	1:A:333:ILE:C	2.43	0.57
1:A:299:MET:HE1	1:A:322:GLY:CA	2.33	0.57
1:A:282:GLN:O	1:A:285:MET:N	2.35	0.57
1:A:337:LEU:HD21	1:A:366:PHE:CG	2.40	0.57
1:A:28:ILE:O	1:A:32:VAL:HG23	2.05	0.57
1:A:82:SER:HB2	1:A:304:GLY:HA3	1.87	0.57
1:A:13:GLU:CG	1:A:314:ARG:HD2	2.34	0.57
1:A:195:VAL:O	1:A:197:GLY:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLY:O	1:A:377:VAL:CG2	2.50	0.57
1:A:38:VAL:HG12	1:A:39:VAL:HG13	1.87	0.57
1:A:120:GLY:O	1:A:121:PRO:C	2.42	0.57
1:A:156:ALA:HB1	1:A:213:VAL:HG11	1.86	0.57
1:A:278:PHE:O	1:A:282:GLN:NE2	2.38	0.57
1:A:353:GLU:CA	1:A:356:GLN:HB2	2.32	0.57
1:A:9:ARG:C	1:A:11:GLY:H	2.08	0.57
1:A:423:PHE:HB2	1:A:424:PRO:CD	2.35	0.57
1:A:428:VAL:CG1	1:A:429:LEU:N	2.68	0.57
1:A:25:PRO:HA	1:A:170:MET:SD	2.44	0.56
1:A:338:MET:HA	1:A:341:PRO:HG3	1.87	0.56
1:A:23:SER:OG	1:A:24:ILE:N	2.38	0.56
1:A:142:PRO:HG2	1:A:199:SER:HB2	1.86	0.56
1:A:87:GLU:H	1:A:308:GLY:HA3	1.71	0.56
1:A:148:ILE:HG13	1:A:149:PHE:CD1	2.40	0.56
1:A:361:ALA:O	1:A:365:LEU:CB	2.54	0.56
1:A:30:MET:HB3	1:A:290:MET:SD	2.45	0.56
1:A:409:ILE:HG22	1:A:409:ILE:O	2.06	0.56
1:A:76:GLY:HA2	1:A:244:VAL:HB	1.88	0.56
1:A:374:ALA:O	1:A:376:ILE:N	2.38	0.56
1:A:420:TRP:HZ3	1:A:421:TRP:CD2	2.24	0.56
1:A:428:VAL:HG13	1:A:432:ILE:CD1	2.36	0.56
1:A:13:GLU:HG3	1:A:15:ILE:HG22	1.87	0.55
1:A:436:VAL:O	1:A:440:ARG:HB2	2.06	0.55
1:A:11:GLY:HA2	1:A:305:TYR:CZ	2.42	0.55
1:A:179:LEU:HD22	1:A:183:LEU:CG	2.35	0.55
1:A:364:ILE:O	1:A:364:ILE:HG22	2.06	0.55
1:A:410:LEU:CD2	1:A:421:TRP:HB2	2.36	0.55
1:A:98:GLY:O	1:A:101:LEU:HB2	2.07	0.55
1:A:157:ASN:HA	1:A:160:ILE:HG12	1.88	0.55
1:A:350:ALA:HB3	1:A:354:VAL:HG21	1.88	0.55
1:A:126:PHE:HB3	1:A:264:SER:HB2	1.89	0.55
1:A:303:VAL:HG13	1:A:315:LEU:HD22	1.89	0.54
1:A:364:ILE:HG22	1:A:420:TRP:HZ2	1.72	0.54
1:A:68:SER:HB2	1:A:252:GLN:HB2	1.88	0.54
1:A:16:PRO:HD2	1:A:17:LYS:N	2.22	0.54
1:A:9:ARG:HH21	1:A:85:LEU:HB3	1.71	0.54
1:A:358:GLY:O	1:A:362:MET:HG2	2.07	0.54
1:A:290:MET:HB3	1:A:291:PRO:HD2	1.89	0.54
1:A:36:TYR:O	1:A:37:ASN:O	2.25	0.54
1:A:327:THR:HA	1:A:330:SER:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLY:HA3	1:A:267:LEU:HG	1.90	0.54
1:A:63:MET:CB	2:A:501:4YH:H24	2.38	0.54
1:A:9:ARG:NH2	1:A:86:GLY:N	2.56	0.54
1:A:345:LEU:HG	1:A:359:VAL:CG2	2.37	0.53
1:A:325:VAL:O	1:A:328:ILE:HG22	2.07	0.53
1:A:13:GLU:CD	1:A:306:ASN:HD21	2.12	0.53
1:A:374:ALA:C	1:A:376:ILE:H	2.12	0.53
1:A:180:ASN:O	1:A:184:ASP:CG	2.47	0.53
1:A:96:VAL:HG13	1:A:100:ILE:HD11	1.90	0.53
1:A:31:PHE:C	1:A:31:PHE:CD2	2.82	0.53
1:A:191:LEU:HB3	1:A:193:MET:HE3	1.91	0.53
1:A:402:PHE:O	1:A:406:LEU:HB2	2.08	0.53
1:A:4:LYS:HD3	1:A:5:GLN:H	1.73	0.53
1:A:31:PHE:CZ	1:A:35:LEU:HD21	2.44	0.52
1:A:365:LEU:HA	1:A:424:PRO:HG3	1.90	0.52
1:A:167:THR:O	1:A:170:MET:HB3	2.09	0.52
1:A:37:ASN:HB2	2:A:501:4YH:C33	2.35	0.52
1:A:302:ILE:HG22	1:A:303:VAL:N	2.24	0.52
1:A:9:ARG:HH22	1:A:86:GLY:H	1.57	0.52
1:A:219:THR:O	1:A:220:GLY:C	2.47	0.52
1:A:283:ARG:CD	1:A:283:ARG:H	2.21	0.52
1:A:84:ARG:HD3	1:A:92:GLU:HG2	1.90	0.52
1:A:46:TYR:CB	1:A:189:PHE:CZ	2.92	0.52
1:A:49:GLY:N	1:A:51:GLU:OE2	2.42	0.52
1:A:410:LEU:O	1:A:414:PHE:N	2.43	0.52
1:A:180:ASN:HA	1:A:183:LEU:HB2	1.92	0.52
1:A:385:LEU:HG	1:A:385:LEU:O	2.09	0.52
1:A:266:LEU:HD22	1:A:278:PHE:CD1	2.45	0.51
1:A:126:PHE:HB3	1:A:264:SER:CB	2.40	0.51
1:A:431:PHE:O	1:A:434:THR:HG22	2.09	0.51
1:A:409:ILE:CG2	1:A:409:ILE:O	2.59	0.51
1:A:420:TRP:CZ3	1:A:421:TRP:CE3	2.97	0.51
1:A:368:VAL:HG21	1:A:424:PRO:HA	1.92	0.51
1:A:97:PHE:CE1	1:A:101:LEU:HD21	2.45	0.51
1:A:302:ILE:C	1:A:304:GLY:N	2.63	0.51
1:A:101:LEU:CA	1:A:104:ILE:HD12	2.38	0.51
1:A:209:VAL:HG23	1:A:210:THR:H	1.76	0.51
1:A:114:SER:HA	1:A:118:LEU:HD12	1.92	0.51
1:A:85:LEU:O	1:A:87:GLU:N	2.44	0.51
1:A:102:THR:CG2	1:A:232:ARG:HD2	2.41	0.51
1:A:252:GLN:O	1:A:254:SER:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ILE:HG22	1:A:114:SER:N	2.25	0.51
1:A:175:VAL:O	1:A:179:LEU:HB2	2.11	0.51
1:A:414:PHE:O	1:A:417:SER:OG	2.29	0.51
1:A:37:ASN:ND2	2:A:501:4YH:O20	2.44	0.50
1:A:152:PHE:O	1:A:155:ALA:HB3	2.11	0.50
1:A:176:PRO:HD3	1:A:209:VAL:CG1	2.41	0.50
1:A:398:ARG:HA	1:A:430:SER:OG	2.12	0.50
1:A:279:GLY:O	1:A:282:GLN:HG2	2.11	0.50
1:A:382:TYR:HE1	1:A:437:LEU:HD13	1.76	0.50
1:A:301:PRO:CD	1:A:302:ILE:H	2.25	0.50
1:A:410:LEU:CB	1:A:418:GLY:HA2	2.42	0.50
1:A:423:PHE:HB2	1:A:424:PRO:HD3	1.94	0.50
1:A:375:GLN:OE1	1:A:431:PHE:HB2	2.12	0.50
1:A:51:GLU:CD	1:A:52:GLY:H	2.14	0.50
1:A:217:PHE:O	1:A:218:LEU:HD23	2.11	0.50
1:A:225:SER:O	1:A:226:LEU:HD23	2.11	0.50
1:A:161:ARG:HD3	1:A:300:GLN:NE2	2.22	0.50
1:A:370:PHE:HD2	1:A:370:PHE:H	1.58	0.50
2:A:501:4YH:H16	2:A:501:4YH:H9	1.94	0.50
1:A:266:LEU:HD13	1:A:278:PHE:HE1	1.77	0.49
1:A:359:VAL:HG13	1:A:359:VAL:O	2.11	0.49
1:A:76:GLY:HA3	1:A:241:VAL:HG13	1.94	0.49
1:A:9:ARG:HD3	1:A:11:GLY:HA3	1.93	0.49
1:A:223:THR:O	1:A:224:LEU:HG	2.11	0.49
1:A:181:ILE:HG22	1:A:182:LEU:HD23	1.94	0.49
1:A:288:VAL:HG13	1:A:333:ILE:HG12	1.94	0.49
1:A:53:VAL:O	1:A:56:VAL:HB	2.13	0.49
1:A:224:LEU:C	1:A:226:LEU:HG	2.27	0.49
1:A:244:VAL:HA	1:A:388:PRO:CG	2.42	0.49
1:A:300:GLN:CB	1:A:301:PRO:CD	2.90	0.49
1:A:423:PHE:O	1:A:424:PRO:C	2.50	0.49
1:A:145:LEU:N	1:A:146:GLY:CA	2.72	0.49
1:A:382:TYR:CD1	1:A:390:GLN:HG3	2.47	0.49
1:A:237:VAL:HA	1:A:240:GLU:CG	2.37	0.49
1:A:169:ALA:O	1:A:170:MET:C	2.51	0.49
1:A:230:ASP:O	1:A:231:LEU:C	2.51	0.49
1:A:27:MET:HE1	1:A:295:ILE:HD13	1.95	0.49
1:A:340:PHE:N	1:A:341:PRO:HD3	2.28	0.49
1:A:293:MET:CE	1:A:376:ILE:HD11	2.43	0.49
1:A:43:PHE:HB3	1:A:188:ILE:HD12	1.93	0.49
1:A:142:PRO:CG	1:A:199:SER:CB	2.90	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:SER:O	1:A:46:TYR:CD1	2.66	0.48
1:A:297:GLN:HA	1:A:300:GLN:HG3	1.95	0.48
1:A:31:PHE:N	1:A:290:MET:SD	2.86	0.48
1:A:32:VAL:O	1:A:35:LEU:N	2.46	0.48
1:A:63:MET:HB3	2:A:501:4YH:H24	1.94	0.48
1:A:15:ILE:O	1:A:15:ILE:CG1	2.60	0.48
1:A:16:PRO:CD	1:A:17:LYS:N	2.65	0.48
1:A:22:LEU:HA	1:A:22:LEU:HD23	1.49	0.48
1:A:102:THR:HG22	1:A:232:ARG:HH11	1.78	0.48
1:A:197:GLY:HA2	1:A:200:ILE:HG12	1.95	0.48
1:A:281:VAL:O	1:A:281:VAL:CG1	2.62	0.48
1:A:321:LEU:O	1:A:322:GLY:C	2.52	0.48
1:A:367:CYS:O	1:A:367:CYS:SG	2.71	0.48
1:A:125:LEU:O	1:A:126:PHE:HB2	2.14	0.48
1:A:150:PHE:CE2	1:A:154:PHE:HE1	2.32	0.47
1:A:221:LYS:HD2	1:A:226:LEU:O	2.14	0.47
1:A:94:ASN:HD21	1:A:227:HIS:HB2	1.78	0.47
2:A:501:4YH:H13	2:A:501:4YH:C25	2.44	0.47
1:A:299:MET:O	1:A:300:GLN:C	2.53	0.47
1:A:254:SER:HB2	1:A:399:GLN:HG2	1.89	0.47
1:A:6:GLN:HG2	1:A:88:ARG:HH21	1.78	0.47
1:A:167:THR:O	1:A:170:MET:CB	2.63	0.47
1:A:31:PHE:HA	1:A:290:MET:CE	2.39	0.47
1:A:255:ALA:O	1:A:258:MET:HG3	2.15	0.47
1:A:416:LEU:HD12	1:A:419:VAL:HB	1.96	0.47
1:A:98:GLY:HA2	1:A:101:LEU:HG	1.96	0.47
1:A:227:HIS:HD2	1:A:231:LEU:HB2	1.71	0.47
1:A:66:MET:CE	1:A:150:PHE:HE2	2.22	0.47
1:A:20:ARG:HD3	1:A:20:ARG:HA	1.69	0.47
1:A:397:SER:HA	1:A:401:ILE:CG1	2.44	0.47
1:A:40:ASP:OD1	1:A:41:THR:HG23	2.15	0.47
1:A:72:ALA:O	1:A:73:LEU:C	2.53	0.47
1:A:179:LEU:HD13	1:A:183:LEU:HD12	1.95	0.47
1:A:431:PHE:C	1:A:431:PHE:CD2	2.88	0.47
1:A:97:PHE:CD1	1:A:97:PHE:C	2.88	0.47
1:A:270:GLY:HA3	1:A:274:TYR:CD1	2.50	0.46
1:A:17:LYS:HA	1:A:20:ARG:HB2	1.97	0.46
1:A:193:MET:HB2	1:A:197:GLY:HA3	1.97	0.46
1:A:259:MET:HA	1:A:262:ILE:CG1	2.42	0.46
1:A:188:ILE:CG2	1:A:189:PHE:N	2.73	0.46
1:A:359:VAL:HA	1:A:362:MET:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ILE:H	1:A:58:ILE:HG13	1.59	0.46
1:A:258:MET:O	1:A:261:ALA:HB3	2.15	0.46
1:A:352:ARG:O	1:A:356:GLN:HG3	2.15	0.46
1:A:9:ARG:HH21	1:A:305:TYR:HB2	1.79	0.46
1:A:66:MET:CE	1:A:67:MET:N	2.59	0.46
1:A:182:LEU:HD23	1:A:182:LEU:N	2.31	0.46
1:A:237:VAL:O	1:A:240:GLU:N	2.48	0.46
1:A:128:ALA:CB	1:A:133:GLN:OE1	2.56	0.46
1:A:169:ALA:C	1:A:171:VAL:N	2.69	0.46
1:A:178:VAL:O	1:A:182:LEU:HG	2.16	0.46
1:A:217:PHE:HD2	1:A:226:LEU:HD13	1.81	0.46
1:A:441:ASP:O	1:A:443:ASN:N	2.42	0.46
1:A:96:VAL:O	1:A:100:ILE:HG12	2.16	0.46
1:A:176:PRO:O	1:A:177:ALA:C	2.53	0.46
1:A:299:MET:HE3	1:A:322:GLY:CA	2.34	0.46
1:A:177:ALA:O	1:A:178:VAL:C	2.55	0.45
1:A:25:PRO:HB2	1:A:166:ALA:HB1	1.97	0.45
1:A:149:PHE:CD2	1:A:207:ALA:CA	2.91	0.45
1:A:66:MET:HE3	1:A:67:MET:CA	2.43	0.45
1:A:93:ALA:O	1:A:96:VAL:N	2.48	0.45
1:A:181:ILE:O	1:A:184:ASP:N	2.49	0.45
1:A:183:LEU:HA	1:A:183:LEU:HD23	1.65	0.45
1:A:192:ASN:O	1:A:194:GLY:N	2.49	0.45
1:A:174:ILE:O	1:A:177:ALA:HB3	2.17	0.45
1:A:310:LYS:HB3	1:A:311:GLN:OE1	2.16	0.45
1:A:163:GLU:HG3	1:A:164:GLY:H	1.81	0.45
1:A:80:VAL:O	1:A:82:SER:N	2.50	0.45
1:A:67:MET:HB3	1:A:67:MET:HE2	1.89	0.45
1:A:120:GLY:N	1:A:121:PRO:HD2	2.32	0.45
1:A:382:TYR:CE1	1:A:437:LEU:HD13	2.51	0.45
1:A:437:LEU:HD23	1:A:437:LEU:HA	1.60	0.45
1:A:187:PHE:CE2	1:A:200:ILE:HD11	2.52	0.45
1:A:306:ASN:HA	1:A:310:LYS:HB2	1.98	0.45
1:A:97:PHE:CD1	1:A:101:LEU:HD21	2.52	0.45
1:A:222:SER:O	1:A:226:LEU:CD1	2.61	0.44
1:A:52:GLY:O	1:A:55:GLY:N	2.50	0.44
1:A:65:ILE:HG13	1:A:66:MET:N	2.32	0.44
1:A:147:SER:O	1:A:150:PHE:CB	2.65	0.44
1:A:181:ILE:N	1:A:181:ILE:HD13	2.33	0.44
1:A:184:ASP:O	1:A:186:LEU:N	2.50	0.44
1:A:187:PHE:O	1:A:188:ILE:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:O	1:A:39:VAL:HG22	2.16	0.44
1:A:428:VAL:HG13	1:A:432:ILE:HD12	1.98	0.44
1:A:193:MET:HE3	1:A:193:MET:H	1.82	0.44
1:A:35:LEU:O	1:A:36:TYR:C	2.54	0.44
1:A:279:GLY:O	1:A:283:ARG:HD2	2.17	0.44
1:A:200:ILE:HG13	1:A:201:ALA:N	2.32	0.44
1:A:6:GLN:HA	1:A:224:LEU:HD21	1.99	0.44
1:A:278:PHE:O	1:A:279:GLY:C	2.56	0.44
1:A:19:LEU:CD2	1:A:298:ALA:HB1	2.48	0.44
1:A:303:VAL:HG12	1:A:303:VAL:O	2.17	0.44
1:A:320:MET:HB2	1:A:445:PHE:CE1	2.45	0.44
1:A:330:SER:OG	1:A:373:GLY:N	2.49	0.44
1:A:96:VAL:O	1:A:97:PHE:C	2.56	0.44
1:A:101:LEU:O	1:A:104:ILE:HB	2.17	0.44
1:A:156:ALA:HB1	1:A:213:VAL:CG1	2.48	0.44
1:A:16:PRO:CD	1:A:17:LYS:H	2.31	0.44
1:A:182:LEU:HD23	1:A:182:LEU:H	1.81	0.44
1:A:339:LEU:C	1:A:341:PRO:CD	2.85	0.44
1:A:400:ILE:O	1:A:402:PHE:N	2.51	0.44
1:A:40:ASP:OD1	1:A:41:THR:N	2.51	0.44
1:A:124:GLN:O	1:A:126:PHE:N	2.51	0.43
1:A:374:ALA:C	1:A:376:ILE:N	2.71	0.43
1:A:88:ARG:C	1:A:90:GLY:H	2.14	0.43
1:A:368:VAL:HG11	1:A:427:ASP:HB2	1.98	0.43
1:A:151:PHE:O	1:A:152:PHE:C	2.56	0.43
1:A:168:PHE:O	1:A:168:PHE:CD2	2.72	0.43
1:A:374:ALA:O	1:A:377:VAL:N	2.51	0.43
1:A:364:ILE:CG2	1:A:420:TRP:HZ2	2.31	0.43
1:A:287:PHE:C	1:A:287:PHE:CD2	2.91	0.43
1:A:302:ILE:O	1:A:304:GLY:N	2.49	0.43
1:A:100:ILE:O	1:A:104:ILE:HG13	2.19	0.43
1:A:27:MET:SD	1:A:27:MET:N	2.91	0.43
1:A:107:LEU:HA	1:A:110:ILE:HD13	2.01	0.43
1:A:203:VAL:C	1:A:205:ALA:N	2.71	0.43
1:A:26:ALA:O	1:A:28:ILE:N	2.51	0.43
1:A:290:MET:CG	1:A:291:PRO:CD	2.96	0.43
1:A:368:VAL:HA	1:A:370:PHE:HE2	1.83	0.43
1:A:420:TRP:O	1:A:421:TRP:C	2.57	0.43
1:A:89:ARG:O	1:A:92:GLU:N	2.50	0.43
1:A:364:ILE:O	1:A:364:ILE:CG2	2.66	0.43
1:A:55:GLY:HA2	1:A:58:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:GLU:O	1:A:243:LEU:HB2	2.18	0.43
1:A:244:VAL:HA	1:A:388:PRO:HG3	2.01	0.43
1:A:288:VAL:O	1:A:288:VAL:HG13	2.19	0.43
1:A:359:VAL:O	1:A:359:VAL:CG1	2.66	0.43
1:A:24:ILE:HA	1:A:27:MET:HB2	2.00	0.43
1:A:51:GLU:CD	1:A:52:GLY:N	2.72	0.43
1:A:104:ILE:O	1:A:107:LEU:N	2.52	0.42
1:A:300:GLN:O	1:A:384:SER:HB3	2.19	0.42
1:A:316:ARG:HA	1:A:319:VAL:HG22	2.00	0.42
1:A:389:LYS:O	1:A:393:ILE:HD12	2.19	0.42
1:A:63:MET:HB2	2:A:501:4YH:H24	2.00	0.42
1:A:266:LEU:HD22	1:A:278:PHE:CE1	2.54	0.42
1:A:387:LYS:C	1:A:389:LYS:H	2.21	0.42
1:A:37:ASN:HB3	1:A:38:VAL:H	1.57	0.42
2:A:501:4YH:H15	2:A:501:4YH:H9	2.02	0.42
1:A:15:ILE:O	1:A:15:ILE:CD1	2.66	0.42
1:A:272:ASP:O	1:A:274:TYR:N	2.53	0.42
1:A:180:ASN:HA	1:A:180:ASN:HD22	1.62	0.42
1:A:193:MET:CE	1:A:193:MET:H	2.33	0.42
1:A:261:ALA:O	1:A:263:ASN:N	2.52	0.42
1:A:120:GLY:O	1:A:123:LEU:N	2.53	0.42
1:A:154:PHE:O	1:A:158:ASN:HB2	2.20	0.42
1:A:283:ARG:O	1:A:287:PHE:CB	2.64	0.42
1:A:215:ARG:C	1:A:217:PHE:H	2.21	0.42
1:A:82:SER:HB2	1:A:304:GLY:CA	2.49	0.42
1:A:372:ILE:O	1:A:372:ILE:HG23	2.19	0.42
1:A:7:SER:CB	1:A:223:THR:O	2.53	0.42
1:A:392:LEU:O	1:A:393:ILE:C	2.58	0.42
1:A:19:LEU:CD2	1:A:298:ALA:CB	2.97	0.42
1:A:62:ILE:HB	1:A:140:LEU:HD21	2.01	0.42
1:A:242:CYS:O	1:A:246:LEU:N	2.48	0.41
1:A:36:TYR:C	1:A:36:TYR:CD2	2.92	0.41
1:A:244:VAL:HA	1:A:388:PRO:HG2	2.00	0.41
1:A:9:ARG:NH2	1:A:86:GLY:H	2.17	0.41
1:A:56:VAL:O	1:A:59:ALA:HB3	2.19	0.41
1:A:119:LEU:HB3	1:A:120:GLY:H	1.63	0.41
1:A:144:LEU:O	1:A:147:SER:OG	2.39	0.41
1:A:224:LEU:HB3	1:A:225:SER:H	1.51	0.41
1:A:252:GLN:C	1:A:254:SER:N	2.74	0.41
1:A:37:ASN:HA	1:A:37:ASN:HD22	1.65	0.41
1:A:364:ILE:C	1:A:420:TRP:HE1	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:C	1:A:109:VAL:N	2.74	0.41
1:A:15:ILE:HD12	1:A:314:ARG:O	2.21	0.41
1:A:206:GLN:HA	1:A:209:VAL:CG2	2.50	0.41
1:A:19:LEU:HD22	1:A:298:ALA:CB	2.51	0.41
1:A:339:LEU:CA	1:A:341:PRO:HD3	2.50	0.41
1:A:214:LEU:O	1:A:218:LEU:N	2.53	0.41
1:A:441:ASP:C	1:A:443:ASN:H	2.23	0.41
1:A:56:VAL:O	1:A:60:PHE:N	2.52	0.41
1:A:9:ARG:C	1:A:11:GLY:N	2.73	0.41
1:A:290:MET:CB	1:A:291:PRO:CD	2.99	0.41
1:A:87:GLU:HB2	1:A:308:GLY:C	2.41	0.41
1:A:172:THR:O	1:A:176:PRO:HD2	2.20	0.41
1:A:155:ALA:O	1:A:156:ALA:C	2.59	0.41
1:A:195:VAL:C	1:A:197:GLY:N	2.73	0.41
1:A:301:PRO:CD	1:A:302:ILE:N	2.83	0.41
1:A:366:PHE:HA	1:A:368:VAL:HG23	2.03	0.41
1:A:58:ILE:O	1:A:61:PRO:HD2	2.21	0.41
1:A:112:PHE:O	1:A:115:ALA:HB3	2.20	0.41
1:A:300:GLN:HB3	1:A:301:PRO:HD3	2.01	0.41
1:A:400:ILE:O	1:A:403:LEU:N	2.54	0.41
1:A:84:ARG:HA	1:A:87:GLU:O	2.21	0.41
1:A:28:ILE:HB	1:A:170:MET:SD	2.61	0.41
1:A:370:PHE:CD2	1:A:371:LEU:N	2.89	0.41
1:A:445:PHE:CE2	1:A:448:LYS:HB3	2.56	0.41
1:A:97:PHE:HD1	1:A:97:PHE:C	2.24	0.41
1:A:285:MET:O	1:A:289:MET:HG2	2.21	0.40
1:A:290:MET:O	1:A:291:PRO:O	2.39	0.40
1:A:290:MET:CB	1:A:291:PRO:HD2	2.51	0.40
1:A:298:ALA:O	1:A:301:PRO:HD2	2.21	0.40
1:A:148:ILE:CG1	1:A:149:PHE:CD1	3.04	0.40
1:A:86:GLY:HA2	1:A:310:LYS:CG	2.51	0.40
1:A:89:ARG:HB3	1:A:92:GLU:HB3	2.03	0.40
1:A:441:ASP:C	1:A:443:ASN:N	2.75	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	444/464 (96%)	251 (56%)	118 (27%)	75 (17%)	0 0

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	15	ILE
1	A	16	PRO
1	A	37	ASN
1	A	38	VAL
1	A	56	VAL
1	A	89	ARG
1	A	90	GLY
1	A	93	ALA
1	A	119	LEU
1	A	170	MET
1	A	174	ILE
1	A	177	ALA
1	A	185	VAL
1	A	188	ILE
1	A	196	LEU
1	A	223	THR
1	A	261	ALA
1	A	291	PRO
1	A	300	GLN
1	A	303	VAL
1	A	375	GLN
1	A	386	GLY
1	A	413	ILE
1	A	6	GLN
1	A	23	SER
1	A	81	ILE
1	A	94	ASN

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Mol	Chain	Res	Type
1	A	126	PHE
1	A	193	MET
1	A	210	THR
1	A	229	SER
1	A	253	SER
1	A	290	MET
1	A	310	LYS
1	A	322	GLY
1	A	342	GLU
1	A	343	ALA
1	A	364	ILE
1	A	392	LEU
1	A	393	ILE
1	A	442	ARG
1	A	10	LEU
1	A	97	PHE
1	A	173	MET
1	A	187	PHE
1	A	262	ILE
1	A	273	PHE
1	A	301	PRO
1	A	420	TRP
1	A	104	ILE
1	A	128	ALA
1	A	164	GLY
1	A	169	ALA
1	A	181	ILE
1	A	279	GLY
1	A	423	PHE
1	A	26	ALA
1	A	102	THR
1	A	121	PRO
1	A	184	ASP
1	A	216	TYR
1	A	283	ARG
1	A	340	PHE
1	A	363	HIS
1	A	410	LEU
1	A	80	VAL
1	A	116	PHE
1	A	194	GLY
1	A	368	VAL

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Mol	Chain	Res	Type
1	A	148	ILE
1	A	32	VAL
1	A	333	ILE
1	A	401	ILE
1	A	195	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	366/383 (96%)	269 (74%)	97 (26%)	0 2

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	15	ILE
1	A	22	LEU
1	A	27	MET
1	A	28	ILE
1	A	37	ASN
1	A	40	ASP
1	A	48	VAL
1	A	50	ILE
1	A	51	GLU
1	A	58	ILE
1	A	66	MET
1	A	67	MET
1	A	85	LEU
1	A	91	GLU
1	A	97	PHE
1	A	99	ASN
1	A	101	LEU
1	A	103	VAL
1	A	108	SER
1	A	109	VAL

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Mol	Chain	Res	Type
1	A	117	THR
1	A	119	LEU
1	A	123	LEU
1	A	126	PHE
1	A	131	VAL
1	A	141	PHE
1	A	147	SER
1	A	148	ILE
1	A	158	ASN
1	A	159	ILE
1	A	167	THR
1	A	168	PHE
1	A	171	VAL
1	A	173	MET
1	A	174	ILE
1	A	175	VAL
1	A	178	VAL
1	A	179	LEU
1	A	180	ASN
1	A	181	ILE
1	A	182	LEU
1	A	186	LEU
1	A	188	ILE
1	A	193	MET
1	A	196	LEU
1	A	203	VAL
1	A	209	VAL
1	A	214	LEU
1	A	222	SER
1	A	223	THR
1	A	224	LEU
1	A	226	LEU
1	A	228	TRP
1	A	230	ASP
1	A	232	ARG
1	A	241	VAL
1	A	246	LEU
1	A	262	ILE
1	A	266	LEU
1	A	267	LEU
1	A	268	ARG
1	A	271	SER

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Mol	Chain	Res	Type
1	A	278	PHE
1	A	283	ARG
1	A	284	ILE
1	A	285	MET
1	A	288	VAL
1	A	291	PRO
1	A	292	MET
1	A	299	MET
1	A	305	TYR
1	A	315	LEU
1	A	327	THR
1	A	330	SER
1	A	331	ILE
1	A	336	LEU
1	A	345	LEU
1	A	348	PHE
1	A	356	GLN
1	A	359	VAL
1	A	363	HIS
1	A	368	VAL
1	A	370	PHE
1	A	372	ILE
1	A	375	GLN
1	A	381	LEU
1	A	384	SER
1	A	406	LEU
1	A	407	VAL
1	A	428	VAL
1	A	429	LEU
1	A	432	ILE
1	A	433	LEU
1	A	434	THR
1	A	441	ASP
1	A	446	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	180	ASN
1	A	227	HIS
1	A	251	GLN

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Mol	Chain	Res	Type
1	A	300	GLN
1	A	306	ASN
1	A	412	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
2	4YH	A	501	-	32,34,34	1.79	5 (15%)	36,46,46	1.78	8 (22%)

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	4YH	A	501	-	-	16/32/35/35	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	4YH	O23-C32	5.76	1.60	1.42
2	A	501	4YH	C1-C2	-4.45	1.44	1.53
2	A	501	4YH	C21-C17	-4.32	1.39	1.51
2	A	501	4YH	C3-N4	3.93	1.20	1.14
2	A	501	4YH	O19-C30	2.01	1.48	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	4YH	C33-O24-C10	-5.45	109.30	117.53
2	A	501	4YH	C30-O19-C6	-3.54	112.19	117.53
2	A	501	4YH	O23-C9-C6	3.43	120.18	115.41
2	A	501	4YH	O24-C10-C7	2.70	119.17	115.41
2	A	501	4YH	O24-C10-C14	-2.68	119.78	124.37
2	A	501	4YH	O20-C7-C10	2.62	119.06	115.41
2	A	501	4YH	C11-C2-C1	2.32	124.68	120.79
2	A	501	4YH	O23-C9-C13	-2.09	120.78	124.37

There are no chirality outliers.

All (16) torsion outliers are listed below:

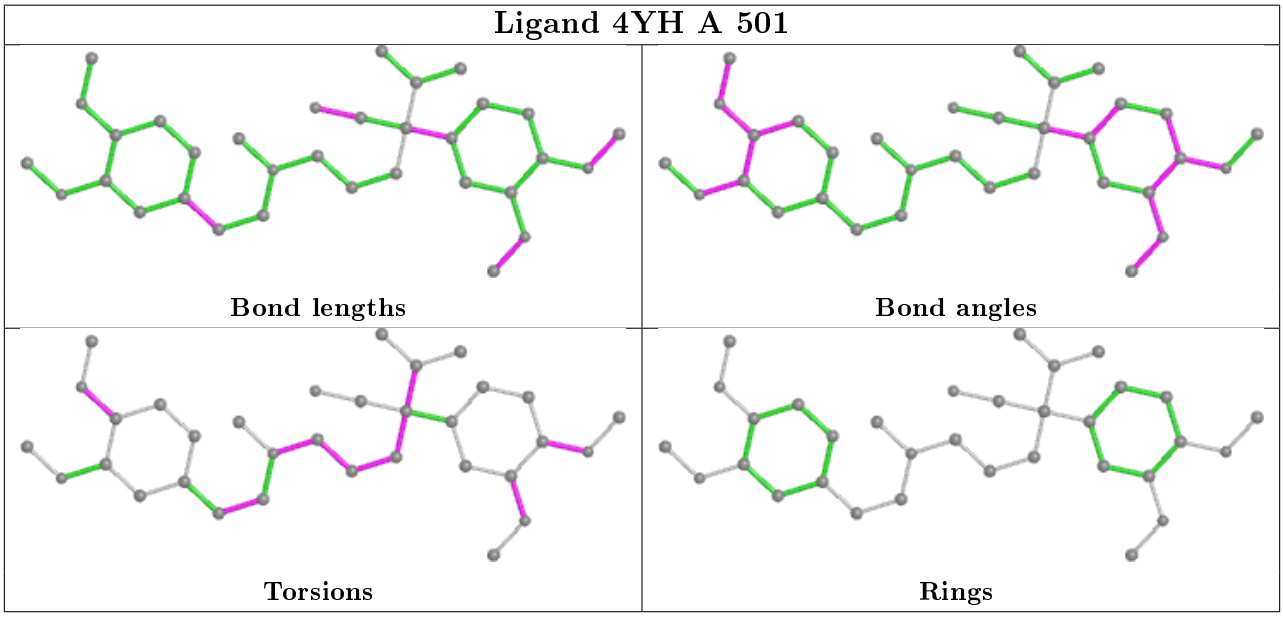
Mol	Chain	Res	Type	Atoms
2	A	501	4YH	C2-C1-C22-C26
2	A	501	4YH	C15-C1-C22-C26
2	A	501	4YH	C3-C1-C22-C26
2	A	501	4YH	C26-C25-N8-C27
2	A	501	4YH	N8-C16-C21-C17
2	A	501	4YH	C5-C6-O19-C30
2	A	501	4YH	C9-C6-O19-C30
2	A	501	4YH	C7-C10-O24-C33
2	A	501	4YH	C14-C10-O24-C33
2	A	501	4YH	C13-C9-O23-C32
2	A	501	4YH	C6-C9-O23-C32
2	A	501	4YH	C26-C25-N8-C16
2	A	501	4YH	N8-C25-C26-C22
2	A	501	4YH	C3-C1-C15-C28
2	A	501	4YH	C1-C22-C26-C25
2	A	501	4YH	C22-C1-C15-C28

There are no ring outliers.

1 monomer is involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	4YH	18	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	446/464 (96%)	0.52	58 (13%) 3 1	139, 230, 336, 469	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	MET	11.5
1	A	447	LEU	10.8
1	A	364	ILE	9.2
1	A	87	GLU	9.1
1	A	235	GLY	8.5
1	A	416	LEU	8.2
1	A	234	LYS	8.1
1	A	271	SER	7.8
1	A	270	GLY	7.0
1	A	269	PHE	6.6
1	A	308	GLY	6.3
1	A	127	GLY	6.1
1	A	229	SER	6.0
1	A	129	THR	6.0
1	A	116	PHE	5.9
1	A	399	GLN	5.6
1	A	227	HIS	5.5
1	A	219	THR	5.5
1	A	162	SER	5.3
1	A	417	SER	5.2
1	A	363	HIS	5.1
1	A	226	LEU	5.1
1	A	343	ALA	4.8
1	A	228	TRP	4.1
1	A	346	ARG	3.9
1	A	352	ARG	3.8
1	A	230	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	411	PRO	3.7
1	A	415	GLY	3.7
1	A	388	PRO	3.6
1	A	49	GLY	3.6
1	A	312	TYR	3.4
1	A	418	GLY	3.3
1	A	191	LEU	3.1
1	A	225	SER	3.0
1	A	149	PHE	3.0
1	A	249	PHE	3.0
1	A	398	ARG	3.0
1	A	386	GLY	3.0
1	A	309	ALA	3.0
1	A	232	ARG	2.9
1	A	409	ILE	2.9
1	A	439	TYR	2.8
1	A	274	TYR	2.7
1	A	440	ARG	2.7
1	A	413	ILE	2.6
1	A	130	SER	2.5
1	A	128	ALA	2.5
1	A	7	SER	2.5
1	A	112	PHE	2.4
1	A	445	PHE	2.2
1	A	105	LEU	2.2
1	A	362	MET	2.1
1	A	236	SER	2.1
1	A	143	ILE	2.1
1	A	94	ASN	2.1
1	A	272	ASP	2.0
1	A	135	TYR	2.0

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

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

6.3 Carbohydrates (i)

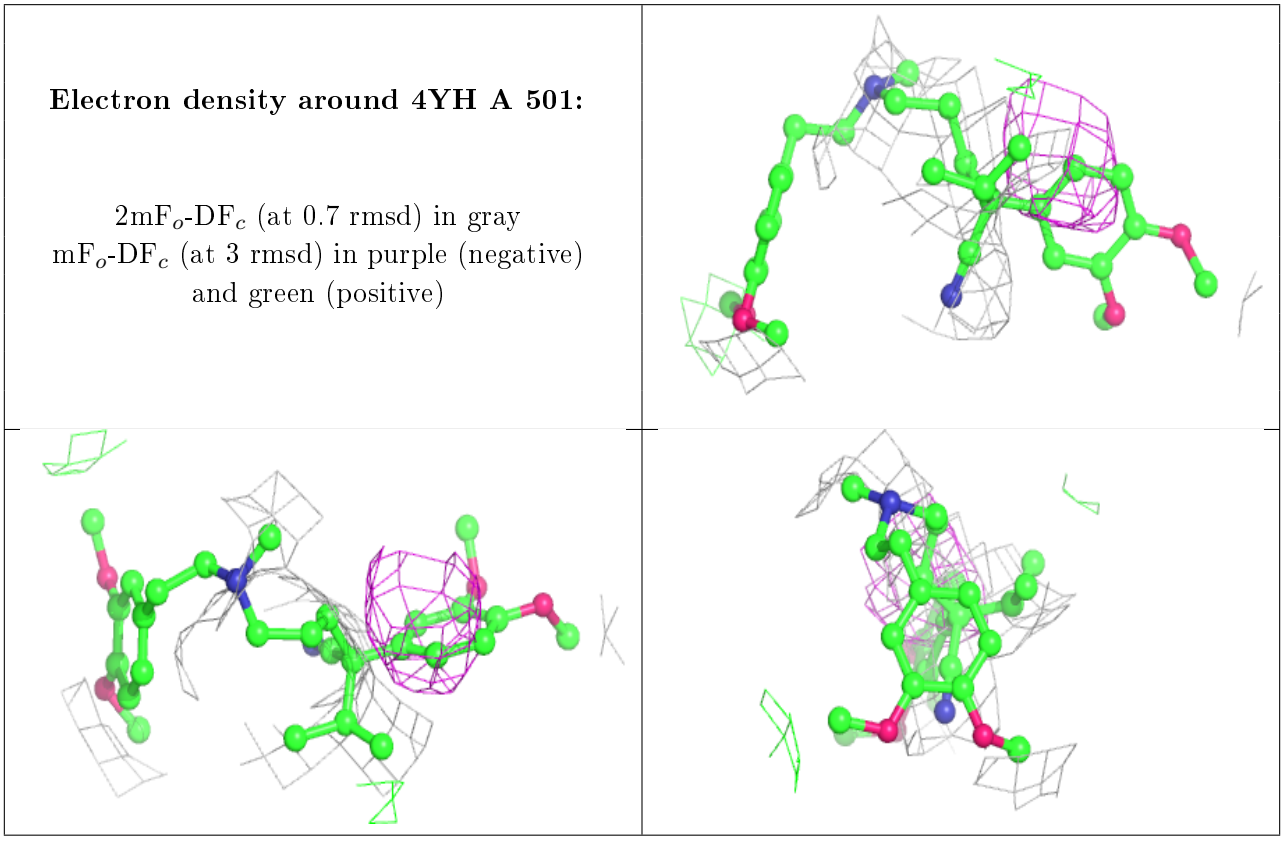
There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	4YH	A	501	33/33	0.31	0.68	379,379,379,379	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers

There are no such residues in this entry.