



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:23 AM UTC

PDB ID : 1B7Y / pdb_00001b7y
Title : PHENYLALANYL TRNA SYNTHETASE COMPLEXED WITH PHENYL
ALANINYL-ADENYLATE
Authors : Reshetnikova, L.; Moor, N.; Lavrik, O.; Vassilyev, D.G.
Deposited on : 1999-01-26
Resolution : 2.50 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

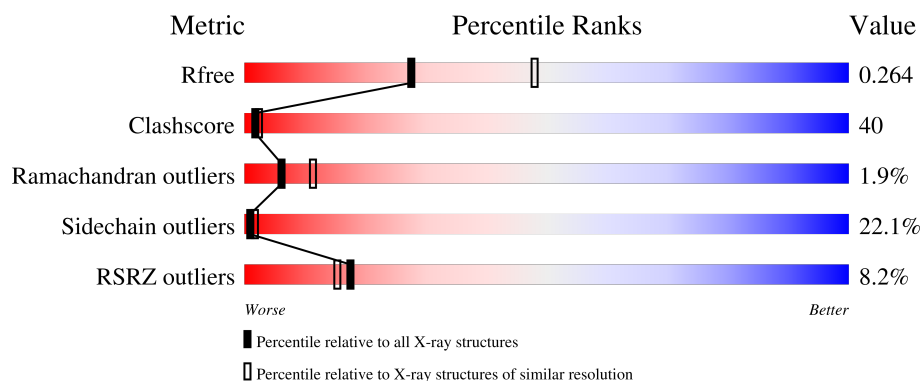
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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	350	 6% 31% 32% 13% 24%
2	B	785	 8% 39% 43% 14% 2%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8439 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 PROTEIN (PHENYLALANYL-TRNA SYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2112	1382	359	364	7			

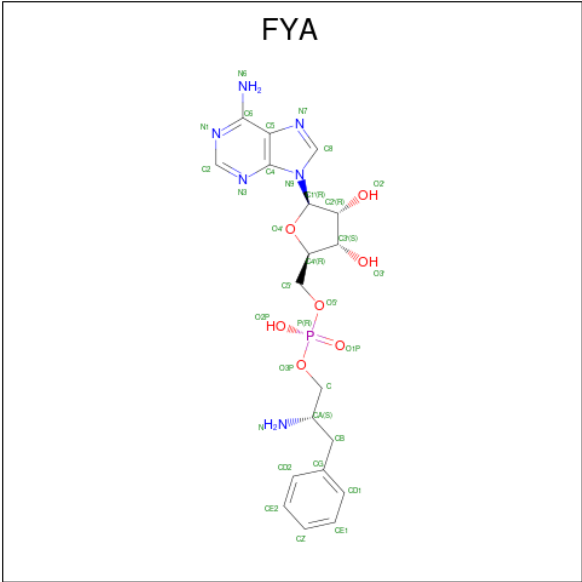
- Molecule 2 is a protein called PROTEIN (PHENYLALANYL-TRNA SYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	775	Total	C	N	O	S	0	0	0
			6054	3879	1078	1087	10			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is ADENOSINE-5'-[PHENYLALANINOL-PHOSPHATE] (CCD ID: FYA) (formula: C₁₉H₂₅N₆O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			33	19	6	7	1		

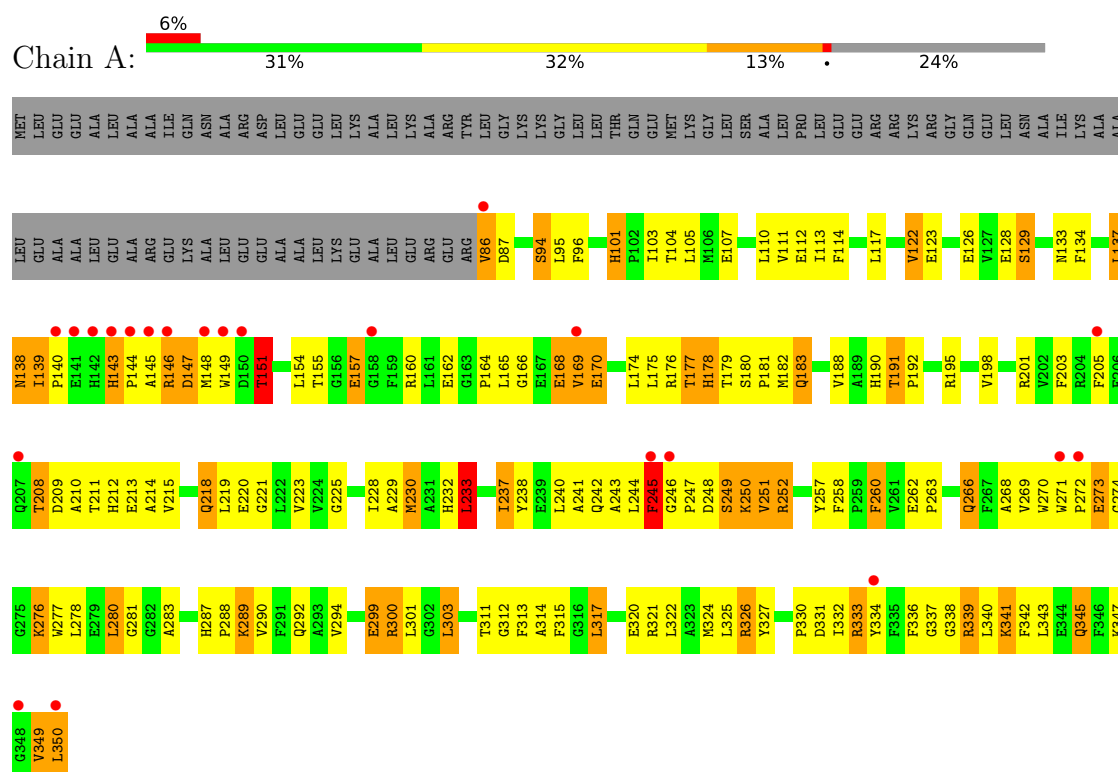
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	48	Total	O	0	0
			48	48		
5	B	191	Total	O	0	0
			191	191		

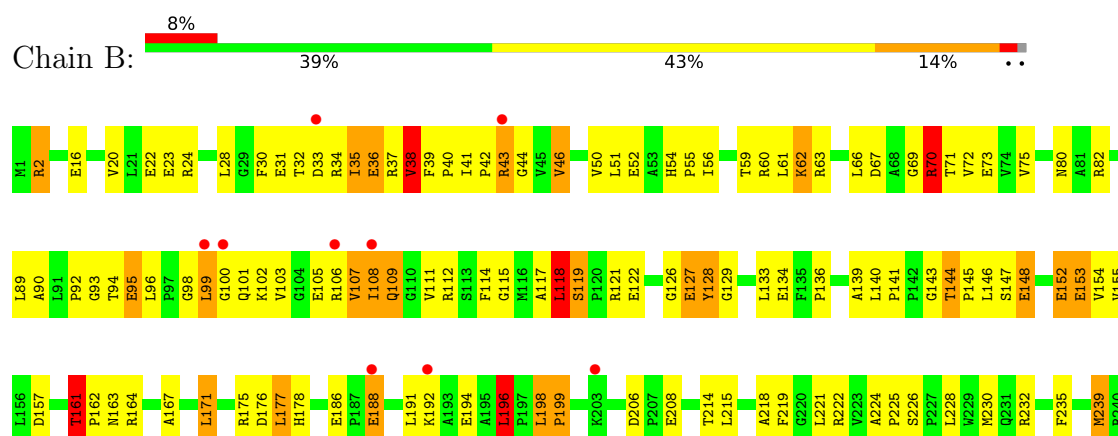
3 Residue-property plots [i](#)

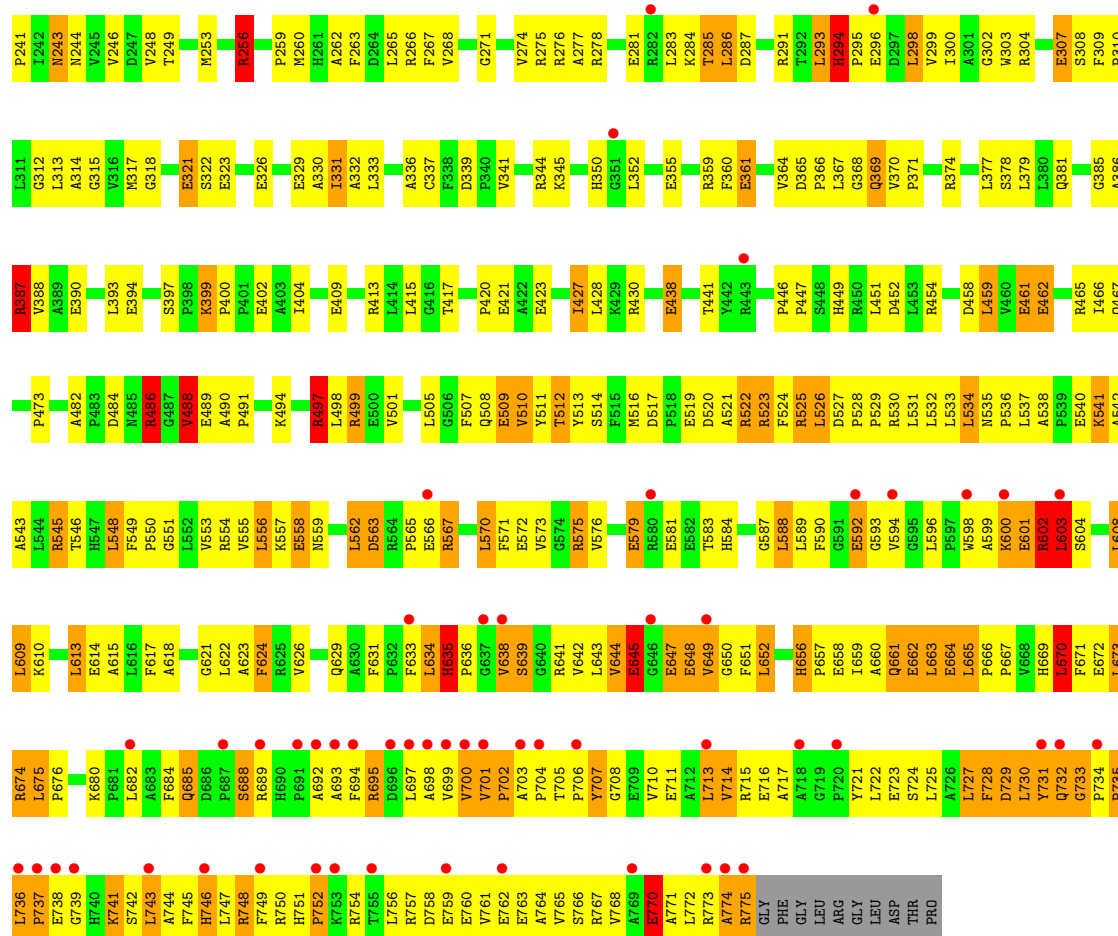
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PROTEIN (PHENYLALANYL-TRNA SYNTHETASE)



• Molecule 2: PROTEIN (PHENYLALANYL-TRNA SYNTHETASE)





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.50Å 174.50Å 140.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.00-2.50) 95.7 (50.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	15112.19 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.230 , 0.267 0.229 , 0.264	Depositor DCC
R_{free} test set	4109 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 81.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.056 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8439	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FYA

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	0.62	0/2180	1.11	14/2957 (0.5%)
2	B	0.63	0/6205	1.20	69/8436 (0.8%)
All	All	0.63	0/8385	1.17	83/11393 (0.7%)

There are no bond length outliers.

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	774	ALA	N-CA-C	-11.48	98.38	112.38
1	A	218	GLN	OE1-CD-NE2	-9.52	113.08	122.60
2	B	198	LEU	CA-C-N	9.06	131.16	119.84
2	B	198	LEU	C-N-CA	9.06	131.16	119.84
1	A	139	ILE	N-CA-C	8.44	116.29	107.76
1	A	151	THR	N-CA-C	8.29	121.74	110.55
2	B	118	LEU	N-CA-C	7.75	122.10	109.85
2	B	350	HIS	N-CA-C	-7.71	98.80	110.14
2	B	294	HIS	N-CA-C	-7.69	99.40	110.40
2	B	196	LEU	CA-C-N	7.61	128.21	120.14
2	B	196	LEU	C-N-CA	7.61	128.21	120.14
2	B	352	LEU	N-CA-C	7.28	121.44	109.06
2	B	736	LEU	N-CA-C	7.08	114.59	108.22
2	B	321	GLU	N-CA-C	7.04	118.61	111.07
2	B	43	ARG	N-CA-C	-7.00	104.00	112.54
2	B	128	TYR	N-CA-C	6.87	125.44	110.80
2	B	601	GLU	CB-CG-CD	-6.81	101.03	112.60
2	B	670	LEU	N-CA-C	6.81	118.85	109.18
1	A	251	VAL	N-CA-C	6.78	118.37	108.53
2	B	100	GLY	N-CA-C	-6.74	106.00	114.16
2	B	365	ASP	CA-C-N	6.67	126.36	119.82
2	B	365	ASP	C-N-CA	6.67	126.36	119.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	GLU	N-CA-C	6.67	118.91	110.24
2	B	177	LEU	N-CA-C	-6.65	103.29	111.33
1	A	280	LEU	N-CA-C	6.56	121.57	112.45
2	B	665	LEU	N-CA-C	6.53	119.32	110.31
2	B	387	ARG	N-CA-C	-6.51	98.64	109.24
2	B	647	GLU	N-CA-C	6.51	119.61	109.52
1	A	208	THR	N-CA-C	6.50	118.50	109.15
2	B	336	ALA	N-CA-C	6.49	118.01	108.86
2	B	546	THR	N-CA-C	-6.43	105.59	113.50
2	B	70	ARG	N-CA-C	-6.43	99.73	109.95
2	B	733	GLY	N-CA-C	6.41	125.42	112.34
2	B	133	LEU	N-CA-C	-6.36	100.16	110.20
2	B	256	ARG	N-CA-C	-6.29	100.39	110.14
2	B	521	ALA	N-CA-C	-6.26	104.74	112.38
2	B	115	GLY	N-CA-C	-6.18	98.54	113.18
2	B	695	ARG	N-CA-C	6.15	118.65	108.99
2	B	602	ARG	N-CA-C	-6.12	100.11	109.41
1	A	218	GLN	CG-CD-NE2	6.01	125.42	116.40
2	B	482	ALA	CA-C-N	6.00	125.48	119.24
2	B	482	ALA	C-N-CA	6.00	125.48	119.24
2	B	369	GLN	N-CA-C	5.99	118.33	111.02
2	B	206	ASP	CA-C-N	5.98	125.60	119.56
2	B	206	ASP	C-N-CA	5.98	125.60	119.56
1	A	266	GLN	N-CA-C	-5.97	100.45	109.95
2	B	489	GLU	N-CA-C	5.96	119.65	112.38
2	B	488	VAL	N-CA-C	5.92	121.66	109.34
2	B	601	GLU	CB-CA-C	-5.89	99.22	109.64
2	B	656	HIS	CA-C-N	5.82	125.95	119.32
2	B	656	HIS	C-N-CA	5.82	125.95	119.32
2	B	37	ARG	CA-C-N	-5.82	111.50	121.97
2	B	37	ARG	C-N-CA	-5.82	111.50	121.97
2	B	635	HIS	N-CA-C	-5.66	102.61	109.57
2	B	107	VAL	N-CA-C	-5.66	100.17	108.54
2	B	665	LEU	CA-C-N	5.63	126.18	120.38
2	B	665	LEU	C-N-CA	5.63	126.18	120.38
2	B	534	LEU	N-CA-C	-5.61	106.28	113.23
2	B	119	SER	N-CA-C	-5.53	102.94	110.36
2	B	497	ARG	N-CA-C	-5.53	105.26	111.28
1	A	190	HIS	N-CA-C	5.49	116.97	109.18
2	B	743	LEU	N-CA-C	5.48	117.27	107.80
2	B	563	ASP	N-CA-C	-5.47	100.85	109.50
1	A	137	LEU	N-CA-C	-5.42	101.64	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	603	LEU	N-CA-C	-5.42	98.42	107.80
2	B	333	LEU	N-CA-C	5.41	117.44	108.20
2	B	38	VAL	N-CA-C	5.38	120.54	109.34
2	B	161	THR	CA-C-N	5.37	125.04	119.56
2	B	161	THR	C-N-CA	5.37	125.04	119.56
2	B	136	PRO	N-CA-C	-5.34	102.30	110.95
2	B	36	GLU	N-CA-C	5.31	117.46	109.23
2	B	729	ASP	N-CA-C	5.29	116.48	108.07
2	B	69	GLY	N-CA-C	-5.27	100.70	113.18
1	A	245	PHE	N-CA-C	-5.23	101.52	108.74
2	B	155	VAL	N-CA-C	5.21	115.35	107.75
2	B	117	ALA	N-CA-C	-5.15	102.90	110.52
2	B	462	GLU	N-CA-C	5.13	116.68	111.14
2	B	608	LEU	N-CA-C	-5.13	105.15	111.40
2	B	228	LEU	N-CA-C	5.12	117.26	111.11
1	A	233	LEU	N-CA-C	-5.08	105.83	111.36
2	B	559	ASN	N-CA-C	-5.00	105.74	111.14
1	A	101	HIS	CA-C-N	5.00	125.02	119.32
1	A	101	HIS	C-N-CA	5.00	125.02	119.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2112	0	2062	171	0
2	B	6054	0	6109	521	0
3	A	1	0	0	0	0
4	A	33	0	24	4	0
5	A	48	0	0	4	0
5	B	191	0	0	6	0
All	All	8439	0	8195	659	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 40.

All (659) 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:262:GLU:HG2	5:A:1015:HOH:O	1.45	1.16
2:B:600:LYS:HG2	2:B:601:GLU:H	1.04	1.14
2:B:75:VAL:HG11	2:B:108:ILE:HG21	1.31	1.12
2:B:285:THR:HG21	2:B:291:ARG:HE	1.20	1.02
2:B:294:HIS:CD2	2:B:296:GLU:H	1.79	1.00
1:A:213:GLU:HG3	1:A:214:ALA:H	1.28	0.99
2:B:601:GLU:O	2:B:602:ARG:HD2	1.64	0.98
2:B:600:LYS:HG2	2:B:601:GLU:N	1.78	0.96
2:B:614:GLU:HG2	2:B:624:PHE:HE1	1.29	0.95
2:B:602:ARG:HG2	2:B:602:ARG:HH11	1.28	0.95
2:B:596:LEU:HB2	2:B:599:ALA:HB3	1.46	0.95
1:A:263:PRO:HG3	2:B:461:GLU:HA	1.50	0.94
1:A:165:LEU:HD12	1:A:301:LEU:HD13	1.51	0.93
1:A:101:HIS:HB2	2:B:509:GLU:HG2	1.50	0.93
1:A:143:HIS:ND1	1:A:144:PRO:HD2	1.84	0.93
2:B:593:GLY:HA3	2:B:604:SER:HB3	1.50	0.92
2:B:707:TYR:HE1	2:B:711:GLU:HB2	1.32	0.91
2:B:764:ALA:HA	2:B:767:ARG:HG2	1.52	0.89
2:B:602:ARG:HH11	2:B:602:ARG:CG	1.84	0.89
2:B:294:HIS:HD2	2:B:296:GLU:H	0.89	0.89
1:A:213:GLU:HG2	1:A:215:VAL:H	1.38	0.88
2:B:673:LEU:N	2:B:673:LEU:HD22	1.90	0.86
2:B:710:VAL:O	2:B:714:VAL:HG23	1.75	0.86
2:B:707:TYR:CE1	2:B:711:GLU:HB2	2.11	0.85
1:A:138:ASN:HD21	1:A:289:LYS:HE2	1.39	0.85
1:A:257:TYR:HB3	2:B:161:THR:HG21	1.59	0.85
1:A:209:ASP:O	1:A:333:ARG:HD2	1.77	0.84
2:B:278:ARG:NH2	2:B:308:SER:HB3	1.92	0.84
2:B:729:ASP:N	2:B:744:ALA:HB3	1.92	0.84
1:A:101:HIS:HD2	1:A:103:ILE:H	1.26	0.83
2:B:596:LEU:CB	2:B:599:ALA:HB3	2.09	0.83
2:B:688:SER:HB3	2:B:752:PRO:HA	1.61	0.83
1:A:213:GLU:CG	1:A:214:ALA:H	1.92	0.82
2:B:497:ARG:O	2:B:501:VAL:HG23	1.78	0.82
1:A:287:HIS:HD2	1:A:289:LYS:H	1.24	0.82
2:B:278:ARG:HH21	2:B:308:SER:HB3	1.42	0.82
2:B:563:ASP:O	2:B:565:PRO:HD3	1.78	0.82
1:A:138:ASN:ND2	1:A:289:LYS:HE2	1.96	0.81
2:B:701:VAL:HG22	2:B:702:PRO:HD2	1.62	0.81
2:B:38:VAL:O	2:B:40:PRO:HD3	1.80	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:ARG:HG3	5:B:974:HOH:O	1.79	0.81
2:B:294:HIS:HD2	2:B:296:GLU:N	1.75	0.81
1:A:311:THR:HG22	1:A:312:GLY:N	1.94	0.81
1:A:140:PRO:O	1:A:146:ARG:HB2	1.81	0.81
2:B:549:PHE:O	2:B:553:VAL:HG23	1.81	0.80
1:A:140:PRO:HD2	1:A:145:ALA:HB3	1.63	0.80
2:B:121:ARG:HD3	2:B:127:GLU:O	1.80	0.80
2:B:751:HIS:HD2	2:B:752:PRO:HD2	1.47	0.80
2:B:198:LEU:HD12	2:B:393:LEU:HD13	1.64	0.79
2:B:730:LEU:C	2:B:730:LEU:HD12	2.07	0.79
2:B:603:LEU:C	2:B:603:LEU:HD12	2.08	0.79
2:B:99:LEU:HD13	2:B:101:GLN:HB2	1.63	0.79
2:B:757:ARG:HG3	2:B:759:GLU:HB2	1.63	0.79
1:A:213:GLU:CG	1:A:214:ALA:N	2.47	0.78
2:B:161:THR:HG22	2:B:162:PRO:HD2	1.64	0.78
2:B:438:GLU:OE1	2:B:438:GLU:HA	1.84	0.78
2:B:519:GLU:HB3	2:B:523:ARG:HH12	1.47	0.77
2:B:643:LEU:HA	2:B:647:GLU:O	1.84	0.77
1:A:250:LYS:H	1:A:270:TRP:HB3	1.48	0.77
1:A:218:GLN:NE2	4:A:1002:FYA:H5'1	1.98	0.77
2:B:427:ILE:HG12	2:B:466:ILE:HG21	1.67	0.76
2:B:239:MET:HE1	2:B:253:MET:HE1	1.66	0.76
2:B:663:LEU:C	2:B:665:LEU:H	1.94	0.76
2:B:614:GLU:HG2	2:B:624:PHE:CE1	2.19	0.76
2:B:656:HIS:HB3	2:B:659:ILE:HD12	1.68	0.75
1:A:311:THR:HG22	1:A:312:GLY:H	1.50	0.75
1:A:160:ARG:HG2	1:A:168:GLU:OE2	1.85	0.75
2:B:490:ALA:HB3	2:B:491:PRO:HD3	1.67	0.75
2:B:672:GLU:C	2:B:673:LEU:HD22	2.12	0.75
2:B:243:ASN:ND2	2:B:246:VAL:H	1.86	0.74
2:B:697:LEU:HD23	2:B:698:ALA:N	2.03	0.74
2:B:728:PHE:HE1	2:B:745:PHE:C	1.96	0.74
2:B:751:HIS:HB3	2:B:754:ARG:O	1.87	0.74
2:B:722:LEU:HD11	2:B:724:SER:O	1.88	0.74
2:B:688:SER:CB	2:B:752:PRO:HA	2.17	0.73
2:B:194:GLU:OE2	2:B:387:ARG:HG2	1.87	0.73
2:B:770:GLU:O	2:B:774:ALA:HB2	1.88	0.73
2:B:404:ILE:HD12	2:B:446:PRO:HD3	1.70	0.73
1:A:263:PRO:HG3	2:B:461:GLU:CA	2.18	0.73
2:B:635:HIS:HB2	2:B:656:HIS:HA	1.70	0.72
2:B:700:VAL:HA	2:B:741:LYS:O	1.88	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:730:LEU:HB2	2:B:742:SER:O	1.89	0.72
2:B:663:LEU:O	2:B:665:LEU:N	2.23	0.72
1:A:262:GLU:OE1	2:B:458:ASP:HA	1.90	0.71
2:B:286:LEU:HB3	2:B:317:MET:HE2	1.72	0.71
2:B:666:PRO:HB2	2:B:667:PRO:CD	2.19	0.71
2:B:38:VAL:HG22	2:B:153:GLU:O	1.89	0.71
2:B:285:THR:HG21	2:B:291:ARG:NE	2.01	0.71
1:A:349:VAL:O	1:A:350:LEU:HD22	1.91	0.71
2:B:178:HIS:O	2:B:430:ARG:NH1	2.24	0.71
2:B:95:GLU:OE2	2:B:102:LYS:HE2	1.91	0.70
2:B:243:ASN:HD21	2:B:246:VAL:H	1.38	0.70
2:B:770:GLU:CG	2:B:771:ALA:N	2.52	0.70
1:A:101:HIS:CD2	1:A:103:ILE:H	2.08	0.70
1:A:103:ILE:HD11	1:A:320:GLU:HG3	1.73	0.70
2:B:736:LEU:HB2	2:B:737:PRO:HD2	1.73	0.70
2:B:761:VAL:HG23	2:B:762:GLU:N	2.06	0.70
1:A:271:TRP:HZ3	1:A:276:LYS:HE2	1.57	0.70
2:B:294:HIS:NE2	2:B:296:GLU:HB2	2.07	0.70
2:B:761:VAL:HG23	2:B:762:GLU:H	1.56	0.70
2:B:589:LEU:HB3	2:B:609:LEU:HD12	1.73	0.70
2:B:602:ARG:CG	2:B:602:ARG:NH1	2.49	0.70
2:B:757:ARG:HD3	2:B:759:GLU:H	1.56	0.70
2:B:303:TRP:HA	2:B:307:GLU:O	1.91	0.69
2:B:583:THR:HG22	2:B:675:LEU:HD12	1.75	0.69
1:A:148:MET:HE2	2:B:162:PRO:HG2	1.75	0.69
1:A:278:LEU:HD13	1:A:325:LEU:HD13	1.74	0.69
1:A:349:VAL:HG12	1:A:350:LEU:HD22	1.75	0.69
1:A:149:TRP:CD1	1:A:177:THR:HG23	2.27	0.69
2:B:588:LEU:C	2:B:588:LEU:HD23	2.18	0.68
2:B:604:SER:HA	2:B:608:LEU:HD22	1.74	0.68
1:A:331:ASP:HB3	1:A:334:TYR:CD2	2.28	0.68
1:A:209:ASP:OD2	1:A:212:HIS:HB2	1.93	0.68
2:B:673:LEU:N	2:B:673:LEU:CD2	2.57	0.68
1:A:271:TRP:CZ3	1:A:274:GLY:HA3	2.29	0.68
2:B:734:PRO:HB2	2:B:735:PRO:HD3	1.76	0.68
2:B:698:ALA:HA	2:B:743:LEU:O	1.94	0.67
2:B:724:SER:HB2	2:B:748:ARG:HB2	1.75	0.67
1:A:155:THR:CG2	2:B:534:LEU:HD21	2.24	0.67
1:A:229:ALA:H	1:A:232:HIS:HD2	1.41	0.67
2:B:610:LYS:O	2:B:614:GLU:HG3	1.94	0.67
1:A:349:VAL:O	1:A:350:LEU:HD13	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:751:HIS:HB2	2:B:756:LEU:CD2	2.25	0.67
1:A:278:LEU:HD13	1:A:325:LEU:CD1	2.25	0.67
2:B:652:LEU:HD12	2:B:670:LEU:O	1.94	0.67
2:B:520:ASP:OD2	2:B:524:PHE:HE1	1.79	0.66
2:B:707:TYR:C	2:B:707:TYR:CD1	2.73	0.66
2:B:707:TYR:C	2:B:707:TYR:HD1	2.03	0.66
2:B:751:HIS:HB2	2:B:756:LEU:HD21	1.77	0.66
1:A:249:SER:HB2	1:A:270:TRP:O	1.96	0.66
2:B:693:ALA:HB3	2:B:749:PHE:HB2	1.77	0.65
1:A:331:ASP:O	1:A:334:TYR:HB2	1.96	0.65
1:A:246:GLY:HA2	1:A:248:ASP:N	2.12	0.65
2:B:243:ASN:C	2:B:243:ASN:HD22	2.05	0.65
1:A:157:GLU:HG3	5:A:1035:HOH:O	1.96	0.65
2:B:767:ARG:HE	2:B:767:ARG:N	1.95	0.65
1:A:205:PHE:O	1:A:205:PHE:CD1	2.50	0.64
1:A:290:VAL:O	1:A:294:VAL:HG23	1.96	0.64
2:B:108:ILE:HG22	2:B:109:GLN:N	2.11	0.64
2:B:557:LYS:HZ3	2:B:663:LEU:HD12	1.63	0.64
2:B:656:HIS:NE2	2:B:658:GLU:HB2	2.12	0.64
1:A:155:THR:HG21	2:B:534:LEU:HD21	1.80	0.64
2:B:645:GLU:OE2	2:B:680:LYS:HB2	1.98	0.64
2:B:194:GLU:HB2	2:B:196:LEU:CD2	2.28	0.64
2:B:108:ILE:O	2:B:109:GLN:HG2	1.98	0.64
2:B:139:ALA:O	2:B:140:LEU:HD12	1.98	0.64
1:A:248:ASP:HB2	5:A:1013:HOH:O	1.98	0.63
2:B:757:ARG:HD2	2:B:759:GLU:HG2	1.81	0.63
2:B:729:ASP:H	2:B:744:ALA:HB3	1.59	0.63
2:B:194:GLU:O	2:B:390:GLU:HG2	1.98	0.63
2:B:516:MET:HE3	2:B:545:ARG:HA	1.81	0.63
2:B:662:GLU:O	2:B:662:GLU:HG3	1.97	0.63
2:B:215:LEU:HB2	2:B:393:LEU:HB2	1.80	0.63
2:B:635:HIS:HB2	2:B:657:PRO:CD	2.28	0.63
2:B:758:ASP:O	2:B:761:VAL:HG22	1.99	0.62
2:B:770:GLU:HG2	2:B:771:ALA:H	1.64	0.62
2:B:299:VAL:HG23	2:B:312:GLY:O	1.98	0.62
2:B:671:PHE:HD1	2:B:673:LEU:HD21	1.64	0.62
2:B:767:ARG:HE	2:B:767:ARG:CA	2.12	0.62
2:B:219:PHE:HE2	2:B:387:ARG:HE	1.47	0.62
2:B:553:VAL:O	2:B:556:LEU:HB3	1.99	0.62
2:B:702:PRO:C	2:B:704:PRO:HD2	2.24	0.62
2:B:600:LYS:CG	2:B:601:GLU:H	1.93	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:751:HIS:CD2	2:B:752:PRO:HD2	2.32	0.62
2:B:767:ARG:HA	2:B:767:ARG:NE	2.14	0.62
1:A:213:GLU:HG2	1:A:215:VAL:N	2.12	0.61
2:B:214:THR:HG22	2:B:394:GLU:HG3	1.82	0.61
2:B:286:LEU:HD11	2:B:323:GLU:CD	2.25	0.61
2:B:517:ASP:HB3	2:B:520:ASP:OD1	1.99	0.61
2:B:671:PHE:CD1	2:B:673:LEU:HD21	2.36	0.61
2:B:381:GLN:HE21	2:B:388:VAL:HG23	1.66	0.61
2:B:551:GLY:O	2:B:555:VAL:HG23	2.01	0.61
2:B:702:PRO:CB	2:B:704:PRO:HD2	2.31	0.61
1:A:137:LEU:O	1:A:139:ILE:N	2.30	0.61
1:A:311:THR:CG2	1:A:312:GLY:N	2.63	0.61
2:B:153:GLU:HG3	2:B:154:VAL:N	2.14	0.61
2:B:508:GLN:O	2:B:570:LEU:HB2	2.01	0.61
2:B:707:TYR:HD1	2:B:707:TYR:O	1.84	0.61
2:B:764:ALA:HA	2:B:767:ARG:CG	2.29	0.61
1:A:205:PHE:HE2	2:B:535:ASN:O	1.84	0.60
1:A:341:LYS:HE3	2:B:563:ASP:OD2	2.01	0.60
2:B:707:TYR:HE1	2:B:711:GLU:CB	2.10	0.60
1:A:311:THR:CG2	1:A:312:GLY:H	2.15	0.60
2:B:589:LEU:CB	2:B:609:LEU:HD12	2.31	0.60
2:B:366:PRO:C	2:B:367:LEU:HD22	2.27	0.60
2:B:757:ARG:HB3	2:B:760:GLU:OE2	2.01	0.60
2:B:762:GLU:O	2:B:765:VAL:HG12	2.02	0.60
2:B:603:LEU:HD12	2:B:603:LEU:O	2.02	0.59
2:B:635:HIS:ND1	2:B:636:PRO:O	2.35	0.59
2:B:38:VAL:C	2:B:40:PRO:HD3	2.27	0.59
2:B:285:THR:CG2	2:B:291:ARG:HE	2.06	0.59
2:B:512:THR:HG22	2:B:545:ARG:HH21	1.68	0.59
2:B:657:PRO:HA	2:B:660:ALA:HB3	1.85	0.59
2:B:281:GLU:HG2	2:B:310:PRO:HG3	1.84	0.59
2:B:771:ALA:HA	2:B:774:ALA:HB3	1.84	0.59
1:A:134:PHE:O	1:A:137:LEU:O	2.21	0.59
2:B:39:PHE:HB2	2:B:152:GLU:HA	1.84	0.59
2:B:629:GLN:O	2:B:639:SER:HB3	2.03	0.59
1:A:331:ASP:OD1	1:A:333:ARG:HD3	2.01	0.59
2:B:409:GLU:OE2	2:B:413:ARG:HD3	2.03	0.59
2:B:519:GLU:HB3	2:B:523:ARG:NH1	2.17	0.59
1:A:165:LEU:HD11	1:A:303:LEU:HD21	1.84	0.59
2:B:656:HIS:CD2	2:B:658:GLU:H	2.20	0.59
2:B:75:VAL:CG1	2:B:108:ILE:HG21	2.21	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:GLU:HB2	2:B:232:ARG:NH2	2.17	0.58
2:B:703:ALA:N	2:B:704:PRO:CD	2.66	0.58
2:B:710:VAL:HG11	2:B:743:LEU:CD1	2.33	0.58
1:A:341:LYS:HE2	1:A:341:LYS:H	1.68	0.58
2:B:731:TYR:HD1	2:B:742:SER:HG	1.51	0.58
1:A:299:GLU:HG3	1:A:300:ARG:N	2.18	0.58
2:B:119:SER:OG	2:B:122:GLU:HG3	2.04	0.58
2:B:259:PRO:HG2	2:B:360:PHE:CE2	2.38	0.58
2:B:649:VAL:HG23	2:B:674:ARG:H	1.69	0.58
2:B:161:THR:HB	2:B:163:ASN:OD1	2.03	0.58
2:B:671:PHE:HD1	2:B:673:LEU:CD2	2.15	0.58
2:B:265:LEU:HD23	2:B:268:VAL:HG21	1.86	0.58
2:B:294:HIS:CD2	2:B:296:GLU:HB2	2.39	0.58
2:B:706:PRO:O	2:B:710:VAL:HG23	2.04	0.58
2:B:99:LEU:HD22	2:B:101:GLN:NE2	2.19	0.57
2:B:108:ILE:CG2	2:B:109:GLN:N	2.67	0.57
2:B:556:LEU:HD12	2:B:556:LEU:C	2.28	0.57
2:B:728:PHE:HD1	2:B:728:PHE:H	1.49	0.57
1:A:148:MET:CE	2:B:162:PRO:HG2	2.34	0.57
2:B:757:ARG:CG	2:B:759:GLU:HB2	2.34	0.57
2:B:669:HIS:C	2:B:670:LEU:HD13	2.29	0.57
2:B:767:ARG:CA	2:B:767:ARG:NE	2.67	0.57
1:A:180:SER:O	1:A:183:GLN:HB2	2.05	0.57
2:B:377:LEU:HD22	2:B:388:VAL:HG13	1.87	0.57
2:B:293:LEU:HD13	2:B:293:LEU:N	2.18	0.57
2:B:635:HIS:HB2	2:B:657:PRO:HD3	1.85	0.57
2:B:729:ASP:CG	2:B:730:LEU:N	2.62	0.57
2:B:657:PRO:HA	2:B:660:ALA:CB	2.35	0.57
1:A:148:MET:HE1	1:A:257:TYR:CE2	2.39	0.57
2:B:557:LYS:NZ	2:B:663:LEU:HD12	2.19	0.57
1:A:162:GLU:CG	1:A:166:GLY:HA2	2.35	0.57
2:B:730:LEU:C	2:B:730:LEU:CD1	2.77	0.57
2:B:287:ASP:HB3	2:B:317:MET:HE1	1.87	0.56
1:A:126:GLU:HG3	2:B:575:ARG:HD2	1.87	0.56
2:B:601:GLU:C	2:B:602:ARG:HD2	2.29	0.56
2:B:707:TYR:HE2	2:B:727:LEU:HD22	1.70	0.56
2:B:38:VAL:O	2:B:40:PRO:CD	2.53	0.56
2:B:697:LEU:HD23	2:B:697:LEU:C	2.29	0.56
1:A:143:HIS:CG	1:A:144:PRO:HD2	2.40	0.56
1:A:252:ARG:HE	1:A:268:ALA:HB3	1.71	0.56
2:B:563:ASP:C	2:B:565:PRO:HD3	2.30	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:702:PRO:HA	2:B:739:GLY:O	2.06	0.56
2:B:758:ASP:HA	2:B:761:VAL:HG22	1.88	0.56
1:A:122:VAL:CG1	2:B:488:VAL:HG13	2.35	0.56
1:A:271:TRP:NE1	1:A:273:GLU:HB2	2.21	0.56
1:A:276:LYS:HG3	1:A:278:LEU:HD21	1.87	0.56
2:B:226:SER:OG	2:B:244:ASN:HA	2.05	0.56
2:B:634:LEU:HB3	2:B:639:SER:OG	2.05	0.56
2:B:71:THR:HG22	2:B:72:VAL:N	2.21	0.56
1:A:238:TYR:HA	1:A:251:VAL:HG11	1.88	0.55
2:B:643:LEU:C	2:B:644:VAL:O	2.47	0.55
2:B:762:GLU:C	2:B:765:VAL:HG12	2.31	0.55
1:A:287:HIS:CD2	1:A:288:PRO:HD2	2.41	0.55
2:B:514:SER:O	2:B:545:ARG:HG2	2.07	0.55
2:B:381:GLN:O	2:B:385:GLY:HA2	2.06	0.55
2:B:55:PRO:HA	2:B:62:LYS:HA	1.89	0.55
2:B:770:GLU:CG	2:B:771:ALA:H	2.19	0.55
2:B:221:LEU:CD2	2:B:386:ALA:HB2	2.36	0.55
2:B:527:ASP:HB3	2:B:528:PRO:HD2	1.89	0.55
1:A:96:PHE:CE1	2:B:567:ARG:HG3	2.42	0.54
1:A:123:GLU:O	1:A:182:MET:HE2	2.06	0.54
1:A:94:SER:HB2	2:B:567:ARG:NH2	2.21	0.54
2:B:458:ASP:O	2:B:462:GLU:HG2	2.08	0.54
1:A:219:LEU:HB3	1:A:317:LEU:CD2	2.37	0.54
1:A:349:VAL:CG1	1:A:350:LEU:HD22	2.38	0.54
2:B:370:VAL:N	2:B:371:PRO:HD2	2.23	0.54
2:B:734:PRO:CB	2:B:735:PRO:HD3	2.37	0.54
2:B:530:ARG:HH11	2:B:530:ARG:HB2	1.72	0.54
1:A:343:LEU:HD13	2:B:509:GLU:O	2.07	0.54
2:B:239:MET:CE	2:B:355:GLU:HG3	2.37	0.54
2:B:509:GLU:HG3	2:B:510:VAL:N	2.22	0.54
2:B:757:ARG:CD	2:B:759:GLU:H	2.21	0.54
2:B:761:VAL:CG2	2:B:762:GLU:H	2.20	0.54
2:B:163:ASN:O	2:B:452:ASP:HB3	2.08	0.54
2:B:224:ALA:HB1	2:B:225:PRO:HD2	1.90	0.54
2:B:194:GLU:HB2	2:B:196:LEU:HD21	1.90	0.54
2:B:239:MET:HE3	2:B:355:GLU:HG3	1.90	0.53
2:B:194:GLU:HB2	2:B:196:LEU:HD23	1.91	0.53
1:A:257:TYR:HB3	2:B:161:THR:CG2	2.36	0.53
2:B:702:PRO:HB2	2:B:704:PRO:HD2	1.90	0.53
2:B:707:TYR:CD1	2:B:707:TYR:O	2.62	0.53
1:A:242:GLN:OE1	1:A:247:PRO:HB3	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:650:GLY:HA3	2:B:673:LEU:HD13	1.90	0.53
2:B:275:ARG:O	2:B:299:VAL:HG12	2.08	0.53
2:B:575:ARG:HG2	2:B:581:GLU:HG2	1.90	0.53
2:B:498:LEU:O	2:B:498:LEU:HD12	2.08	0.52
2:B:523:ARG:NH1	2:B:523:ARG:HG3	2.23	0.52
1:A:281:GLY:HA2	4:A:1002:FYA:O3'	2.09	0.52
2:B:617:PHE:HB3	2:B:622:LEU:O	2.09	0.52
1:A:96:PHE:CZ	2:B:567:ARG:HG3	2.43	0.52
2:B:263:PHE:O	2:B:331:ILE:HB	2.10	0.52
2:B:663:LEU:C	2:B:665:LEU:N	2.62	0.52
2:B:728:PHE:CD1	2:B:728:PHE:N	2.78	0.52
2:B:20:VAL:O	2:B:24:ARG:HG2	2.10	0.52
2:B:285:THR:HG23	2:B:287:ASP:OD1	2.09	0.52
2:B:459:LEU:O	2:B:462:GLU:HB2	2.10	0.52
2:B:761:VAL:CG2	2:B:762:GLU:N	2.73	0.52
2:B:51:LEU:HD21	2:B:67:ASP:HB2	1.91	0.52
2:B:267:PHE:CE2	2:B:321:GLU:HG2	2.45	0.52
2:B:549:PHE:CG	2:B:550:PRO:HD3	2.45	0.52
2:B:671:PHE:CD1	2:B:673:LEU:CD2	2.92	0.52
2:B:733:GLY:HA3	2:B:736:LEU:HD21	1.92	0.52
2:B:447:PRO:HB2	2:B:449:HIS:CE1	2.45	0.52
2:B:699:VAL:HG12	2:B:773:ARG:NH2	2.25	0.52
1:A:165:LEU:HD12	1:A:301:LEU:CD1	2.33	0.51
2:B:63:ARG:HD2	2:B:73:GLU:OE2	2.10	0.51
2:B:621:GLY:O	2:B:680:LYS:HE2	2.10	0.51
2:B:666:PRO:HB2	2:B:667:PRO:HD2	1.92	0.51
2:B:191:LEU:HD13	2:B:378:SER:HA	1.91	0.51
2:B:359:ARG:HG3	2:B:359:ARG:HH11	1.75	0.51
1:A:246:GLY:HA2	1:A:248:ASP:H	1.74	0.51
2:B:671:PHE:CD1	2:B:671:PHE:C	2.88	0.51
2:B:107:VAL:HA	2:B:112:ARG:HA	1.92	0.51
2:B:224:ALA:HB1	2:B:225:PRO:CD	2.41	0.51
2:B:635:HIS:HB2	2:B:657:PRO:HD2	1.91	0.51
1:A:175:LEU:HB3	1:A:203:PHE:CD2	2.45	0.51
1:A:209:ASP:C	1:A:333:ARG:HD2	2.35	0.51
2:B:243:ASN:ND2	2:B:243:ASN:C	2.69	0.51
2:B:538:ALA:HB1	2:B:540:GLU:OE1	2.10	0.51
2:B:548:LEU:HD13	2:B:576:VAL:CG1	2.41	0.51
2:B:644:VAL:HG22	2:B:645:GLU:H	1.74	0.51
2:B:337:CYS:HB2	2:B:369:GLN:NE2	2.25	0.51
2:B:770:GLU:O	2:B:774:ALA:CB	2.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:770:GLU:HG2	2:B:771:ALA:N	2.24	0.51
2:B:773:ARG:C	2:B:775:ARG:N	2.62	0.51
1:A:283:ALA:HB2	1:A:315:PHE:CB	2.40	0.51
2:B:285:THR:HG22	2:B:291:ARG:HG3	1.93	0.51
2:B:723:GLU:OE1	2:B:750:ARG:HD2	2.10	0.51
2:B:770:GLU:HG3	2:B:771:ALA:N	2.24	0.51
1:A:94:SER:O	2:B:594:VAL:HB	2.11	0.51
1:A:271:TRP:CH2	1:A:274:GLY:HA3	2.45	0.51
2:B:409:GLU:OE1	2:B:413:ARG:NH1	2.43	0.51
2:B:530:ARG:HB2	2:B:530:ARG:NH1	2.25	0.50
2:B:635:HIS:CE1	2:B:636:PRO:O	2.64	0.50
1:A:101:HIS:CD2	1:A:103:ILE:HB	2.46	0.50
1:A:270:TRP:O	1:A:272:PRO:HD3	2.10	0.50
1:A:110:LEU:HD11	1:A:322:LEU:HD23	1.93	0.50
5:A:1006:HOH:O	2:B:31:GLU:HG3	2.11	0.50
2:B:661:GLN:C	2:B:663:LEU:N	2.68	0.50
2:B:773:ARG:HB2	2:B:773:ARG:NH1	2.27	0.50
2:B:105:GLU:HG3	2:B:114:PHE:CD1	2.47	0.50
2:B:36:GLU:O	2:B:154:VAL:HA	2.11	0.50
2:B:299:VAL:HG22	2:B:300:ILE:N	2.26	0.50
2:B:656:HIS:HB3	2:B:659:ILE:CD1	2.39	0.50
2:B:30:PHE:HA	5:B:976:HOH:O	2.10	0.50
2:B:2:ARG:HD2	5:B:828:HOH:O	2.12	0.50
2:B:262:ALA:HB1	2:B:331:ILE:HG13	1.94	0.50
2:B:274:VAL:HG12	2:B:298:LEU:HD21	1.92	0.50
1:A:105:LEU:HD22	1:A:349:VAL:CG1	2.41	0.50
2:B:253:MET:HG3	2:B:259:PRO:HA	1.93	0.50
2:B:557:LYS:HE3	2:B:664:GLU:OE2	2.11	0.50
1:A:315:PHE:CD1	1:A:315:PHE:C	2.89	0.50
2:B:72:VAL:HG21	2:B:114:PHE:CD2	2.47	0.50
2:B:649:VAL:CG2	2:B:674:ARG:H	2.24	0.50
2:B:188:GLU:HG3	2:B:188:GLU:O	2.12	0.49
1:A:101:HIS:CB	2:B:509:GLU:HG2	2.32	0.49
1:A:198:VAL:N	1:A:220:GLU:O	2.38	0.49
2:B:46:VAL:HB	2:B:143:GLY:O	2.12	0.49
2:B:92:PRO:HG3	2:B:114:PHE:O	2.13	0.49
2:B:598:TRP:CZ3	2:B:599:ALA:HB2	2.47	0.49
2:B:710:VAL:HG11	2:B:743:LEU:HD12	1.94	0.49
1:A:122:VAL:HG13	2:B:488:VAL:HG13	1.94	0.49
2:B:520:ASP:HA	2:B:523:ARG:HB2	1.94	0.49
2:B:688:SER:OG	2:B:752:PRO:HA	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:VAL:HA	2:B:66:LEU:HD23	1.93	0.49
2:B:692:ALA:HA	2:B:749:PHE:O	2.12	0.49
1:A:134:PHE:CZ	1:A:151:THR:HG21	2.48	0.49
2:B:517:ASP:OD1	2:B:519:GLU:HB2	2.13	0.49
2:B:287:ASP:N	2:B:317:MET:HE2	2.27	0.49
1:A:114:PHE:HA	1:A:117:LEU:HD13	1.95	0.49
2:B:765:VAL:HG13	2:B:766:SER:N	2.28	0.49
2:B:286:LEU:HB2	2:B:318:GLY:O	2.13	0.48
2:B:609:LEU:HD21	2:B:671:PHE:HD2	1.77	0.48
2:B:538:ALA:HB3	2:B:541:LYS:HG2	1.95	0.48
2:B:603:LEU:C	2:B:603:LEU:CD1	2.82	0.48
2:B:613:LEU:O	2:B:617:PHE:HD1	1.96	0.48
1:A:268:ALA:HA	1:A:278:LEU:O	2.12	0.48
2:B:355:GLU:O	2:B:359:ARG:HG3	2.13	0.48
2:B:532:LEU:N	2:B:532:LEU:HD22	2.28	0.48
2:B:509:GLU:HA	2:B:571:PHE:CE1	2.47	0.48
2:B:575:ARG:HG2	2:B:581:GLU:CG	2.44	0.48
2:B:587:GLY:HA3	2:B:671:PHE:CE2	2.47	0.48
1:A:277:TRP:C	1:A:278:LEU:HD23	2.39	0.48
1:A:283:ALA:HB2	1:A:315:PHE:HB3	1.95	0.48
1:A:213:GLU:HG2	1:A:214:ALA:N	2.28	0.48
1:A:86:VAL:HG23	1:A:87:ASP:N	2.29	0.48
1:A:104:THR:HG1	2:B:511:TYR:HH	1.62	0.48
2:B:119:SER:OG	2:B:129:GLY:HA2	2.14	0.48
2:B:721:TYR:CD1	2:B:721:TYR:N	2.81	0.48
2:B:549:PHE:CD1	2:B:549:PHE:C	2.92	0.47
2:B:703:ALA:N	2:B:704:PRO:HD2	2.28	0.47
2:B:331:ILE:HG12	2:B:332:ALA:N	2.29	0.47
1:A:271:TRP:CZ3	1:A:276:LYS:HE2	2.43	0.47
2:B:287:ASP:CB	2:B:317:MET:HE1	2.44	0.47
2:B:596:LEU:HD13	2:B:598:TRP:CH2	2.50	0.47
1:A:205:PHE:O	1:A:205:PHE:HD1	1.97	0.47
1:A:342:PHE:O	1:A:345:GLN:HB2	2.15	0.47
2:B:303:TRP:CA	2:B:307:GLU:O	2.61	0.47
2:B:642:VAL:HG23	2:B:651:PHE:HA	1.96	0.47
1:A:337:GLY:O	1:A:339:ARG:N	2.41	0.47
1:A:339:ARG:NH1	2:B:562:LEU:HD22	2.30	0.47
2:B:498:LEU:HD12	2:B:498:LEU:C	2.39	0.47
2:B:244:ASN:O	2:B:248:VAL:HG23	2.15	0.47
2:B:486:ARG:HA	2:B:486:ARG:HD3	1.73	0.47
2:B:650:GLY:HA3	2:B:672:GLU:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:717:ALA:C	2:B:768:VAL:HG22	2.40	0.47
2:B:642:VAL:HG23	2:B:651:PHE:CA	2.45	0.47
1:A:208:THR:HG22	1:A:213:GLU:HA	1.96	0.47
2:B:293:LEU:N	2:B:293:LEU:CD1	2.78	0.47
2:B:609:LEU:HD22	2:B:652:LEU:CD1	2.45	0.47
2:B:105:GLU:HG3	2:B:114:PHE:HD1	1.79	0.47
2:B:286:LEU:HB3	2:B:317:MET:CE	2.42	0.47
2:B:615:ALA:O	2:B:618:ALA:HB3	2.15	0.47
2:B:702:PRO:O	2:B:741:LYS:HE2	2.15	0.47
2:B:751:HIS:HD2	2:B:752:PRO:CD	2.22	0.47
2:B:523:ARG:HG3	2:B:523:ARG:HH11	1.79	0.46
2:B:533:LEU:HB2	2:B:536:PRO:HG3	1.97	0.46
2:B:651:PHE:CE2	2:B:672:GLU:HB3	2.50	0.46
2:B:765:VAL:CG1	2:B:766:SER:N	2.78	0.46
2:B:536:PRO:HB3	2:B:542:ALA:HA	1.97	0.46
1:A:221:GLY:O	1:A:314:ALA:HA	2.14	0.46
1:A:260:PHE:CD1	1:A:260:PHE:N	2.82	0.46
2:B:556:LEU:HD22	2:B:588:LEU:HD21	1.96	0.46
2:B:675:LEU:HB3	2:B:676:PRO:HA	1.96	0.46
2:B:731:TYR:CE2	2:B:733:GLY:HA2	2.50	0.46
2:B:374:ARG:HA	2:B:374:ARG:HD3	1.77	0.46
2:B:537:LEU:HA	2:B:537:LEU:HD23	1.60	0.46
1:A:94:SER:HB2	2:B:567:ARG:CZ	2.46	0.46
1:A:147:ASP:OD1	1:A:147:ASP:N	2.49	0.46
1:A:215:VAL:HG21	2:B:513:TYR:CD2	2.51	0.46
2:B:266:ARG:NH1	2:B:267:PHE:CE1	2.83	0.46
1:A:134:PHE:HZ	1:A:151:THR:HG21	1.81	0.46
2:B:93:GLY:O	2:B:102:LYS:HD3	2.16	0.46
2:B:417:THR:HG22	2:B:473:PRO:HD2	1.97	0.46
2:B:636:PRO:C	2:B:638:VAL:H	2.24	0.46
2:B:669:HIS:C	2:B:670:LEU:CD1	2.89	0.46
1:A:164:PRO:HG2	1:A:188:VAL:HG11	1.97	0.46
2:B:294:HIS:CD2	2:B:296:GLU:N	2.63	0.46
2:B:695:ARG:HH22	2:B:761:VAL:HG21	1.80	0.46
2:B:631:PHE:HB2	2:B:634:LEU:HB2	1.97	0.46
1:A:219:LEU:HB3	1:A:317:LEU:HD22	1.97	0.45
2:B:730:LEU:HD12	2:B:730:LEU:O	2.16	0.45
2:B:766:SER:C	2:B:768:VAL:N	2.72	0.45
1:A:169:VAL:HG22	1:A:170:GLU:N	2.31	0.45
1:A:191:THR:HG22	1:A:192:PRO:HD2	1.98	0.45
1:A:238:TYR:HA	1:A:251:VAL:CG1	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:PHE:CZ	2:B:387:ARG:HB3	2.51	0.45
2:B:287:ASP:H	2:B:317:MET:HE2	1.81	0.45
2:B:549:PHE:CD2	2:B:550:PRO:HD3	2.51	0.45
2:B:660:ALA:O	2:B:663:LEU:O	2.34	0.45
1:A:270:TRP:HA	1:A:270:TRP:CE3	2.51	0.45
2:B:164:ARG:O	2:B:167:ALA:HB3	2.16	0.45
2:B:243:ASN:HD21	2:B:246:VAL:HG23	1.82	0.45
2:B:695:ARG:HB2	2:B:747:LEU:HB2	1.99	0.45
2:B:509:GLU:HB2	2:B:571:PHE:CE1	2.52	0.45
2:B:588:LEU:C	2:B:588:LEU:CD2	2.88	0.45
2:B:600:LYS:HD2	2:B:600:LYS:N	2.31	0.45
2:B:617:PHE:HD2	2:B:622:LEU:HB2	1.81	0.45
2:B:757:ARG:HD3	2:B:758:ASP:N	2.31	0.45
1:A:287:HIS:CD2	1:A:289:LYS:H	2.16	0.45
1:A:271:TRP:HB2	1:A:278:LEU:HD11	1.98	0.45
2:B:531:LEU:C	2:B:532:LEU:HD22	2.42	0.45
1:A:260:PHE:C	1:A:287:HIS:HB2	2.42	0.45
2:B:219:PHE:CE2	2:B:387:ARG:NE	2.82	0.45
2:B:300:ILE:HD13	2:B:314:ALA:HA	1.97	0.45
1:A:258:PHE:CZ	4:A:1002:FYA:HD1	2.52	0.45
2:B:44:GLY:HA3	2:B:94:THR:OG1	2.17	0.45
2:B:427:ILE:HG22	2:B:428:LEU:N	2.32	0.45
2:B:520:ASP:C	2:B:522:ARG:N	2.72	0.45
1:A:336:PHE:HB3	2:B:513:TYR:CE1	2.51	0.45
2:B:219:PHE:HE2	2:B:387:ARG:NE	2.12	0.45
2:B:399:LYS:HA	2:B:400:PRO:HD3	1.82	0.45
2:B:556:LEU:HD12	2:B:556:LEU:O	2.17	0.45
1:A:126:GLU:HB3	1:A:203:PHE:HE2	1.83	0.44
1:A:169:VAL:CG2	1:A:170:GLU:N	2.80	0.44
2:B:28:LEU:HD13	2:B:176:ASP:HB3	1.98	0.44
2:B:218:ALA:O	2:B:330:ALA:HA	2.17	0.44
2:B:623:ALA:O	2:B:645:GLU:HA	2.17	0.44
2:B:635:HIS:ND1	2:B:635:HIS:C	2.75	0.44
1:A:218:GLN:NE2	4:A:1002:FYA:C5'	2.75	0.44
1:A:317:LEU:C	1:A:317:LEU:HD23	2.42	0.44
2:B:2:ARG:CG	2:B:2:ARG:HH11	2.30	0.44
2:B:35:ILE:C	2:B:36:GLU:HG2	2.42	0.44
2:B:121:ARG:HA	2:B:126:GLY:O	2.17	0.44
2:B:701:VAL:CG2	2:B:702:PRO:HD2	2.42	0.44
1:A:105:LEU:HD22	1:A:349:VAL:HG12	1.98	0.44
1:A:349:VAL:O	1:A:349:VAL:CG1	2.63	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:ILE:O	2:B:36:GLU:HG2	2.16	0.44
2:B:657:PRO:O	2:B:660:ALA:HB3	2.18	0.44
2:B:725:LEU:C	2:B:725:LEU:HD23	2.42	0.44
1:A:180:SER:N	1:A:181:PRO:HD2	2.32	0.44
2:B:271:GLY:O	2:B:302:GLY:HA2	2.17	0.44
2:B:651:PHE:C	2:B:651:PHE:CD1	2.95	0.44
2:B:759:GLU:O	2:B:763:GLU:HB2	2.18	0.44
1:A:245:PHE:HE2	1:A:269:VAL:HG11	1.82	0.44
2:B:359:ARG:HH11	2:B:359:ARG:CG	2.30	0.44
2:B:548:LEU:HD22	2:B:584:HIS:CB	2.48	0.44
2:B:549:PHE:CD1	2:B:550:PRO:N	2.86	0.44
2:B:700:VAL:CG1	2:B:736:LEU:HD13	2.47	0.44
2:B:721:TYR:CD2	2:B:756:LEU:HD21	2.53	0.44
1:A:241:ALA:O	1:A:242:GLN:C	2.59	0.44
1:A:242:GLN:O	1:A:245:PHE:O	2.35	0.44
1:A:321:ARG:HA	1:A:324:MET:HE2	1.99	0.44
1:A:326:ARG:HG2	1:A:327:TYR:CD1	2.52	0.44
2:B:235:PHE:CZ	2:B:241:PRO:HD2	2.53	0.44
2:B:609:LEU:CD2	2:B:652:LEU:HD13	2.47	0.44
2:B:695:ARG:HH12	2:B:761:VAL:HG23	1.82	0.44
2:B:730:LEU:HD12	2:B:731:TYR:N	2.33	0.44
1:A:160:ARG:N	2:B:579:GLU:O	2.45	0.44
1:A:225:GLY:O	1:A:228:ILE:HG12	2.17	0.44
2:B:643:LEU:HD13	2:B:648:GLU:HA	2.00	0.44
2:B:707:TYR:O	2:B:710:VAL:HB	2.18	0.44
1:A:143:HIS:CB	1:A:144:PRO:HD2	2.48	0.44
1:A:339:ARG:NH1	2:B:563:ASP:OD1	2.51	0.44
2:B:198:LEU:HA	2:B:199:PRO:HD2	1.54	0.44
2:B:728:PHE:O	2:B:729:ASP:HB2	2.18	0.44
1:A:277:TRP:O	1:A:278:LEU:HD23	2.17	0.43
2:B:42:PRO:HA	2:B:43:ARG:NH1	2.33	0.43
2:B:523:ARG:HH11	2:B:523:ARG:CG	2.30	0.43
2:B:557:LYS:HA	2:B:665:LEU:HD11	2.00	0.43
2:B:656:HIS:CD2	2:B:656:HIS:C	2.95	0.43
2:B:659:ILE:O	2:B:660:ALA:C	2.61	0.43
2:B:732:GLN:OE1	2:B:732:GLN:HA	2.14	0.43
2:B:276:ARG:NH1	2:B:296:GLU:O	2.38	0.43
2:B:368:GLY:O	2:B:371:PRO:HG2	2.17	0.43
2:B:598:TRP:CE3	2:B:599:ALA:HB2	2.53	0.43
1:A:145:ALA:C	1:A:147:ASP:N	2.76	0.43
2:B:253:MET:O	2:B:256:ARG:O	2.35	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:TRP:HB2	2:B:307:GLU:O	2.18	0.43
2:B:92:PRO:HD3	2:B:114:PHE:O	2.19	0.43
2:B:420:PRO:O	2:B:421:GLU:C	2.62	0.43
2:B:694:PHE:C	2:B:695:ARG:HG2	2.43	0.43
2:B:705:THR:HG23	2:B:706:PRO:HD2	2.00	0.43
2:B:90:ALA:HB2	2:B:118:LEU:HD11	2.00	0.43
2:B:575:ARG:HD3	2:B:581:GLU:OE2	2.18	0.43
1:A:237:ILE:O	1:A:240:LEU:HB3	2.18	0.43
2:B:72:VAL:HG22	2:B:73:GLU:N	2.34	0.43
2:B:379:LEU:HD23	2:B:379:LEU:HA	1.92	0.43
1:A:149:TRP:CD1	1:A:177:THR:CG2	2.98	0.43
1:A:229:ALA:H	1:A:232:HIS:CD2	2.27	0.43
1:A:230:MET:HB2	2:B:415:LEU:HA	2.01	0.43
2:B:265:LEU:HD23	2:B:265:LEU:HA	1.81	0.43
2:B:600:LYS:HG2	2:B:601:GLU:HG3	2.00	0.43
2:B:309:PHE:CD1	2:B:309:PHE:N	2.87	0.43
2:B:520:ASP:OD2	2:B:554:ARG:NH1	2.49	0.43
2:B:768:VAL:O	2:B:772:LEU:HB2	2.19	0.43
1:A:201:ARG:HD2	1:A:215:VAL:CG1	2.48	0.43
2:B:535:ASN:OD1	2:B:535:ASN:N	2.52	0.43
2:B:589:LEU:HB3	2:B:609:LEU:CD1	2.43	0.43
1:A:233:LEU:HB2	1:A:313:PHE:CG	2.54	0.43
1:A:341:LYS:HA	1:A:341:LYS:HD3	1.87	0.43
2:B:498:LEU:O	2:B:499:ARG:C	2.61	0.43
2:B:729:ASP:CG	2:B:730:LEU:H	2.25	0.43
2:B:377:LEU:HD22	2:B:388:VAL:CG1	2.47	0.42
2:B:579:GLU:H	2:B:579:GLU:HG2	1.38	0.42
2:B:650:GLY:CA	2:B:672:GLU:O	2.67	0.42
2:B:713:LEU:O	2:B:714:VAL:C	2.62	0.42
1:A:122:VAL:HG13	2:B:488:VAL:CG1	2.49	0.42
2:B:80:ASN:HD22	2:B:134:GLU:HG3	1.84	0.42
2:B:520:ASP:OD2	2:B:524:PHE:CE1	2.67	0.42
2:B:600:LYS:HE2	2:B:600:LYS:HB3	1.78	0.42
1:A:107:GLU:O	1:A:111:VAL:HG23	2.20	0.42
1:A:210:ALA:C	1:A:332:ILE:HG22	2.44	0.42
1:A:339:ARG:HH12	2:B:562:LEU:HD22	1.85	0.42
2:B:176:ASP:OD2	2:B:465:ARG:NH2	2.53	0.42
2:B:276:ARG:HB3	2:B:295:PRO:O	2.19	0.42
2:B:337:CYS:HB2	2:B:369:GLN:HE22	1.84	0.42
2:B:555:VAL:HA	2:B:558:GLU:CD	2.44	0.42
2:B:602:ARG:NH1	2:B:602:ARG:HG3	2.31	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:703:ALA:HA	2:B:741:LYS:HG2	2.00	0.42
1:A:177:THR:HG22	1:A:178:HIS:CD2	2.54	0.42
2:B:22:GLU:HG3	2:B:32:THR:HB	2.00	0.42
2:B:80:ASN:O	2:B:82:ARG:HD3	2.19	0.42
2:B:514:SER:C	2:B:545:ARG:HG2	2.43	0.42
2:B:16:GLU:CD	2:B:20:VAL:HG11	2.44	0.42
2:B:171:LEU:HD23	2:B:171:LEU:HA	1.74	0.42
2:B:307:GLU:OE1	2:B:307:GLU:HA	2.14	0.42
2:B:589:LEU:HD21	2:B:608:LEU:HD23	2.01	0.42
2:B:651:PHE:O	2:B:671:PHE:HA	2.19	0.42
2:B:98:GLY:HA3	5:B:975:HOH:O	2.19	0.42
2:B:249:THR:HB	2:B:260:MET:HG3	2.02	0.42
2:B:430:ARG:NH2	5:B:786:HOH:O	2.53	0.42
2:B:700:VAL:HG12	2:B:736:LEU:CD1	2.49	0.42
2:B:706:PRO:O	2:B:707:TYR:C	2.61	0.42
1:A:113:ILE:O	1:A:117:LEU:HD12	2.19	0.42
1:A:148:MET:HE1	1:A:257:TYR:HE2	1.81	0.42
1:A:111:VAL:O	1:A:112:GLU:C	2.63	0.42
2:B:538:ALA:HB3	2:B:541:LYS:CG	2.50	0.42
2:B:692:ALA:CA	2:B:749:PHE:O	2.68	0.42
2:B:524:PHE:O	2:B:526:LEU:HG	2.20	0.42
2:B:643:LEU:N	2:B:643:LEU:HD22	2.35	0.42
1:A:128:GLU:HG3	1:A:129:SER:H	1.84	0.41
2:B:509:GLU:CA	2:B:571:PHE:CE1	3.03	0.41
2:B:519:GLU:O	2:B:522:ARG:HB2	2.20	0.41
2:B:535:ASN:N	2:B:536:PRO:HD3	2.35	0.41
2:B:727:LEU:HA	2:B:744:ALA:O	2.20	0.41
2:B:277:ALA:O	2:B:295:PRO:HA	2.19	0.41
2:B:467:GLN:OE1	2:B:467:GLN:HA	2.20	0.41
2:B:661:GLN:C	2:B:663:LEU:H	2.27	0.41
2:B:684:PHE:C	2:B:685:GLN:HG2	2.44	0.41
1:A:271:TRP:CE3	1:A:274:GLY:HA3	2.55	0.41
2:B:294:HIS:CD2	2:B:296:GLU:CB	3.03	0.41
2:B:549:PHE:O	2:B:550:PRO:C	2.63	0.41
2:B:265:LEU:HD23	2:B:268:VAL:CG2	2.50	0.41
1:A:179:THR:C	1:A:181:PRO:HD2	2.46	0.41
1:A:180:SER:O	1:A:181:PRO:C	2.62	0.41
2:B:177:LEU:HD23	2:B:177:LEU:HA	1.83	0.41
2:B:572:GLU:HG3	2:B:573:VAL:N	2.36	0.41
2:B:51:LEU:HD11	2:B:67:ASP:HB2	2.03	0.41
2:B:82:ARG:HH12	2:B:134:GLU:CD	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:505:LEU:HD12	2:B:505:LEU:HA	1.84	0.41
2:B:512:THR:HB	2:B:572:GLU:OE2	2.21	0.41
2:B:52:GLU:HB3	2:B:54:HIS:CE1	2.55	0.41
2:B:304:ARG:O	2:B:307:GLU:HB2	2.20	0.41
2:B:344:ARG:HG3	2:B:361:GLU:OE2	2.21	0.41
2:B:402:GLU:HG3	5:B:903:HOH:O	2.21	0.41
2:B:529:PRO:CB	2:B:543:ALA:HB1	2.50	0.41
2:B:600:LYS:HD2	2:B:600:LYS:H	1.85	0.41
1:A:144:PRO:HB2	2:B:162:PRO:HB3	2.03	0.41
2:B:286:LEU:CB	2:B:317:MET:HE2	2.47	0.41
2:B:633:PHE:HD1	2:B:634:LEU:HD13	1.85	0.41
2:B:704:PRO:O	2:B:705:THR:C	2.64	0.41
1:A:133:ASN:OD1	1:A:176:ARG:HA	2.21	0.41
1:A:133:ASN:HD21	1:A:177:THR:HB	1.85	0.41
2:B:71:THR:CG2	2:B:72:VAL:N	2.83	0.41
2:B:145:PRO:O	2:B:148:GLU:HB2	2.21	0.41
2:B:520:ASP:HB3	2:B:524:PHE:CD1	2.55	0.41
2:B:609:LEU:HD23	2:B:613:LEU:CD2	2.51	0.41
2:B:710:VAL:O	2:B:711:GLU:C	2.64	0.41
2:B:746:HIS:C	2:B:747:LEU:HD12	2.46	0.41
1:A:126:GLU:CG	2:B:575:ARG:HD2	2.50	0.41
2:B:90:ALA:O	2:B:103:VAL:HG11	2.21	0.41
2:B:146:LEU:O	2:B:147:SER:C	2.62	0.41
2:B:267:PHE:CD2	2:B:321:GLU:HG2	2.56	0.41
2:B:699:VAL:CG1	2:B:773:ARG:NH2	2.84	0.41
2:B:728:PHE:HE1	2:B:746:HIS:N	2.19	0.41
2:B:756:LEU:HA	2:B:756:LEU:HD23	1.82	0.41
2:B:278:ARG:NH2	2:B:308:SER:O	2.55	0.40
2:B:549:PHE:N	2:B:550:PRO:CD	2.84	0.40
2:B:656:HIS:HD2	2:B:657:PRO:CD	2.34	0.40
2:B:764:ALA:O	2:B:767:ARG:HB2	2.21	0.40
2:B:566:GLU:CG	2:B:592:GLU:HG2	2.51	0.40
1:A:244:LEU:O	1:A:326:ARG:NH2	2.53	0.40
1:A:278:LEU:HD13	1:A:325:LEU:HD11	2.01	0.40
2:B:41:ILE:HA	2:B:42:PRO:HD2	1.92	0.40
2:B:108:ILE:HG22	2:B:109:GLN:H	1.81	0.40
2:B:507:PHE:CD1	2:B:507:PHE:N	2.89	0.40
2:B:761:VAL:C	2:B:763:GLU:H	2.28	0.40
2:B:761:VAL:C	2:B:763:GLU:N	2.78	0.40
2:B:141:PRO:HG2	2:B:144:THR:CG2	2.51	0.40
2:B:773:ARG:HB2	2:B:773:ARG:HH11	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ILE:HD13	1:A:243:ALA:CB	2.52	0.40
1:A:195:ARG:HG2	1:A:223:VAL:HG22	2.03	0.40
2:B:381:GLN:NE2	2:B:388:VAL:HG23	2.33	0.40
2:B:522:ARG:O	2:B:523:ARG:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	263/350 (75%)	244 (93%)	14 (5%)	5 (2%)	6	11
2	B	773/785 (98%)	695 (90%)	63 (8%)	15 (2%)	6	11
All	All	1036/1135 (91%)	939 (91%)	77 (7%)	20 (2%)	6	11

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
2	B	488	VAL
2	B	664	GLU
1	A	338	GLY
2	B	708	GLY
1	A	94	SER
1	A	330	PRO
2	B	128	TYR
2	B	199	PRO
2	B	525	ARG
2	B	702	PRO
2	B	735	PRO
2	B	770	GLU
1	A	273	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	737	PRO
2	B	752	PRO
2	B	486	ARG
2	B	645	GLU
2	B	315	GLY
2	B	644	VAL

5.3.2 Protein sidechains ⓘ

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	213/277 (77%)	168 (79%)	45 (21%)	1	2
2	B	623/630 (99%)	483 (78%)	140 (22%)	1	1
All	All	836/907 (92%)	651 (78%)	185 (22%)	1	2

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	VAL
1	A	95	LEU
1	A	122	VAL
1	A	129	SER
1	A	143	HIS
1	A	146	ARG
1	A	147	ASP
1	A	151	THR
1	A	154	LEU
1	A	157	GLU
1	A	168	GLU
1	A	169	VAL
1	A	170	GLU
1	A	174	LEU
1	A	177	THR
1	A	178	HIS
1	A	183	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	191	THR
1	A	211	THR
1	A	230	MET
1	A	233	LEU
1	A	237	ILE
1	A	245	PHE
1	A	249	SER
1	A	250	LYS
1	A	252	ARG
1	A	260	PHE
1	A	266	GLN
1	A	276	LYS
1	A	280	LEU
1	A	289	LYS
1	A	292	GLN
1	A	299	GLU
1	A	300	ARG
1	A	303	LEU
1	A	317	LEU
1	A	326	ARG
1	A	333	ARG
1	A	339	ARG
1	A	340	LEU
1	A	341	LYS
1	A	345	GLN
1	A	347	LYS
1	A	349	VAL
1	A	350	LEU
2	B	2	ARG
2	B	23	GLU
2	B	33	ASP
2	B	34	ARG
2	B	35	ILE
2	B	38	VAL
2	B	46	VAL
2	B	56	ILE
2	B	59	THR
2	B	60	ARG
2	B	61	LEU
2	B	62	LYS
2	B	70	ARG
2	B	89	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	95	GLU
2	B	96	LEU
2	B	99	LEU
2	B	106	ARG
2	B	108	ILE
2	B	109	GLN
2	B	111	VAL
2	B	118	LEU
2	B	127	GLU
2	B	144	THR
2	B	148	GLU
2	B	152	GLU
2	B	153	GLU
2	B	157	ASP
2	B	161	THR
2	B	171	LEU
2	B	175	ARG
2	B	186	GLU
2	B	188	GLU
2	B	192	LYS
2	B	196	LEU
2	B	208	GLU
2	B	222	ARG
2	B	230	MET
2	B	239	MET
2	B	243	ASN
2	B	256	ARG
2	B	283	LEU
2	B	284	LYS
2	B	285	THR
2	B	286	LEU
2	B	293	LEU
2	B	294	HIS
2	B	298	LEU
2	B	307	GLU
2	B	313	LEU
2	B	322	SER
2	B	326	GLU
2	B	329	GLU
2	B	331	ILE
2	B	339	ASP
2	B	341	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	345	LYS
2	B	361	GLU
2	B	364	VAL
2	B	387	ARG
2	B	397	SER
2	B	399	LYS
2	B	423	GLU
2	B	427	ILE
2	B	438	GLU
2	B	441	THR
2	B	451	LEU
2	B	454	ARG
2	B	459	LEU
2	B	461	GLU
2	B	484	ASP
2	B	486	ARG
2	B	494	LYS
2	B	497	ARG
2	B	499	ARG
2	B	509	GLU
2	B	510	VAL
2	B	512	THR
2	B	522	ARG
2	B	523	ARG
2	B	525	ARG
2	B	526	LEU
2	B	541	LYS
2	B	545	ARG
2	B	548	LEU
2	B	556	LEU
2	B	558	GLU
2	B	562	LEU
2	B	567	ARG
2	B	570	LEU
2	B	575	ARG
2	B	579	GLU
2	B	588	LEU
2	B	590	PHE
2	B	592	GLU
2	B	600	LYS
2	B	602	ARG
2	B	603	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	609	LEU
2	B	613	LEU
2	B	624	PHE
2	B	626	VAL
2	B	634	LEU
2	B	635	HIS
2	B	638	VAL
2	B	639	SER
2	B	641	ARG
2	B	645	GLU
2	B	648	GLU
2	B	649	VAL
2	B	652	LEU
2	B	661	GLN
2	B	662	GLU
2	B	663	LEU
2	B	670	LEU
2	B	673	LEU
2	B	674	ARG
2	B	675	LEU
2	B	682	LEU
2	B	685	GLN
2	B	688	SER
2	B	689	ARG
2	B	700	VAL
2	B	701	VAL
2	B	707	TYR
2	B	713	LEU
2	B	714	VAL
2	B	715	ARG
2	B	716	GLU
2	B	727	LEU
2	B	728	PHE
2	B	730	LEU
2	B	731	TYR
2	B	732	GLN
2	B	738	GLU
2	B	741	LYS
2	B	746	HIS
2	B	748	ARG
2	B	770	GLU
2	B	775	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	A	138	ASN
1	A	142	HIS
1	A	178	HIS
1	A	190	HIS
1	A	218	GLN
1	A	232	HIS
1	A	254	GLN
1	A	287	HIS
2	B	54	HIS
2	B	109	GLN
2	B	178	HIS
2	B	212	HIS
2	B	231	GLN
2	B	243	ASN
2	B	258	GLN
2	B	261	HIS
2	B	294	HIS
2	B	350	HIS
2	B	358	HIS
2	B	449	HIS
2	B	485	ASN
2	B	496	GLN
2	B	656	HIS
2	B	746	HIS
2	B	751	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	FYA	A	1002	-	36,36,36	1.06	1 (2%)	48,52,52	0.62	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	FYA	A	1002	-	-	4/20/36/36	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	FYA	O3P-C	-4.48	1.27	1.44

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

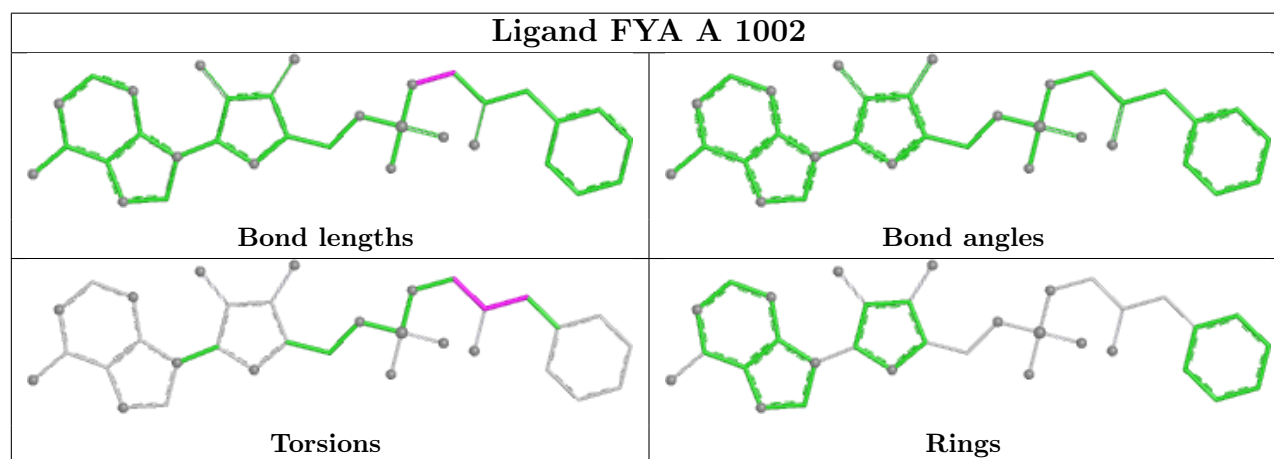
Mol	Chain	Res	Type	Atoms
4	A	1002	FYA	O3P-C-CA-N
4	A	1002	FYA	O3P-C-CA-CB
4	A	1002	FYA	C-CA-CB-CG
4	A	1002	FYA	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	FYA	4	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 than 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

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, 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	265/350 (75%)	0.27	22 (8%) 17 15	27, 54, 103, 129	0
2	B	775/785 (98%)	0.27	63 (8%) 18 15	21, 59, 108, 128	0
All	All	1040/1135 (91%)	0.27	85 (8%) 17 15	21, 58, 107, 129	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	LEU	7.0
1	A	149	TRP	6.4
1	A	143	HIS	5.1
2	B	701	VAL	4.1
1	A	142	HIS	4.1
1	A	246	GLY	4.0
1	A	148	MET	4.0
2	B	696	ASP	3.8
1	A	150	ASP	3.8
2	B	734	PRO	3.7
2	B	775	ARG	3.7
1	A	86	VAL	3.6
2	B	732	GLN	3.5
1	A	144	PRO	3.4
2	B	753	LYS	3.4
2	B	106	ARG	3.4
2	B	700	VAL	3.2
1	A	205	PHE	3.2
2	B	637	GLY	3.2
2	B	773	ARG	3.1
2	B	698	ALA	3.0
2	B	731	TYR	3.0
2	B	646	GLY	3.0
2	B	649	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	718	ALA	2.9
2	B	694	PHE	2.9
1	A	158	GLY	2.9
1	A	145	ALA	2.8
2	B	282	ARG	2.8
1	A	140	PRO	2.8
2	B	755	THR	2.8
2	B	697	LEU	2.8
2	B	736	LEU	2.8
1	A	207	GLN	2.8
2	B	99	LEU	2.7
2	B	693	ALA	2.7
1	A	348	GLY	2.7
2	B	739	GLY	2.7
2	B	296	GLU	2.6
1	A	271	TRP	2.6
2	B	749	PHE	2.6
2	B	100	GLY	2.5
2	B	192	LYS	2.5
2	B	699	VAL	2.5
2	B	737	PRO	2.4
2	B	351	GLY	2.4
2	B	638	VAL	2.4
1	A	141	GLU	2.4
2	B	743	LEU	2.4
2	B	774	ALA	2.4
2	B	443	ARG	2.3
2	B	600	LYS	2.3
2	B	682	LEU	2.3
2	B	759	GLU	2.3
2	B	687	PRO	2.3
2	B	598	TRP	2.3
2	B	203	LYS	2.3
2	B	592	GLU	2.3
2	B	738	GLU	2.3
2	B	594	VAL	2.2
2	B	689	ARG	2.2
1	A	146	ARG	2.2
2	B	720	PRO	2.2
2	B	580	ARG	2.2
2	B	703	ALA	2.1
1	A	272	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	691	PRO	2.1
2	B	706	PRO	2.1
1	A	169	VAL	2.1
2	B	713	LEU	2.1
2	B	566	GLU	2.1
2	B	762	GLU	2.1
2	B	704	PRO	2.1
2	B	633	PHE	2.1
2	B	692	ALA	2.1
2	B	108	ILE	2.1
1	A	334	TYR	2.1
2	B	769	ALA	2.1
2	B	43	ARG	2.1
2	B	188	GLU	2.1
2	B	752	PRO	2.1
2	B	746	HIS	2.0
1	A	245	PHE	2.0
2	B	603	LEU	2.0
2	B	33	ASP	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 oligosaccharides in this entry.

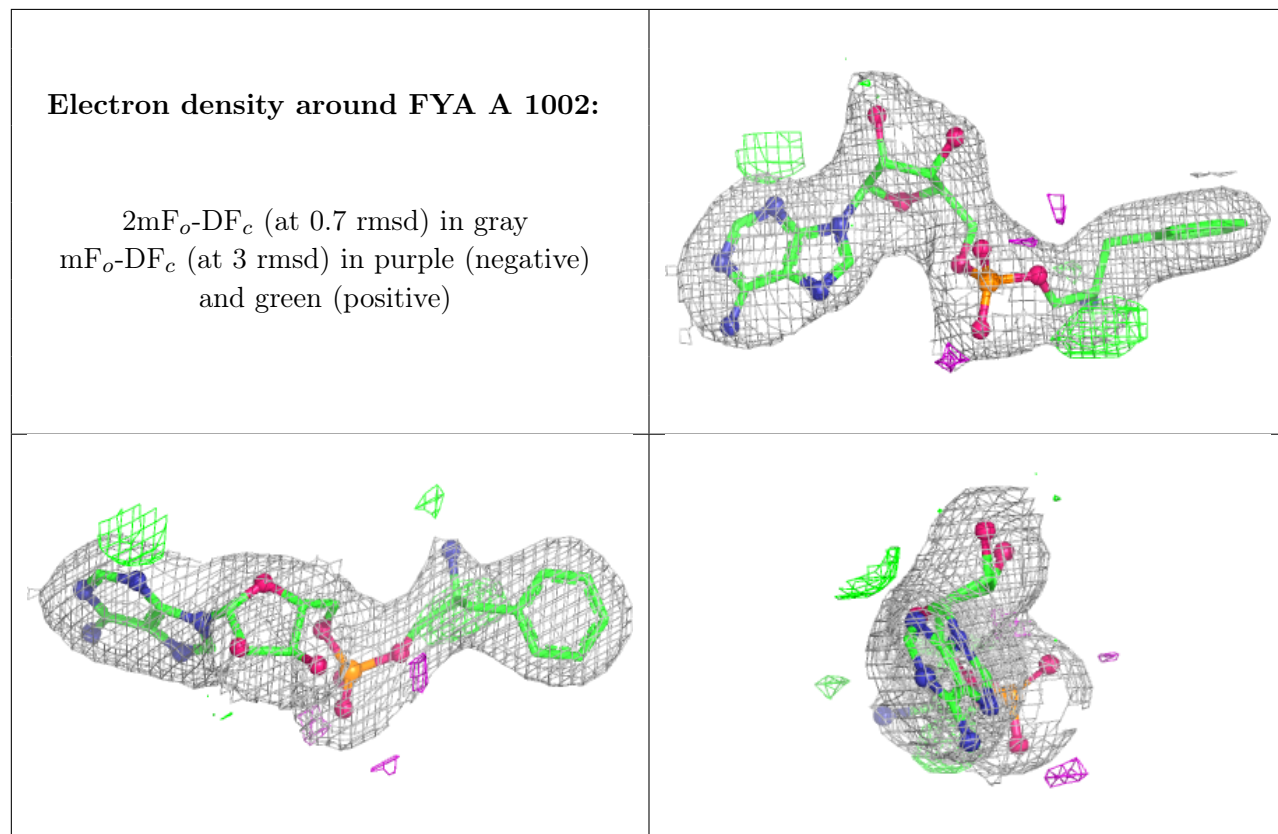
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
3	MG	A	1001	1/1	0.81	0.22	42,42,42,42	0
4	FYA	A	1002	33/33	0.95	0.10	40,65,73,76	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 [i](#)

There are no such residues in this entry.