Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 05:26 AM EDT

PDB ID	:	1K7W
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 (i) symbol.

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

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

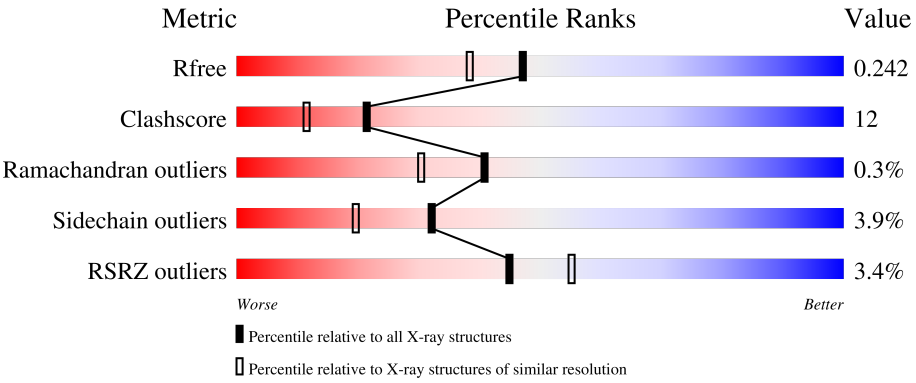
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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 <=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	4% 72% 23%
1	B	468	5% 71% 22%
1	C	468	2% 74% 20%
1	D	468	2% 72% 21%

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 (i)

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.

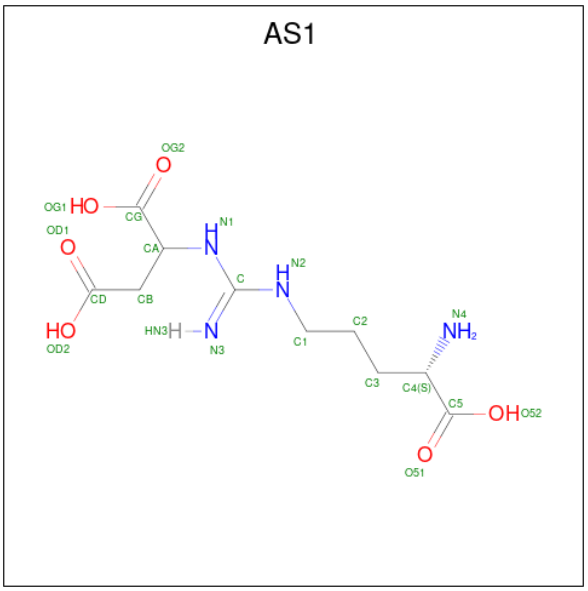
- Molecule 1 is a protein called delta 2 crystallin.

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 (three-letter code: AS1) (formula: $C_{10}H_{18}N_4O_6$).



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

- Molecule 3 is water.

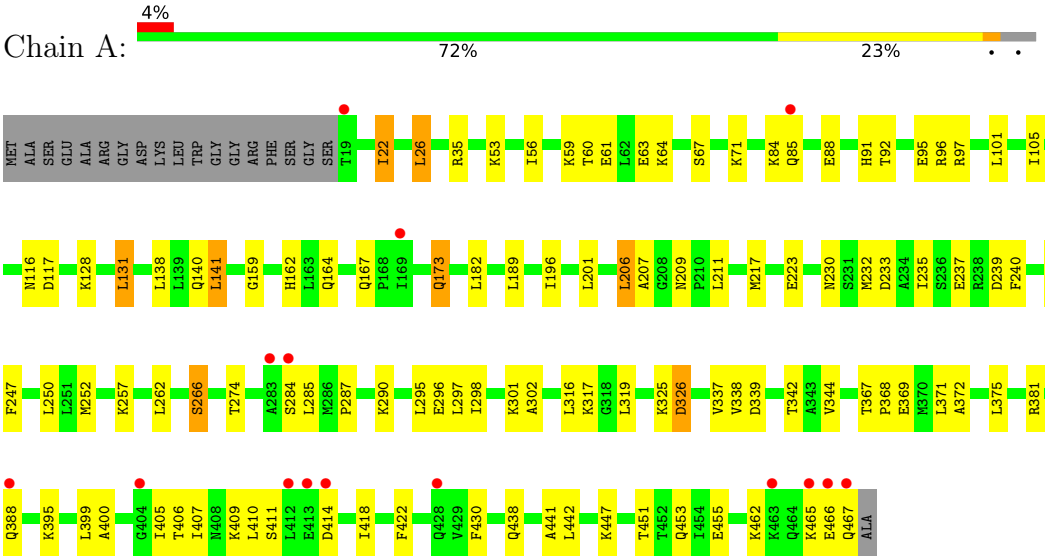
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	211	Total O 211 211	0	0
3	B	137	Total O 137 137	0	0
3	C	191	Total O 191 191	0	0
3	D	168	Total O 168 168	0	0

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.

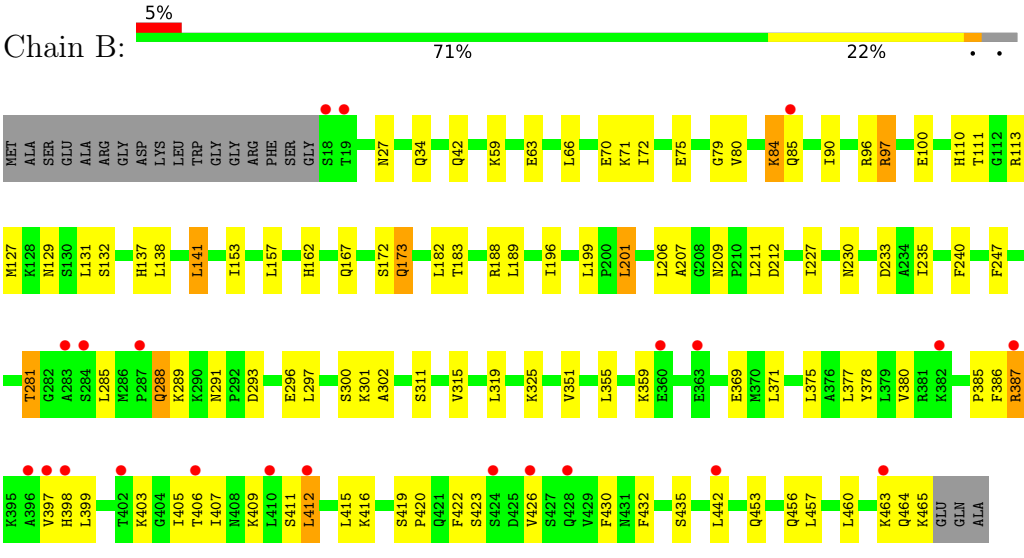
• Molecule 1: delta 2 crystallin

Chain A:



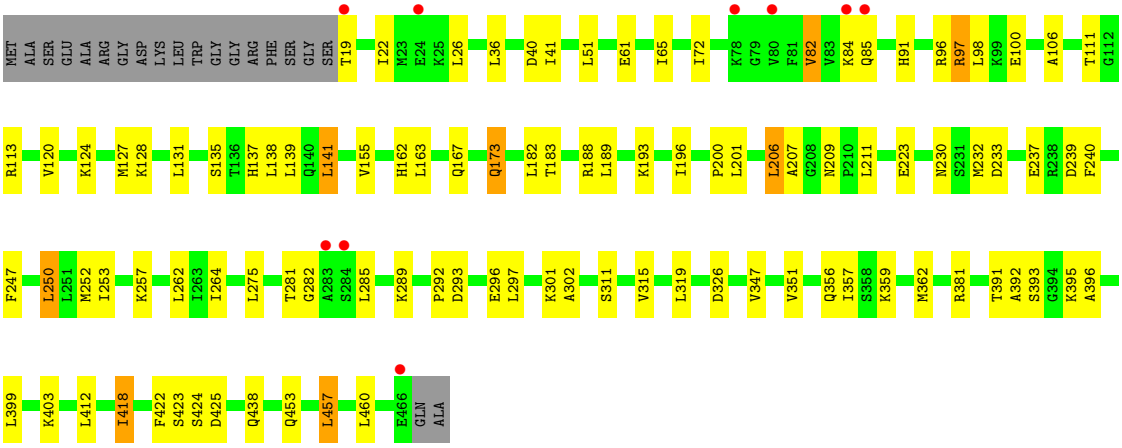
• Molecule 1: delta 2 crystallin

Chain B:



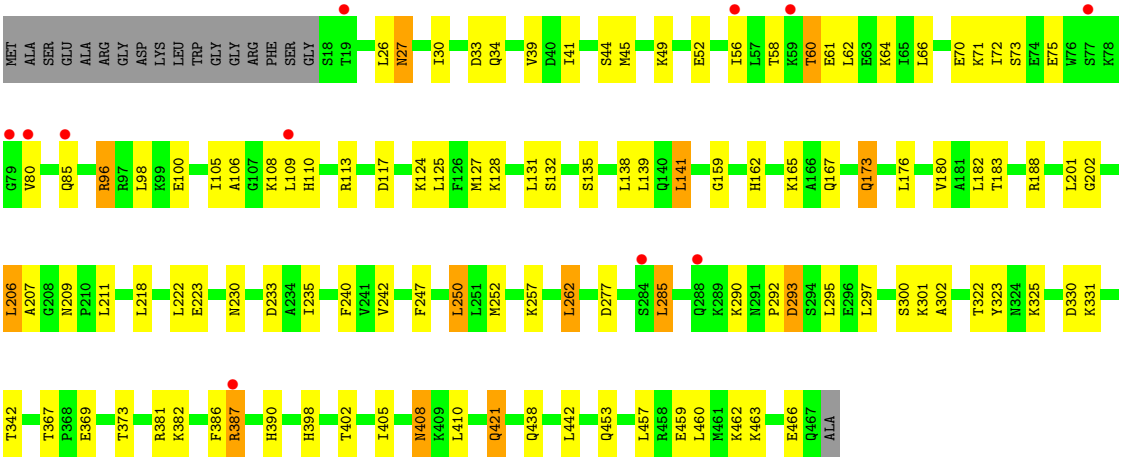
• Molecule 1: delta 2 crystallin

Chain C:



- Molecule 1: delta 2 crystallin

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.65 (at 1.96Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.253 0.198 , 0.242	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)	0.39 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.49	1/3529 (0.0%)	0.64	1/4759 (0.0%)
1	B	0.43	0/3517	0.63	0/4743
1	C	0.47	0/3527	0.65	0/4756
1	D	0.45	0/3537	0.63	1/4770 (0.0%)
All	All	0.46	1/14110 (0.0%)	0.64	2/19028 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	GLU	CB-CG	-5.20	1.42	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	159	GLY	N-CA-C	-5.18	100.15	113.10
1	D	159	GLY	N-CA-C	-5.15	100.23	113.10

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	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3473	0	3595	94	0
1	C	3482	0	3603	81	0
1	D	3492	0	3607	101	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	11	0
3	B	137	0	0	5	0
3	C	191	0	0	8	0
3	D	168	0	0	6	0
All	All	14719	0	14465	343	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 12.

All (343) 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	0.79
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:B:230:ASN:HD22	1:B:233:ASP:H	1.35	0.74
1:C:359:LYS:HA	1:C:362:MET:HE3	1.70	0.74

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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: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: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:85:GLN:CD	1:D:85:GLN:H	1.99	0.65
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
1:B:463:LYS:C	1:B:465:LYS:H	2.02	0.61

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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: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: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: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
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:A:369:GLU:H	1:A:369:GLU:CD	2.09	0.56
1:C:61:GLU:O	1:C:65:ILE:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:TYR:CZ	1:B:426:VAL:HG22	2.39	0.56
1:B:355:LEU:HD12	1:B:355:LEU:C	2.26	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: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: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: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:189:LEU:HD23	1:B:189:LEU:C	2.29	0.52
1:D:27:ASN:HD21	1:D:325:LYS:HZ3	1.54	0.52
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:369:GLU:CD	1:B:369:GLU:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:288:GLN:H	1:B:288:GLN:CD	2.16	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:386:PHE:N	1:D:108:LYS:HZ2	2.11	0.48
1:B:387:ARG:O	1:B:391:THR:HG23	2.13	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:A:245:LEU:CD2	1:A:337:VAL:HG21	2.43	0.48
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: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:408:ASN:N	1:D:408:ASN:ND2	2.62	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:322:THR:OG1	1:D:323:TYR:N	2.47	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:B:111:THR:HG22	1:B:211:LEU:HD11	1.98	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: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:B:385:PRO:HA	1:D:108:LYS:HZ3	1.81	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:C:393:SER:HB3	1:D:285:LEU:HD11	1.99	0.44
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:B:463:LYS:C	1:B:465:LYS:N	2.69	0.44
1:D:39:VAL:HG23	1:D:125:LEU:CD1	2.48	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:C:357:ILE:HB	1:C:362:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:189:LEU:HD23	1:A:189:LEU:C	2.38	0.43
1:A:296:GLU:OE2	1:B:162:HIS:HA	2.19	0.43
1:A:317:LYS:HD3	1:A:317:LYS:C	2.39	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:A:35:ARG:NH2	1:A:339:ASP:OD2	2.51	0.43
1:A:465:LYS:C	1:A:467:GLN:H	2.22	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:D:201:LEU:HD23	1:D:201:LEU:C	2.40	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
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:C:189:LEU:HD23	1:C:189:LEU:C	2.40	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:ARG:HD2	1:D:387:ARG:H	1.84	0.41
1:B:375:LEU:O	1:B:378:TYR:HB3	2.20	0.41
1:D:58:THR:HG1	1:D:60:THR:HG23	1.85	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:397:VAL:HG23	1:B:398:HIS:N	2.35	0.41
1:B:415:LEU:HB3	1:B:422:PHE:CD2	2.56	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:D:369:GLU:CD	1:D:369:GLU:H	2.24	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:D:27:ASN:HD21	1:D:325:LYS:HE2	1.86	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:316:LEU:HA	1:A:319:LEU:HD12	2.04	0.40
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:B:386:PHE:N	1:D:108:LYS:NZ	2.69	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:B:386:PHE:H	1:D:108:LYS:CD	2.34	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	447/468 (96%)	439 (98%)	7 (2%)	1 (0%)	47	38
1	B	446/468 (95%)	434 (97%)	10 (2%)	2 (0%)	34	22
1	C	446/468 (95%)	439 (98%)	5 (1%)	2 (0%)	34	22
1	D	448/468 (96%)	438 (98%)	9 (2%)	1 (0%)	47	38
All	All	1787/1872 (96%)	1750 (98%)	31 (2%)	6 (0%)	41	30

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	391/404 (97%)	377 (96%)	14 (4%)	35	23
1	B	390/404 (96%)	373 (96%)	17 (4%)	28	15
1	C	391/404 (97%)	377 (96%)	14 (4%)	35	23
1	D	391/404 (97%)	375 (96%)	16 (4%)	30	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1563/1616 (97%)	1502 (96%)	61 (4%)	32 19

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	26	LEU
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	247	PHE
1	A	250	LEU
1	A	266	SER
1	A	285	LEU
1	A	326	ASP
1	A	399	LEU
1	B	84	LYS
1	B	85	GLN
1	B	97	ARG
1	B	138	LEU
1	B	141	LEU
1	B	157	LEU
1	B	173	GLN
1	B	201	LEU
1	B	212	ASP
1	B	247	PHE
1	B	250	LEU
1	B	281	THR
1	B	288	GLN
1	B	387	ARG
1	B	412	LEU
1	B	442	LEU
1	B	457	LEU
1	C	19	THR
1	C	36	LEU
1	C	51	LEU
1	C	82	VAL
1	C	97	ARG
1	C	138	LEU

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Mol	Chain	Res	Type
1	C	141	LEU
1	C	173	GLN
1	C	201	LEU
1	C	247	PHE
1	C	250	LEU
1	C	262	LEU
1	C	418	ILE
1	C	457	LEU
1	D	27	ASN
1	D	60	THR
1	D	96	ARG
1	D	132	SER
1	D	138	LEU
1	D	141	LEU
1	D	173	GLN
1	D	247	PHE
1	D	250	LEU
1	D	262	LEU
1	D	285	LEU
1	D	293	ASP
1	D	387	ARG
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 (50) 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	167	GLN
1	A	173	GLN
1	A	209	ASN
1	A	230	ASN
1	A	388	GLN
1	A	390	HIS
1	A	421	GLN
1	A	438	GLN
1	A	464	GLN
1	B	42	GLN

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Mol	Chain	Res	Type
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	390	HIS
1	B	438	GLN
1	B	456	GLN
1	C	85	GLN
1	C	91	HIS
1	C	137	HIS
1	C	167	GLN
1	C	173	GLN
1	C	209	ASN
1	C	230	ASN
1	C	288	GLN
1	C	438	GLN
1	D	27	ASN
1	D	91	HIS
1	D	110	HIS
1	D	137	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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	D	1002	-	17,19,19	2.33	5 (29%)	22,24,24	4.47	13 (59%)
2	AS1	A	1004	-	17,19,19	2.40	5 (29%)	22,24,24	4.37	13 (59%)
2	AS1	C	1001	-	17,19,19	2.40	5 (29%)	22,24,24	4.44	13 (59%)
2	AS1	B	1003	-	17,19,19	2.48	5 (29%)	22,24,24	4.42	11 (50%)

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	D	1002	-	1/1/6/8	8/23/23/23	-
2	AS1	A	1004	-	1/1/6/8	6/23/23/23	-
2	AS1	C	1001	-	1/1/6/8	8/23/23/23	-
2	AS1	B	1003	-	1/1/6/8	8/23/23/23	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	AS1	C-N3	6.23	1.46	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1003	AS1	C-N3	6.08	1.46	1.29
2	A	1004	AS1	C-N3	6.06	1.46	1.29
2	D	1002	AS1	C-N3	6.00	1.46	1.29
2	B	1003	AS1	C-N1	5.24	1.47	1.34
2	A	1004	AS1	C-N1	4.89	1.46	1.34
2	D	1002	AS1	C-N1	4.74	1.45	1.34
2	C	1001	AS1	C-N1	4.69	1.45	1.34
2	A	1004	AS1	OG2-CG	3.07	1.31	1.22
2	B	1003	AS1	OG2-CG	2.99	1.31	1.22
2	B	1003	AS1	CA-N1	2.93	1.52	1.45
2	D	1002	AS1	OG2-CG	2.91	1.31	1.22
2	C	1001	AS1	OG2-CG	2.87	1.30	1.22
2	A	1004	AS1	OD1-CD	2.79	1.31	1.22
2	C	1001	AS1	CA-N1	2.74	1.51	1.45
2	A	1004	AS1	CA-N1	2.73	1.51	1.45
2	B	1003	AS1	OD1-CD	2.61	1.30	1.22
2	D	1002	AS1	CA-N1	2.61	1.51	1.45
2	C	1001	AS1	OD1-CD	2.55	1.30	1.22
2	D	1002	AS1	OD1-CD	2.46	1.30	1.22

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1002	AS1	CA-N1-C	13.69	148.91	122.06
2	C	1001	AS1	CA-N1-C	13.62	148.76	122.06
2	B	1003	AS1	CA-N1-C	13.14	147.82	122.06
2	A	1004	AS1	CA-N1-C	12.88	147.31	122.06
2	B	1003	AS1	CB-CA-N1	8.43	127.11	110.60
2	A	1004	AS1	CB-CA-N1	8.37	126.98	110.60
2	C	1001	AS1	CB-CA-N1	8.15	126.56	110.60
2	D	1002	AS1	CB-CA-N1	8.00	126.26	110.60
2	A	1004	AS1	N2-C-N1	5.95	130.66	116.82
2	B	1003	AS1	N2-C-N1	5.86	130.46	116.82
2	D	1002	AS1	N2-C-N1	5.54	129.70	116.82
2	B	1003	AS1	C3-C2-C1	5.52	128.61	112.05
2	C	1001	AS1	OD2-CD-CB	-5.44	96.62	114.07
2	A	1004	AS1	OD2-CD-CB	-5.42	96.68	114.07
2	C	1001	AS1	N2-C-N1	5.42	129.42	116.82
2	B	1003	AS1	C2-C1-N2	5.38	127.58	112.21
2	A	1004	AS1	C2-C1-N2	5.38	127.58	112.21
2	D	1002	AS1	OD2-CD-CB	-5.37	96.88	114.07
2	B	1003	AS1	OD2-CD-CB	-5.33	97.00	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1002	AS1	C3-C2-C1	5.31	127.98	112.05
2	D	1002	AS1	C2-C1-N2	5.28	127.32	112.21
2	C	1001	AS1	C2-C1-N2	5.19	127.04	112.21
2	C	1001	AS1	C3-C2-C1	4.68	126.10	112.05
2	A	1004	AS1	C3-C2-C1	4.67	126.05	112.05
2	C	1001	AS1	CG-CA-N1	4.63	121.53	110.55
2	D	1002	AS1	CG-CA-N1	4.62	121.49	110.55
2	B	1003	AS1	CG-CA-N1	4.26	120.63	110.55
2	A	1004	AS1	CG-CA-N1	4.23	120.56	110.55
2	C	1001	AS1	O52-C5-C4	3.32	124.68	113.38
2	D	1002	AS1	O52-C5-C4	3.24	124.43	113.38
2	A	1004	AS1	O52-C5-C4	3.22	124.35	113.38
2	B	1003	AS1	O52-C5-C4	3.00	123.61	113.38
2	C	1001	AS1	O51-C5-C4	-2.66	112.76	122.14
2	D	1002	AS1	OD1-CD-CB	-2.65	114.31	122.80
2	A	1004	AS1	OD1-CD-CB	-2.62	114.39	122.80
2	C	1001	AS1	C2-C3-C4	-2.62	104.93	113.35
2	C	1001	AS1	OD1-CD-CB	-2.61	114.45	122.80
2	A	1004	AS1	O51-C5-C4	-2.60	112.95	122.14
2	D	1002	AS1	O51-C5-C4	-2.58	113.04	122.14
2	A	1004	AS1	C2-C3-C4	-2.56	105.10	113.35
2	B	1003	AS1	OD1-CD-CB	-2.56	114.59	122.80
2	D	1002	AS1	C2-C3-C4	-2.47	105.41	113.35
2	C	1001	AS1	CA-CB-CD	-2.41	105.86	112.88
2	B	1003	AS1	O51-C5-C4	-2.38	113.72	122.14
2	B	1003	AS1	OD2-CD-OD1	-2.38	117.38	123.30
2	D	1002	AS1	CA-CB-CD	-2.34	106.05	112.88
2	A	1004	AS1	CA-CB-CD	-2.26	106.28	112.88
2	D	1002	AS1	OD2-CD-OD1	-2.20	117.81	123.30
2	A	1004	AS1	OD2-CD-OD1	-2.12	118.01	123.30
2	C	1001	AS1	OD2-CD-OD1	-2.12	118.01	123.30

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 (30) 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	D	1002	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	N1-CA-CG-OG1
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	D	1002	AS1	N1-CA-CG-OG2
2	C	1001	AS1	N1-CA-CG-OG2
2	A	1004	AS1	C2-C3-C4-N4
2	A	1004	AS1	N1-CA-CG-OG2
2	A	1004	AS1	N1-CA-CG-OG1
2	C	1001	AS1	C2-C3-C4-N4
2	D	1002	AS1	CG-CA-N1-C
2	D	1002	AS1	C1-C2-C3-C4
2	C	1001	AS1	CA-CB-CD-OD2
2	B	1003	AS1	C1-C2-C3-C4
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	C	1001	AS1	CA-CB-CD-OD1

There are no ring outliers.

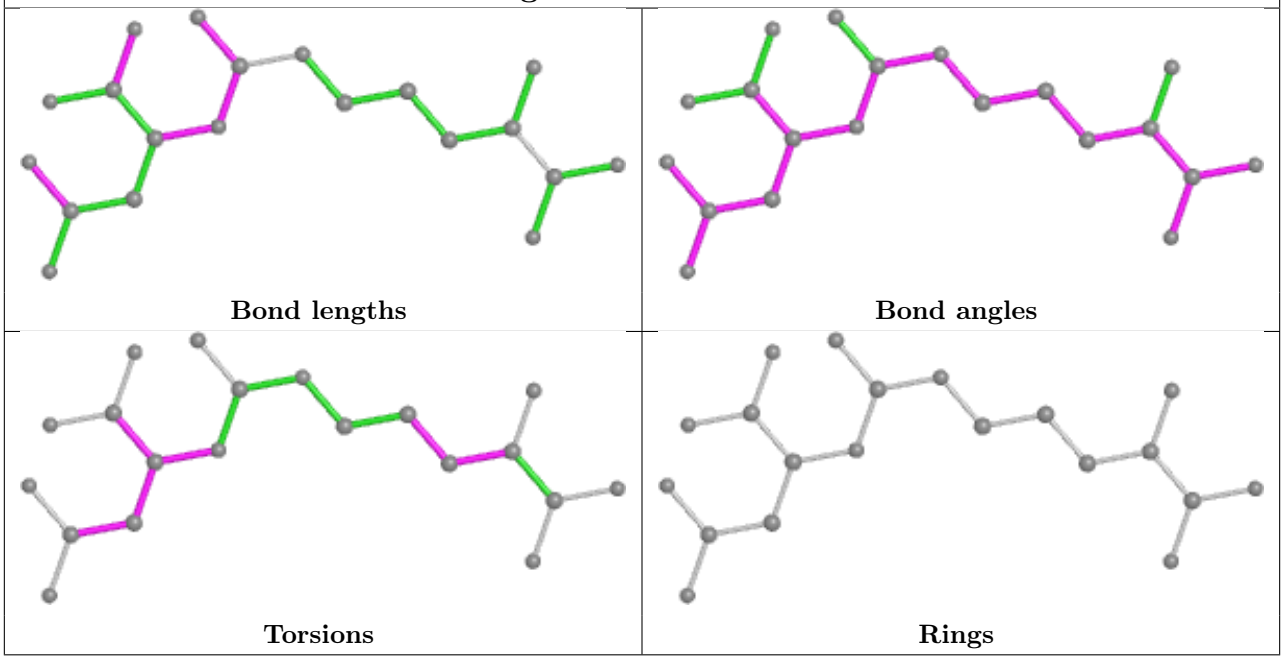
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1002	AS1	1	0
2	B	1003	AS1	1	0

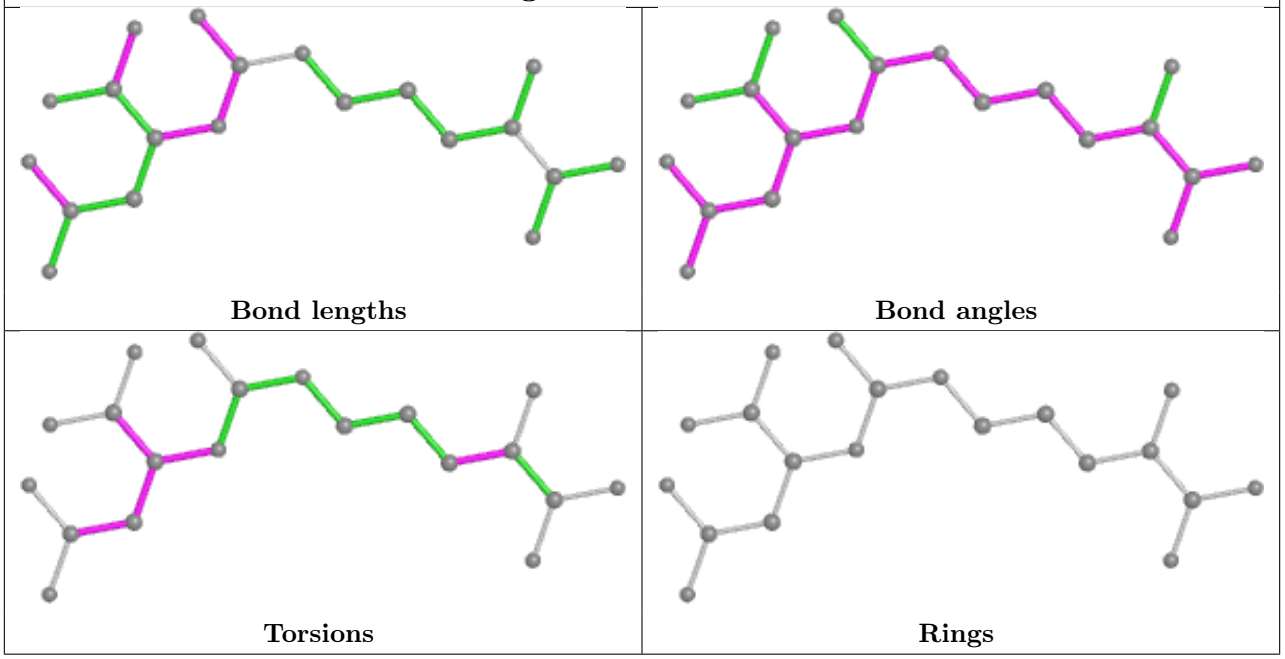
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

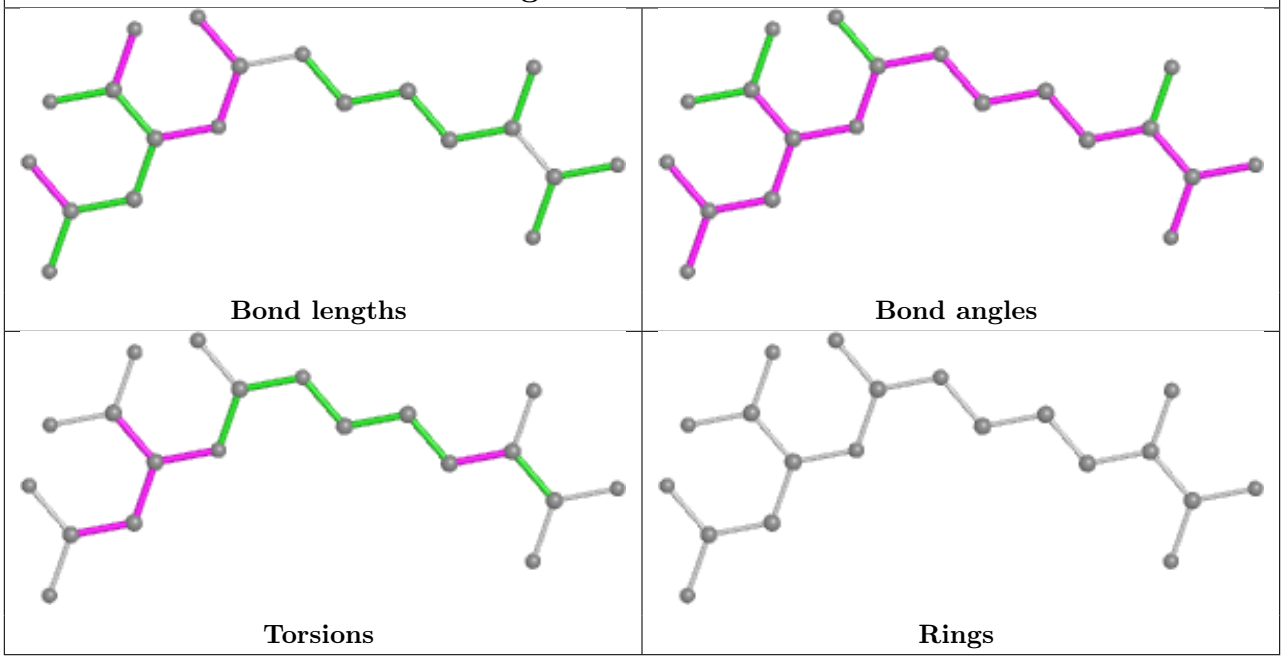
Ligand AS1 D 1002



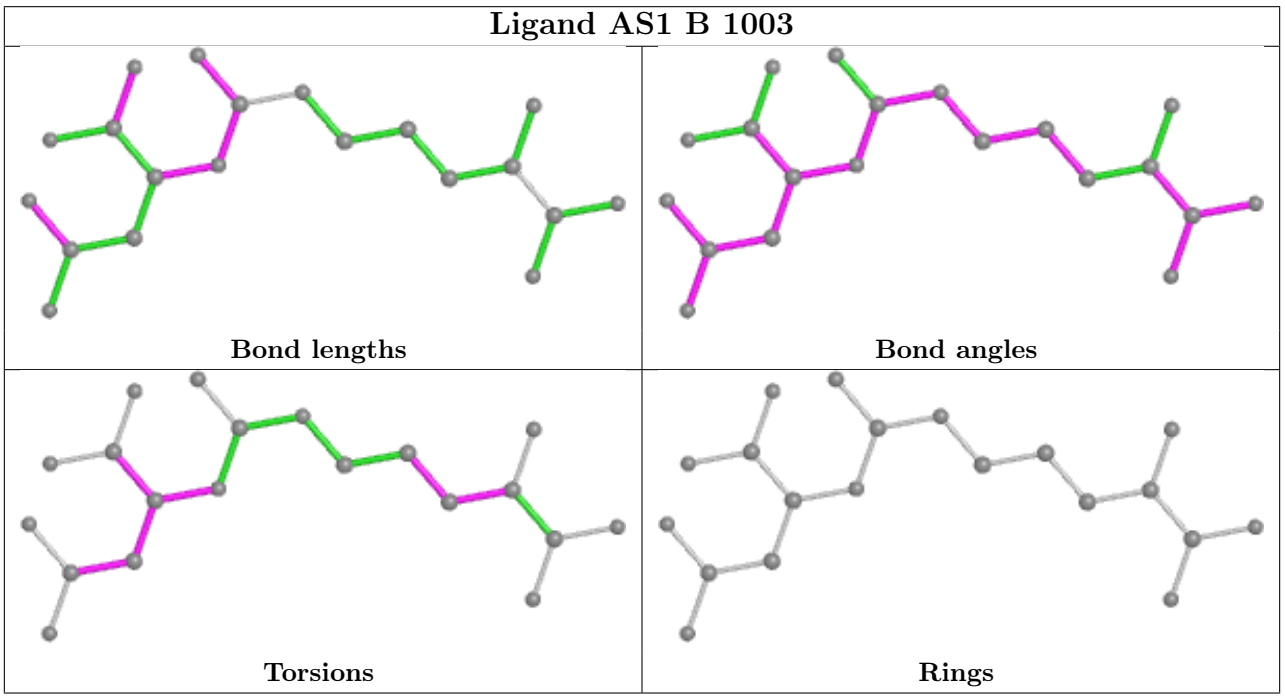
Ligand AS1 A 1004



Ligand AS1 C 1001



Ligand AS1 B 1003



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	449/468 (95%)	-0.01	17 (3%) 40 50	15, 25, 53, 71	0
1	B	448/468 (95%)	0.19	24 (5%) 25 34	16, 31, 53, 66	0
1	C	448/468 (95%)	-0.08	9 (2%) 65 73	13, 25, 45, 62	0
1	D	450/468 (96%)	0.05	11 (2%) 59 68	15, 28, 50, 62	0
All	All	1795/1872 (95%)	0.04	61 (3%) 45 55	13, 27, 51, 71	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	80	VAL	4.9
1	B	18	SER	4.6
1	A	19	THR	4.5
1	A	467	GLN	4.1
1	B	402	THR	3.9
1	C	284	SER	3.6
1	A	283	ALA	3.5
1	A	284	SER	3.5
1	D	79	GLY	3.5
1	C	85	GLN	3.4
1	B	463	LYS	3.4
1	B	284	SER	3.4
1	B	398	HIS	3.3
1	C	466	GLU	3.3
1	B	85	GLN	3.2
1	D	85	GLN	3.2
1	B	390	HIS	3.2
1	B	391	THR	3.1
1	A	466	GLU	3.1
1	A	387	ARG	3.1
1	A	384	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	59	LYS	3.0
1	B	283	ALA	3.0
1	B	287	PRO	2.9
1	B	442	LEU	2.8
1	D	284	SER	2.8
1	B	397	VAL	2.8
1	B	382	LYS	2.7
1	B	412	LEU	2.7
1	A	463	LYS	2.7
1	C	84	LYS	2.7
1	A	388	GLN	2.6
1	D	77	SER	2.5
1	A	412	LEU	2.5
1	C	78	LYS	2.4
1	B	426	VAL	2.4
1	B	363	GLU	2.4
1	B	428	GLN	2.4
1	A	413	GLU	2.3
1	B	19	THR	2.3
1	B	360	GLU	2.3
1	B	406	THR	2.3
1	C	80	VAL	2.3
1	C	19	THR	2.2
1	D	288	GLN	2.2
1	A	428	GLN	2.2
1	B	424	SER	2.2
1	D	387	ARG	2.2
1	C	24	GLU	2.2
1	A	465	LYS	2.2
1	A	85	GLN	2.2
1	D	56	ILE	2.1
1	A	414	ASP	2.1
1	A	404	GLY	2.1
1	B	410	LEU	2.1
1	D	109	LEU	2.1
1	D	19	THR	2.0
1	B	387	ARG	2.0
1	A	169	ILE	2.0
1	B	396	ALA	2.0
1	C	283	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

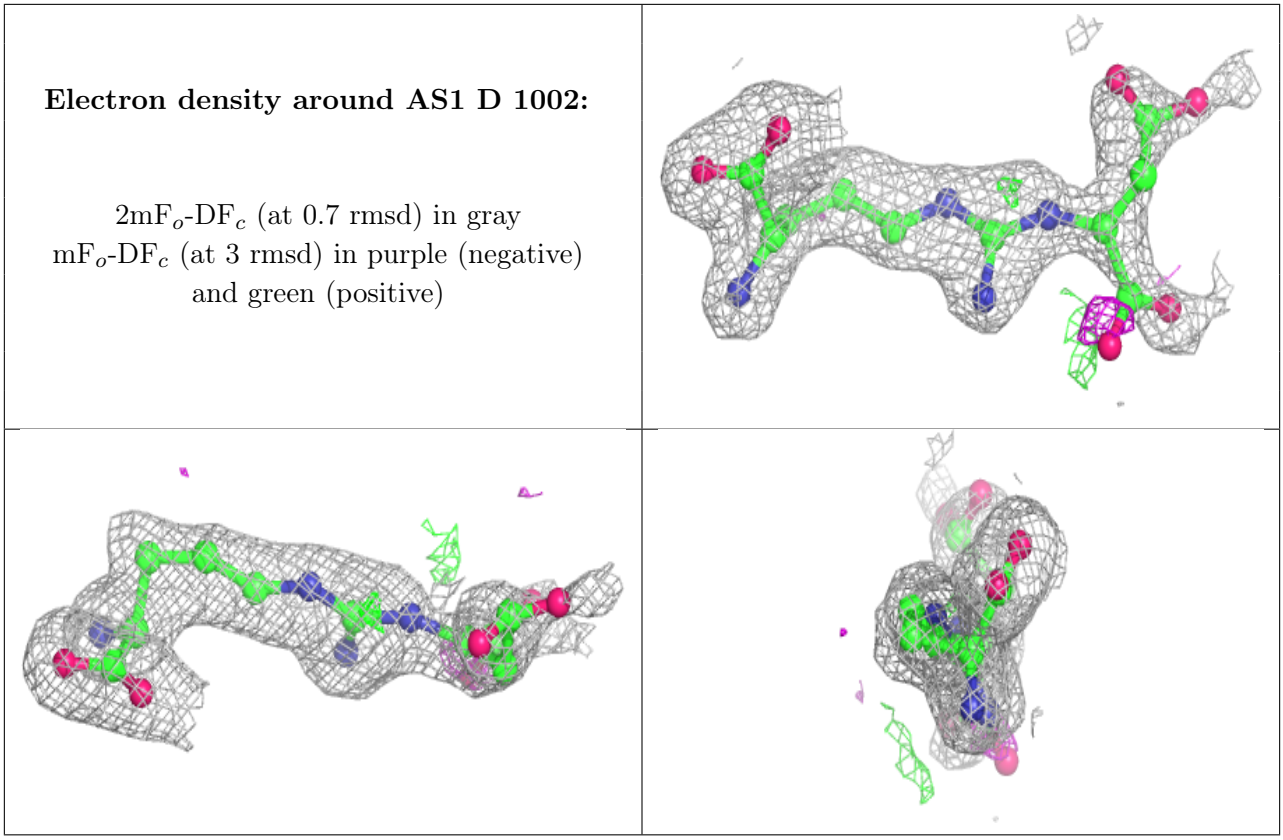
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AS1	D	1002	20/20	0.81	0.20	22,48,67,67	0
2	AS1	A	1004	20/20	0.86	0.18	17,40,60,60	0
2	AS1	C	1001	20/20	0.87	0.18	17,40,57,57	0
2	AS1	B	1003	20/20	0.87	0.17	18,39,61,62	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.

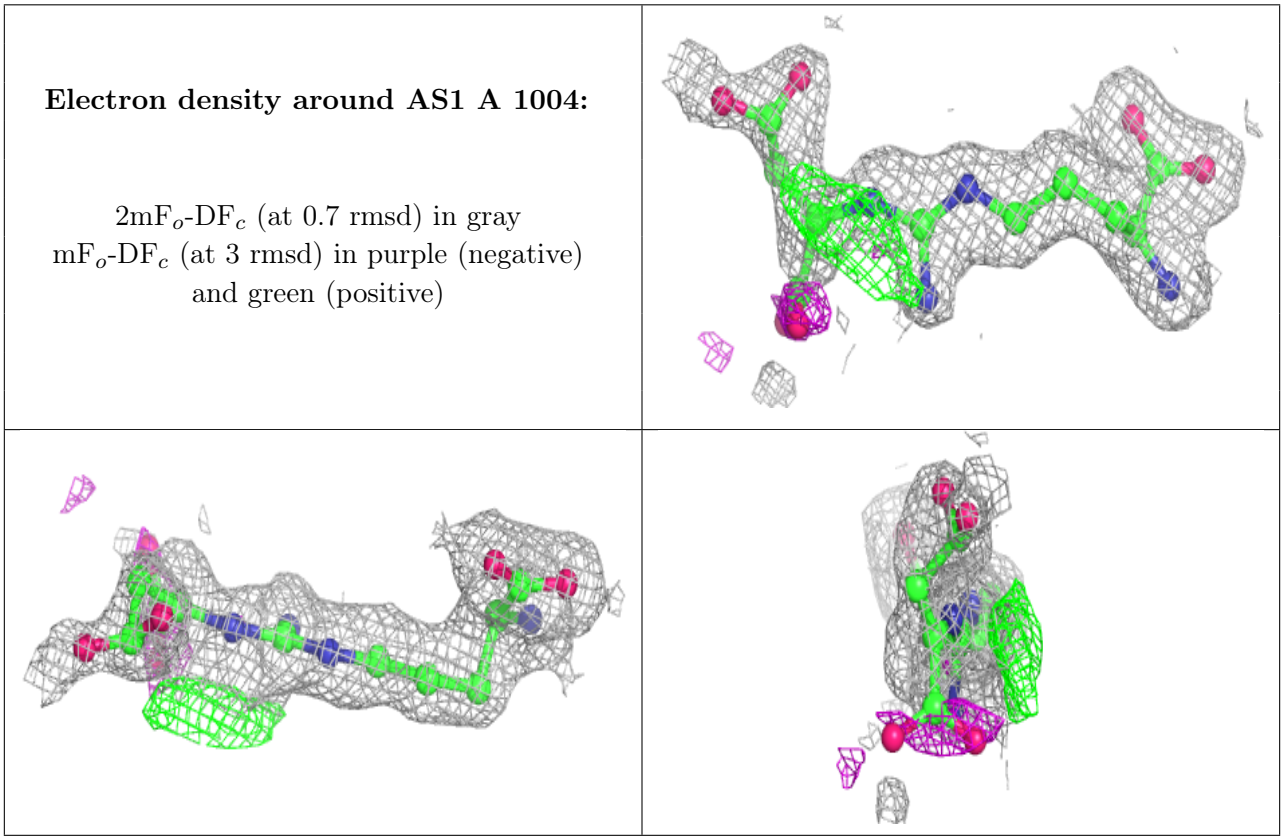
Electron density around AS1 D 1002:

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



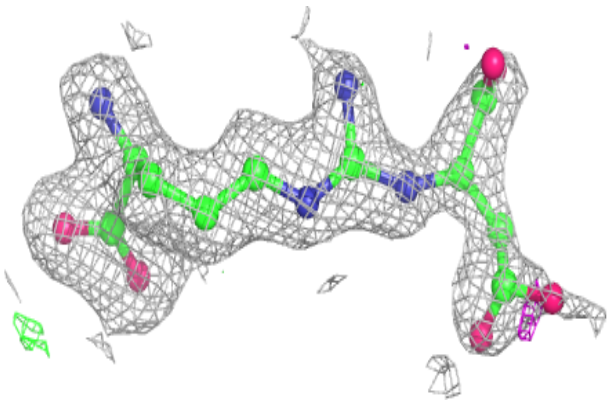
Electron density around AS1 A 1004:

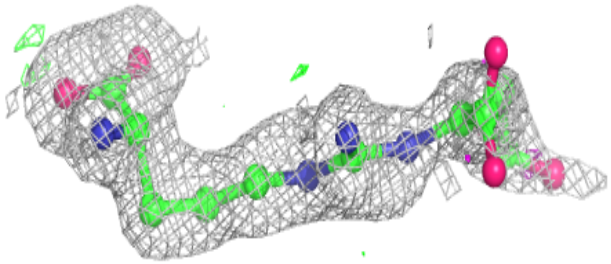
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

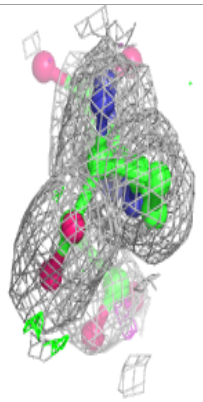


Electron density around AS1 C 1001:

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

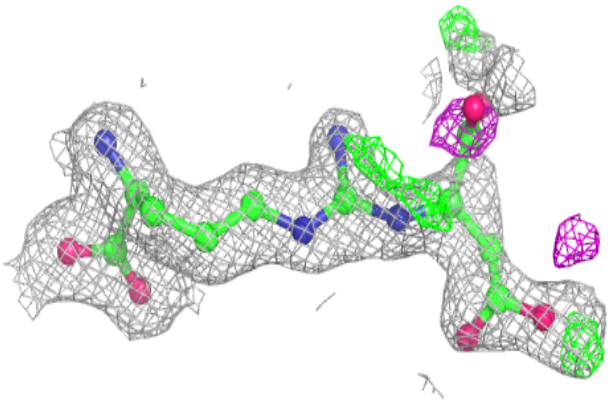


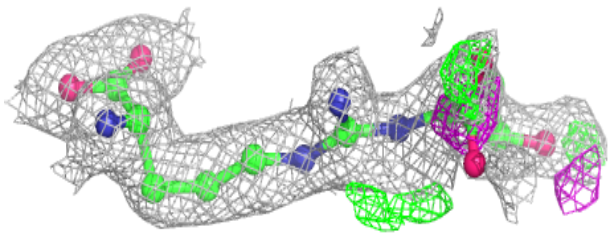


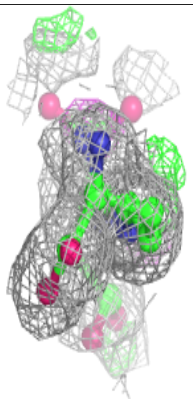


Electron density around AS1 B 1003:

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







6.5 Other polymers (i)

There are no such residues in this entry.