



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 12:01 PM UTC

PDB ID : 1K7W / pdb_00001k7w
Title : Crystal Structure of S283A Duck Delta 2 Crystallin Mutant
Authors : Sampaleanu, L.M.; Yu, B.; Howell, P.L.
Deposited on : 2001-10-22
Resolution : 1.96 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

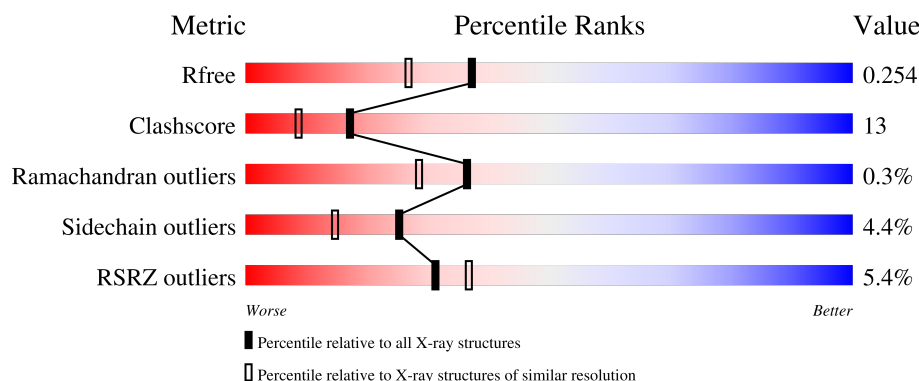
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	468	5% 70% 24% • •
1	B	468	8% 67% 26% • •
1	C	468	2% 71% 23% • •
1	D	468	6% 71% 22% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AS1	A	1004	X	-	-	-
2	AS1	B	1003	X	-	-	-
2	AS1	C	1001	X	-	-	-
2	AS1	D	1002	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14719 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.

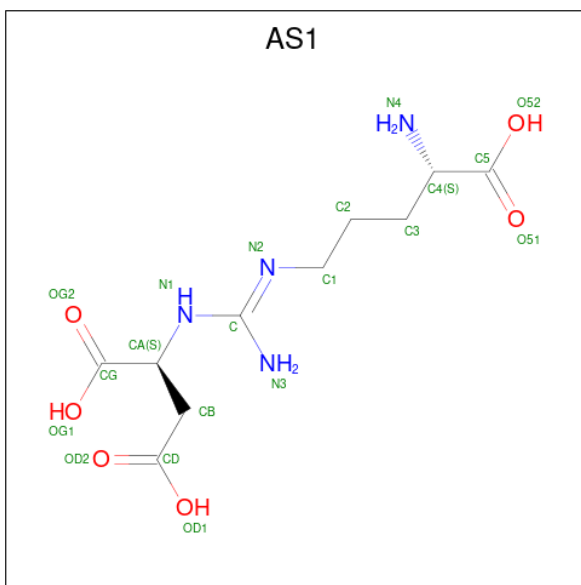
- Molecule 1 is a protein called delta 2 crystallin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3485	2205	591	677	12			
1	B	448	Total	C	N	O	S	0	0	0
			3473	2198	589	674	12			
1	C	448	Total	C	N	O	S	0	0	0
			3482	2206	589	675	12			
1	D	450	Total	C	N	O	S	0	0	0
			3492	2212	591	677	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	ALA	SER	engineered mutation	UNP P24058
A	443	GLY	ALA	conflict	UNP P24058
B	283	ALA	SER	engineered mutation	UNP P24058
B	443	GLY	ALA	conflict	UNP P24058
C	283	ALA	SER	engineered mutation	UNP P24058
C	443	GLY	ALA	conflict	UNP P24058
D	283	ALA	SER	engineered mutation	UNP P24058
D	443	GLY	ALA	conflict	UNP P24058

- Molecule 2 is ARGININOSUCCINATE (CCD ID: AS1) (formula: C₁₀H₁₈N₄O₆).



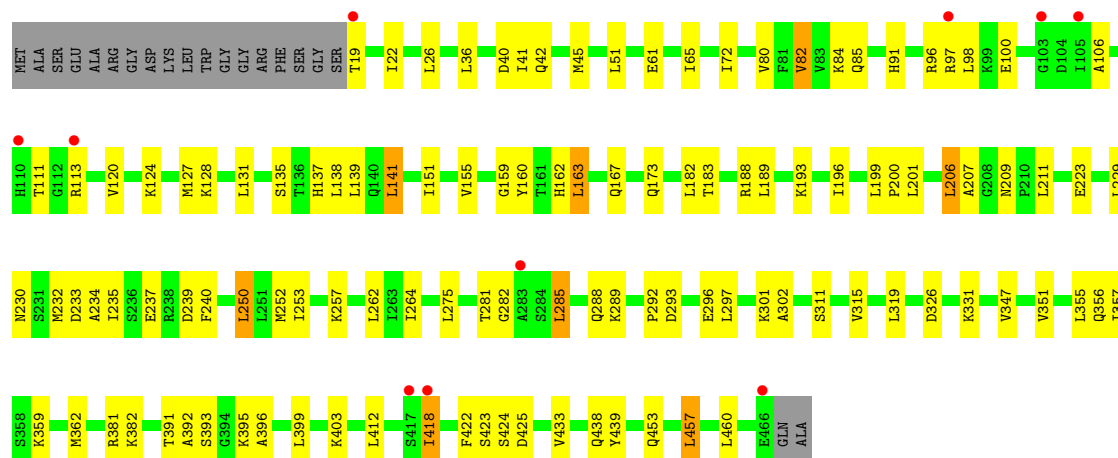
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 20	C 10	N 4	O 6	0	0
2	B	1	Total 20	C 10	N 4	O 6	0	0
2	C	1	Total 20	C 10	N 4	O 6	0	0
2	D	1	Total 20	C 10	N 4	O 6	0	0

- Molecule 3 is water.

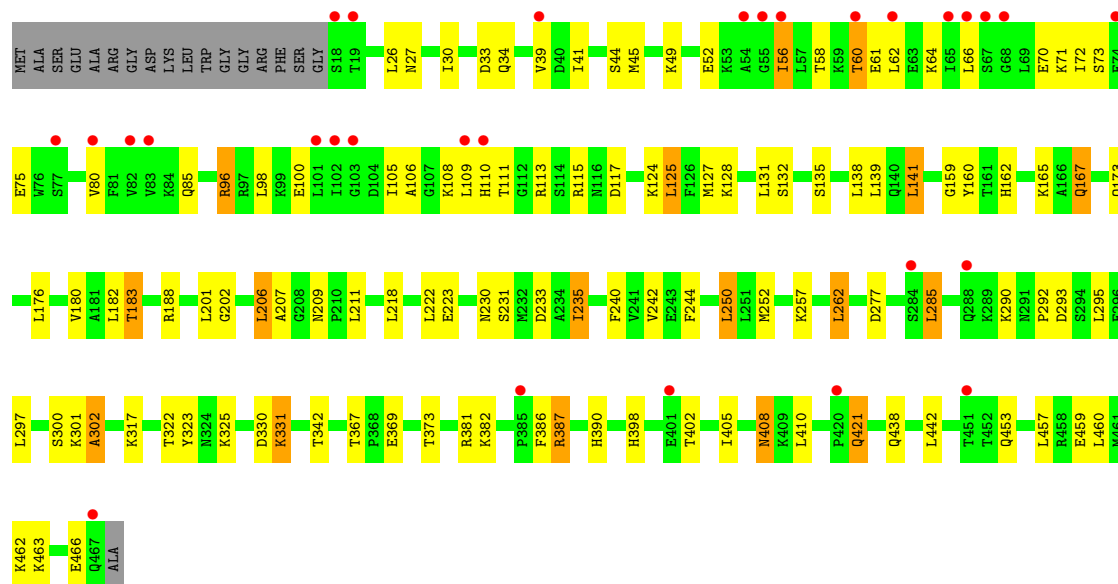
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	211	Total O 211 211	0	0
3	B	137	Total O 137 137	0	0
3	C	191	Total O 191 191	0	0
3	D	168	Total O 168 168	0	0



• Molecule 1: delta 2 crystallin



• Molecule 1: delta 2 crystallin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.76Å 98.64Å 106.15Å 90.00° 101.30° 90.00°	Depositor
Resolution (Å)	19.81 – 1.96 19.81 – 1.96	Depositor EDS
% Data completeness (in resolution range)	92.0 (19.81-1.96) 92.0 (19.81-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 1.96Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.253 0.207 , 0.254	Depositor DCC
R_{free} test set	12678 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14719	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: AS1

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.61	1/3529 (0.0%)	0.96	14/4759 (0.3%)
1	B	0.54	0/3517	0.97	14/4743 (0.3%)
1	C	0.57	0/3527	0.97	8/4756 (0.2%)
1	D	0.56	0/3537	0.95	9/4770 (0.2%)
All	All	0.57	1/14110 (0.0%)	0.96	45/19028 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	MET	SD-CE	6.02	1.94	1.79

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	LYS	N-CA-C	8.38	120.03	111.07
1	D	167	GLN	N-CA-C	8.26	115.65	108.22
1	D	244	PHE	N-CA-C	-7.85	102.67	111.07
1	A	331	LYS	N-CA-C	7.47	119.06	111.07
1	C	331	LYS	N-CA-C	7.29	118.87	111.07
1	C	439	TYR	N-CA-C	6.74	121.14	110.70
1	D	302	ALA	N-CA-C	-6.48	104.22	111.28
1	D	331	LYS	N-CA-C	6.30	117.81	111.07
1	B	286	MET	CA-C-N	6.25	125.94	119.56
1	B	286	MET	C-N-CA	6.25	125.94	119.56
1	A	159	GLY	N-CA-C	-6.20	100.15	111.25
1	D	159	GLY	N-CA-C	-6.16	100.23	111.25
1	A	286	MET	CA-C-N	6.07	125.75	119.56
1	A	286	MET	C-N-CA	6.07	125.75	119.56
1	A	302	ALA	N-CA-C	-5.86	104.97	111.36
1	A	209	ASN	N-CA-C	-5.82	102.45	109.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	234	ALA	N-CA-C	5.79	117.59	111.28
1	B	242	VAL	CB-CA-C	-5.74	104.54	111.88
1	D	115	ARG	N-CA-C	-5.60	105.71	112.54
1	C	159	GLY	N-CA-C	-5.55	101.32	111.25
1	C	160	TYR	N-CA-C	5.54	118.75	109.95
1	D	231	SER	N-CA-C	5.50	116.95	111.07
1	A	160	TYR	N-CA-C	5.48	118.66	109.95
1	B	115	ARG	N-CA-C	-5.45	105.89	112.54
1	A	439	TYR	N-CA-C	5.41	118.20	110.68
1	B	263	ILE	N-CA-C	-5.37	105.30	110.72
1	A	389	ALA	N-CA-C	-5.34	105.54	111.36
1	C	229	LEU	N-CA-C	5.31	118.92	112.23
1	B	202	GLY	N-CA-C	-5.30	107.90	115.64
1	B	159	GLY	N-CA-C	-5.28	101.32	110.71
1	B	40	ASP	N-CA-C	-5.24	105.64	111.36
1	B	302	ALA	N-CA-C	-5.23	105.66	111.36
1	C	151	ILE	N-CA-C	5.21	115.43	110.53
1	B	412	LEU	N-CA-C	-5.18	105.75	111.71
1	D	125	LEU	N-CA-C	-5.16	105.74	111.36
1	A	102	ILE	N-CA-C	5.15	118.10	113.10
1	A	367	THR	CA-C-N	5.13	124.75	119.05
1	A	367	THR	C-N-CA	5.13	124.75	119.05
1	B	160	TYR	N-CA-C	5.12	117.90	109.72
1	B	224	PHE	N-CA-C	-5.11	102.95	110.52
1	A	319	LEU	CA-C-N	-5.08	115.49	120.52
1	A	319	LEU	C-N-CA	-5.08	115.49	120.52
1	B	244	PHE	N-CA-C	-5.04	105.98	111.82
1	C	433	VAL	N-CA-C	-5.04	105.80	110.53
1	D	160	TYR	N-CA-C	5.03	117.95	109.95

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	3485	0	3604	105	0
1	B	3473	0	3595	100	0
1	C	3482	0	3603	86	0
1	D	3492	0	3607	100	0
2	A	20	0	14	0	0
2	B	20	0	14	1	0
2	C	20	0	14	0	0
2	D	20	0	14	1	0
3	A	211	0	0	12	0
3	B	137	0	0	5	0
3	C	191	0	0	9	0
3	D	168	0	0	6	0
All	All	14719	0	14465	359	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 13.

All (359) 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:C:183:THR:HG21	1:C:460:LEU:HD13	1.29	1.06
1:C:285:LEU:HD21	1:D:390:HIS:NE2	1.71	1.06
1:B:423:SER:O	1:B:426:VAL:HG23	1.71	0.91
1:D:183:THR:HG21	1:D:460:LEU:HD13	1.51	0.90
1:D:201:LEU:HD22	1:D:218:LEU:HD13	1.56	0.86
1:B:117:ASP:HB3	1:B:235:ILE:HD11	1.61	0.82
1:A:406:THR:OG1	1:A:409:LYS:HE2	1.80	0.82
1:C:173:GLN:HE22	1:C:453:GLN:HE22	1.27	0.81
1:D:408:ASN:H	1:D:408:ASN:HD22	1.26	0.80
1:C:357:ILE:HD12	1:C:362:MET:HE1	1.63	0.80
1:A:117:ASP:HB3	1:A:235:ILE:HD11	1.64	0.79
1:B:377:LEU:O	1:B:380:VAL:HG22	1.83	0.79
1:A:110:HIS:HD2	1:A:113:ARG:HE	1.31	0.79
1:B:72:ILE:HG12	1:B:97:ARG:HG2	1.64	0.78
1:A:381:ARG:HH22	1:A:438:GLN:HE21	1.29	0.78
1:D:201:LEU:HD23	1:D:202:GLY:N	1.99	0.78
1:B:412:LEU:HD22	1:B:416:LYS:HG3	1.66	0.78
1:A:85:GLN:HG3	3:A:1138:HOH:O	1.84	0.77
1:C:285:LEU:H	1:C:285:LEU:HD22	1.49	0.75
1:C:285:LEU:HD22	1:C:285:LEU:N	2.02	0.74
1:C:359:LYS:HA	1:C:362:MET:HE3	1.69	0.74
1:B:230:ASN:HD22	1:B:233:ASP:H	1.35	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ASN:HD22	1:A:233:ASP:H	1.34	0.74
1:C:183:THR:CG2	1:C:460:LEU:HD13	2.14	0.74
1:D:27:ASN:HD21	1:D:325:LYS:NZ	1.86	0.74
1:A:97:ARG:CZ	1:A:101:LEU:HD11	2.18	0.73
1:A:61:GLU:HG2	1:A:105:ILE:HG21	1.70	0.73
1:B:110:HIS:HD2	1:B:113:ARG:HE	1.36	0.73
1:C:230:ASN:HD22	1:C:233:ASP:H	1.37	0.73
1:D:30:ILE:O	1:D:34:GLN:HG3	1.90	0.72
1:D:39:VAL:HG21	1:D:125:LEU:HB2	1.71	0.71
1:D:381:ARG:HH22	1:D:438:GLN:HE21	1.35	0.71
1:D:85:GLN:CD	1:D:85:GLN:H	1.99	0.70
1:B:84:LYS:HB2	1:B:96:ARG:NH2	2.06	0.70
1:B:281:THR:HB	1:B:293:ASP:OD2	1.91	0.70
1:A:395:LYS:HD2	1:A:418:ILE:HG23	1.75	0.69
1:C:381:ARG:HH22	1:C:438:GLN:HE21	1.41	0.68
1:B:463:LYS:C	1:B:465:LYS:H	2.02	0.68
1:B:412:LEU:HD13	1:B:416:LYS:HE2	1.77	0.67
1:A:97:ARG:O	1:A:101:LEU:HD13	1.93	0.67
1:B:84:LYS:HB2	1:B:96:ARG:HH21	1.59	0.67
1:D:117:ASP:HB3	1:D:235:ILE:HD11	1.76	0.67
1:D:408:ASN:HD22	1:D:408:ASN:N	1.92	0.67
1:C:418:ILE:HD11	1:C:422:PHE:HE2	1.60	0.66
1:D:173:GLN:HE22	1:D:453:GLN:HE22	1.41	0.66
1:B:173:GLN:HE22	1:B:453:GLN:HE22	1.42	0.66
1:B:297:LEU:O	1:B:301:LYS:HG2	1.93	0.66
1:A:173:GLN:HE22	1:A:453:GLN:HE22	1.42	0.66
1:D:421:GLN:HE21	1:D:421:GLN:N	1.94	0.65
1:B:183:THR:HG21	1:B:460:LEU:HD13	1.78	0.65
1:C:113:ARG:HA	3:C:1190:HOH:O	1.96	0.65
1:A:116:ASN:HB3	1:A:235:ILE:CG2	2.27	0.65
1:C:285:LEU:HD21	1:D:390:HIS:CE1	2.31	0.64
1:D:58:THR:OG1	1:D:60:THR:HG23	1.98	0.64
1:A:405:ILE:HD11	1:A:410:LEU:HD12	1.80	0.64
2:D:1002:AS1:HB1	3:D:1151:HOH:O	1.98	0.64
1:D:41:ILE:HD11	1:D:72:ILE:HG22	1.79	0.63
1:B:412:LEU:CD1	1:B:416:LYS:HE2	2.28	0.63
1:B:189:LEU:O	1:B:189:LEU:HD23	1.98	0.62
1:B:141:LEU:HD13	1:B:182:LEU:HD13	1.82	0.62
1:B:207:ALA:HB3	1:D:167:GLN:NE2	2.14	0.62
1:B:209:ASN:ND2	1:B:211:LEU:H	1.96	0.62
1:A:141:LEU:HD13	1:A:182:LEU:HD13	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:THR:CG2	1:D:460:LEU:HD13	2.28	0.61
1:A:209:ASN:ND2	1:A:211:LEU:H	1.98	0.61
1:A:369:GLU:H	1:A:369:GLU:CD	2.09	0.61
1:B:59:LYS:O	1:B:63:GLU:HG3	2.01	0.61
1:C:135:SER:O	1:C:139:LEU:HD23	2.01	0.61
1:D:44:SER:HB3	1:D:109:LEU:HD21	1.82	0.60
1:D:173:GLN:HE21	1:D:173:GLN:HA	1.66	0.60
1:B:127:MET:O	1:B:131:LEU:HD13	2.00	0.60
1:B:355:LEU:HD12	1:B:355:LEU:C	2.26	0.60
1:B:386:PHE:N	1:D:108:LYS:HZ2	1.98	0.60
1:C:41:ILE:HD11	1:C:72:ILE:HG22	1.83	0.60
1:A:381:ARG:HH22	1:A:438:GLN:NE2	2.00	0.60
1:D:421:GLN:HE21	1:D:421:GLN:H	1.48	0.60
1:A:297:LEU:O	1:A:301:LYS:HG2	2.02	0.60
1:D:277:ASP:OD1	1:D:290:LYS:HE2	2.02	0.60
1:B:453:GLN:HA	1:B:456:GLN:HE21	1.66	0.60
1:B:173:GLN:HA	1:B:173:GLN:HE21	1.67	0.59
1:B:250:LEU:HG	1:D:242:VAL:HG11	1.85	0.59
1:C:418:ILE:HG21	3:C:1167:HOH:O	2.01	0.59
1:A:35:ARG:O	1:A:35:ARG:HG3	2.02	0.59
1:A:173:GLN:HA	1:A:173:GLN:HE21	1.68	0.59
1:B:281:THR:HG22	1:B:291:ASN:HD22	1.68	0.59
1:C:297:LEU:O	1:C:301:LYS:HG2	2.02	0.58
1:A:164:GLN:HB3	1:B:289:LYS:HD3	1.85	0.58
1:C:423:SER:HB2	1:C:425:ASP:OD2	2.04	0.58
1:D:405:ILE:HD11	1:D:410:LEU:HD23	1.85	0.58
1:A:116:ASN:HB3	1:A:235:ILE:HG21	1.85	0.58
1:D:41:ILE:HG21	1:D:73:SER:HB2	1.85	0.58
1:A:451:THR:O	1:A:455:GLU:HG3	2.05	0.57
1:B:189:LEU:HD23	1:B:189:LEU:C	2.29	0.57
1:A:84:LYS:HD3	1:A:96:ARG:CZ	2.35	0.57
1:B:397:VAL:HG12	1:B:407:ILE:HG21	1.86	0.57
1:D:128:LYS:NZ	1:D:223:GLU:O	2.38	0.57
1:C:392:ALA:O	1:C:418:ILE:HD12	2.05	0.57
1:A:59:LYS:O	1:A:63:GLU:HG3	2.04	0.57
1:A:110:HIS:CD2	1:A:113:ARG:HE	2.17	0.57
1:D:398:HIS:O	1:D:402:THR:HG23	2.04	0.57
1:A:342:THR:HG21	3:A:1108:HOH:O	2.05	0.56
1:A:406:THR:H	1:A:409:LYS:CE	2.18	0.56
1:D:230:ASN:HD22	1:D:233:ASP:H	1.53	0.56
1:A:442:LEU:HD23	3:C:1022:HOH:O	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:GLN:HE22	1:C:453:GLN:NE2	2.02	0.56
1:B:301:LYS:HE3	1:C:26:LEU:HD21	1.87	0.56
1:C:61:GLU:O	1:C:65:ILE:HG12	2.06	0.56
1:B:378:TYR:CZ	1:B:426:VAL:HG22	2.39	0.56
1:D:141:LEU:HD13	1:D:182:LEU:HD13	1.88	0.56
1:A:110:HIS:HE1	3:A:1186:HOH:O	1.90	0.55
1:B:209:ASN:HD22	1:B:211:LEU:H	1.54	0.55
1:B:34:GLN:HA	1:B:90:ILE:HD13	1.88	0.55
1:C:141:LEU:HD13	1:C:182:LEU:HD13	1.88	0.55
1:D:209:ASN:ND2	1:D:211:LEU:H	2.04	0.55
1:B:371:LEU:HD13	1:B:430:PHE:HA	1.88	0.55
1:B:405:ILE:HD12	1:B:409:LYS:HB2	1.89	0.54
1:B:42:GLN:NE2	3:B:1051:HOH:O	2.40	0.54
1:A:60:THR:O	1:A:64:LYS:HG2	2.08	0.54
1:C:209:ASN:ND2	1:C:211:LEU:H	2.05	0.54
1:D:39:VAL:CG2	1:D:125:LEU:HB2	2.35	0.54
1:A:206:LEU:HD21	1:C:167:GLN:HG2	1.89	0.54
1:A:230:ASN:HD21	1:A:232:MET:HB2	1.72	0.54
1:B:463:LYS:O	1:B:465:LYS:N	2.41	0.54
1:A:406:THR:HG1	1:A:409:LYS:HE2	1.69	0.54
1:C:230:ASN:HD21	1:C:232:MET:HB2	1.73	0.54
1:D:52:GLU:HG3	1:D:62:LEU:HD22	1.88	0.54
1:D:61:GLU:HB3	1:D:105:ILE:HD11	1.89	0.54
1:A:67:SER:O	1:A:71:LYS:HG3	2.09	0.53
1:B:369:GLU:CD	1:B:369:GLU:H	2.16	0.53
1:D:297:LEU:O	1:D:301:LYS:HG2	2.09	0.53
1:B:387:ARG:HE	1:B:387:ARG:HA	1.73	0.53
1:C:285:LEU:H	1:C:285:LEU:CD2	2.20	0.53
1:B:288:GLN:CD	1:B:288:GLN:H	2.16	0.53
1:B:252:MET:HB3	1:B:302:ALA:HA	1.91	0.53
1:B:117:ASP:CB	1:B:235:ILE:HD11	2.36	0.53
1:C:137:HIS:HE1	3:C:1130:HOH:O	1.91	0.53
1:B:378:TYR:CE2	1:B:426:VAL:HG22	2.43	0.53
1:C:399:LEU:HD11	1:C:403:LYS:HE2	1.91	0.53
1:A:257:LYS:HG3	1:C:319:LEU:O	2.08	0.53
1:A:301:LYS:HE3	1:D:26:LEU:HD11	1.89	0.53
1:D:62:LEU:O	1:D:66:LEU:HD13	2.09	0.53
1:D:80:VAL:O	1:D:80:VAL:HG22	2.09	0.53
1:B:359:LYS:NZ	1:B:359:LYS:HB3	2.24	0.52
1:D:381:ARG:HH22	1:D:438:GLN:NE2	2.06	0.52
1:A:257:LYS:HD3	3:A:1123:HOH:O	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:LEU:HD11	1:A:422:PHE:CZ	2.45	0.52
1:A:338:VAL:O	1:A:342:THR:HG23	2.10	0.52
1:C:173:GLN:HA	1:C:173:GLN:HE21	1.75	0.52
1:A:400:ALA:HB2	1:A:410:LEU:HD13	1.92	0.51
1:A:117:ASP:CB	1:A:235:ILE:HD11	2.35	0.51
1:D:27:ASN:HD21	1:D:325:LYS:CE	2.23	0.51
1:B:167:GLN:NE2	1:D:207:ALA:HB3	2.25	0.51
1:A:61:GLU:HG2	1:A:105:ILE:CG2	2.41	0.51
1:B:411:SER:O	1:B:415:LEU:HD22	2.11	0.51
1:A:196:ILE:HG12	1:A:240:PHE:HB2	1.92	0.51
1:A:116:ASN:HB3	1:A:235:ILE:HG23	1.92	0.51
1:C:155:VAL:HG22	1:C:359:LYS:HE2	1.90	0.51
1:B:230:ASN:ND2	1:B:233:ASP:H	2.05	0.51
1:C:120:VAL:O	1:C:124:LYS:HG3	2.11	0.51
1:C:252:MET:HB3	1:C:302:ALA:HA	1.92	0.51
1:C:183:THR:HG21	1:C:460:LEU:CD1	2.22	0.51
1:A:325:LYS:NZ	1:D:293:ASP:OD2	2.44	0.50
1:B:355:LEU:HD12	1:B:355:LEU:O	2.11	0.50
1:B:399:LEU:HD11	1:B:403:LYS:HE2	1.94	0.50
1:D:183:THR:HG22	3:D:1105:HOH:O	2.11	0.50
1:D:387:ARG:HD2	1:D:387:ARG:N	2.26	0.50
1:B:377:LEU:HA	1:B:380:VAL:HG22	1.93	0.50
1:B:311:SER:O	1:B:315:VAL:HG23	2.10	0.50
1:C:359:LYS:NZ	1:C:359:LYS:HB3	2.26	0.50
1:D:135:SER:O	1:D:139:LEU:HD23	2.11	0.50
1:D:176:LEU:O	1:D:180:VAL:HG23	2.11	0.50
1:A:91:HIS:HE1	3:A:1140:HOH:O	1.95	0.50
1:B:66:LEU:O	1:B:70:GLU:HG3	2.11	0.50
1:B:96:ARG:O	1:B:100:GLU:HG3	2.10	0.50
1:D:342:THR:HG22	3:D:1123:HOH:O	2.11	0.50
1:A:388:GLN:HA	1:A:388:GLN:NE2	2.27	0.50
1:D:373:THR:HB	3:D:1118:HOH:O	2.12	0.50
1:A:26:LEU:HD12	1:D:297:LEU:HD13	1.94	0.50
1:D:459:GLU:O	1:D:463:LYS:HG2	2.11	0.50
1:B:79:GLY:HA2	3:B:1103:HOH:O	2.11	0.49
1:D:71:LYS:O	1:D:75:GLU:HG3	2.13	0.49
1:A:405:ILE:HD11	1:A:410:LEU:CD1	2.42	0.49
1:A:209:ASN:HD22	1:A:211:LEU:H	1.60	0.49
1:B:80:VAL:HG12	1:B:80:VAL:O	2.11	0.49
1:B:227:ILE:HD11	1:D:442:LEU:HD13	1.94	0.49
1:C:82:VAL:HG22	1:C:82:VAL:O	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:SER:O	1:A:287:PRO:HD3	2.12	0.48
1:A:368:PRO:O	1:A:407:ILE:HD11	2.13	0.48
1:A:97:ARG:NE	1:A:101:LEU:HD11	2.28	0.48
1:D:382:LYS:HE2	1:D:421:GLN:O	2.13	0.48
1:A:22:ILE:HD12	3:A:1168:HOH:O	2.12	0.48
1:A:128:LYS:NZ	1:A:223:GLU:O	2.45	0.48
1:B:27:ASN:OD1	1:B:325:LYS:HE2	2.14	0.48
1:B:281:THR:HG21	3:B:1131:HOH:O	2.12	0.48
1:A:35:ARG:HD2	3:A:1206:HOH:O	2.12	0.48
1:A:274:THR:CG2	1:A:290:LYS:HD2	2.43	0.48
1:A:442:LEU:H	1:A:442:LEU:HD22	1.78	0.48
1:B:387:ARG:O	1:B:391:THR:HG23	2.13	0.48
1:A:189:LEU:HD23	1:A:189:LEU:C	2.38	0.48
1:A:317:LYS:HD3	1:A:317:LYS:C	2.39	0.48
1:A:326:ASP:HA	1:D:300:SER:HB3	1.95	0.48
1:A:462:LYS:O	1:A:466:GLU:HG2	2.14	0.48
1:C:173:GLN:NE2	1:C:453:GLN:HE22	2.04	0.48
1:C:22:ILE:N	1:C:22:ILE:HD12	2.28	0.48
1:D:56:ILE:HG23	1:D:108:LYS:HE3	1.95	0.48
1:D:98:LEU:HD23	1:D:106:ALA:HB1	1.95	0.48
1:A:88:GLU:OE1	1:A:92:THR:HG21	2.14	0.48
1:B:406:THR:OG1	1:B:409:LYS:HG2	2.13	0.48
1:B:463:LYS:C	1:B:465:LYS:N	2.69	0.48
1:A:245:LEU:CD2	1:A:337:VAL:HG21	2.43	0.48
1:A:465:LYS:C	1:A:467:GLN:H	2.22	0.47
1:C:296:GLU:OE2	1:D:162:HIS:HA	2.15	0.47
1:D:188:ARG:NH2	1:D:250:LEU:HD13	2.29	0.47
1:A:381:ARG:NH2	1:A:438:GLN:HE21	2.06	0.47
1:A:262:LEU:HB2	1:A:295:LEU:HD13	1.96	0.47
1:B:196:ILE:HG12	1:B:240:PHE:HB2	1.97	0.47
1:C:396:ALA:HA	3:C:1167:HOH:O	2.15	0.47
1:D:201:LEU:HD23	1:D:201:LEU:C	2.40	0.47
1:A:162:HIS:HA	1:B:296:GLU:OE2	2.15	0.47
1:C:128:LYS:NZ	1:C:223:GLU:O	2.48	0.47
1:D:367:THR:HB	1:D:369:GLU:OE1	2.15	0.47
1:D:110:HIS:HD2	1:D:113:ARG:HH21	1.61	0.47
1:B:188:ARG:NH2	1:B:250:LEU:HD13	2.30	0.47
1:A:124:LYS:NZ	3:A:1029:HOH:O	2.35	0.47
1:A:447:LYS:O	1:A:451:THR:HG23	2.15	0.47
1:C:111:THR:HG22	1:C:211:LEU:HD11	1.96	0.47
1:C:189:LEU:HD23	1:C:189:LEU:C	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:MET:HB3	1:D:302:ALA:HA	1.96	0.47
1:C:97:ARG:O	1:C:97:ARG:HD3	2.15	0.46
1:B:300:SER:HB3	1:C:326:ASP:HA	1.96	0.46
1:C:252:MET:HE2	1:C:301:LYS:HB2	1.97	0.46
1:C:418:ILE:CD1	1:C:422:PHE:HE2	2.28	0.46
1:A:230:ASN:ND2	1:A:233:ASP:H	2.09	0.46
1:A:367:THR:HB	1:A:369:GLU:OE2	2.16	0.46
1:D:30:ILE:HA	1:D:33:ASP:OD2	2.16	0.46
1:B:275:LEU:HD22	1:B:351:VAL:HG13	1.97	0.46
1:C:196:ILE:HG12	1:C:240:PHE:HB2	1.98	0.46
1:C:237:GLU:OE2	1:C:239:ASP:HB2	2.16	0.46
1:C:281:THR:CG2	1:C:282:GLY:N	2.78	0.46
1:A:411:SER:O	1:A:414:ASP:HB2	2.15	0.46
1:B:137:HIS:HE1	3:B:1118:HOH:O	1.99	0.46
1:C:42:GLN:HA	1:C:45:MET:HE2	1.98	0.46
1:B:111:THR:HG22	1:B:211:LEU:HD11	1.98	0.46
1:D:369:GLU:CD	1:D:369:GLU:H	2.24	0.46
1:A:465:LYS:HE2	3:A:1154:HOH:O	2.16	0.46
1:B:110:HIS:CD2	1:B:113:ARG:HE	2.24	0.46
1:A:372:ALA:HB3	1:B:285:LEU:HB3	1.97	0.45
1:B:153:ILE:HA	1:B:172:SER:OG	2.16	0.45
1:C:418:ILE:HD11	1:C:422:PHE:CE2	2.46	0.45
1:B:359:LYS:HB3	1:B:359:LYS:HZ3	1.80	0.45
1:C:127:MET:O	1:C:131:LEU:HD13	2.17	0.45
1:C:230:ASN:ND2	1:C:233:ASP:H	2.09	0.45
1:D:61:GLU:CB	1:D:105:ILE:HD11	2.46	0.45
1:D:386:PHE:HD2	1:D:387:ARG:HE	1.61	0.45
1:A:53:LYS:HD3	1:A:217:MET:SD	2.57	0.45
1:C:357:ILE:HB	1:C:362:MET:CE	2.46	0.45
1:A:405:ILE:HB	1:A:409:LYS:HE3	1.99	0.45
1:C:84:LYS:NZ	1:C:85:GLN:HE21	2.14	0.45
1:D:96:ARG:O	1:D:100:GLU:HG3	2.17	0.45
1:C:289:LYS:HE2	1:D:165:LYS:O	2.17	0.45
1:D:462:LYS:O	1:D:466:GLU:HG3	2.18	0.45
1:A:252:MET:HB3	1:A:302:ALA:HA	1.98	0.44
1:A:372:ALA:CB	1:B:285:LEU:HB3	2.46	0.44
1:C:188:ARG:NH2	1:C:250:LEU:HD13	2.32	0.44
1:B:384:VAL:O	1:B:385:PRO:C	2.60	0.44
1:D:317:LYS:C	1:D:317:LYS:HD3	2.42	0.44
1:B:357:ILE:HB	1:B:362:MET:HE3	1.99	0.44
1:C:393:SER:HB3	1:D:285:LEU:HD11	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:PHE:O	1:B:435:SER:HB3	2.18	0.44
1:B:463:LYS:NZ	1:B:463:LYS:HB3	2.33	0.44
1:C:193:LYS:HD2	3:C:1112:HOH:O	2.16	0.44
1:B:319:LEU:O	1:D:257:LYS:HG3	2.18	0.44
1:D:39:VAL:HG23	1:D:125:LEU:CD1	2.48	0.44
1:D:322:THR:OG1	1:D:323:TYR:N	2.47	0.44
1:B:124:LYS:HE2	1:B:240:PHE:CD2	2.53	0.44
1:D:66:LEU:O	1:D:70:GLU:HG2	2.17	0.44
1:A:56:ILE:HD12	1:A:56:ILE:N	2.33	0.44
1:A:298:ILE:HG12	1:A:344:VAL:HG13	1.99	0.44
1:B:377:LEU:C	1:B:380:VAL:HG22	2.42	0.44
1:D:39:VAL:HG23	1:D:125:LEU:HD13	1.99	0.44
1:C:206:LEU:HD23	1:C:206:LEU:N	2.32	0.43
1:C:412:LEU:HD22	1:C:424:SER:HA	2.00	0.43
1:D:110:HIS:CD2	1:D:113:ARG:HH21	2.35	0.43
1:D:325:LYS:CE	3:D:1159:HOH:O	2.65	0.43
1:D:325:LYS:HE2	3:D:1159:HOH:O	2.16	0.43
1:A:167:GLN:NE2	1:C:207:ALA:HB3	2.32	0.43
1:C:163:LEU:HD11	1:C:264:ILE:HD13	2.00	0.43
1:A:296:GLU:OE2	1:B:162:HIS:HA	2.19	0.43
1:C:391:THR:O	1:C:395:LYS:HG3	2.18	0.43
1:C:311:SER:O	1:C:315:VAL:HG23	2.18	0.43
1:A:131:LEU:HD12	1:A:131:LEU:HA	1.82	0.43
1:C:235:ILE:C	1:C:235:ILE:HD12	2.44	0.43
1:A:35:ARG:NH2	1:A:339:ASP:OD2	2.51	0.43
1:A:117:ASP:HA	1:A:235:ILE:CD1	2.49	0.43
1:C:292:PRO:HD2	1:D:162:HIS:HB3	2.00	0.43
1:C:281:THR:HB	1:C:293:ASP:OD1	2.19	0.42
1:D:45:MET:O	1:D:49:LYS:HG3	2.19	0.42
1:A:274:THR:HG23	1:A:290:LYS:HD2	2.00	0.42
1:B:199:LEU:HD11	1:B:201:LEU:HB2	2.01	0.42
1:C:347:VAL:O	1:C:351:VAL:HG23	2.19	0.42
1:C:356:GLN:HG3	3:C:1162:HOH:O	2.19	0.42
1:A:314:MET:HA	1:B:314:MET:HE2	2.01	0.42
1:A:371:LEU:HD13	1:A:430:PHE:HA	2.01	0.42
1:D:127:MET:O	1:D:131:LEU:HD13	2.19	0.42
1:D:110:HIS:CD2	1:D:113:ARG:HE	2.37	0.42
2:B:1003:AS1:HB1	3:C:1188:HOH:O	2.20	0.42
1:C:457:LEU:HD12	1:C:457:LEU:HA	1.84	0.42
1:D:222:LEU:O	1:D:223:GLU:HB2	2.20	0.42
1:A:388:GLN:HA	1:A:388:GLN:HE21	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ALA:CB	1:D:167:GLN:NE2	2.81	0.42
1:B:394:GLY:O	1:B:397:VAL:HG22	2.19	0.42
1:D:61:GLU:O	1:D:64:LYS:HB3	2.20	0.42
1:C:275:LEU:HD22	1:C:351:VAL:HG13	2.00	0.42
3:B:1089:HOH:O	1:C:26:LEU:HD23	2.19	0.41
1:C:355:LEU:C	1:C:355:LEU:HD12	2.45	0.41
1:D:285:LEU:HD12	1:D:285:LEU:HA	1.90	0.41
1:B:167:GLN:HG2	1:D:206:LEU:HD21	2.01	0.41
1:D:124:LYS:HE2	1:D:240:PHE:CD2	2.55	0.41
1:D:387:ARG:HD2	1:D:387:ARG:H	1.84	0.41
1:B:189:LEU:C	1:B:189:LEU:CD2	2.92	0.41
1:B:375:LEU:O	1:B:378:TYR:HB3	2.20	0.41
1:A:375:LEU:HD13	1:A:375:LEU:O	2.20	0.41
1:A:406:THR:H	1:A:409:LYS:HE2	1.83	0.41
1:C:96:ARG:O	1:C:100:GLU:HG3	2.19	0.41
1:D:262:LEU:HB3	1:D:295:LEU:CD1	2.50	0.41
1:A:105:ILE:HB	3:A:1178:HOH:O	2.20	0.41
1:A:319:LEU:O	1:C:257:LYS:HG3	2.21	0.41
1:A:441:ALA:HB3	3:A:1078:HOH:O	2.20	0.41
1:B:273:LEU:HD12	1:B:273:LEU:C	2.45	0.41
1:B:397:VAL:HG23	1:B:398:HIS:N	2.35	0.41
1:D:85:GLN:CD	1:D:85:GLN:N	2.75	0.41
1:B:415:LEU:HB3	1:B:422:PHE:CD2	2.56	0.41
1:D:27:ASN:HD21	1:D:325:LYS:HZ3	1.65	0.41
1:B:71:LYS:O	1:B:75:GLU:HG3	2.21	0.41
1:B:419:SER:HA	1:B:420:PRO:HD3	1.91	0.41
1:C:40:ASP:OD2	1:C:91:HIS:HD2	2.04	0.41
1:A:237:GLU:OE2	1:A:239:ASP:HB2	2.21	0.41
1:C:162:HIS:HB3	1:D:292:PRO:HD2	2.01	0.41
1:C:253:ILE:HD13	1:C:253:ILE:HA	1.92	0.41
1:A:207:ALA:HB3	1:C:167:GLN:HE21	1.85	0.41
1:A:262:LEU:O	1:A:266:SER:HB3	2.20	0.41
1:A:400:ALA:HB1	1:A:405:ILE:O	2.21	0.41
1:C:281:THR:HG22	1:C:282:GLY:N	2.35	0.41
1:C:357:ILE:HB	1:C:362:MET:HE2	2.02	0.41
1:D:27:ASN:HD21	1:D:325:LYS:HE2	1.86	0.41
1:A:252:MET:HE2	1:A:301:LYS:HB2	2.03	0.41
1:B:129:ASN:O	1:B:132:SER:HB3	2.21	0.41
1:D:135:SER:O	1:D:139:LEU:CD2	2.69	0.41
1:A:116:ASN:C	1:A:235:ILE:HD12	2.46	0.40
1:A:316:LEU:HA	1:A:319:LEU:HD12	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:VAL:O	1:B:80:VAL:CG1	2.69	0.40
1:D:330:ASP:OD1	1:D:331:LYS:N	2.55	0.40
1:D:108:LYS:O	1:D:111:THR:OG1	2.33	0.40
1:A:95:GLU:HG3	3:A:1082:HOH:O	2.21	0.40
1:A:162:HIS:CG	1:B:291:ASN:HB3	2.56	0.40
1:C:98:LEU:HD23	1:C:106:ALA:HB1	2.04	0.40
1:C:124:LYS:NZ	3:C:1068:HOH:O	2.49	0.40
1:B:33:ASP:OD1	1:B:33:ASP:C	2.64	0.40
1:B:386:PHE:H	1:D:108:LYS:CD	2.34	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	447/468 (96%)	439 (98%)	7 (2%)	1 (0%)	43	36
1	B	446/468 (95%)	434 (97%)	10 (2%)	2 (0%)	30	21
1	C	446/468 (95%)	439 (98%)	5 (1%)	2 (0%)	30	21
1	D	448/468 (96%)	438 (98%)	9 (2%)	1 (0%)	43	36
All	All	1787/1872 (96%)	1750 (98%)	31 (2%)	6 (0%)	36	28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	206	LEU
1	A	206	LEU
1	B	206	LEU
1	C	206	LEU
1	B	464	GLN
1	C	200	PRO

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	391/404 (97%)	375 (96%)	16 (4%)	27	17
1	B	390/404 (96%)	369 (95%)	21 (5%)	20	9
1	C	391/404 (97%)	374 (96%)	17 (4%)	26	15
1	D	391/404 (97%)	376 (96%)	15 (4%)	29	19
All	All	1563/1616 (97%)	1494 (96%)	69 (4%)	25	15

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	26	LEU
1	A	34	GLN
1	A	35	ARG
1	A	110	HIS
1	A	131	LEU
1	A	138	LEU
1	A	140	GLN
1	A	141	LEU
1	A	173	GLN
1	A	201	LEU
1	A	250	LEU
1	A	266	SER
1	A	285	LEU
1	A	364	LYS
1	A	399	LEU
1	B	84	LYS
1	B	85	GLN
1	B	97	ARG
1	B	101	LEU
1	B	105	ILE
1	B	138	LEU
1	B	139	LEU
1	B	141	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	173	GLN
1	B	201	LEU
1	B	212	ASP
1	B	250	LEU
1	B	262	LEU
1	B	281	THR
1	B	288	GLN
1	B	325	LYS
1	B	387	ARG
1	B	412	LEU
1	B	415	LEU
1	B	442	LEU
1	B	457	LEU
1	C	19	THR
1	C	36	LEU
1	C	51	LEU
1	C	80	VAL
1	C	82	VAL
1	C	138	LEU
1	C	141	LEU
1	C	163	LEU
1	C	199	LEU
1	C	201	LEU
1	C	250	LEU
1	C	262	LEU
1	C	285	LEU
1	C	288	GLN
1	C	382	LYS
1	C	418	ILE
1	C	457	LEU
1	D	56	ILE
1	D	60	THR
1	D	96	ARG
1	D	132	SER
1	D	138	LEU
1	D	141	LEU
1	D	183	THR
1	D	235	ILE
1	D	250	LEU
1	D	262	LEU
1	D	285	LEU
1	D	387	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	408	ASN
1	D	421	GLN
1	D	457	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	HIS
1	A	110	HIS
1	A	129	ASN
1	A	137	HIS
1	A	140	GLN
1	A	167	GLN
1	A	173	GLN
1	A	209	ASN
1	A	230	ASN
1	A	324	ASN
1	A	388	GLN
1	A	390	HIS
1	A	398	HIS
1	A	421	GLN
1	A	438	GLN
1	A	464	GLN
1	B	42	GLN
1	B	85	GLN
1	B	91	HIS
1	B	110	HIS
1	B	129	ASN
1	B	137	HIS
1	B	167	GLN
1	B	173	GLN
1	B	209	ASN
1	B	230	ASN
1	B	291	ASN
1	B	324	ASN
1	B	390	HIS
1	B	398	HIS
1	B	438	GLN
1	B	456	GLN
1	C	85	GLN
1	C	91	HIS
1	C	118	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	137	HIS
1	C	173	GLN
1	C	209	ASN
1	C	230	ASN
1	C	288	GLN
1	C	324	ASN
1	C	390	HIS
1	C	438	GLN
1	D	27	ASN
1	D	91	HIS
1	D	110	HIS
1	D	167	GLN
1	D	173	GLN
1	D	209	ASN
1	D	230	ASN
1	D	356	GLN
1	D	388	GLN
1	D	408	ASN
1	D	421	GLN
1	D	438	GLN
1	D	464	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
2	AS1	A	1004	-	18,19,19	2.59	5 (27%)	19,24,24	3.99	9 (47%)
2	AS1	B	1003	-	18,19,19	2.78	5 (27%)	19,24,24	3.99	8 (42%)
2	AS1	D	1002	-	18,19,19	2.59	5 (27%)	19,24,24	3.94	8 (42%)
2	AS1	C	1001	-	18,19,19	2.60	5 (27%)	19,24,24	3.94	8 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AS1	A	1004	-	1/1/6/7	7/21/23/23	-
2	AS1	B	1003	-	1/1/6/7	9/21/23/23	-
2	AS1	D	1002	-	1/1/6/7	9/21/23/23	-
2	AS1	C	1001	-	1/1/6/7	8/21/23/23	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1003	AS1	C-N2	6.83	1.45	1.28
2	D	1002	AS1	C-N2	6.39	1.44	1.28
2	A	1004	AS1	C-N2	6.11	1.43	1.28
2	C	1001	AS1	C-N2	6.06	1.43	1.28
2	B	1003	AS1	C-N1	5.52	1.47	1.34
2	C	1001	AS1	C-N3	5.42	1.46	1.34
2	B	1003	AS1	C-N3	5.24	1.46	1.34
2	A	1004	AS1	C-N3	5.21	1.46	1.34
2	A	1004	AS1	C-N1	5.15	1.46	1.34
2	D	1002	AS1	C-N3	5.14	1.46	1.34
2	D	1002	AS1	C-N1	4.99	1.45	1.34
2	C	1001	AS1	C-N1	4.94	1.45	1.34
2	A	1004	AS1	OG2-CG	3.17	1.31	1.22
2	B	1003	AS1	OG2-CG	3.09	1.31	1.22
2	D	1002	AS1	OG2-CG	3.01	1.31	1.22
2	C	1001	AS1	OG2-CG	2.97	1.30	1.22
2	B	1003	AS1	CA-N1	2.96	1.52	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	AS1	CA-N1	2.77	1.51	1.45
2	A	1004	AS1	CA-N1	2.75	1.51	1.45
2	D	1002	AS1	CA-N1	2.63	1.51	1.45

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1003	AS1	C2-C1-N2	9.55	127.58	110.67
2	A	1004	AS1	C2-C1-N2	9.55	127.58	110.67
2	D	1002	AS1	C2-C1-N2	9.40	127.32	110.67
2	C	1001	AS1	C2-C1-N2	9.24	127.04	110.67
2	B	1003	AS1	CB-CA-N1	8.64	127.11	110.64
2	A	1004	AS1	CB-CA-N1	8.57	126.98	110.64
2	C	1001	AS1	OD2-CD-CB	-8.54	96.62	122.84
2	A	1004	AS1	OD2-CD-CB	-8.52	96.68	122.84
2	D	1002	AS1	OD2-CD-CB	-8.46	96.88	122.84
2	B	1003	AS1	OD2-CD-CB	-8.42	97.00	122.84
2	C	1001	AS1	CB-CA-N1	8.34	126.56	110.64
2	D	1002	AS1	CB-CA-N1	8.19	126.26	110.64
2	C	1001	AS1	CG-CA-N1	4.72	121.53	110.57
2	D	1002	AS1	CG-CA-N1	4.71	121.49	110.57
2	B	1003	AS1	CG-CA-N1	4.34	120.63	110.57
2	A	1004	AS1	CG-CA-N1	4.31	120.56	110.57
2	B	1003	AS1	N3-C-N1	-3.99	111.22	118.86
2	A	1004	AS1	N3-C-N1	-3.81	111.56	118.86
2	D	1002	AS1	N3-C-N1	-3.77	111.64	118.86
2	C	1001	AS1	N3-C-N1	-3.40	112.34	118.86
2	C	1001	AS1	C2-C3-C4	-2.57	104.93	113.22
2	A	1004	AS1	C2-C3-C4	-2.52	105.10	113.22
2	C	1001	AS1	CA-CB-CD	-2.45	105.86	112.75
2	D	1002	AS1	C2-C3-C4	-2.42	105.41	113.22
2	D	1002	AS1	CA-CB-CD	-2.38	106.05	112.75
2	A	1004	AS1	N1-C-N2	2.34	130.66	125.00
2	B	1003	AS1	OD1-CD-OD2	-2.32	117.38	123.33
2	A	1004	AS1	CA-CB-CD	-2.30	106.28	112.75
2	B	1003	AS1	N1-C-N2	2.26	130.46	125.00
2	D	1002	AS1	OD1-CD-OD2	-2.15	117.81	123.33
2	A	1004	AS1	OD1-CD-OD2	-2.07	118.01	123.33
2	C	1001	AS1	OD1-CD-OD2	-2.07	118.01	123.33
2	B	1003	AS1	CA-CB-CD	-2.01	107.08	112.75

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1004	AS1	CA
2	B	1003	AS1	CA
2	C	1001	AS1	CA
2	D	1002	AS1	CA

All (33) torsion outliers are listed below:

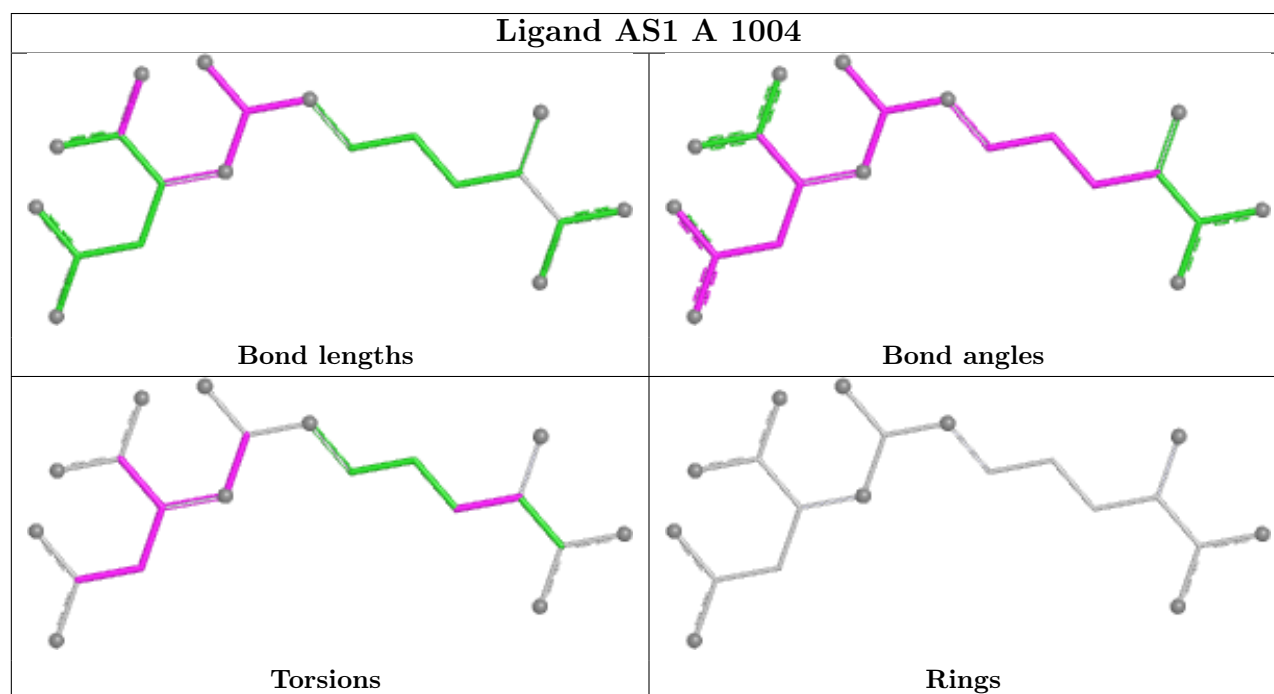
Mol	Chain	Res	Type	Atoms
2	A	1004	AS1	CG-CA-N1-C
2	B	1003	AS1	C2-C3-C4-N4
2	B	1003	AS1	CG-CA-N1-C
2	C	1001	AS1	CG-CA-N1-C
2	D	1002	AS1	C2-C3-C4-N4
2	A	1004	AS1	CA-CB-CD-OD2
2	B	1003	AS1	CA-CB-CD-OD2
2	A	1004	AS1	CG-CA-CB-CD
2	B	1003	AS1	CG-CA-CB-CD
2	C	1001	AS1	CG-CA-CB-CD
2	D	1002	AS1	CG-CA-CB-CD
2	D	1002	AS1	CA-CB-CD-OD2
2	D	1002	AS1	N1-CA-CG-OG1
2	D	1002	AS1	N1-CA-CG-OG2
2	C	1001	AS1	CA-CB-CD-OD2
2	B	1003	AS1	N2-C-N1-CA
2	D	1002	AS1	N2-C-N1-CA
2	D	1002	AS1	CG-CA-N1-C
2	A	1004	AS1	C2-C3-C4-N4
2	C	1001	AS1	C2-C3-C4-N4
2	B	1003	AS1	N1-CA-CG-OG2
2	B	1003	AS1	N1-CA-CG-OG1
2	C	1001	AS1	N1-CA-CG-OG1
2	C	1001	AS1	N1-CA-CG-OG2
2	D	1002	AS1	C1-C2-C3-C4
2	A	1004	AS1	N1-CA-CG-OG2
2	A	1004	AS1	N1-CA-CG-OG1
2	B	1003	AS1	C2-C3-C4-C5
2	C	1001	AS1	C2-C3-C4-C5
2	D	1002	AS1	C2-C3-C4-C5
2	A	1004	AS1	N2-C-N1-CA
2	C	1001	AS1	N2-C-N1-CA
2	B	1003	AS1	C1-C2-C3-C4

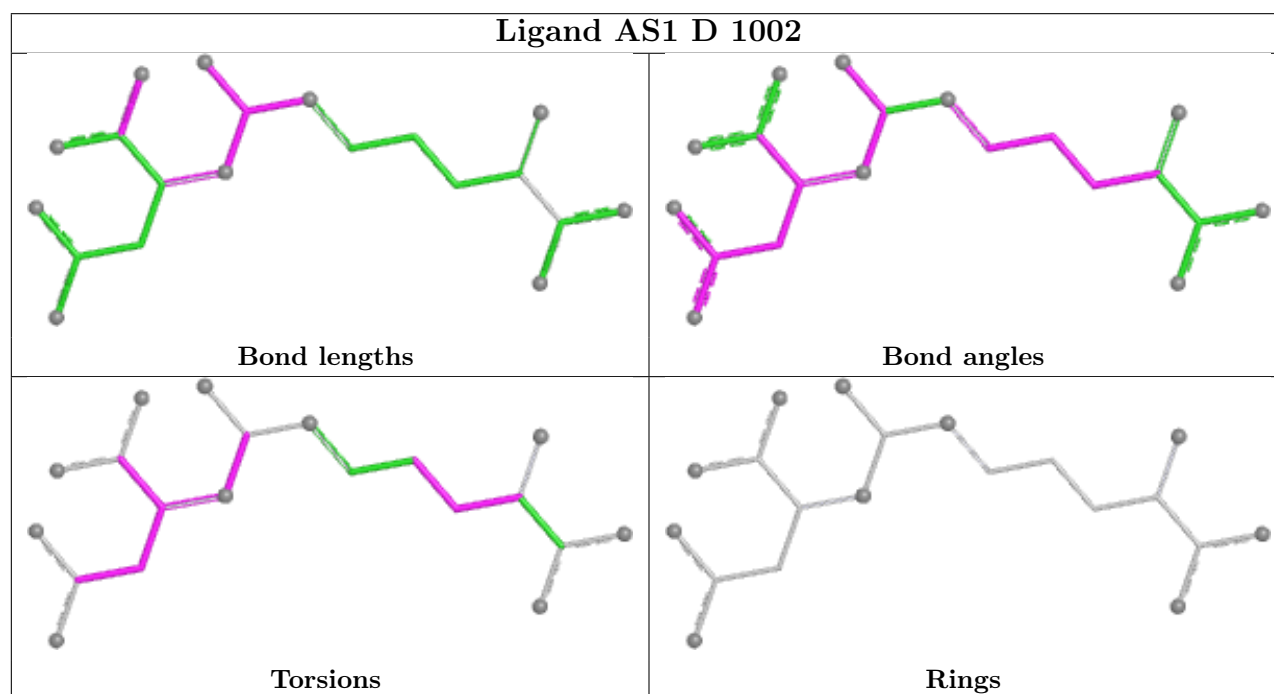
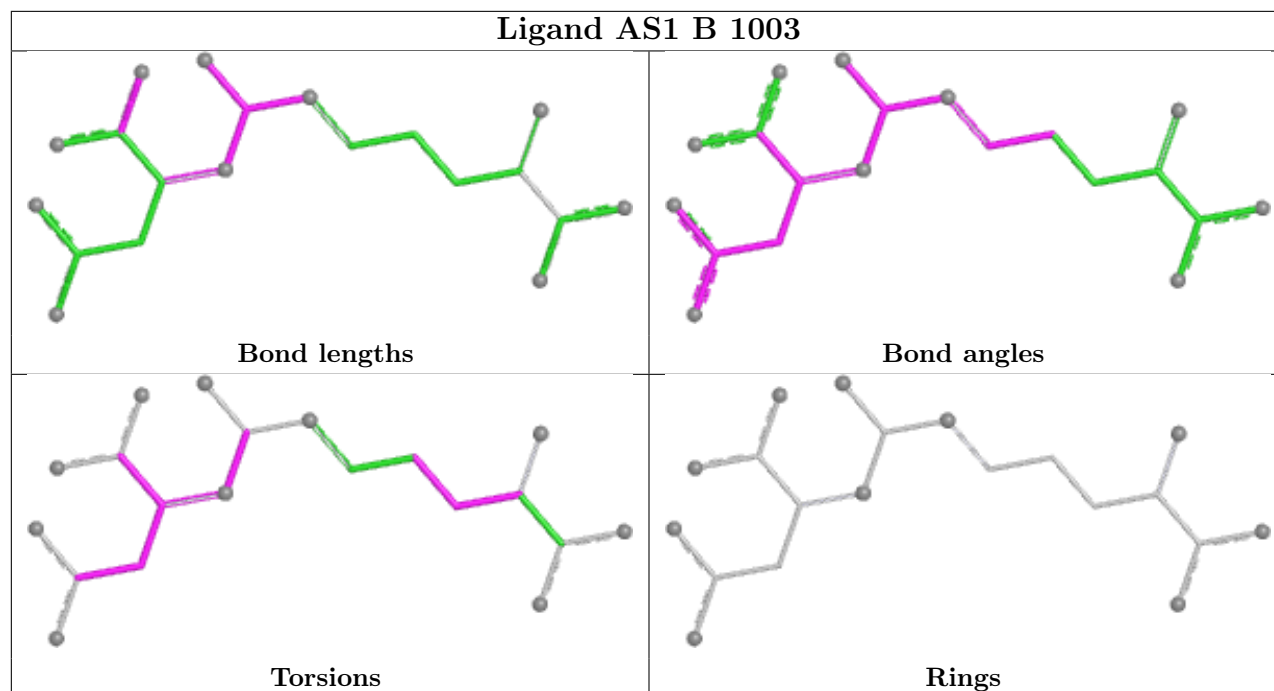
There are no ring outliers.

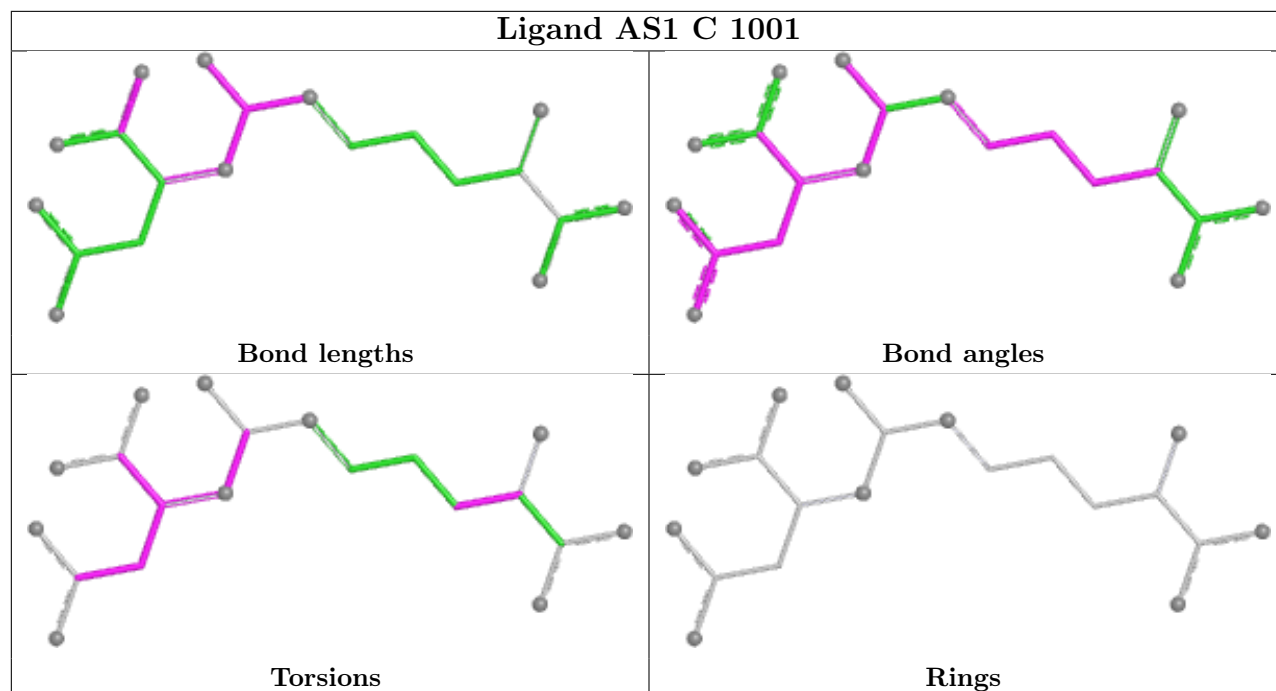
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1003	AS1	1	0
2	D	1002	AS1	1	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	449/468 (95%)	0.35	22 (4%) 35 41	15, 25, 53, 71	0
1	B	448/468 (95%)	0.63	36 (8%) 18 21	16, 31, 53, 66	0
1	C	448/468 (95%)	0.26	10 (2%) 62 69	13, 25, 45, 62	0
1	D	450/468 (96%)	0.46	29 (6%) 25 29	15, 28, 50, 62	0
All	All	1795/1872 (95%)	0.43	97 (5%) 31 37	13, 27, 51, 71	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	384	VAL	4.6
1	D	60	THR	4.3
1	A	283	ALA	4.2
1	A	467	GLN	4.1
1	B	378	TYR	4.1
1	C	283	ALA	4.0
1	B	386	PHE	3.7
1	D	103	GLY	3.7
1	B	402	THR	3.7
1	B	397	VAL	3.7
1	D	420	PRO	3.7
1	D	80	VAL	3.5
1	D	467	GLN	3.4
1	D	55	GLY	3.3
1	A	411	SER	3.3
1	C	418	ILE	3.2
1	B	399	LEU	3.2
1	B	424	SER	3.1
1	D	54	ALA	3.1
1	D	77	SER	3.1
1	B	465	LYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	56	ILE	2.9
1	B	415	LEU	2.9
1	D	101	LEU	2.9
1	B	426	VAL	2.8
1	D	82	VAL	2.8
1	D	68	GLY	2.8
1	A	403	LYS	2.8
1	A	380	VAL	2.8
1	A	388	GLN	2.8
1	A	19	THR	2.8
1	B	431	ASN	2.7
1	B	433	VAL	2.7
1	B	282	GLY	2.6
1	C	97	ARG	2.6
1	B	390	HIS	2.6
1	B	380	VAL	2.6
1	B	283	ALA	2.6
1	B	377	LEU	2.6
1	D	39	VAL	2.6
1	D	83	VAL	2.6
1	B	212	ASP	2.5
1	B	410	LEU	2.5
1	B	389	ALA	2.5
1	B	400	ALA	2.5
1	D	62	LEU	2.5
1	D	65	ILE	2.5
1	D	102	ILE	2.5
1	C	466	GLU	2.5
1	B	18	SER	2.4
1	D	67	SER	2.4
1	B	406	THR	2.4
1	A	410	LEU	2.4
1	B	418	ILE	2.4
1	B	436	VAL	2.4
1	C	103	GLY	2.4
1	C	19	THR	2.3
1	D	19	THR	2.3
1	B	213	ILE	2.3
1	B	398	HIS	2.3
1	A	424	SER	2.3
1	C	113	ARG	2.3
1	B	285	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	66	LEU	2.3
1	D	109	LEU	2.3
1	A	418	ILE	2.3
1	D	18	SER	2.3
1	B	363	GLU	2.3
1	C	110	HIS	2.3
1	D	110	HIS	2.3
1	A	422	PHE	2.3
1	A	420	PRO	2.3
1	B	391	THR	2.2
1	B	284	SER	2.2
1	A	383	GLY	2.2
1	D	385	PRO	2.2
1	A	398	HIS	2.1
1	A	386	PHE	2.1
1	D	401	GLU	2.1
1	B	367	THR	2.1
1	C	105	ILE	2.1
1	C	417	SER	2.1
1	D	451	THR	2.1
1	A	404	GLY	2.1
1	B	287	PRO	2.1
1	A	400	ALA	2.1
1	A	414	ASP	2.1
1	A	449	SER	2.1
1	A	285	LEU	2.1
1	D	284	SER	2.0
1	D	74	GLU	2.0
1	A	416	LYS	2.0
1	B	358	SER	2.0
1	B	105	ILE	2.0
1	B	19	THR	2.0
1	D	288	GLN	2.0
1	B	368	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

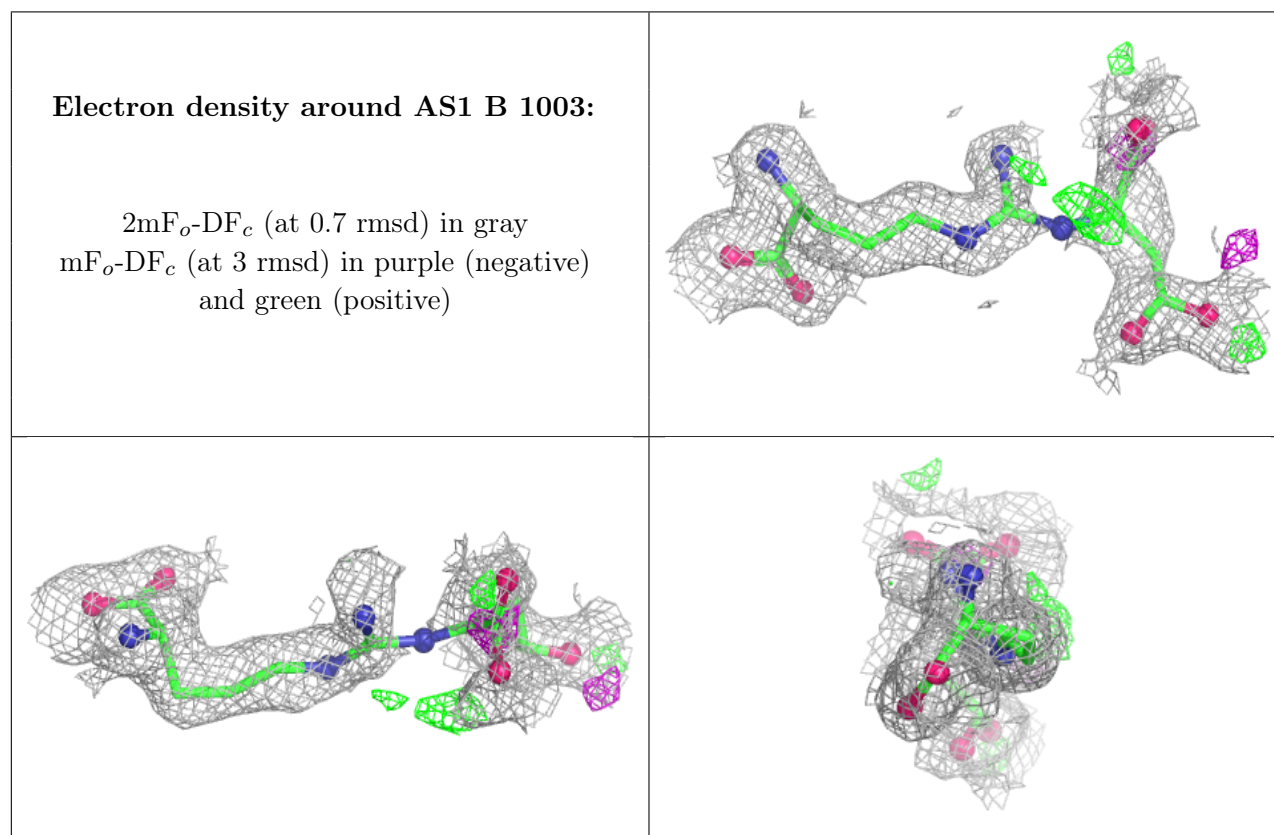
There are no oligosaccharides in this entry.

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.

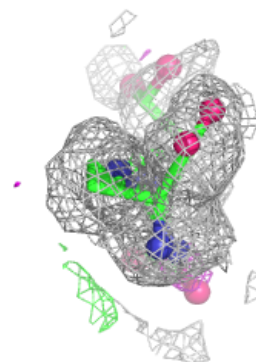
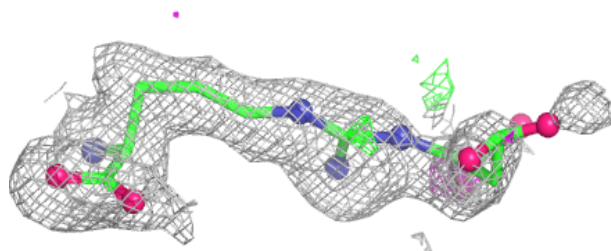
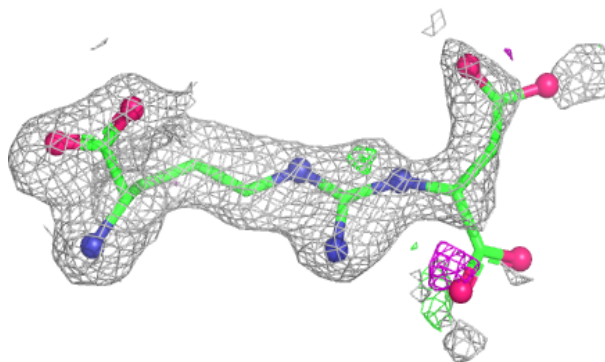
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AS1	B	1003	20/20	0.88	0.13	18,39,61,62	0
2	AS1	D	1002	20/20	0.88	0.15	22,48,67,67	0
2	AS1	C	1001	20/20	0.90	0.11	17,40,57,57	0
2	AS1	A	1004	20/20	0.90	0.15	17,40,60,60	0

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.

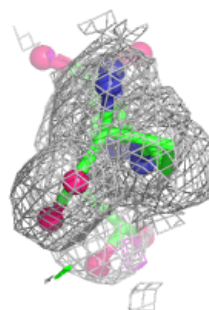
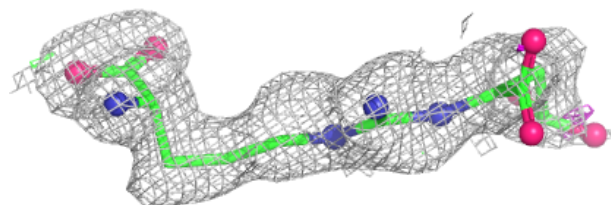
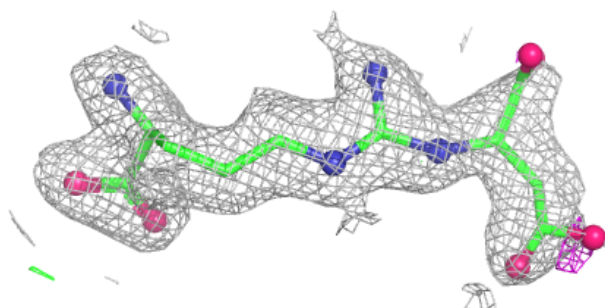


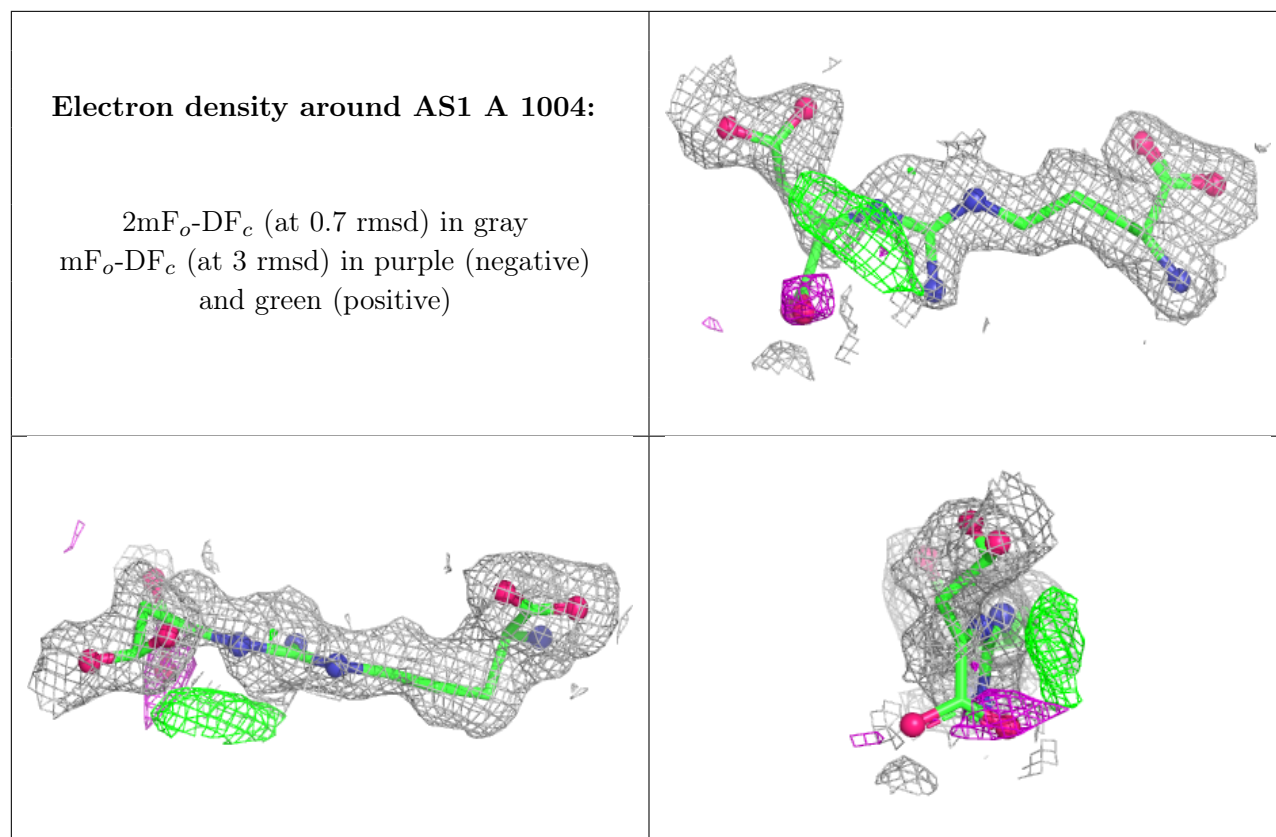
Electron density around AS1 D 1002:

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

**Electron density around AS1 C 1001:**

$2mF_o-DF_c$ (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.