Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 11:09 PM EDT

PDB ID	:	4AGW
Title	:	Discovery of a small molecule type II inhibitor of wild-type and gatekeeper mutants of BCR-ABL, PDGFRalpha, Kit, and Src kinases
Authors	:	Weisberg, E.; Choi, H.G.; Seeliger, M.; Gray, N.; Griffin, J.D.
Deposited on	:	2012-02-01
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

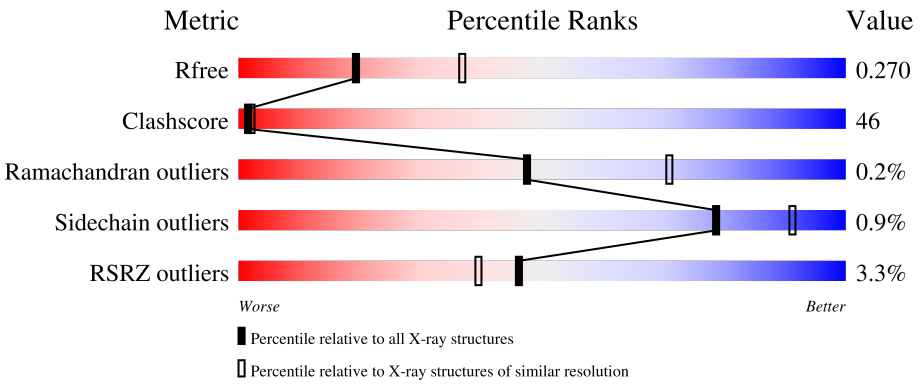
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	286	5% 32% 56% • 10%
1	B	286	% 31% 57% • 10%

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	MES	A	1535	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4419 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.

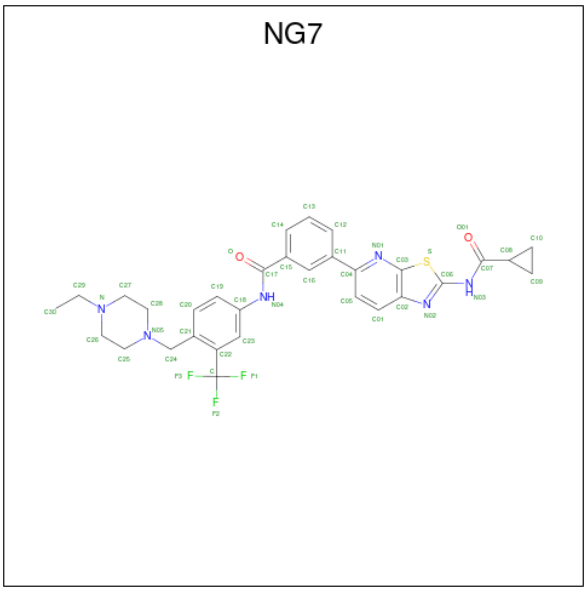
- Molecule 1 is a protein called PROTO-ONCOGENE TYROSINE-PROTEIN KINASE SRC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	258	2080	1334	347	382	17	0	0	0
1	B	257	2071	1328	345	381	17	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

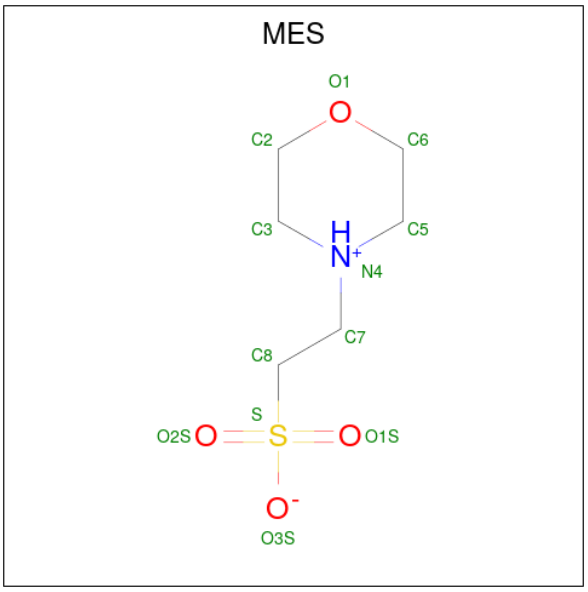
Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	expression tag	UNP P00523
A	249	HIS	-	expression tag	UNP P00523
A	250	MET	-	expression tag	UNP P00523
B	248	GLY	-	expression tag	UNP P00523
B	249	HIS	-	expression tag	UNP P00523
B	250	MET	-	expression tag	UNP P00523

- Molecule 2 is 3-{2-[(cyclopropylcarbonyl)amino][1,3]thiazolo[5,4-b]pyridin-5-yl}-N-{4-[(4-ethylpiperazin-1-yl)methyl]-3-(trifluoromet hyl)phenyl}benzamide (three-letter code: NG7) (formula: $C_{31}H_{31}F_3N_6O_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
2	A	1	43	31	3	6	2	1	0	0
			Total	C	F	N	O	S		
2	B	1	43	31	3	6	2	1	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



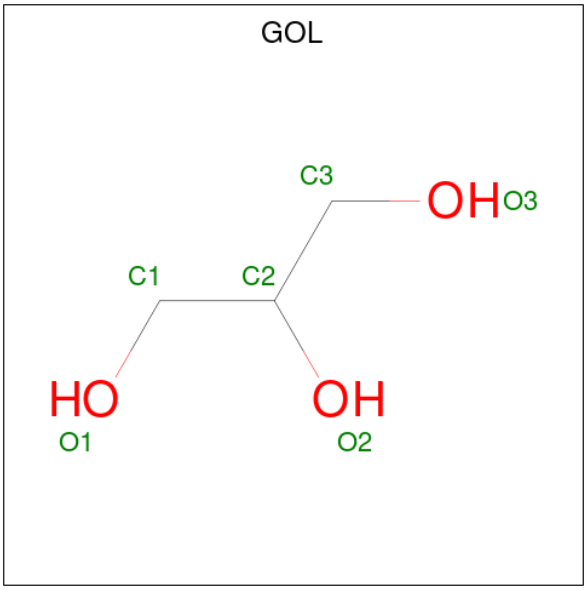
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	12	6	1	4	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	B	1	12	6	1	4	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	A	1	6	3	3		0	0

- Molecule 5 is water.

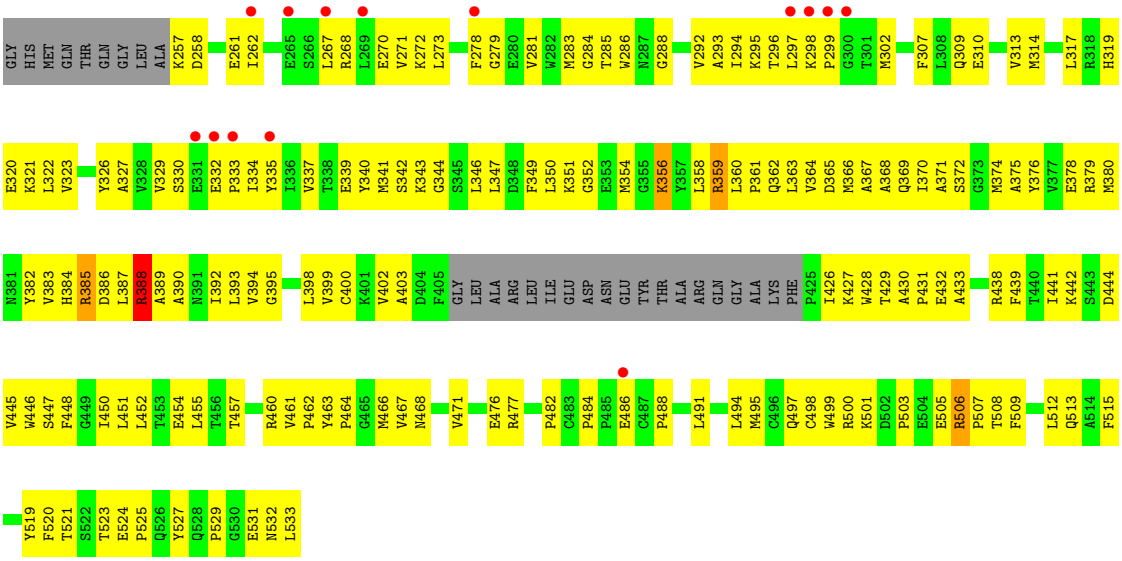
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O			
5	A	74	74	74		0	0
			Total	O			
5	B	78	78	78		0	0

3 Residue-property plots (i)

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

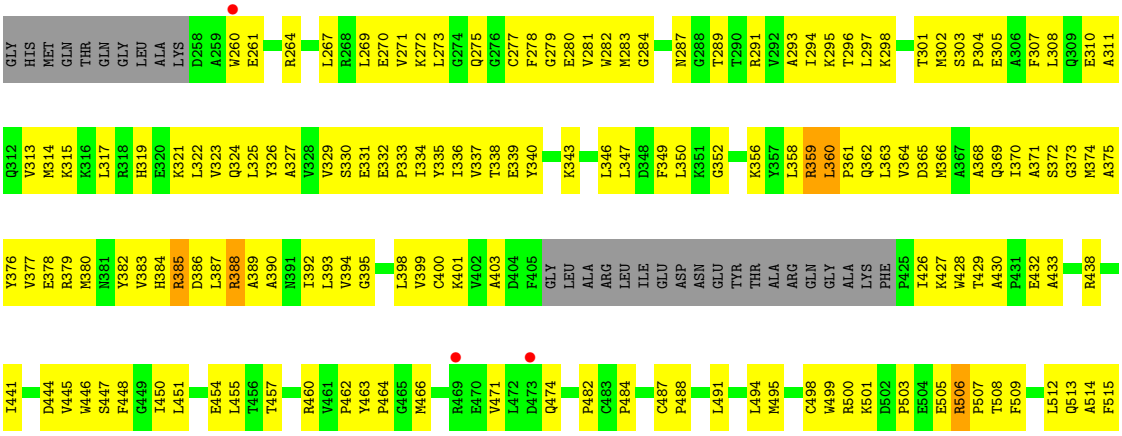
• Molecule 1: PROTO-ONCOGENE TYROSINE-PROTEIN KINASE SRC

Chain A:



• Molecule 1: PROTO-ONCOGENE TYROSINE-PROTEIN KINASE SRC

Chain B:



D518
Y519
F520
T521
S522
T523
E524
P525
Q526
Y527
Q528
P529
G530
E531
N532
L533

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	40.74Å 61.39Å 71.81Å 79.57° 89.10° 90.14°	Depositor
Resolution (Å)	42.27 – 2.60 42.27 – 2.36	Depositor EDS
% Data completeness (in resolution range)	92.2 (42.27-2.60) 81.8 (42.27-2.36)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.62 (at 2.37Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.226 , 0.271 0.226 , 0.270	Depositor DCC
R_{free} test set	2010 reflections (8.00%)	wwPDB-VP
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4419	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.5126e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, NG7, GOL

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	0.50	0/2131	0.98	14/2884 (0.5%)
1	B	0.52	0/2122	0.92	14/2873 (0.5%)
All	All	0.51	0/4253	0.95	28/5757 (0.5%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	379	ARG	NE-CZ-NH2	-13.60	113.50	120.30
1	A	359	ARG	NE-CZ-NH2	-13.34	113.63	120.30
1	A	359	ARG	NE-CZ-NH1	13.32	126.96	120.30
1	A	388	ARG	NE-CZ-NH2	-13.29	113.66	120.30
1	A	379	ARG	NE-CZ-NH1	13.23	126.92	120.30
1	A	388	ARG	NE-CZ-NH1	12.96	126.78	120.30
1	B	385	ARG	NE-CZ-NH2	-12.90	113.85	120.30
1	B	359	ARG	NE-CZ-NH2	-12.88	113.86	120.30
1	B	379	ARG	NE-CZ-NH1	11.82	126.21	120.30
1	B	379	ARG	NE-CZ-NH2	-11.78	114.41	120.30
1	B	359	ARG	NE-CZ-NH1	11.69	126.14	120.30
1	A	385	ARG	NE-CZ-NH2	-11.62	114.49	120.30
1	A	506	ARG	NE-CZ-NH2	-11.11	114.74	120.30
1	A	385	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	B	385	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	B	388	ARG	NE-CZ-NH2	-10.63	114.99	120.30
1	B	388	ARG	NE-CZ-NH1	10.10	125.35	120.30
1	A	506	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	B	506	ARG	NE-CZ-NH2	-8.33	116.13	120.30
1	B	506	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	379	ARG	CD-NE-CZ	6.82	133.15	123.60
1	A	359	ARG	CD-NE-CZ	6.40	132.56	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	359	ARG	CD-NE-CZ	6.16	132.22	123.60
1	B	379	ARG	CD-NE-CZ	6.00	132.00	123.60
1	A	388	ARG	CD-NE-CZ	5.79	131.70	123.60
1	B	385	ARG	CD-NE-CZ	5.56	131.39	123.60
1	A	385	ARG	CD-NE-CZ	5.49	131.28	123.60
1	B	388	ARG	CD-NE-CZ	5.47	131.26	123.60

There are no chirality outliers.

There are no planarity outliers.

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	2080	0	2067	204	0
1	B	2071	0	2054	179	0
2	A	43	0	30	20	0
2	B	43	0	31	8	0
3	A	12	0	12	6	0
3	B	12	0	12	5	0
4	A	6	0	8	0	0
5	A	74	0	0	16	0
5	B	78	0	0	7	0
All	All	4419	0	4214	388	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 46.

All (388) 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:295:LYS:HB2	2:A:1534:NG7:H13	1.34	1.04
1:A:460:ARG:NE	1:B:518:ASP:OD2	1.95	1.00
1:A:383:VAL:H	3:A:1535:MES:H21	1.31	0.96
1:B:273:LEU:HB2	1:B:281:VAL:HG12	1.51	0.92
1:A:363:LEU:HD23	1:A:366:MET:CE	2.00	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:LEU:HD23	1:B:366:MET:CE	2.01	0.90
1:B:362:GLN:O	1:B:366:MET:HG3	1.74	0.88
1:A:362:GLN:O	1:A:366:MET:HG3	1.74	0.88
1:A:494:LEU:HD22	1:A:515:PHE:CE1	2.10	0.87
1:A:385:ARG:HD3	2:A:1534:NG7:H29	1.58	0.85
1:B:273:LEU:HD11	1:B:283:MET:HB2	1.60	0.84
1:A:297:LEU:HD23	1:A:334:ILE:HD12	1.60	0.83
2:B:1534:NG7:H26	3:B:1535:MES:H61	1.60	0.83
2:A:1534:NG7:C20	2:A:1534:NG7:H28A	2.06	0.82
1:B:349:PHE:HE1	1:B:358:LEU:HD11	1.45	0.80
1:A:385:ARG:CD	2:A:1534:NG7:H29	2.12	0.80
1:A:349:PHE:HE1	1:A:358:LEU:HD11	1.46	0.79
1:B:321:LYS:HD2	1:B:369:GLN:HB3	1.65	0.78
1:A:310:GLU:HB3	5:A:2004:HOH:O	1.84	0.77
1:B:295:LYS:O	1:B:335:TYR:HA	1.84	0.77
1:A:374:MET:HB3	1:A:509:PHE:CD2	2.20	0.76
1:B:494:LEU:HD22	1:B:515:PHE:CE1	2.21	0.75
1:B:501:LYS:HG2	5:B:2058:HOH:O	1.86	0.75
1:A:363:LEU:HD23	1:A:366:MET:HE2	1.68	0.74
2:A:1534:NG7:H28A	2:A:1534:NG7:H20	1.68	0.73
1:B:466:MET:HE2	1:B:471:VAL:HG22	1.71	0.73
1:A:262:ILE:HG12	1:A:327:ALA:HB1	1.70	0.73
1:B:349:PHE:CE1	1:B:358:LEU:HD11	2.24	0.73
1:B:332:GLU:HG2	1:B:334:ILE:HG13	1.71	0.73
1:A:349:PHE:CE1	1:A:358:LEU:HD11	2.24	0.72
1:A:494:LEU:HD22	1:A:515:PHE:CD1	2.24	0.72
1:A:383:VAL:HG12	1:A:385:ARG:HG3	1.71	0.72
1:A:295:LYS:CB	2:A:1534:NG7:H13	2.16	0.72
1:A:521:THR:O	1:A:525:PRO:HG3	1.89	0.71
1:A:466:MET:HE2	1:A:471:VAL:HG22	1.71	0.70
1:A:356:LYS:O	1:A:359:ARG:NH2	2.20	0.70
1:B:521:THR:O	1:B:525:PRO:HG3	1.91	0.70
1:A:461:VAL:HG21	1:B:521:THR:HB	1.74	0.70
1:B:494:LEU:HD22	1:B:515:PHE:CD1	2.27	0.69
1:A:283:MET:HG3	1:A:340:TYR:CE1	2.27	0.69
1:A:383:VAL:N	3:A:1535:MES:H21	2.04	0.69
1:B:303:SER:OG	1:B:305:GLU:HG2	1.93	0.69
1:A:486:GLU:OE1	5:A:2060:HOH:O	2.11	0.69
1:A:491:LEU:O	1:A:495:MET:HG3	1.91	0.69
1:A:320:GLU:HG2	1:A:321:LYS:HD3	1.74	0.68
1:A:477:ARG:NH1	5:A:2049:HOH:O	2.17	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:LEU:HD23	1:B:366:MET:HE2	1.75	0.68
1:B:428:TRP:HE1	1:B:454:GLU:CD	1.97	0.68
1:A:387:LEU:O	1:A:447:SER:HB3	1.93	0.67
1:B:313:VAL:HG11	2:B:1534:NG7:H25	1.77	0.67
1:B:491:LEU:O	1:B:495:MET:HG3	1.95	0.67
1:A:313:VAL:HG11	2:A:1534:NG7:H25	1.76	0.67
1:B:278:PHE:CD1	1:B:302:MET:HB2	2.29	0.67
1:B:500:ARG:HD2	1:B:505:GLU:HB3	1.77	0.67
2:B:1534:NG7:H26	3:B:1535:MES:C6	2.24	0.67
1:B:374:MET:HB3	1:B:509:PHE:CD2	2.30	0.67
1:B:314:MET:HE2	1:B:325:LEU:HB2	1.76	0.67
1:B:323:VAL:CG2	1:B:393:LEU:HD12	2.25	0.66
1:A:294:ILE:HG12	1:A:337:VAL:HG22	1.78	0.66
1:A:428:TRP:HE1	1:A:454:GLU:CD	1.97	0.66
1:B:501:LYS:O	1:B:503:PRO:HD3	1.95	0.66
1:B:384:HIS:O	1:B:385:ARG:HB2	1.96	0.66
1:B:297:LEU:HB3	1:B:334:ILE:HB	1.79	0.65
1:A:273:LEU:HD11	1:A:283:MET:HB2	1.79	0.65
1:A:296:THR:HG22	1:A:335:TYR:CD1	2.31	0.65
1:A:432:GLU:OE2	1:A:506:ARG:NH2	2.29	0.65
1:A:500:ARG:HD2	1:A:505:GLU:HB3	1.79	0.65
1:A:354:MET:SD	5:A:2009:HOH:O	2.55	0.64
1:B:324:GLN:H	1:B:339:GLU:HG2	1.63	0.64
1:B:388:ARG:HD3	5:B:2034:HOH:O	1.96	0.64
1:A:329:VAL:HB	1:A:335:TYR:H	1.62	0.64
1:A:323:VAL:HG21	1:A:403:ALA:HB2	1.78	0.64
1:A:515:PHE:O	5:A:2066:HOH:O	2.15	0.64
1:A:344:GLY:HA2	2:A:1534:NG7:C07	2.29	0.63
1:A:446:TRP:CE3	1:A:499:TRP:HA	2.34	0.63
1:B:386:ASP:O	1:B:388:ARG:HG2	1.99	0.63
1:B:329:VAL:HA	5:B:2002:HOH:O	1.97	0.63
1:B:366:MET:O	1:B:370:ILE:HG13	1.99	0.63
1:B:387:LEU:O	1:B:447:SER:HB3	1.99	0.63
1:B:365:ASP:O	1:B:369:GLN:HG3	1.98	0.62
1:A:386:ASP:O	1:A:388:ARG:HG2	1.99	0.62
1:B:280:GLU:H	1:B:296:THR:HB	1.65	0.62
1:B:362:GLN:HB3	1:B:398:LEU:HD13	1.81	0.62
1:A:278:PHE:O	1:A:297:LEU:HD12	2.00	0.62
1:A:388:ARG:HD3	5:A:2026:HOH:O	1.98	0.61
1:B:323:VAL:HG21	1:B:403:ALA:HB2	1.81	0.61
1:A:321:LYS:HE3	1:A:369:GLN:HB3	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:GLY:HA3	5:A:2011:HOH:O	1.99	0.61
1:A:393:LEU:HD13	2:A:1534:NG7:C01	2.30	0.61
1:A:393:LEU:O	1:A:400:CYS:HA	2.00	0.61
1:A:384:HIS:O	1:A:385:ARG:HB2	2.01	0.61
1:B:298:LYS:HD3	1:B:301:THR:HG21	1.82	0.61
1:A:501:LYS:O	1:A:503:PRO:HD3	2.01	0.61
1:A:376:TYR:O	1:A:380:MET:HG2	2.00	0.60
1:B:393:LEU:O	1:B:400:CYS:HA	2.02	0.60
1:A:385:ARG:HD3	2:A:1534:NG7:C29	2.30	0.60
1:B:323:VAL:HG21	1:B:393:LEU:HD12	1.83	0.60
1:A:378:GLU:HB3	5:A:2019:HOH:O	2.02	0.60
1:A:346:LEU:HD21	1:A:455:LEU:HD21	1.83	0.60
1:A:362:GLN:HB3	1:A:398:LEU:HD13	1.84	0.59
1:A:267:LEU:HD11	1:A:337:VAL:HG21	1.84	0.59
1:A:309:GLN:HG3	5:A:2003:HOH:O	2.02	0.59
1:B:283:MET:HG3	1:B:340:TYR:CE1	2.38	0.59
1:B:310:GLU:O	1:B:314:MET:HG3	2.02	0.59
1:A:362:GLN:HB3	1:A:398:LEU:CD1	2.32	0.59
1:B:376:TYR:O	1:B:380:MET:HG2	2.03	0.58
1:A:346:LEU:N	1:A:392:ILE:O	2.35	0.58
1:B:297:LEU:HD23	1:B:334:ILE:HD12	1.83	0.58
1:B:310:GLU:CG	2:B:1534:NG7:H19	2.33	0.58
1:A:432:GLU:HB2	1:A:438:ARG:HD2	1.86	0.58
1:B:361:PRO:HD3	1:B:527:TYR:CZ	2.39	0.58
1:B:326:TYR:CE1	1:B:339:GLU:HB3	2.38	0.58
1:B:446:TRP:CE3	1:B:499:TRP:HA	2.37	0.58
1:A:366:MET:O	1:A:370:ILE:HG13	2.04	0.57
1:A:344:GLY:HA3	2:A:1534:NG7:H09	1.86	0.57
1:B:346:LEU:HD21	1:B:455:LEU:HD21	1.86	0.57
1:B:323:VAL:CG2	1:B:403:ALA:HB2	2.34	0.57
1:A:430:ALA:HB2	1:A:446:TRP:CB	2.34	0.57
1:A:295:LYS:HB2	2:A:1534:NG7:C13	2.23	0.57
1:B:311:ALA:HB2	1:B:336:ILE:CD1	2.34	0.57
1:B:329:VAL:HB	1:B:335:TYR:HB2	1.87	0.57
1:B:363:LEU:HD23	1:B:366:MET:HE3	1.84	0.57
1:A:283:MET:HG3	1:A:340:TYR:CZ	2.39	0.56
1:B:520:PHE:O	1:B:525:PRO:HA	2.05	0.56
1:A:360:LEU:HD23	1:A:520:PHE:CE1	2.39	0.56
1:A:395:GLY:N	1:A:399:VAL:O	2.30	0.56
1:B:362:GLN:HB3	1:B:398:LEU:CD1	2.35	0.56
1:B:432:GLU:HB2	1:B:438:ARG:HD2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ASP:O	1:A:369:GLN:HG3	2.04	0.56
1:B:514:ALA:HB2	5:B:2070:HOH:O	2.06	0.56
1:A:375:ALA:HA	1:A:509:PHE:HB2	1.87	0.56
1:B:372:SER:HA	1:B:513:GLN:OE1	2.05	0.56
1:A:520:PHE:O	1:A:525:PRO:HA	2.07	0.55
1:B:269:LEU:HB3	1:B:282:TRP:CE3	2.41	0.55
1:B:360:LEU:HD13	1:B:520:PHE:CZ	2.41	0.55
1:B:346:LEU:N	1:B:392:ILE:O	2.32	0.55
1:B:375:ALA:HA	1:B:509:PHE:HB2	1.88	0.55
1:A:372:SER:HA	1:A:513:GLN:OE1	2.06	0.55
1:A:323:VAL:CG2	1:A:403:ALA:HB2	2.37	0.55
1:A:332:GLU:HA	1:A:333:PRO:C	2.28	0.55
1:A:445:VAL:HG13	1:A:512:LEU:HD11	1.88	0.55
1:A:363:LEU:HD13	1:A:455:LEU:O	2.07	0.55
1:B:395:GLY:N	1:B:399:VAL:O	2.33	0.55
1:A:486:GLU:HA	5:A:2059:HOH:O	2.05	0.54
1:A:310:GLU:O	1:A:314:MET:HG3	2.07	0.54
1:A:494:LEU:HD11	1:A:512:LEU:HD23	1.89	0.54
1:B:304:PRO:HB3	1:B:334:ILE:HD11	1.90	0.54
1:A:361:PRO:HD3	1:A:527:TYR:CZ	2.41	0.54
1:A:330:SER:O	1:A:334:ILE:HG12	2.07	0.54
1:A:344:GLY:CA	2:A:1534:NG7:H09	2.37	0.54
1:A:441:ILE:O	1:A:444:ASP:HB2	2.08	0.54
1:A:532:ASN:O	1:A:533:LEU:HD23	2.08	0.53
1:A:273:LEU:HB2	1:A:281:VAL:HG12	1.90	0.53
1:B:466:MET:HE2	1:B:471:VAL:CG2	2.38	0.53
1:B:445:VAL:HG13	1:B:512:LEU:HD11	1.91	0.53
1:A:426:ILE:C	1:A:426:ILE:HD12	2.29	0.53
1:B:311:ALA:O	1:B:315:LYS:HG3	2.09	0.53
1:A:486:GLU:CD	5:A:2060:HOH:O	2.47	0.53
1:A:524:GLU:HA	5:A:2071:HOH:O	2.08	0.52
1:B:302:MET:SD	1:B:307:PHE:HB2	2.49	0.52
1:B:500:ARG:CD	1:B:505:GLU:HB3	2.39	0.52
1:B:383:VAL:H	3:B:1535:MES:C6	2.23	0.52
1:B:441:ILE:O	1:B:444:ASP:HB2	2.09	0.52
1:A:267:LEU:HD21	1:A:337:VAL:HG21	1.91	0.52
1:B:445:VAL:HG22	1:B:509:PHE:CE1	2.44	0.52
1:A:500:ARG:CD	1:A:505:GLU:HB3	2.40	0.52
1:B:293:ALA:HB3	1:B:338:THR:OG1	2.10	0.52
1:B:310:GLU:HG2	2:B:1534:NG7:H19	1.91	0.52
1:A:531:GLU:OE1	1:A:531:GLU:HA	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ALA:HB2	1:B:446:TRP:CB	2.40	0.52
1:B:332:GLU:HA	1:B:333:PRO:C	2.29	0.52
1:A:382:TYR:HA	3:A:1535:MES:H32	1.91	0.52
1:B:264:ARG:NH2	1:B:331:GLU:O	2.43	0.52
1:A:319:HIS:CD2	1:A:376:TYR:HB2	2.45	0.52
1:A:344:GLY:N	2:A:1534:NG7:H09	2.25	0.52
1:B:457:THR:HB	1:B:460:ARG:HB2	1.92	0.52
1:A:273:LEU:HD12	1:A:281:VAL:HG12	1.92	0.51
1:A:359:ARG:HB3	1:A:533:LEU:OXT	2.09	0.51
1:A:359:ARG:O	1:A:363:LEU:HG	2.10	0.51
1:A:273:LEU:N	1:A:281:VAL:O	2.43	0.51
1:A:279:GLY:HA2	1:A:298:LYS:HG3	1.92	0.51
1:A:297:LEU:HD21	1:A:302:MET:O	2.11	0.51
1:B:494:LEU:HD11	1:B:512:LEU:HD23	1.92	0.51
1:A:271:VAL:HG12	1:A:272:LYS:O	2.11	0.51
1:A:361:PRO:HA	1:A:520:PHE:CE2	2.46	0.51
1:B:532:ASN:O	1:B:533:LEU:HD23	2.11	0.51
1:B:361:PRO:HA	1:B:520:PHE:CE2	2.46	0.51
2:B:1534:NG7:H20	2:B:1534:NG7:H28A	1.92	0.51
1:A:428:TRP:HA	1:A:450:ILE:HG13	1.92	0.50
1:A:445:VAL:HG22	1:A:509:PHE:CE1	2.46	0.50
1:B:363:LEU:HD13	1:B:455:LEU:O	2.11	0.50
1:A:297:LEU:HD11	1:A:302:MET:HB3	1.93	0.50
1:A:363:LEU:HD23	1:A:366:MET:HE3	1.90	0.50
1:B:369:GLN:O	1:B:372:SER:HB3	2.11	0.50
1:A:508:THR:O	1:A:512:LEU:HG	2.11	0.50
1:B:352:GLY:HA3	5:B:2014:HOH:O	2.12	0.50
1:A:363:LEU:HA	1:A:366:MET:HE3	1.93	0.50
1:A:446:TRP:HA	1:A:498:CYS:O	2.11	0.50
1:B:297:LEU:HB2	1:B:307:PHE:CD2	2.47	0.50
1:B:445:VAL:CG2	1:B:509:PHE:CE1	2.95	0.50
1:A:364:VAL:HB	1:A:520:PHE:HE2	1.77	0.49
1:B:426:ILE:HD12	1:B:426:ILE:C	2.32	0.49
1:A:341:MET:O	2:A:1534:NG7:N03	2.45	0.49
1:B:359:ARG:O	1:B:363:LEU:HG	2.12	0.49
1:B:375:ALA:O	1:B:378:GLU:HB3	2.12	0.49
1:A:257:LYS:N	1:A:257:LYS:HD2	2.27	0.49
1:A:314:MET:HB3	5:A:2005:HOH:O	2.12	0.49
1:A:388:ARG:HB3	1:A:428:TRP:CD1	2.47	0.49
1:B:531:GLU:HA	1:B:531:GLU:OE1	2.13	0.49
1:B:363:LEU:HA	1:B:366:MET:HE3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:VAL:CG2	1:A:509:PHE:CE1	2.96	0.49
1:A:482:PRO:O	1:A:484:PRO:HD3	2.13	0.49
1:B:261:GLU:OE1	1:B:330:SER:OG	2.28	0.49
1:B:278:PHE:HD1	1:B:302:MET:HB2	1.77	0.49
1:B:383:VAL:H	3:B:1535:MES:H62	1.78	0.48
1:A:329:VAL:O	1:A:334:ILE:HA	2.13	0.48
1:A:365:ASP:O	1:A:368:ALA:HB3	2.12	0.48
1:A:430:ALA:HB2	1:A:446:TRP:HB3	1.95	0.48
1:B:291:ARG:HG2	1:B:340:TYR:CD2	2.48	0.48
1:A:360:LEU:HD23	1:A:520:PHE:CZ	2.48	0.48
1:B:317:LEU:HB3	1:B:322:LEU:HD23	1.95	0.48
1:B:389:ALA:HB3	1:B:454:GLU:OE2	2.13	0.48
1:B:270:GLU:H	1:B:284:GLY:HA2	1.79	0.48
1:A:383:VAL:H	3:A:1535:MES:C2	2.15	0.48
1:B:302:MET:HG2	1:B:303:SER:N	2.27	0.48
1:A:326:TYR:CZ	1:A:339:GLU:HB3	2.49	0.48
1:B:487:CYS:SG	1:B:491:LEU:HB3	2.54	0.48
1:A:375:ALA:O	1:A:378:GLU:HB3	2.14	0.47
1:A:283:MET:CG	1:A:340:TYR:CE1	2.95	0.47
1:A:360:LEU:HB3	1:A:361:PRO:HD3	1.96	0.47
2:B:1534:NG7:O01	2:B:1534:NG7:S	2.73	0.47
1:B:430:ALA:HB2	1:B:446:TRP:HB3	1.97	0.47
1:A:386:ASP:HA	5:A:2026:HOH:O	2.14	0.47
1:B:383:VAL:HG12	1:B:385:ARG:HG3	1.96	0.47
1:B:487:CYS:SG	1:B:488:PRO:CD	3.03	0.47
1:A:441:ILE:HG13	1:A:509:PHE:CE1	2.50	0.47
1:B:363:LEU:HD12	1:B:533:LEU:HD22	1.97	0.47
1:A:374:MET:HB3	1:A:509:PHE:CE2	2.49	0.47
1:B:364:VAL:HB	1:B:520:PHE:HE2	1.80	0.47
1:A:374:MET:CB	1:A:509:PHE:CD2	2.96	0.46
1:A:293:ALA:C	1:A:294:ILE:HG13	2.35	0.46
1:B:370:ILE:HD13	1:B:392:ILE:HG13	1.97	0.46
1:A:347:LEU:HD22	1:A:390:ALA:HB2	1.96	0.46
1:A:351:LYS:HD2	1:B:522:SER:HB3	1.98	0.46
1:B:482:PRO:O	1:B:484:PRO:HD3	2.15	0.46
1:B:267:LEU:HD22	1:B:294:ILE:HD13	1.96	0.46
1:B:441:ILE:HG13	1:B:509:PHE:CE1	2.51	0.46
1:B:491:LEU:HA	1:B:491:LEU:HD12	1.72	0.46
1:A:297:LEU:HD22	1:A:307:PHE:CB	2.45	0.46
1:A:343:LYS:HD2	5:A:2009:HOH:O	2.14	0.46
1:A:446:TRP:CZ3	1:A:499:TRP:O	2.68	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:CYS:SG	1:B:488:PRO:HD2	2.56	0.46
1:A:503:PRO:O	1:A:506:ARG:HB2	2.15	0.46
1:B:304:PRO:HB3	1:B:334:ILE:CD1	2.46	0.46
1:B:360:LEU:HB3	1:B:361:PRO:HD3	1.98	0.46
1:B:426:ILE:HA	1:B:429:THR:HB	1.97	0.46
1:B:446:TRP:O	1:B:450:ILE:HG12	2.15	0.46
1:A:466:MET:HE2	1:A:471:VAL:CG2	2.42	0.46
1:B:347:LEU:HD22	1:B:390:ALA:HB2	1.97	0.46
1:B:509:PHE:HA	1:B:512:LEU:HB2	1.98	0.46
1:B:326:TYR:CZ	1:B:339:GLU:HA	2.51	0.45
1:A:383:VAL:N	3:A:1535:MES:C2	2.78	0.45
1:A:457:THR:HB	1:A:460:ARG:HB2	1.98	0.45
1:B:296:THR:HA	1:B:335:TYR:HD1	1.81	0.45
1:A:519:TYR:CZ	1:A:524:GLU:HG2	2.51	0.45
1:B:321:LYS:HA	1:B:401:LYS:HG2	1.98	0.45
1:A:383:VAL:CG1	1:A:385:ARG:HG3	2.44	0.45
1:B:308:LEU:HD21	1:B:334:ILE:CG2	2.47	0.45
1:A:460:ARG:HH21	1:B:518:ASP:CG	2.19	0.45
1:A:519:TYR:CZ	1:A:524:GLU:CG	3.00	0.45
1:B:428:TRP:HA	1:B:450:ILE:HG13	1.97	0.45
1:A:268:ARG:O	1:A:284:GLY:CA	2.64	0.45
1:A:314:MET:O	5:A:2005:HOH:O	2.20	0.45
1:A:363:LEU:HD12	1:A:533:LEU:HD22	1.98	0.45
1:B:277:CYS:O	1:B:301:THR:HB	2.17	0.45
1:A:451:LEU:O	1:A:451:LEU:HD23	2.15	0.45
1:B:506:ARG:HA	1:B:507:PRO:HD3	1.79	0.45
1:A:370:ILE:O	1:A:371:ALA:C	2.56	0.44
1:B:311:ALA:HB2	1:B:336:ILE:HG12	2.00	0.44
1:B:463:TYR:N	1:B:464:PRO:HD3	2.32	0.44
1:B:487:CYS:SG	1:B:488:PRO:N	2.90	0.44
1:A:267:LEU:CD1	1:A:337:VAL:HG21	2.48	0.44
1:A:445:VAL:O	1:A:448:PHE:HB3	2.16	0.44
1:B:455:LEU:HA	1:B:455:LEU:HD23	1.64	0.44
1:A:430:ALA:O	1:A:433:ALA:HB3	2.16	0.44
1:B:279:GLY:HA3	1:B:296:THR:O	2.17	0.44
1:B:365:ASP:O	1:B:368:ALA:HB3	2.17	0.44
1:B:466:MET:CE	1:B:471:VAL:HA	2.47	0.44
1:A:497:GLN:O	1:A:506:ARG:HG3	2.17	0.44
1:A:341:MET:HG2	2:A:1534:NG7:H01	1.99	0.44
1:B:508:THR:O	1:B:512:LEU:HG	2.18	0.44
1:B:523:THR:C	1:B:525:PRO:HD3	2.38	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLN:O	1:A:372:SER:HB3	2.18	0.44
1:A:350:LEU:HD13	1:A:454:GLU:O	2.18	0.44
1:A:445:VAL:HG21	1:A:507:PRO:O	2.18	0.43
1:B:260:TRP:O	1:B:327:ALA:HB1	2.18	0.43
1:B:438:ARG:NH1	5:B:2042:HOH:O	2.51	0.43
1:A:385:ARG:HG2	1:A:439:PHE:HB3	2.00	0.43
1:A:366:MET:O	1:A:367:ALA:C	2.57	0.43
1:B:362:GLN:H	1:B:362:GLN:CD	2.22	0.43
1:B:519:TYR:CZ	1:B:524:GLU:HG2	2.53	0.43
1:A:447:SER:O	1:A:450:ILE:N	2.51	0.43
1:B:451:LEU:HD23	1:B:451:LEU:O	2.17	0.43
2:A:1534:NG7:H20	2:A:1534:NG7:C28	2.45	0.43
1:B:446:TRP:HA	1:B:498:CYS:O	2.19	0.43
1:A:455:LEU:HD23	1:A:455:LEU:HA	1.72	0.43
1:B:291:ARG:HG2	1:B:340:TYR:CG	2.54	0.43
1:B:370:ILE:O	1:B:371:ALA:C	2.56	0.43
1:B:382:TYR:HA	3:B:1535:MES:H62	2.00	0.43
1:B:445:VAL:O	1:B:448:PHE:HB3	2.18	0.43
1:A:374:MET:HG3	1:A:387:LEU:HD22	2.00	0.43
1:B:310:GLU:HG3	2:B:1534:NG7:H19	2.00	0.43
1:B:319:HIS:CD2	1:B:376:TYR:HB2	2.53	0.43
1:B:430:ALA:O	1:B:433:ALA:HB3	2.18	0.43
1:A:392:ILE:CG2	1:A:400:CYS:HB3	2.49	0.43
1:A:426:ILE:HA	1:A:429:THR:HB	2.00	0.43
1:B:343:LYS:HB2	1:B:394:VAL:HB	2.00	0.43
1:B:271:VAL:HG12	1:B:272:LYS:O	2.19	0.43
1:B:427:LYS:HD3	1:B:462:PRO:O	2.18	0.43
1:B:329:VAL:O	1:B:334:ILE:HA	2.19	0.42
1:B:365:ASP:OD1	1:B:369:GLN:NE2	2.50	0.42
1:B:386:ASP:OD1	1:B:388:ARG:HD2	2.19	0.42
1:A:466:MET:CE	1:A:471:VAL:HA	2.49	0.42
3:A:1535:MES:H32	3:A:1535:MES:H82	1.89	0.42
1:B:527:TYR:OH	1:B:529:PRO:HA	2.19	0.42
1:A:322:LEU:HD22	1:A:402:VAL:HB	2.01	0.42
1:A:442:LYS:HD3	1:A:442:LYS:HA	1.85	0.42
1:B:275:GLN:HA	1:B:280:GLU:HA	2.02	0.42
1:B:322:LEU:O	1:B:323:VAL:C	2.57	0.42
1:B:373:GLY:O	1:B:377:VAL:HG23	2.19	0.42
1:B:380:MET:HB3	1:B:382:TYR:CD1	2.54	0.42
1:B:474:GLN:NE2	5:B:2056:HOH:O	2.51	0.42
1:A:491:LEU:HA	1:A:491:LEU:HD12	1.74	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ALA:O	1:B:337:VAL:HB	2.19	0.42
1:A:296:THR:HG22	1:A:335:TYR:HD1	1.80	0.42
1:B:283:MET:HG3	1:B:340:TYR:CZ	2.54	0.42
1:B:287:ASN:C	1:B:289:THR:H	2.24	0.42
1:A:297:LEU:O	1:A:299:PRO:HD3	2.20	0.42
1:A:343:LYS:C	2:A:1534:NG7:H09	2.39	0.42
1:A:378:GLU:HG3	1:A:441:ILE:HG12	2.02	0.42
2:A:1534:NG7:C20	2:A:1534:NG7:C28	2.87	0.42
1:B:326:TYR:CE2	1:B:339:GLU:HA	2.55	0.42
1:A:389:ALA:HB3	1:A:454:GLU:OE2	2.20	0.41
1:A:463:TYR:N	1:A:464:PRO:HD3	2.35	0.41
1:A:433:ALA:HB1	1:A:439:PHE:CE2	2.56	0.41
1:A:509:PHE:HA	1:A:512:LEU:HB2	2.02	0.41
1:B:488:PRO:O	1:B:491:LEU:N	2.51	0.41
1:B:519:TYR:CZ	1:B:524:GLU:CG	3.02	0.41
1:A:527:TYR:OH	1:A:529:PRO:HA	2.20	0.41
1:A:343:LYS:HB2	1:A:394:VAL:HB	2.02	0.41
1:A:467:VAL:O	1:A:468:ASN:C	2.59	0.41
1:A:431:PRO:HB3	1:A:476:GLU:OE2	2.21	0.41
1:A:512:LEU:O	1:A:513:GLN:C	2.58	0.41
1:B:524:GLU:N	1:B:525:PRO:HD3	2.35	0.41
1:A:286:TRP:HB2	1:A:292:VAL:HG11	2.02	0.41
1:A:344:GLY:CA	2:A:1534:NG7:C07	2.97	0.41
1:A:356:LYS:HB3	1:A:356:LYS:HE2	1.88	0.41
1:B:267:LEU:HD21	1:B:337:VAL:HG21	2.01	0.41
1:B:374:MET:HG3	1:B:387:LEU:HD22	2.02	0.41
1:A:258:ASP:O	1:A:261:GLU:HB2	2.21	0.41
1:A:362:GLN:H	1:A:362:GLN:CD	2.24	0.41
1:A:427:LYS:HD3	1:A:462:PRO:O	2.20	0.41
1:A:452:LEU:HA	1:A:452:LEU:HD23	1.73	0.41
1:B:448:PHE:CD2	1:B:512:LEU:HD13	2.56	0.41
1:A:457:THR:O	1:A:460:ARG:HG2	2.21	0.41
1:A:270:GLU:OE2	1:A:285:THR:OG1	2.39	0.40
1:B:346:LEU:O	1:B:350:LEU:HG	2.21	0.40
1:B:488:PRO:HB2	1:B:519:TYR:OH	2.21	0.40
1:A:326:TYR:CE2	1:A:339:GLU:HA	2.56	0.40
1:A:431:PRO:C	1:A:433:ALA:N	2.75	0.40
1:A:267:LEU:CD2	1:A:337:VAL:HG21	2.52	0.40
1:A:297:LEU:CD2	1:A:334:ILE:HD12	2.42	0.40
1:A:317:LEU:HD23	1:A:380:MET:HG3	2.03	0.40
1:A:340:TYR:CE2	1:A:342:SER:HA	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:MET:HB3	1:A:382:TYR:CD1	2.56	0.40
1:B:359:ARG:HA	1:B:359:ARG:HD3	1.72	0.40
1:B:378:GLU:HG3	1:B:441:ILE:HG12	2.02	0.40
1:B:512:LEU:HD23	1:B:512:LEU:HA	1.87	0.40
1:A:364:VAL:HB	1:A:520:PHE:CE2	2.55	0.40
1:A:506:ARG:HA	1:A:507:PRO:HD3	1.85	0.40
1:A:512:LEU:HD23	1:A:512:LEU:HA	1.89	0.40
1:A:523:THR:C	1:A:525:PRO:HD3	2.41	0.40
1:B:346:LEU:HB3	1:B:392:ILE:HB	2.03	0.40
1:A:350:LEU:HD11	1:A:455:LEU:HD23	2.04	0.40
1:A:388:ARG:CB	1:A:428:TRP:CD1	3.04	0.40
1:A:488:PRO:HB2	1:A:519:TYR:OH	2.22	0.40
1:A:519:TYR:OH	1:A:524:GLU:HG3	2.22	0.40
1:B:264:ARG:CZ	1:B:333:PRO:HD2	2.52	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	254/286 (89%)	232 (91%)	21 (8%)	1 (0%)	34 57
1	B	253/286 (88%)	231 (91%)	22 (9%)	0	100 100
All	All	507/572 (89%)	463 (91%)	43 (8%)	1 (0%)	47 71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	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	225/245 (92%)	223 (99%)	2 (1%)	78	91
1	B	224/245 (91%)	222 (99%)	2 (1%)	78	91
All	All	449/490 (92%)	445 (99%)	4 (1%)	78	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	356	LYS
1	A	388	ARG
1	B	356	LYS
1	B	360	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	312	GLN
1	A	526	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
4	GOL	A	1536	-	5,5,5	0.37	0	5,5,5	0.33	0
2	NG7	B	1534	-	45,48,48	2.11	14 (31%)	61,70,70	2.95	30 (49%)
2	NG7	A	1534	-	45,48,48	2.05	13 (28%)	61,70,70	3.00	29 (47%)
3	MES	B	1535	-	12,12,12	2.31	1 (8%)	15,16,16	6.26	12 (80%)
3	MES	A	1535	-	12,12,12	2.24	1 (8%)	15,16,16	6.14	10 (66%)

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	GOL	A	1536	-	-	2/4/4/4	-
2	NG7	B	1534	-	-	11/30/44/44	0/6/6/6
2	NG7	A	1534	-	-	11/30/44/44	0/6/6/6
3	MES	B	1535	-	-	4/6/14/14	0/1/1/1
3	MES	A	1535	-	-	5/6/14/14	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1535	MES	C8-S	-7.57	1.67	1.77
3	A	1535	MES	C8-S	-7.31	1.67	1.77
2	B	1534	NG7	C11-C04	5.58	1.57	1.49
2	A	1534	NG7	C11-C04	5.54	1.57	1.49
2	B	1534	NG7	C15-C17	5.19	1.61	1.50
2	A	1534	NG7	C15-C17	4.79	1.60	1.50
2	B	1534	NG7	C04-N01	4.76	1.40	1.33
2	A	1534	NG7	C04-N01	4.41	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1534	NG7	C07-N03	4.15	1.45	1.35
2	B	1534	NG7	C07-N03	4.10	1.44	1.35
2	B	1534	NG7	C17-N04	3.86	1.46	1.35
2	A	1534	NG7	C17-N04	3.85	1.46	1.35
2	A	1534	NG7	C06-N03	3.46	1.42	1.36
2	B	1534	NG7	C06-N03	3.32	1.42	1.36
2	A	1534	NG7	C18-N04	2.96	1.47	1.41
2	B	1534	NG7	C18-N04	2.80	1.47	1.41
2	B	1534	NG7	C16-C15	2.76	1.43	1.39
2	A	1534	NG7	C16-C15	2.73	1.43	1.39
2	A	1534	NG7	C01-C05	2.35	1.41	1.36
2	B	1534	NG7	C23-C18	2.33	1.43	1.39
2	B	1534	NG7	C16-C11	2.33	1.43	1.39
2	A	1534	NG7	C16-C11	2.32	1.43	1.39
2	A	1534	NG7	C24-N05	2.29	1.51	1.47
2	B	1534	NG7	C24-C21	2.28	1.55	1.51
2	B	1534	NG7	C01-C05	2.27	1.41	1.36
2	B	1534	NG7	C24-N05	2.24	1.51	1.47
2	B	1534	NG7	C02-N02	2.11	1.45	1.38
2	A	1534	NG7	C24-C21	2.08	1.55	1.51
2	A	1534	NG7	C02-N02	2.04	1.45	1.38

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1535	MES	O1S-S-C8	-13.59	86.20	106.73
3	B	1535	MES	O2S-S-C8	-13.45	86.40	106.73
3	A	1535	MES	O2S-S-C8	-13.44	86.42	106.73
3	A	1535	MES	O1S-S-C8	-12.40	87.99	106.73
3	A	1535	MES	O3S-S-C8	-10.51	85.44	106.00
3	B	1535	MES	O3S-S-C8	-10.14	86.18	106.00
2	A	1534	NG7	C20-C21-C22	-7.43	111.69	118.75
2	B	1534	NG7	C20-C21-C22	-7.43	111.69	118.75
2	A	1534	NG7	C19-C18-C23	-6.53	111.76	119.66
2	A	1534	NG7	C09-C08-C07	6.51	123.60	117.24
2	B	1534	NG7	C19-C18-C23	-6.35	111.98	119.66
2	B	1534	NG7	C11-C16-C15	6.11	127.58	121.04
2	A	1534	NG7	C15-C17-N04	6.09	130.70	115.90
2	A	1534	NG7	C11-C16-C15	6.07	127.54	121.04
2	B	1534	NG7	C15-C17-N04	5.71	129.77	115.90
3	B	1535	MES	C6-C5-N4	-5.48	101.80	110.12
2	B	1534	NG7	C03-C02-N02	5.42	119.94	108.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1534	NG7	C03-C02-N02	5.24	119.56	108.19
2	B	1534	NG7	C27-C28-N05	4.99	120.72	110.65
3	B	1535	MES	C5-N4-C3	4.99	119.59	108.84
3	A	1535	MES	C6-C5-N4	-4.81	102.81	110.12
2	B	1534	NG7	C24-N05-C28	4.63	121.03	111.07
2	A	1534	NG7	C27-C28-N05	4.62	119.97	110.65
3	A	1535	MES	C2-C3-N4	-4.60	103.13	110.12
2	A	1534	NG7	C01-C02-C03	-4.44	112.73	120.53
2	B	1534	NG7	C11-C04-N01	4.41	122.91	117.05
3	A	1535	MES	C5-N4-C3	4.39	118.30	108.84
2	B	1534	NG7	C08-C07-N03	4.28	123.43	115.16
2	A	1534	NG7	C08-C07-N03	4.28	123.42	115.16
2	A	1534	NG7	C26-C25-N05	4.27	119.25	110.65
3	A	1535	MES	C7-N4-C3	4.22	122.49	111.24
2	B	1534	NG7	C01-C02-C03	-4.21	113.12	120.53
2	A	1534	NG7	O01-C07-N03	-4.06	115.34	123.92
2	B	1534	NG7	C24-N05-C25	4.03	119.73	111.07
2	A	1534	NG7	O-C17-C15	-4.02	112.93	120.90
2	B	1534	NG7	C26-C25-N05	3.94	118.59	110.65
2	B	1534	NG7	C14-C15-C16	-3.90	114.74	119.25
2	A	1534	NG7	C24-N05-C25	3.83	119.30	111.07
2	B	1534	NG7	C28-N05-C25	3.80	117.02	108.84
2	A	1534	NG7	C14-C15-C16	-3.77	114.89	119.25
2	B	1534	NG7	O-C17-C15	-3.63	113.70	120.90
2	A	1534	NG7	C23-C22-C21	3.60	123.53	119.15
2	A	1534	NG7	C16-C11-C04	3.57	125.59	120.59
3	A	1535	MES	O3S-S-O2S	3.56	120.31	111.40
2	A	1534	NG7	C24-N05-C28	3.48	118.56	111.07
2	B	1534	NG7	O01-C07-N03	-3.47	116.59	123.92
2	B	1534	NG7	F2-C-C22	3.47	118.80	112.65
2	A	1534	NG7	C28-N05-C25	3.46	116.30	108.84
3	B	1535	MES	C7-N4-C5	3.39	120.28	111.24
2	B	1534	NG7	C23-C22-C21	3.39	123.27	119.15
2	A	1534	NG7	C-C22-C21	-3.38	117.83	121.06
2	B	1534	NG7	C16-C11-C04	3.37	125.30	120.59
2	B	1534	NG7	C12-C11-C16	-3.36	113.60	118.23
3	B	1535	MES	C7-N4-C3	3.33	120.12	111.24
2	B	1534	NG7	C19-C20-C21	3.31	125.72	121.39
3	B	1535	MES	O3S-S-O2S	3.28	119.60	111.40
2	A	1534	NG7	C12-C11-C16	-3.22	113.81	118.23
2	B	1534	NG7	C09-C08-C07	3.20	120.37	117.24
2	B	1534	NG7	C-C22-C21	-3.19	118.02	121.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1534	NG7	C11-C04-N01	3.17	121.26	117.05
2	A	1534	NG7	C20-C19-C18	3.10	123.86	120.30
2	A	1534	NG7	C14-C13-C12	3.07	124.19	120.24
2	A	1534	NG7	C19-C20-C21	3.01	125.33	121.39
3	A	1535	MES	C7-N4-C5	2.99	119.20	111.24
2	A	1534	NG7	O-C17-N04	-2.95	116.27	123.75
2	B	1534	NG7	C20-C19-C18	2.94	123.69	120.30
3	A	1535	MES	O3S-S-O1S	2.94	118.75	111.40
3	B	1535	MES	O3S-S-O1S	2.92	118.71	111.40
2	A	1534	NG7	C05-C04-N01	-2.90	116.90	122.18
3	B	1535	MES	C2-C3-N4	-2.86	105.78	110.12
2	B	1534	NG7	C05-C04-N01	-2.85	116.99	122.18
2	B	1534	NG7	O-C17-N04	-2.85	116.53	123.75
2	A	1534	NG7	F2-C-C22	2.77	117.56	112.65
2	B	1534	NG7	C14-C13-C12	2.65	123.65	120.24
2	A	1534	NG7	O01-C07-C08	-2.47	118.37	122.19
3	B	1535	MES	C8-C7-N4	-2.43	103.17	112.36
2	A	1534	NG7	C18-C23-C22	2.40	123.81	120.82
2	B	1534	NG7	C18-C23-C22	2.27	123.65	120.82
2	B	1534	NG7	C01-C05-C04	2.15	123.02	119.38
3	B	1535	MES	O2S-S-O1S	2.03	120.42	113.82
2	B	1534	NG7	O01-C07-C08	-2.02	119.07	122.19

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1534	NG7	O01-C07-C08-C09
2	A	1534	NG7	N03-C07-C08-C09
2	A	1534	NG7	N03-C07-C08-C10
2	B	1534	NG7	O01-C07-C08-C09
2	B	1534	NG7	O01-C07-C08-C10
2	B	1534	NG7	N03-C07-C08-C09
2	B	1534	NG7	N03-C07-C08-C10
3	A	1535	MES	C8-C7-N4-C3
3	A	1535	MES	C7-C8-S-O1S
3	A	1535	MES	C7-C8-S-O3S
3	B	1535	MES	C7-C8-S-O1S
3	B	1535	MES	C7-C8-S-O3S
4	A	1536	GOL	O1-C1-C2-O2
4	A	1536	GOL	O1-C1-C2-C3
2	B	1534	NG7	N01-C04-C11-C12

Continued on next page...

Continued from previous page...

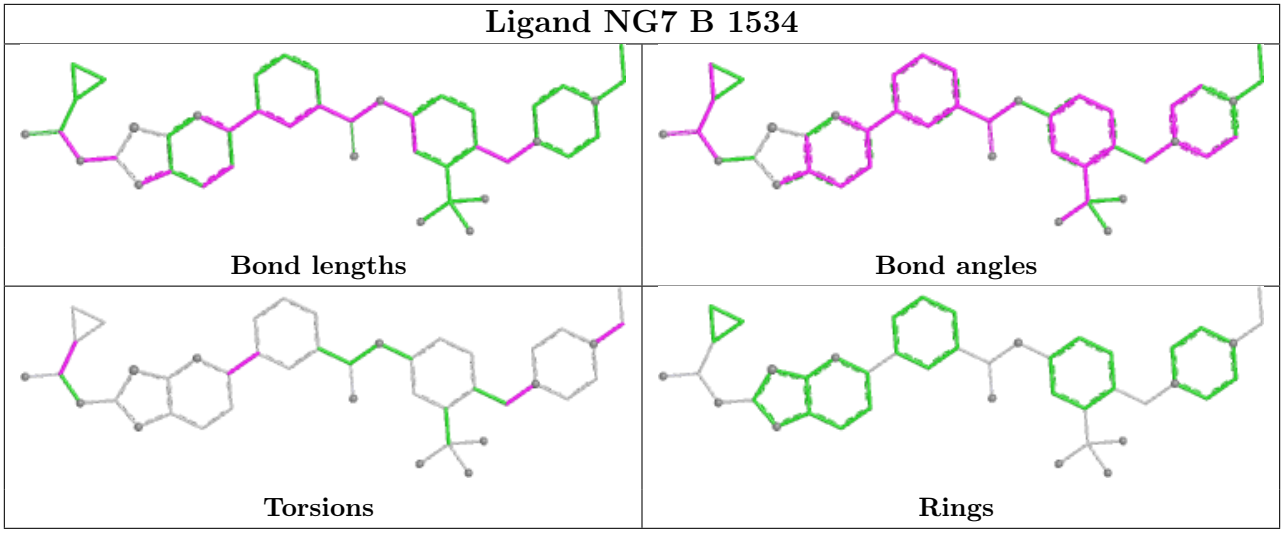
Mol	Chain	Res	Type	Atoms
2	A	1534	NG7	C21-C24-N05-C25
2	B	1534	NG7	C05-C04-C11-C12
2	A	1534	NG7	C21-C24-N05-C28
2	B	1534	NG7	N01-C04-C11-C16
2	B	1534	NG7	C05-C04-C11-C16
2	A	1534	NG7	C30-C29-N-C26
2	A	1534	NG7	N01-C04-C11-C12
2	A	1534	NG7	N01-C04-C11-C16
2	A	1534	NG7	C05-C04-C11-C16
2	A	1534	NG7	C30-C29-N-C27
2	A	1534	NG7	C05-C04-C11-C12
3	B	1535	MES	C8-C7-N4-C5
2	B	1534	NG7	C21-C24-N05-C25
2	B	1534	NG7	C30-C29-N-C26
3	A	1535	MES	C7-C8-S-O2S
3	B	1535	MES	C7-C8-S-O2S
3	A	1535	MES	C8-C7-N4-C5
2	B	1534	NG7	C30-C29-N-C27

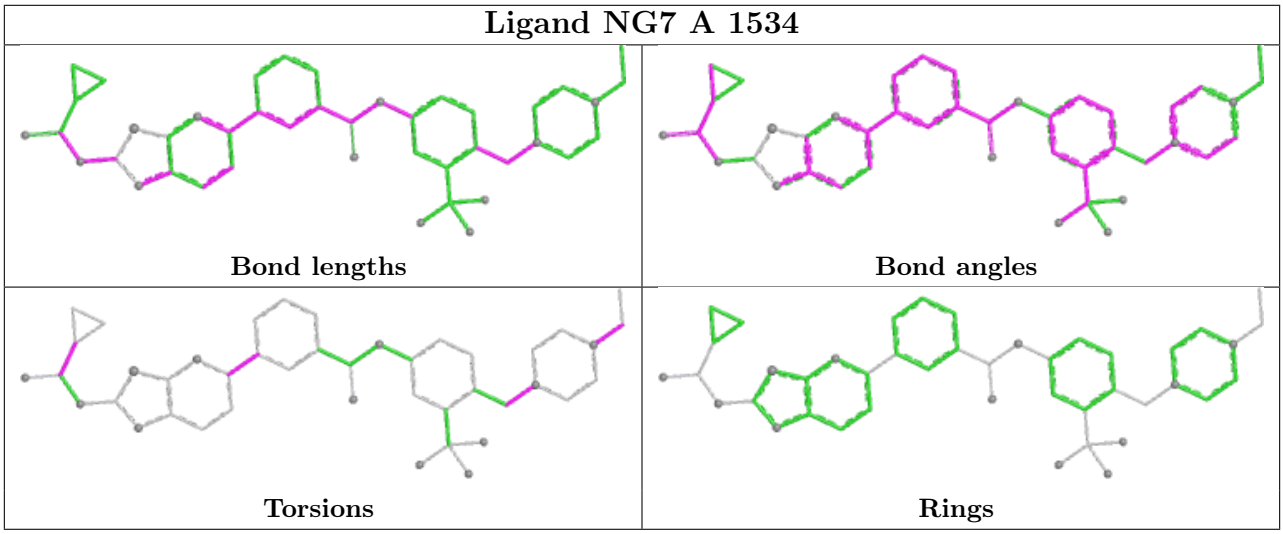
There are no ring outliers.

4 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1534	NG7	8	0
2	A	1534	NG7	20	0
3	B	1535	MES	5	0
3	A	1535	MES	6	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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	258/286 (90%)	0.20	14 (5%)	25	20	29, 49, 107, 122	0
1	B	257/286 (89%)	0.07	3 (1%)	79	76	30, 49, 91, 109	0
All	All	515/572 (90%)	0.13	17 (3%)	46	39	29, 49, 99, 122	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	TYR	5.2
1	A	267	LEU	4.2
1	A	332	GLU	3.7
1	A	269	LEU	3.4
1	A	278	PHE	2.9
1	A	300	GLY	2.8
1	A	265	GLU	2.8
1	B	469	ARG	2.7
1	A	298	LYS	2.7
1	A	297	LEU	2.6
1	A	299	PRO	2.5
1	A	333	PRO	2.3
1	B	473	ASP	2.3
1	B	260	TRP	2.2
1	A	262	ILE	2.2
1	A	331	GLU	2.1
1	A	486	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

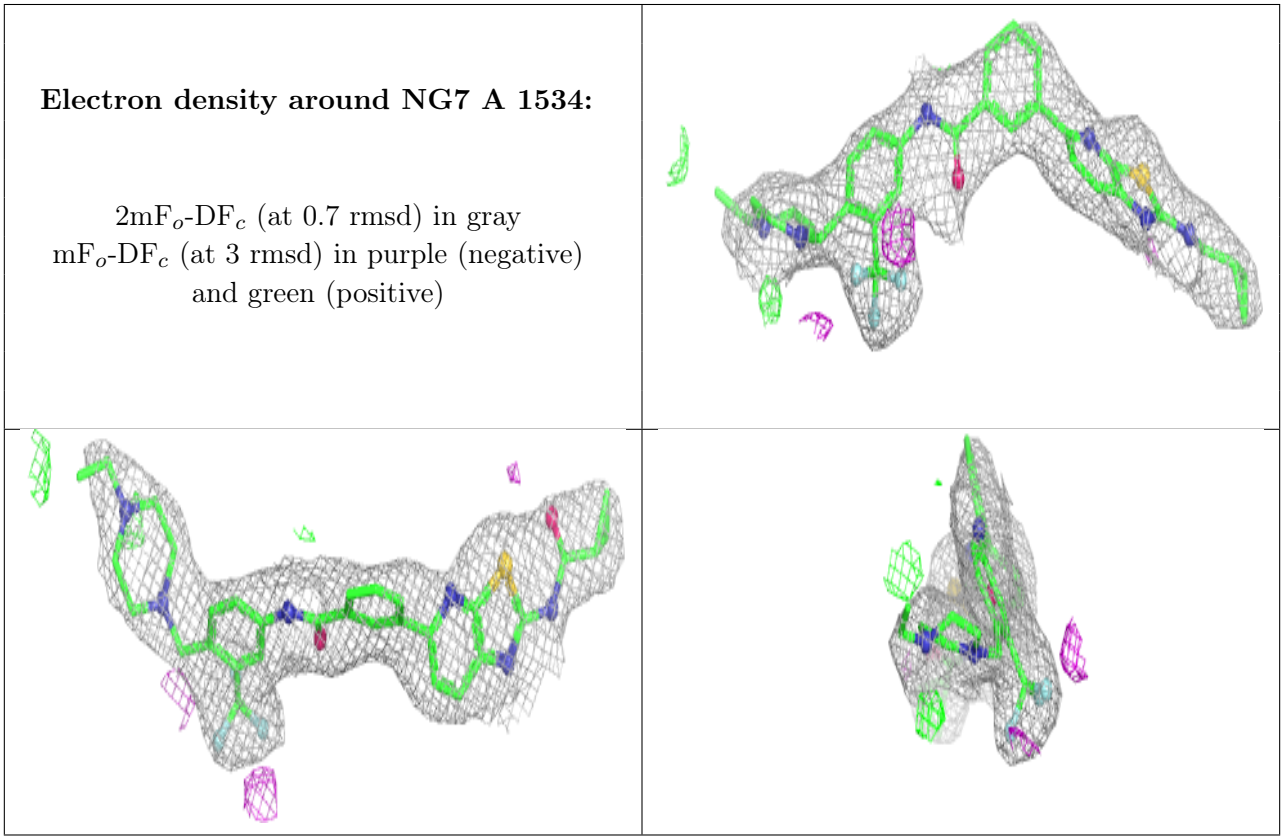
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MES	A	1535	12/12	0.86	0.24	53,77,87,102	0
3	MES	B	1535	12/12	0.87	0.20	50,81,91,99	0
2	NG7	A	1534	43/43	0.93	0.20	37,56,69,74	0
2	NG7	B	1534	43/43	0.94	0.20	32,51,67,76	0
4	GOL	A	1536	6/6	0.94	0.17	42,43,52,55	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.

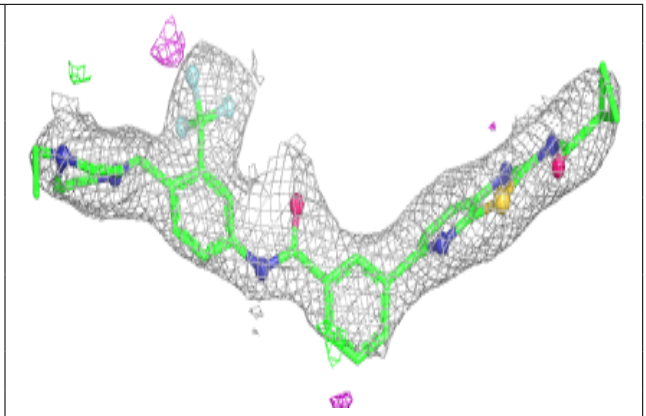
Electron density around NG7 A 1534:

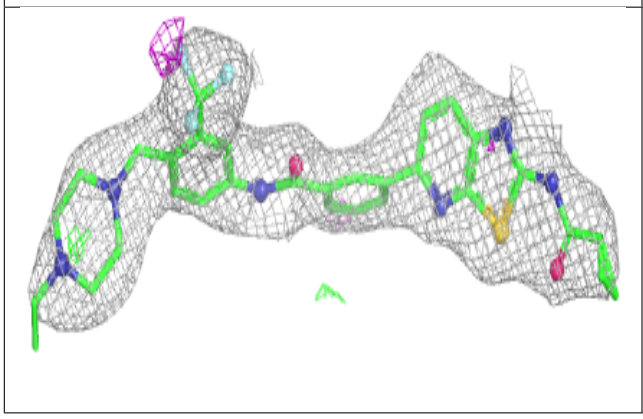
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

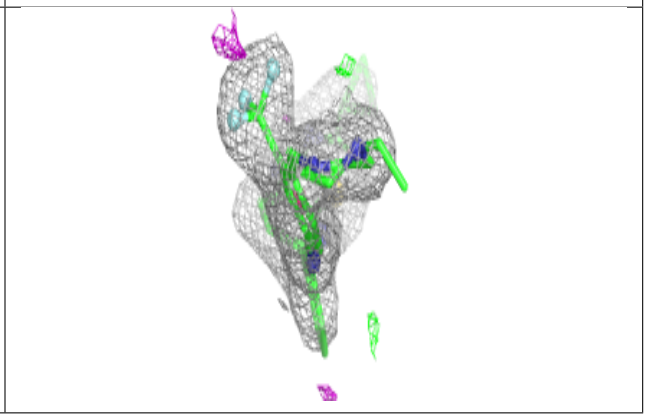


Electron density around NG7 B 1534:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.