



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:56 PM UTC

PDB ID : 1TJW / pdb_00001tjw
Title : Crystal Structure of T161D Duck Delta 2 Crystallin Mutant with bound argininosuccinate
Authors : Sampaleanu, L.M.; Coddling, P.W.; Lobsanov, Y.D.; Tsai, M.; Smith, G.D.; Horvatin, C.; Howell, P.L.
Deposited on : 2004-06-07
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

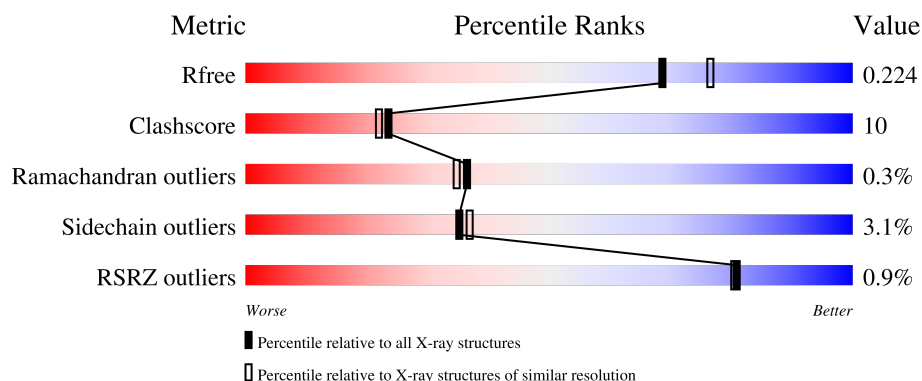
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	474	76% 17% • 5%
1	B	474	73% 18% • 5%
1	C	474	77% 16% • 5%
1	D	474	75% 17% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	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 14819 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 crystallin II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3464	2195	588	669	12			
1	B	448	Total	C	N	O	S	0	0	0
			3441	2179	581	669	12			
1	C	449	Total	C	N	O	S	0	0	0
			3456	2190	585	669	12			
1	D	449	Total	C	N	O	S	0	0	0
			3468	2194	586	676	12			

There are 28 discrepancies between the modelled and reference sequences:

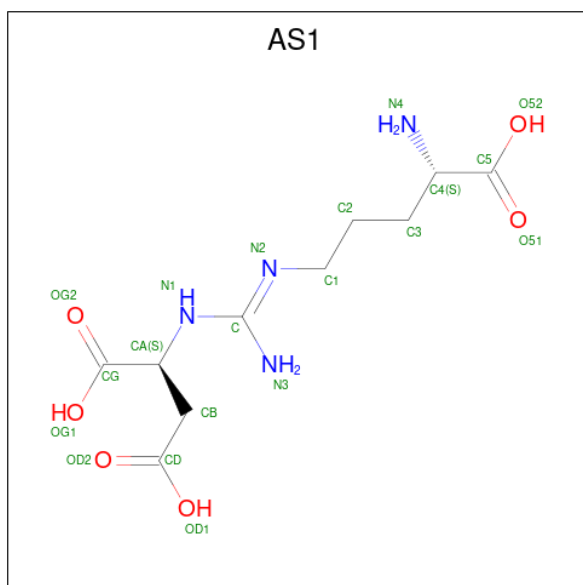
Chain	Residue	Modelled	Actual	Comment	Reference
A	161	ASP	THR	engineered mutation	UNP P24058
B	161	ASP	THR	engineered mutation	UNP P24058
C	161	ASP	THR	engineered mutation	UNP P24058
D	161	ASP	THR	engineered mutation	UNP P24058
A	469	HIS	-	expression tag	UNP P24058
A	470	HIS	-	expression tag	UNP P24058
A	471	HIS	-	expression tag	UNP P24058
A	472	HIS	-	expression tag	UNP P24058
A	473	HIS	-	expression tag	UNP P24058
A	474	HIS	-	expression tag	UNP P24058
B	469	HIS	-	expression tag	UNP P24058
B	470	HIS	-	expression tag	UNP P24058
B	471	HIS	-	expression tag	UNP P24058
B	472	HIS	-	expression tag	UNP P24058
B	473	HIS	-	expression tag	UNP P24058
B	474	HIS	-	expression tag	UNP P24058
C	469	HIS	-	expression tag	UNP P24058
C	470	HIS	-	expression tag	UNP P24058
C	471	HIS	-	expression tag	UNP P24058
C	472	HIS	-	expression tag	UNP P24058
C	473	HIS	-	expression tag	UNP P24058

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Chain	Residue	Modelled	Actual	Comment	Reference
C	474	HIS	-	expression tag	UNP P24058
D	469	HIS	-	expression tag	UNP P24058
D	470	HIS	-	expression tag	UNP P24058
D	471	HIS	-	expression tag	UNP P24058
D	472	HIS	-	expression tag	UNP P24058
D	473	HIS	-	expression tag	UNP P24058
D	474	HIS	-	expression tag	UNP P24058

- Molecule 2 is ARGININOSUCCINATE (CCD ID: AS1) (formula: $C_{10}H_{18}N_4O_6$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	253	Total	O	0	0
			253	253		
3	B	196	Total	O	0	0
			196	196		

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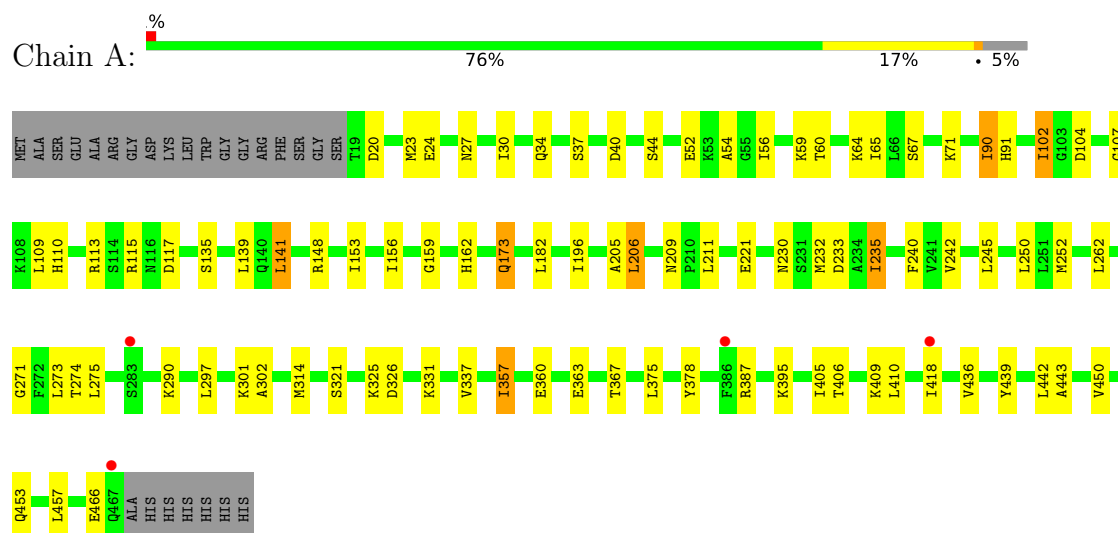
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	258	Total 258	O 258	0	0
3	D	203	Total 203	O 203	0	0

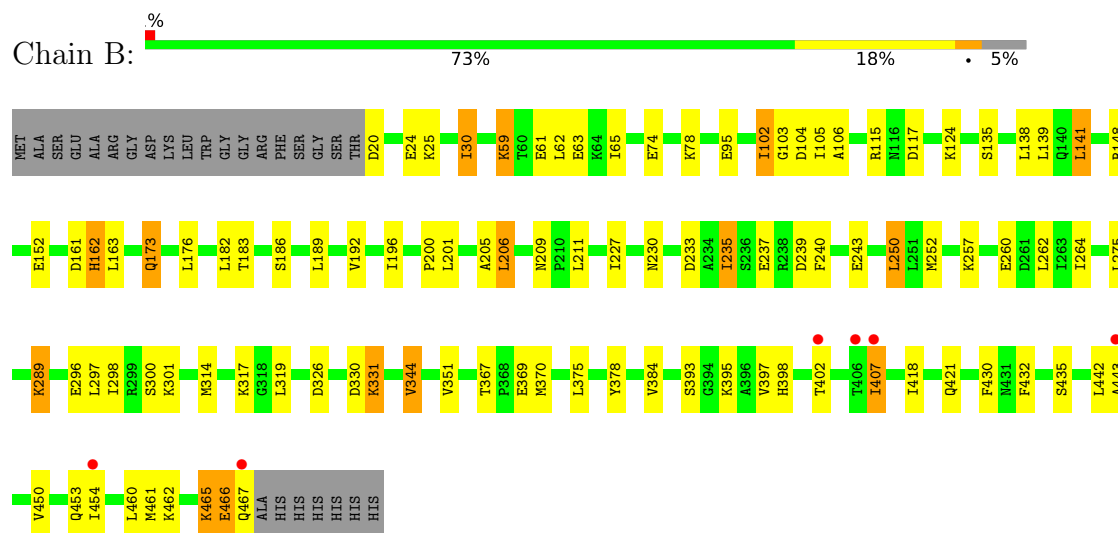
3 Residue-property plots [i](#)

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

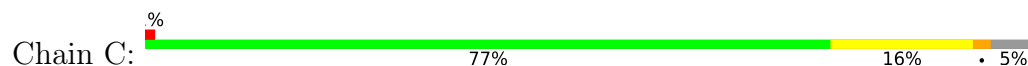
• Molecule 1: Delta crystallin II

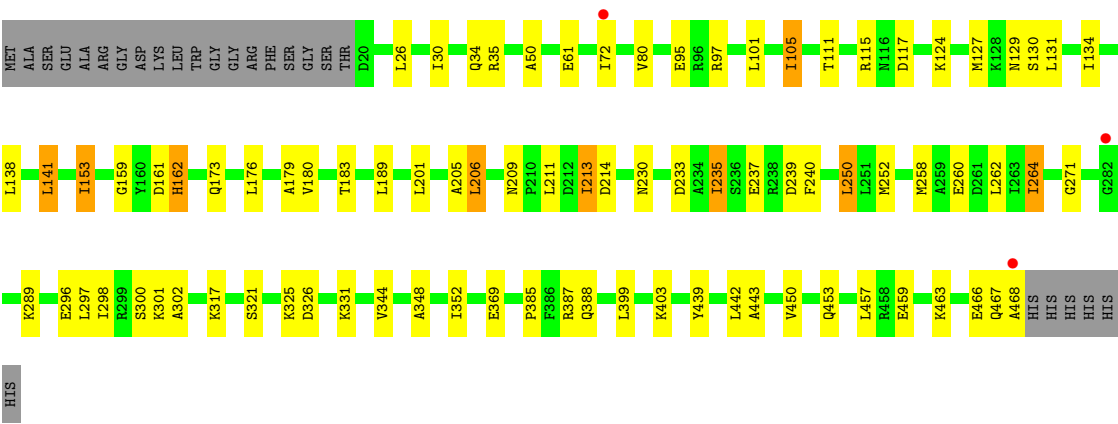


• Molecule 1: Delta crystallin II

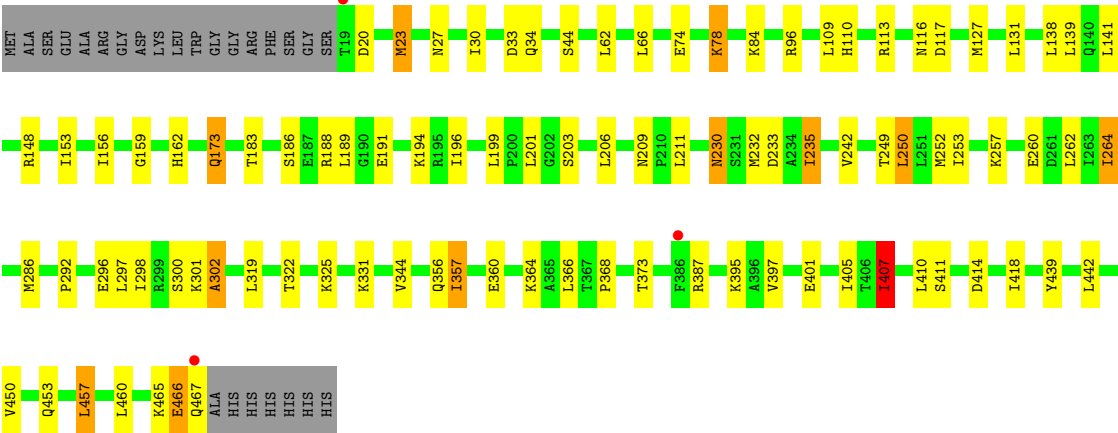
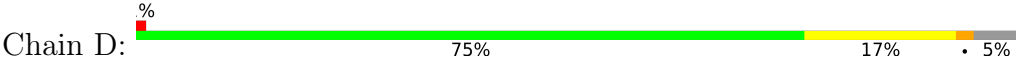


• Molecule 1: Delta crystallin II





● Molecule 1: Delta crystallin II



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.00Å 98.81Å 106.39Å 90.00° 101.34° 90.00°	Depositor
Resolution (Å)	41.76 – 2.00 41.76 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.76-2.00) 99.6 (41.76-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.190 , 0.225 0.190 , 0.224	Depositor DCC
R_{free} test set	12767 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14819	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.54	0/3509	0.92	9/4733 (0.2%)
1	B	0.50	0/3486	0.91	4/4708 (0.1%)
1	C	0.54	0/3501	0.92	5/4727 (0.1%)
1	D	0.53	0/3513	0.90	7/4743 (0.1%)
All	All	0.53	0/14009	0.92	25/18911 (0.1%)

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

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

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	LYS	N-CA-C	7.44	119.03	111.07
1	A	104	ASP	N-CA-C	7.05	119.86	111.33
1	B	331	LYS	N-CA-C	6.74	118.28	111.07
1	B	115	ARG	N-CA-C	-6.25	104.91	112.54
1	B	104	ASP	N-CA-C	6.21	119.70	111.75
1	C	321	SER	N-CA-C	-6.08	101.93	110.50
1	A	102	ILE	N-CA-C	6.02	118.94	113.10
1	C	439	TYR	N-CA-C	6.00	119.02	110.68
1	D	331	LYS	N-CA-C	5.99	117.48	111.07
1	C	162	HIS	N-CA-C	-5.97	105.95	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	GLY	N-CA-C	-5.77	100.93	111.25
1	D	302	ALA	N-CA-C	-5.75	105.01	111.28
1	D	407	ILE	N-CA-C	5.69	118.16	111.05
1	A	439	TYR	N-CA-C	5.69	118.58	110.68
1	A	115	ARG	N-CA-C	-5.49	105.84	112.54
1	A	321	SER	N-CA-C	-5.45	102.41	110.48
1	D	466	GLU	N-CA-C	-5.45	105.89	112.54
1	C	331	LYS	N-CA-C	5.24	117.42	111.02
1	C	159	GLY	N-CA-C	-5.21	101.93	111.25
1	A	367	THR	CA-C-N	5.17	124.78	119.05
1	A	367	THR	C-N-CA	5.17	124.78	119.05
1	D	199	LEU	N-CA-C	5.07	116.93	109.42
1	D	159	GLY	N-CA-C	-5.07	102.66	111.62
1	D	439	TYR	N-CA-C	5.02	117.66	110.68
1	B	162	HIS	N-CA-C	-5.01	107.12	113.23

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	105	ILE	CB
1	B	405	ILE	CB
1	D	105	ILE	CB

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	3464	0	3570	67	0
1	B	3441	0	3512	80	0
1	C	3456	0	3545	75	0
1	D	3468	0	3547	76	0
2	A	20	0	14	1	0
2	B	20	0	14	0	0
2	C	20	0	14	1	0
2	D	20	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	253	0	0	8	0
3	B	196	0	0	5	0
3	C	258	0	0	9	0
3	D	203	0	0	5	0
All	All	14819	0	14230	286	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 10.

All (286) 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:B:102:ILE:HD11	1:B:106:ALA:HB2	1.42	1.00
1:A:110:HIS:HD2	1:A:113:ARG:HE	1.16	0.93
1:A:30:ILE:O	1:A:34:GLN:HG3	1.69	0.93
1:C:50:ALA:HB1	1:C:213:ILE:HD11	1.50	0.92
1:D:110:HIS:HD2	1:D:113:ARG:HE	1.17	0.92
1:D:260:GLU:O	1:D:264:ILE:HD13	1.72	0.88
1:C:173:GLN:HE22	1:C:453:GLN:HE22	1.21	0.87
1:D:357:ILE:HD13	1:D:357:ILE:H	1.43	0.83
1:D:27:ASN:OD1	1:D:325:LYS:HE2	1.77	0.83
1:B:173:GLN:HE22	1:B:453:GLN:HE22	1.23	0.82
1:C:298:ILE:HD12	1:C:344:VAL:HG13	1.59	0.82
1:D:110:HIS:CD2	1:D:113:ARG:HE	1.98	0.82
1:D:153:ILE:HD13	1:D:450:VAL:HG11	1.62	0.80
1:A:135:SER:O	1:A:139:LEU:HD23	1.82	0.80
1:D:173:GLN:HE22	1:D:453:GLN:HE22	1.31	0.78
1:C:50:ALA:CB	1:C:213:ILE:HD11	2.14	0.77
1:A:110:HIS:CD2	1:A:113:ARG:HE	2.02	0.77
1:D:395:LYS:HB3	1:D:418:ILE:HD12	1.65	0.77
1:A:406:THR:OG1	1:A:409:LYS:HD3	1.86	0.76
1:C:399:LEU:HD11	1:C:403:LYS:HE2	1.67	0.76
1:B:395:LYS:HE3	1:B:418:ILE:HG23	1.68	0.75
1:A:117:ASP:HB3	1:A:235:ILE:HD11	1.69	0.74
1:C:348:ALA:O	1:C:352:ILE:HD12	1.89	0.73
1:B:183:THR:HG21	1:B:460:LEU:HD13	1.72	0.72
1:A:65:ILE:HD13	1:A:102:ILE:HD11	1.71	0.71
1:D:183:THR:HG21	1:D:460:LEU:HD13	1.72	0.71
1:A:230:ASN:HD22	1:A:233:ASP:H	1.38	0.71
1:A:173:GLN:HE22	1:A:453:GLN:HE22	1.38	0.70
1:B:230:ASN:HD22	1:B:233:ASP:H	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:ALA:HB1	1:C:213:ILE:CD1	2.21	0.70
1:C:230:ASN:HD22	1:C:233:ASP:H	1.40	0.70
1:A:405:ILE:HD11	1:A:410:LEU:HD23	1.74	0.70
1:A:357:ILE:HD13	1:A:357:ILE:H	1.57	0.69
3:C:1131:HOH:O	1:D:286:MET:HE2	1.91	0.69
1:B:289:LYS:HE3	3:B:1198:HOH:O	1.92	0.69
1:B:465:LYS:C	1:B:467:GLN:H	2.01	0.69
1:B:59:LYS:O	1:B:63:GLU:HG3	1.93	0.68
1:A:395:LYS:HB3	1:A:418:ILE:HD12	1.74	0.68
1:A:153:ILE:HD13	1:A:450:VAL:HG11	1.75	0.68
1:A:65:ILE:HD13	1:A:102:ILE:CD1	2.23	0.68
1:C:117:ASP:HB3	1:C:235:ILE:HD11	1.76	0.68
1:B:209:ASN:ND2	1:B:211:LEU:H	1.92	0.67
1:D:357:ILE:HD13	3:D:1152:HOH:O	1.93	0.67
1:C:213:ILE:HD13	1:C:214:ASP:H	1.60	0.67
1:C:72:ILE:CD1	1:C:97:ARG:HG3	2.25	0.66
1:C:153:ILE:HD13	1:C:450:VAL:HG11	1.78	0.66
1:D:153:ILE:CD1	1:D:450:VAL:HG11	2.25	0.66
1:D:230:ASN:HD22	1:D:233:ASP:H	1.43	0.65
1:A:153:ILE:CD1	1:A:450:VAL:HG11	2.27	0.65
1:D:360:GLU:O	1:D:364:LYS:HD3	1.95	0.65
1:B:30:ILE:HD13	1:B:30:ILE:O	1.97	0.64
1:B:117:ASP:HB3	1:B:235:ILE:HD11	1.79	0.64
1:C:209:ASN:ND2	1:C:211:LEU:H	1.96	0.64
1:C:442:LEU:HD23	3:C:1061:HOH:O	1.97	0.64
1:D:117:ASP:HB3	1:D:235:ILE:HD11	1.80	0.63
1:A:221:GLU:HG2	3:A:1251:HOH:O	1.98	0.63
1:B:102:ILE:HD11	1:B:106:ALA:CB	2.25	0.62
1:A:67:SER:O	1:A:71:LYS:HG2	2.00	0.62
1:A:209:ASN:ND2	1:A:211:LEU:H	1.98	0.61
1:A:442:LEU:O	1:A:443:ALA:HB3	2.00	0.61
1:B:250:LEU:HG	1:D:242:VAL:HG11	1.83	0.61
1:D:30:ILE:O	1:D:34:GLN:HB2	2.00	0.61
1:C:72:ILE:HD12	1:C:97:ARG:HG3	1.82	0.60
1:C:466:GLU:C	1:C:468:ALA:H	2.10	0.60
1:B:102:ILE:HD13	1:B:105:ILE:CG1	2.32	0.59
1:B:297:LEU:O	1:B:301:LYS:HG2	2.01	0.59
1:A:52:GLU:OE1	1:A:59:LYS:HD2	2.02	0.59
1:B:298:ILE:HD13	1:B:344:VAL:HG22	1.85	0.59
1:D:196:ILE:HG13	3:D:1160:HOH:O	2.02	0.59
1:C:179:ALA:O	1:C:183:THR:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:LYS:O	1:B:467:GLN:HG3	2.02	0.59
1:C:213:ILE:HD13	1:C:214:ASP:N	2.17	0.59
1:D:173:GLN:HE21	1:D:173:GLN:HA	1.67	0.59
1:D:407:ILE:HD12	3:D:1091:HOH:O	2.03	0.58
1:C:35:ARG:HD3	3:C:1123:HOH:O	2.03	0.58
1:C:72:ILE:HD12	1:C:97:ARG:CG	2.34	0.58
1:A:252:MET:HE2	1:A:301:LYS:HB2	1.86	0.58
1:C:30:ILE:O	1:C:34:GLN:HG3	2.04	0.58
1:B:176:LEU:HD21	1:B:454:ILE:HD13	1.86	0.57
1:D:127:MET:O	1:D:131:LEU:HD13	2.04	0.57
1:B:442:LEU:O	1:B:443:ALA:HB3	2.05	0.57
1:D:298:ILE:HG12	1:D:344:VAL:HG13	1.87	0.57
1:D:235:ILE:HG22	1:D:322:THR:HG22	1.86	0.57
1:B:102:ILE:CD1	1:B:106:ALA:HB2	2.25	0.57
1:B:462:LYS:O	1:B:466:GLU:HG3	2.05	0.56
1:D:110:HIS:HD2	1:D:113:ARG:NE	1.96	0.56
1:B:74:GLU:OE1	1:B:78:LYS:HE3	2.05	0.56
1:D:189:LEU:C	1:D:189:LEU:HD23	2.31	0.56
1:B:102:ILE:C	1:B:102:ILE:HD12	2.31	0.56
1:D:148:ARG:HH21	1:D:357:ILE:HD12	1.70	0.55
1:B:462:LYS:HA	1:B:465:LYS:HZ2	1.71	0.55
1:B:407:ILE:N	1:B:407:ILE:HD13	2.22	0.55
1:A:27:ASN:OD1	1:A:325:LYS:HE2	2.07	0.55
1:B:257:LYS:HG3	1:D:319:LEU:O	2.06	0.55
1:D:364:LYS:HD3	1:D:364:LYS:N	2.21	0.55
1:C:387:ARG:HH21	1:C:387:ARG:HG2	1.73	0.54
1:A:230:ASN:HD21	1:A:232:MET:HB2	1.72	0.54
1:B:95:GLU:HG3	3:B:1098:HOH:O	2.07	0.54
1:C:298:ILE:CD1	1:C:344:VAL:HG22	2.37	0.54
1:D:139:LEU:HD13	1:D:465:LYS:HE2	1.89	0.54
1:A:173:GLN:HA	1:A:173:GLN:HE21	1.73	0.54
1:B:398:HIS:O	1:B:402:THR:HG23	2.08	0.54
1:C:258:MET:O	1:C:262:LEU:HD13	2.08	0.54
1:D:407:ILE:HD13	1:D:407:ILE:N	2.23	0.54
1:B:65:ILE:HD11	1:B:105:ILE:HG22	1.90	0.54
1:B:319:LEU:O	1:D:257:LYS:HG3	2.07	0.54
1:C:205:ALA:O	1:C:206:LEU:HB3	2.08	0.54
1:C:105:ILE:HG22	3:C:1177:HOH:O	2.08	0.54
1:D:357:ILE:H	1:D:357:ILE:CD1	2.19	0.53
1:C:258:MET:HE1	1:C:352:ILE:HD11	1.90	0.53
1:A:357:ILE:H	1:A:357:ILE:CD1	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:LEU:O	1:D:301:LYS:HG2	2.09	0.53
1:A:141:LEU:HD13	1:A:182:LEU:HD13	1.91	0.52
1:C:153:ILE:HD12	1:C:153:ILE:O	2.09	0.52
1:D:230:ASN:ND2	1:D:233:ASP:H	2.07	0.52
1:A:110:HIS:HD2	1:A:113:ARG:NE	1.96	0.52
1:B:102:ILE:CD1	1:B:102:ILE:C	2.82	0.52
1:C:258:MET:CE	1:C:352:ILE:HD11	2.39	0.52
1:D:84:LYS:HD2	1:D:96:ARG:HD2	1.91	0.52
1:A:162:HIS:HA	1:B:296:GLU:OE1	2.10	0.52
1:B:189:LEU:O	1:B:189:LEU:HD23	2.09	0.52
1:C:252:MET:HB3	1:C:302:ALA:HA	1.92	0.52
1:B:330:ASP:OD1	1:B:331:LYS:N	2.43	0.52
1:A:360:GLU:O	1:A:363:GLU:HG3	2.10	0.52
1:B:173:GLN:HA	1:B:173:GLN:HE21	1.74	0.52
1:C:129:ASN:HB3	3:C:1210:HOH:O	2.09	0.52
2:A:1004:AS1:HA	3:C:1106:HOH:O	2.10	0.52
1:C:80:VAL:HG22	1:C:80:VAL:O	2.09	0.52
1:D:209:ASN:ND2	1:D:211:LEU:H	2.07	0.52
1:B:407:ILE:HG12	1:B:430:PHE:HE2	1.75	0.51
1:A:375:LEU:O	1:A:378:TYR:HB3	2.10	0.51
1:C:173:GLN:HE22	1:C:453:GLN:NE2	2.01	0.51
1:D:405:ILE:HD11	1:D:410:LEU:HD23	1.92	0.51
1:B:135:SER:O	1:B:139:LEU:HD23	2.11	0.51
1:C:289:LYS:HE3	3:C:1219:HOH:O	2.10	0.51
1:D:252:MET:HB3	1:D:302:ALA:HA	1.91	0.51
1:C:271:GLY:HA2	3:C:1075:HOH:O	2.11	0.51
1:C:252:MET:HE2	1:C:301:LYS:HB2	1.93	0.51
1:D:466:GLU:O	1:D:467:GLN:HB2	2.10	0.51
3:A:1078:HOH:O	2:C:1001:AS1:HA	2.10	0.51
1:A:357:ILE:HD13	1:A:357:ILE:N	2.25	0.51
1:B:61:GLU:O	1:B:65:ILE:HG12	2.10	0.50
1:C:442:LEU:O	1:C:443:ALA:HB3	2.10	0.50
1:A:90:ILE:C	1:A:90:ILE:HD13	2.36	0.50
1:D:138:LEU:CD1	1:D:186:SER:HB2	2.42	0.50
1:A:90:ILE:HD13	1:A:90:ILE:O	2.11	0.50
1:B:384:VAL:CG2	1:B:421:GLN:HG3	2.42	0.50
1:C:466:GLU:C	1:C:468:ALA:N	2.69	0.50
1:A:274:THR:CG2	1:A:290:LYS:HD2	2.41	0.49
1:D:357:ILE:HD13	1:D:357:ILE:N	2.18	0.49
1:B:369:GLU:HG3	3:B:1062:HOH:O	2.11	0.49
1:D:44:SER:HB3	1:D:109:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:ILE:HD12	3:B:1062:HOH:O	2.12	0.49
1:C:297:LEU:O	1:C:301:LYS:HG2	2.13	0.49
1:A:357:ILE:HD13	3:A:1132:HOH:O	2.12	0.48
1:D:74:GLU:O	1:D:78:LYS:HG2	2.13	0.48
1:A:37:SER:HA	1:A:90:ILE:HD11	1.94	0.48
1:A:40:ASP:OD1	1:A:91:HIS:HD2	1.96	0.48
1:B:192:VAL:HG22	1:B:243:GLU:HB3	1.95	0.48
1:A:117:ASP:CB	1:A:235:ILE:HD11	2.42	0.48
1:B:461:MET:O	1:B:465:LYS:HD3	2.13	0.48
1:D:188:ARG:NH2	1:D:250:LEU:HD13	2.29	0.48
1:B:189:LEU:HD23	1:B:189:LEU:C	2.38	0.48
1:C:206:LEU:C	1:C:206:LEU:HD12	2.38	0.48
1:A:44:SER:HB3	1:A:109:LEU:HD21	1.96	0.48
1:B:117:ASP:CB	1:B:235:ILE:HD11	2.44	0.47
1:B:393:SER:O	1:B:397:VAL:HG23	2.14	0.47
1:D:407:ILE:HD13	1:D:407:ILE:H	1.79	0.47
1:A:443:ALA:HB3	3:A:1072:HOH:O	2.15	0.47
3:B:1064:HOH:O	2:D:1002:AS1:HA	2.14	0.47
1:D:364:LYS:N	1:D:364:LYS:CD	2.77	0.47
1:A:242:VAL:HG11	1:C:250:LEU:HG	1.97	0.47
1:C:162:HIS:HB3	1:D:292:PRO:HD2	1.96	0.47
1:C:111:THR:HG22	1:C:211:LEU:HD11	1.97	0.47
1:D:360:GLU:HG3	1:D:364:LYS:HE2	1.96	0.47
1:A:148:ARG:HH21	1:A:357:ILE:HD12	1.79	0.47
1:B:260:GLU:O	1:B:264:ILE:HG12	2.14	0.47
1:B:407:ILE:HG12	1:B:430:PHE:CE2	2.50	0.47
1:D:407:ILE:H	1:D:407:ILE:CD1	2.28	0.47
1:C:176:LEU:O	1:C:180:VAL:HG23	2.14	0.47
1:C:260:GLU:O	1:C:264:ILE:HD13	2.15	0.47
1:D:194:LYS:HE2	3:D:1020:HOH:O	2.14	0.47
1:A:60:THR:CG2	1:A:64:LYS:NZ	2.78	0.47
1:C:127:MET:O	1:C:131:LEU:HD13	2.15	0.47
1:C:189:LEU:HD23	1:C:189:LEU:C	2.40	0.47
1:D:20:ASP:HB3	1:D:23:MET:HB2	1.97	0.47
1:C:130:SER:O	1:C:134:ILE:HG12	2.14	0.47
1:D:33:ASP:OD2	1:D:33:ASP:C	2.58	0.47
1:A:60:THR:CG2	1:A:64:LYS:HZ2	2.28	0.46
1:D:373:THR:HB	3:D:1125:HOH:O	2.15	0.46
1:A:466:GLU:O	1:A:466:GLU:HG3	2.15	0.46
1:B:252:MET:HE2	1:B:301:LYS:HB2	1.96	0.46
1:C:237:GLU:OE2	1:C:239:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ARG:HE	1:B:152:GLU:CD	2.24	0.46
1:C:230:ASN:ND2	1:C:233:ASP:H	2.09	0.46
1:C:61:GLU:CB	1:C:105:ILE:HD11	2.46	0.46
1:C:153:ILE:CD1	1:C:450:VAL:HG11	2.46	0.46
1:A:297:LEU:O	1:A:301:LYS:HG2	2.16	0.46
1:B:375:LEU:O	1:B:378:TYR:HB3	2.16	0.46
1:A:442:LEU:O	1:A:443:ALA:CB	2.64	0.45
1:B:176:LEU:HD21	1:B:454:ILE:CD1	2.47	0.45
1:A:156:ILE:HD12	1:A:436:VAL:HG11	1.99	0.45
1:A:245:LEU:CD2	1:A:337:VAL:HG21	2.47	0.45
1:D:191:GLU:HA	1:D:194:LYS:HD3	1.97	0.45
1:B:450:VAL:O	1:B:454:ILE:HG12	2.16	0.45
1:C:467:GLN:O	1:C:468:ALA:HB3	2.17	0.45
1:A:252:MET:HB3	1:A:302:ALA:HA	1.97	0.45
1:B:59:LYS:NZ	1:B:62:LEU:HD23	2.32	0.45
1:B:102:ILE:HD12	1:B:103:GLY:N	2.32	0.45
1:C:173:GLN:HA	1:C:173:GLN:HE21	1.82	0.45
1:D:230:ASN:HD21	1:D:232:MET:HB2	1.81	0.45
1:C:105:ILE:HG12	1:C:105:ILE:O	2.17	0.44
1:B:317:LYS:HD3	1:B:317:LYS:C	2.41	0.44
1:A:387:ARG:HH21	1:A:387:ARG:HG3	1.82	0.44
1:A:326:ASP:HA	1:D:300:SER:HB3	2.00	0.44
1:B:300:SER:HB3	1:C:326:ASP:HA	1.98	0.44
1:D:138:LEU:HD11	1:D:186:SER:HB2	1.98	0.44
1:A:56:ILE:HD12	1:A:56:ILE:N	2.32	0.44
1:A:107:GLY:HA2	1:C:387:ARG:HH22	1.83	0.44
1:B:138:LEU:HD11	1:B:186:SER:HB2	1.98	0.44
1:B:407:ILE:N	1:B:407:ILE:CD1	2.80	0.44
1:B:326:ASP:HA	1:C:300:SER:HB3	2.00	0.44
1:C:298:ILE:HD13	1:C:344:VAL:HG22	1.99	0.44
1:C:442:LEU:CD2	1:C:442:LEU:H	2.31	0.44
1:A:205:ALA:O	1:A:206:LEU:HB3	2.18	0.44
1:A:273:LEU:C	1:A:273:LEU:HD12	2.43	0.44
1:B:161:ASP:O	1:B:162:HIS:HB2	2.17	0.44
1:A:196:ILE:HG12	1:A:240:PHE:HB2	2.00	0.43
1:D:249:THR:O	1:D:253:ILE:HG12	2.17	0.43
1:B:205:ALA:O	1:B:206:LEU:HB3	2.18	0.43
1:B:25:LYS:O	1:B:25:LYS:HD3	2.18	0.43
1:B:465:LYS:C	1:B:467:GLN:N	2.69	0.43
1:B:367:THR:OG1	1:B:370:MET:HG3	2.18	0.43
1:D:387:ARG:NH2	1:D:387:ARG:HG3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:LYS:HE3	1:C:26:LEU:HD11	2.01	0.43
1:A:196:ILE:HG13	3:A:1051:HOH:O	2.18	0.43
1:C:385:PRO:HB2	1:C:388:GLN:OE1	2.18	0.43
1:D:156:ILE:HG22	1:D:366:LEU:HD11	2.00	0.43
1:D:387:ARG:HG3	1:D:387:ARG:HH21	1.84	0.43
1:B:138:LEU:CD1	1:B:186:SER:HB2	2.49	0.43
1:C:124:LYS:HE2	1:C:240:PHE:CD2	2.54	0.43
1:B:20:ASP:O	1:B:24:GLU:HG2	2.19	0.43
1:A:357:ILE:CD1	3:A:1132:HOH:O	2.67	0.42
1:A:395:LYS:CB	1:A:418:ILE:HD12	2.44	0.42
1:C:463:LYS:HE2	1:C:463:LYS:HB3	1.76	0.42
1:B:432:PHE:O	1:B:435:SER:HB3	2.19	0.42
1:D:397:VAL:O	1:D:401:GLU:HG3	2.19	0.42
1:C:162:HIS:HA	1:D:296:GLU:OE1	2.20	0.42
1:C:317:LYS:HD3	1:C:317:LYS:C	2.44	0.42
1:D:368:PRO:O	1:D:407:ILE:HD11	2.18	0.42
1:D:189:LEU:HD23	1:D:189:LEU:O	2.19	0.42
1:B:141:LEU:HD13	1:B:182:LEU:HD13	2.02	0.42
1:D:62:LEU:O	1:D:66:LEU:HG	2.19	0.42
1:D:209:ASN:HD22	1:D:211:LEU:H	1.68	0.42
1:A:110:HIS:HE1	3:A:1215:HOH:O	2.01	0.42
1:B:442:LEU:O	1:B:443:ALA:CB	2.68	0.42
1:A:20:ASP:O	1:A:24:GLU:HG2	2.20	0.42
1:C:442:LEU:N	1:C:442:LEU:HD22	2.35	0.42
1:C:95:GLU:CD	1:C:115:ARG:HH12	2.25	0.42
1:B:196:ILE:HG12	1:B:240:PHE:HB2	2.01	0.41
1:D:264:ILE:N	1:D:264:ILE:HD12	2.33	0.41
1:C:369:GLU:HG3	3:C:1187:HOH:O	2.19	0.41
1:B:163:LEU:HD12	1:B:163:LEU:HA	1.91	0.41
1:A:387:ARG:HG3	1:A:387:ARG:NH2	2.36	0.41
1:C:72:ILE:HD11	1:C:101:LEU:HD12	2.02	0.41
1:C:459:GLU:O	1:C:463:LYS:HG2	2.21	0.41
1:D:411:SER:O	1:D:414:ASP:HB2	2.19	0.41
1:A:230:ASN:ND2	1:A:233:ASP:H	2.13	0.41
1:C:141:LEU:HD21	1:C:352:ILE:HD13	2.01	0.41
1:C:296:GLU:OE1	1:D:162:HIS:HA	2.20	0.41
1:C:161:ASP:O	1:C:162:HIS:HB2	2.20	0.41
1:A:54:ALA:HB3	1:A:56:ILE:HD13	2.03	0.41
1:B:227:ILE:HD11	1:D:442:LEU:HD12	2.03	0.41
1:D:203:SER:HB2	1:D:235:ILE:HD13	2.03	0.41
1:D:264:ILE:N	1:D:264:ILE:CD1	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:LYS:HE2	1:B:240:PHE:CE2	2.56	0.41
1:B:237:GLU:OE2	1:B:239:ASP:HB2	2.21	0.41
1:B:466:GLU:O	1:B:467:GLN:O	2.39	0.41
1:D:116:ASN:HB3	1:D:235:ILE:HG13	2.03	0.41
1:D:457:LEU:HD12	1:D:457:LEU:HA	1.94	0.41
1:B:30:ILE:HD13	1:B:30:ILE:C	2.46	0.40
1:B:275:LEU:HD22	1:B:351:VAL:HG13	2.02	0.40
1:A:271:GLY:HA2	3:A:1176:HOH:O	2.21	0.40
1:A:314:MET:HA	1:B:314:MET:HE2	2.04	0.40
1:C:80:VAL:O	1:C:80:VAL:CG2	2.69	0.40
1:D:203:SER:HB2	1:D:235:ILE:CD1	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	447/474 (94%)	440 (98%)	6 (1%)	1 (0%)	43	42
1	B	446/474 (94%)	438 (98%)	5 (1%)	3 (1%)	18	14
1	C	447/474 (94%)	439 (98%)	7 (2%)	1 (0%)	43	42
1	D	447/474 (94%)	437 (98%)	9 (2%)	1 (0%)	43	42
All	All	1787/1896 (94%)	1754 (98%)	27 (2%)	6 (0%)	36	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	LEU
1	B	206	LEU
1	C	206	LEU
1	B	466	GLU

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Mol	Chain	Res	Type
1	D	206	LEU
1	B	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	386/411 (94%)	376 (97%)	10 (3%)	40	44
1	B	380/411 (92%)	367 (97%)	13 (3%)	32	33
1	C	383/411 (93%)	372 (97%)	11 (3%)	37	40
1	D	386/411 (94%)	372 (96%)	14 (4%)	31	31
All	All	1535/1644 (93%)	1487 (97%)	48 (3%)	35	37

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	MET
1	A	90	ILE
1	A	141	LEU
1	A	173	GLN
1	A	235	ILE
1	A	250	LEU
1	A	262	LEU
1	A	275	LEU
1	A	357	ILE
1	A	457	LEU
1	B	30	ILE
1	B	59	LYS
1	B	102	ILE
1	B	141	LEU
1	B	173	GLN
1	B	201	LEU
1	B	235	ILE
1	B	250	LEU
1	B	262	LEU

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Mol	Chain	Res	Type
1	B	289	LYS
1	B	344	VAL
1	B	407	ILE
1	B	465	LYS
1	C	105	ILE
1	C	138	LEU
1	C	141	LEU
1	C	153	ILE
1	C	201	LEU
1	C	213	ILE
1	C	235	ILE
1	C	250	LEU
1	C	264	ILE
1	C	325	LYS
1	C	457	LEU
1	D	23	MET
1	D	78	LYS
1	D	141	LEU
1	D	173	GLN
1	D	201	LEU
1	D	230	ASN
1	D	235	ILE
1	D	250	LEU
1	D	262	LEU
1	D	264	ILE
1	D	356	GLN
1	D	357	ILE
1	D	407	ILE
1	D	457	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	42	GLN
1	A	91	HIS
1	A	110	HIS
1	A	140	GLN
1	A	173	GLN
1	A	209	ASN
1	A	230	ASN
1	A	388	GLN

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Mol	Chain	Res	Type
1	A	421	GLN
1	A	464	GLN
1	B	34	GLN
1	B	91	HIS
1	B	173	GLN
1	B	209	ASN
1	B	230	ASN
1	B	291	ASN
1	B	356	GLN
1	B	388	GLN
1	B	390	HIS
1	B	464	GLN
1	C	173	GLN
1	C	209	ASN
1	C	230	ASN
1	C	464	GLN
1	D	110	HIS
1	D	140	GLN
1	D	167	GLN
1	D	173	GLN
1	D	209	ASN
1	D	230	ASN
1	D	388	GLN
1	D	421	GLN

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 ⓘ

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	C	1001	-	18,19,19	1.02	1 (5%)	19,24,24	1.37	2 (10%)
2	AS1	D	1002	-	18,19,19	1.08	0	19,24,24	1.25	2 (10%)
2	AS1	A	1004	-	18,19,19	1.05	0	19,24,24	1.57	2 (10%)
2	AS1	B	1003	-	18,19,19	1.02	0	19,24,24	1.34	2 (10%)

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	C	1001	-	1/1/6/7	10/21/23/23	-
2	AS1	D	1002	-	1/1/6/7	10/21/23/23	-
2	AS1	A	1004	-	1/1/6/7	12/21/23/23	-
2	AS1	B	1003	-	1/1/6/7	10/21/23/23	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	AS1	C-N2	2.01	1.33	1.28

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1004	AS1	CG-CA-N1	4.74	121.56	110.57
2	B	1003	AS1	CG-CA-N1	3.63	119.00	110.57
2	C	1001	AS1	CG-CA-N1	3.35	118.35	110.57
2	A	1004	AS1	N1-C-N2	-3.09	117.50	125.00
2	B	1003	AS1	N1-C-N2	-2.87	118.06	125.00
2	C	1001	AS1	N1-C-N2	-2.87	118.06	125.00
2	D	1002	AS1	CG-CA-N1	2.80	117.06	110.57
2	D	1002	AS1	N1-C-N2	-2.67	118.54	125.00

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 (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1004	AS1	N3-C-N1-CA
2	A	1004	AS1	CG-CA-N1-C
2	A	1004	AS1	N1-CA-CB-CD
2	B	1003	AS1	N3-C-N1-CA
2	B	1003	AS1	CG-CA-N1-C
2	B	1003	AS1	N1-CA-CB-CD
2	C	1001	AS1	N3-C-N1-CA
2	C	1001	AS1	CG-CA-N1-C
2	C	1001	AS1	N1-CA-CB-CD
2	D	1002	AS1	N3-C-N1-CA
2	D	1002	AS1	CG-CA-N1-C
2	D	1002	AS1	N1-CA-CB-CD
2	B	1003	AS1	N1-CA-CG-OG2
2	B	1003	AS1	N1-CA-CG-OG1
2	D	1002	AS1	CG-CA-CB-CD
2	D	1002	AS1	N1-CA-CG-OG2
2	C	1001	AS1	N1-CA-CG-OG2
2	C	1001	AS1	N1-CA-CG-OG1
2	D	1002	AS1	N1-CA-CG-OG1
2	C	1001	AS1	CB-CA-CG-OG1
2	B	1003	AS1	CB-CA-CG-OG1
2	C	1001	AS1	CB-CA-CG-OG2
2	D	1002	AS1	CB-CA-CG-OG2
2	B	1003	AS1	N2-C1-C2-C3
2	C	1001	AS1	N2-C1-C2-C3
2	D	1002	AS1	N2-C1-C2-C3
2	D	1002	AS1	CB-CA-CG-OG1
2	A	1004	AS1	C2-C3-C4-N4
2	B	1003	AS1	C2-C3-C4-N4
2	B	1003	AS1	CB-CA-CG-OG2
2	C	1001	AS1	CA-CB-CD-OD2
2	A	1004	AS1	CA-CB-CD-OD2
2	A	1004	AS1	N1-CA-CG-OG2
2	C	1001	AS1	CA-CB-CD-OD1

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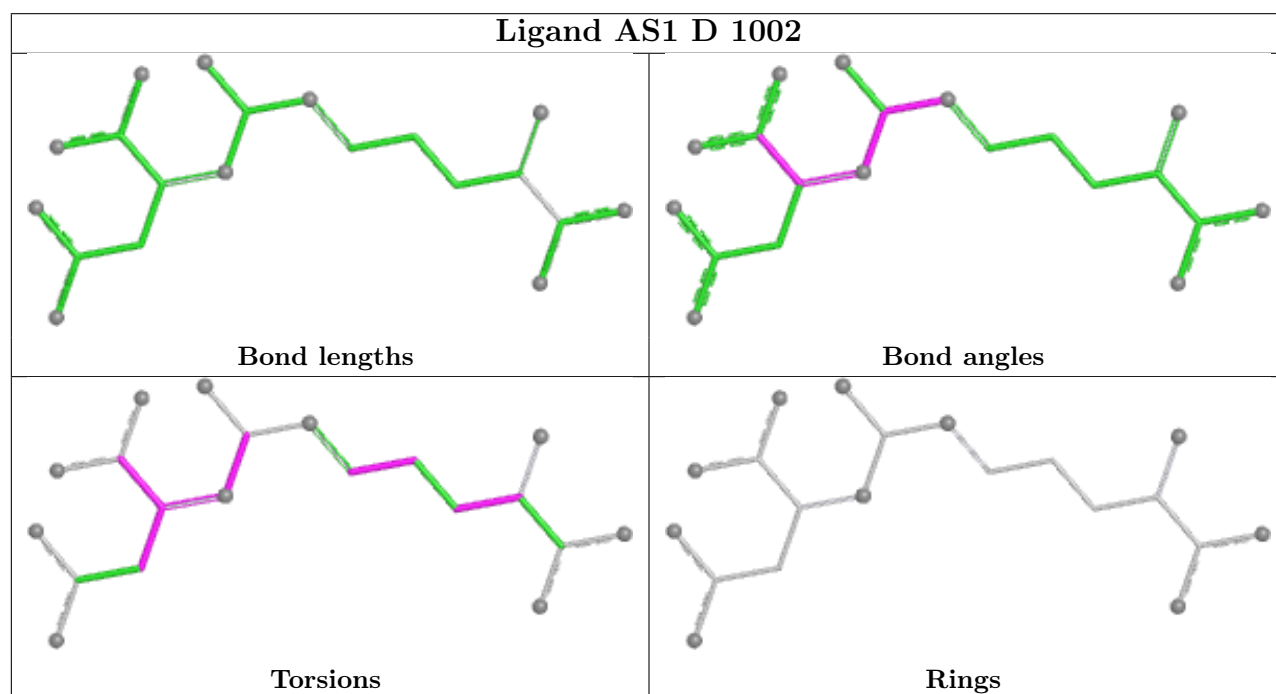
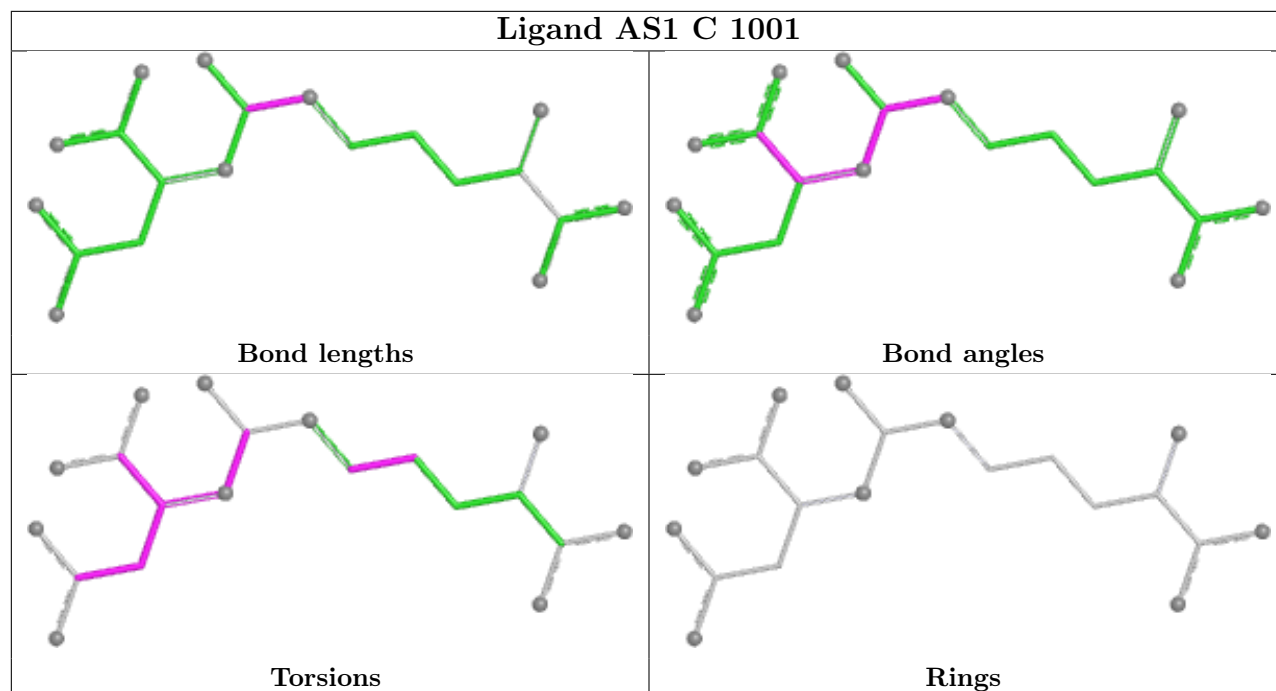
Mol	Chain	Res	Type	Atoms
2	A	1004	AS1	N1-CA-CG-OG1
2	A	1004	AS1	CB-CA-CG-OG2
2	A	1004	AS1	C2-C3-C4-C5
2	A	1004	AS1	N2-C1-C2-C3
2	A	1004	AS1	CA-CB-CD-OD1
2	A	1004	AS1	CB-CA-CG-OG1
2	D	1002	AS1	C2-C3-C4-N4
2	B	1003	AS1	CA-CB-CD-OD2

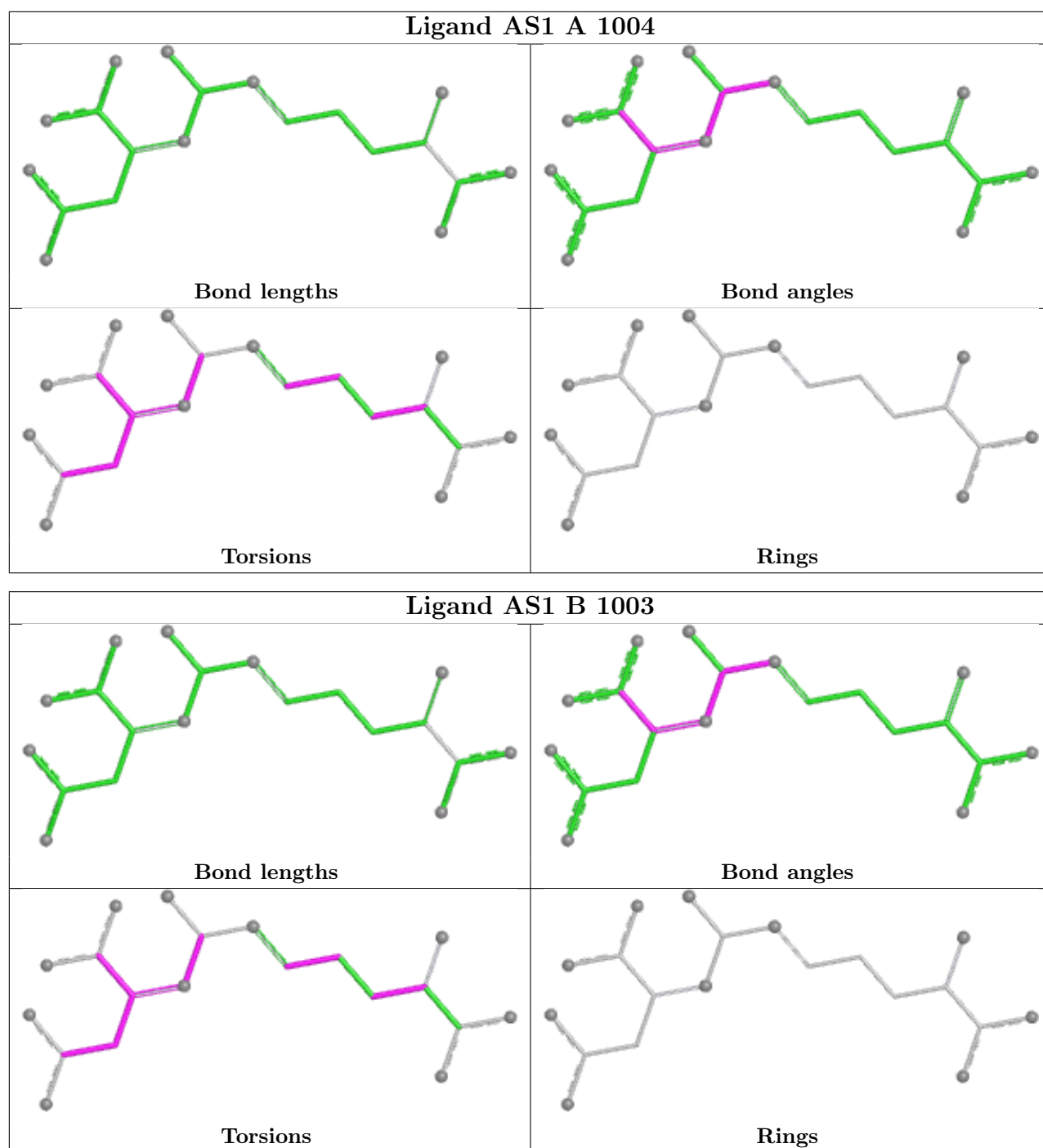
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	AS1	1	0
2	D	1002	AS1	1	0
2	A	1004	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	449/474 (94%)	-0.17	4 (0%) 81 80	10, 19, 41, 55	0
1	B	448/474 (94%)	0.04	6 (1%) 75 74	10, 24, 40, 56	0
1	C	449/474 (94%)	-0.16	3 (0%) 84 84	10, 19, 36, 57	0
1	D	449/474 (94%)	-0.06	3 (0%) 84 84	11, 21, 37, 50	0
All	All	1795/1896 (94%)	-0.09	16 (0%) 81 80	10, 21, 39, 57	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	468	ALA	7.6
1	D	467	GLN	3.3
1	B	407	ILE	3.3
1	A	467	GLN	3.1
1	B	467	GLN	3.1
1	A	418	ILE	2.7
1	C	72	ILE	2.5
1	B	402	THR	2.4
1	D	19	THR	2.4
1	C	282	GLY	2.4
1	D	386	PHE	2.2
1	B	443	ALA	2.2
1	A	386	PHE	2.2
1	B	406	THR	2.2
1	B	454	ILE	2.0
1	A	283	SER	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](#)

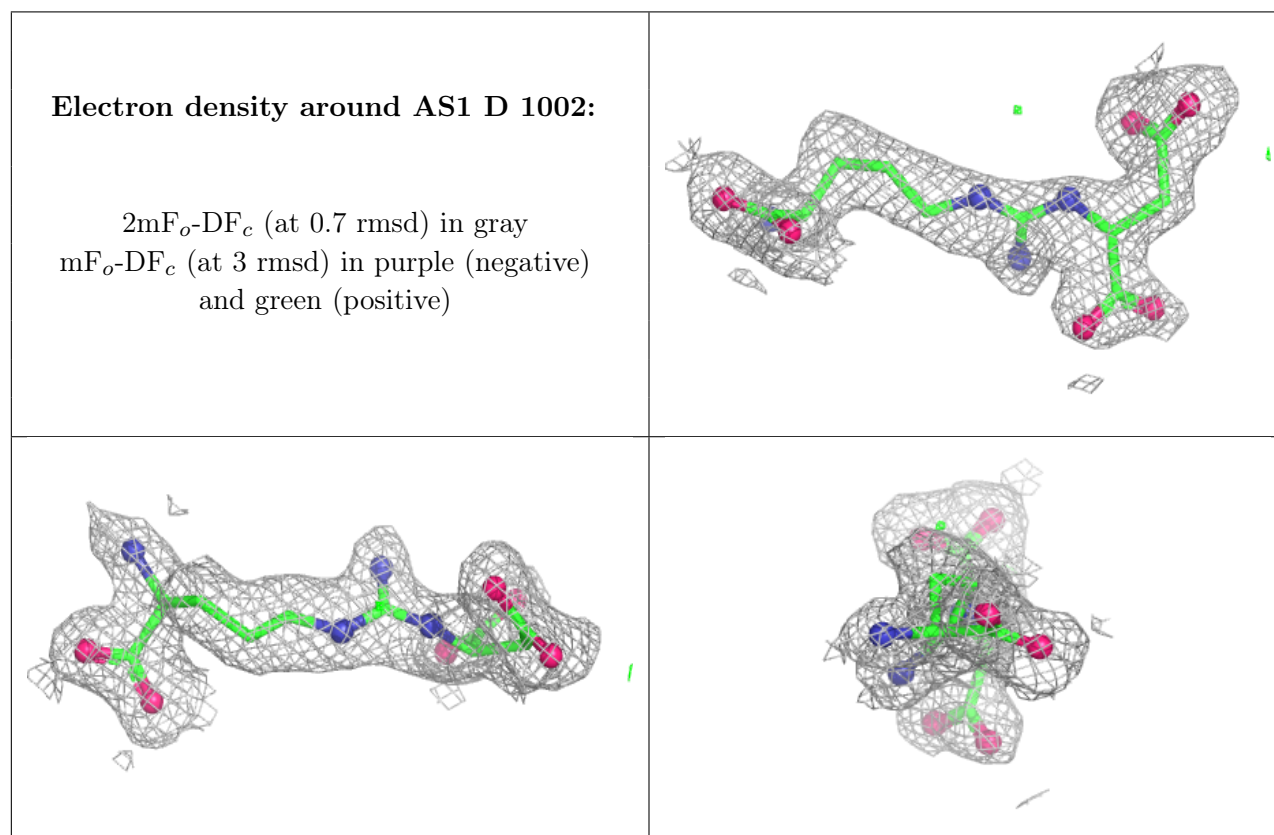
There are no oligosaccharides in this entry.

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.

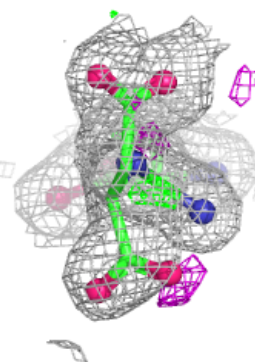
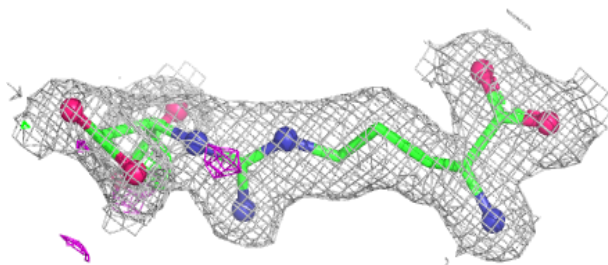
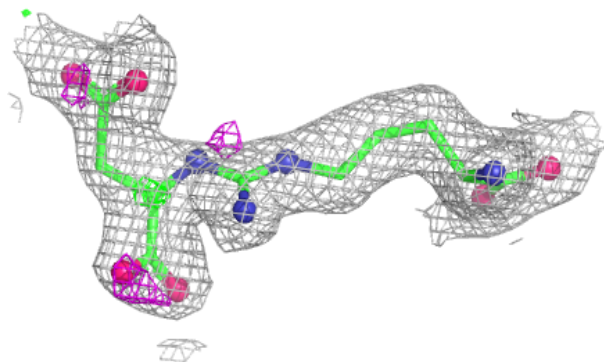
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AS1	D	1002	20/20	0.88	0.11	24,31,38,38	0
2	AS1	B	1003	20/20	0.90	0.11	15,23,35,37	0
2	AS1	C	1001	20/20	0.91	0.09	18,30,36,36	0
2	AS1	A	1004	20/20	0.92	0.08	18,24,30,31	0

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.

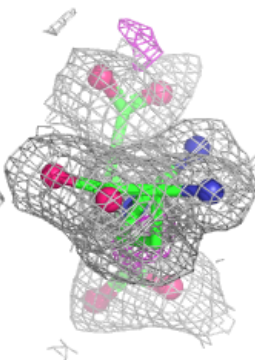
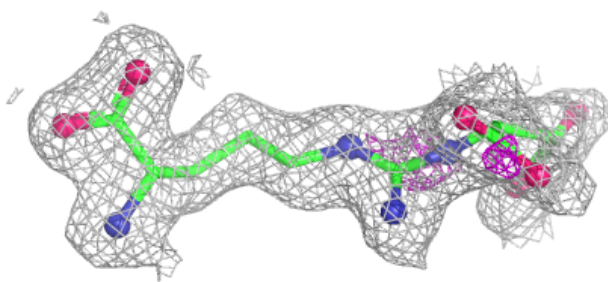
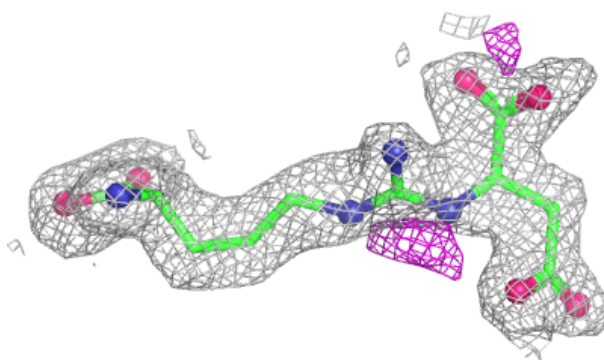


Electron density around AS1 B 1003:

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

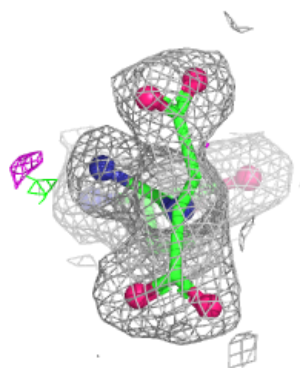
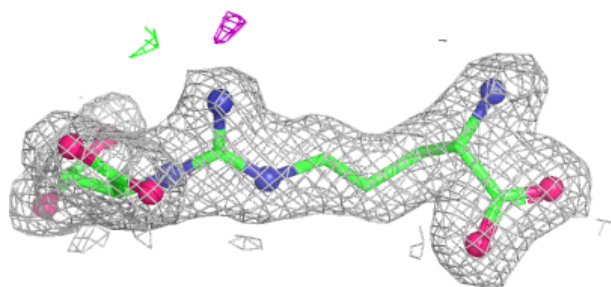
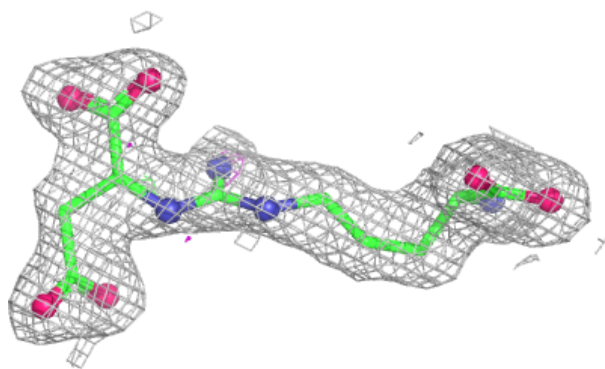
**Electron density around AS1 C 1001:**

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



Electron density around AS1 A 1004:

$2mF_o-DF_c$ (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.