



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:03 PM UTC

PDB ID : 6V5F / pdb_00006v5f
Title : L-asparaginase from Escherichia coli
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Deposited on : 2019-12-04
Resolution : 2.10 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

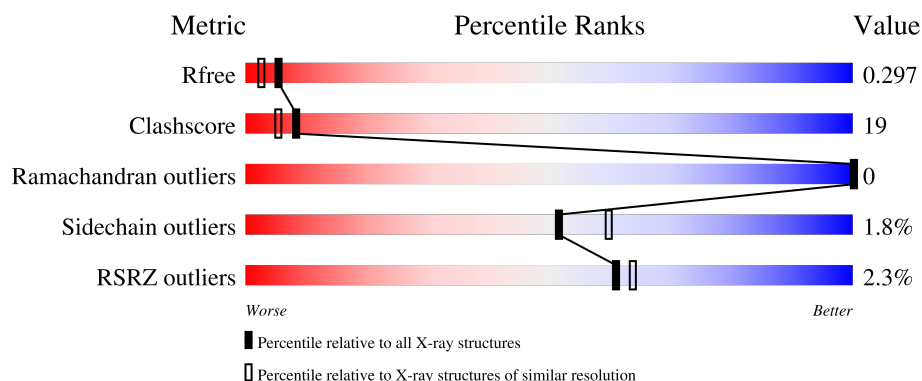
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	326	
1	B	326	
1	C	326	
1	D	326	

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	ASP	A	401	-	-	X	-
2	ASP	D	401	-	-	X	-
3	SIN	B	401	-	X	-	-

2 Entry composition [i](#)

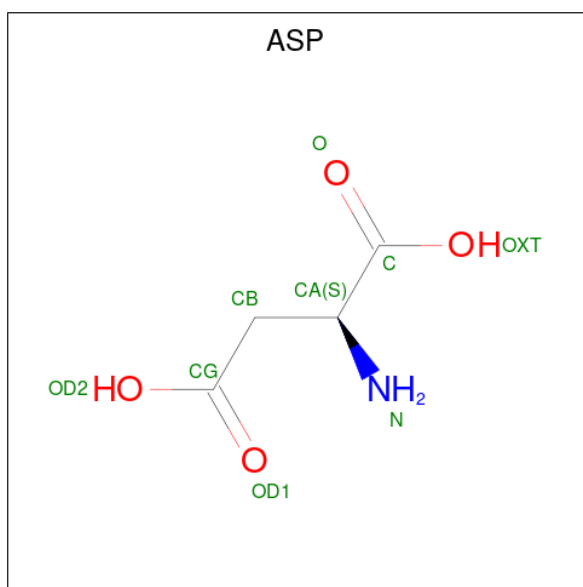
There are 4 unique types of molecules in this entry. The entry contains 9423 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-asparaginase 2.

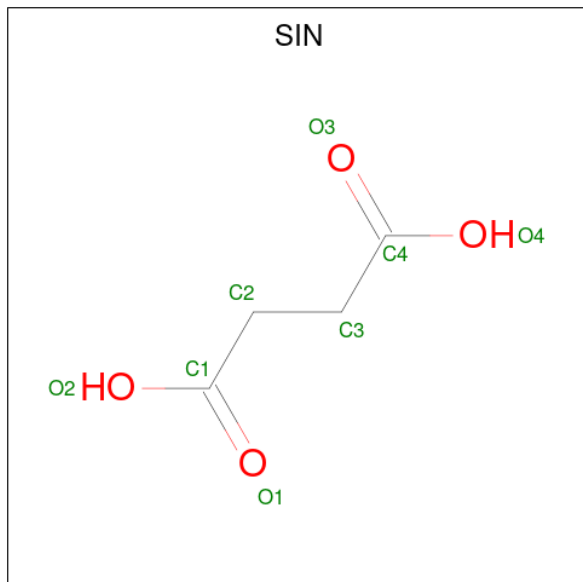
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	44	0	0
			2404	1502	411	483	8			
1	B	300	Total	C	N	O	S	15	0	0
			2255	1412	385	450	8			
1	C	295	Total	C	N	O	S	17	0	0
			2210	1382	376	444	8			
1	D	309	Total	C	N	O	S	12	0	0
			2310	1447	396	459	8			

- Molecule 2 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	1	4		
2	D	1	Total	C	N	O	0	0
			9	4	1	4		

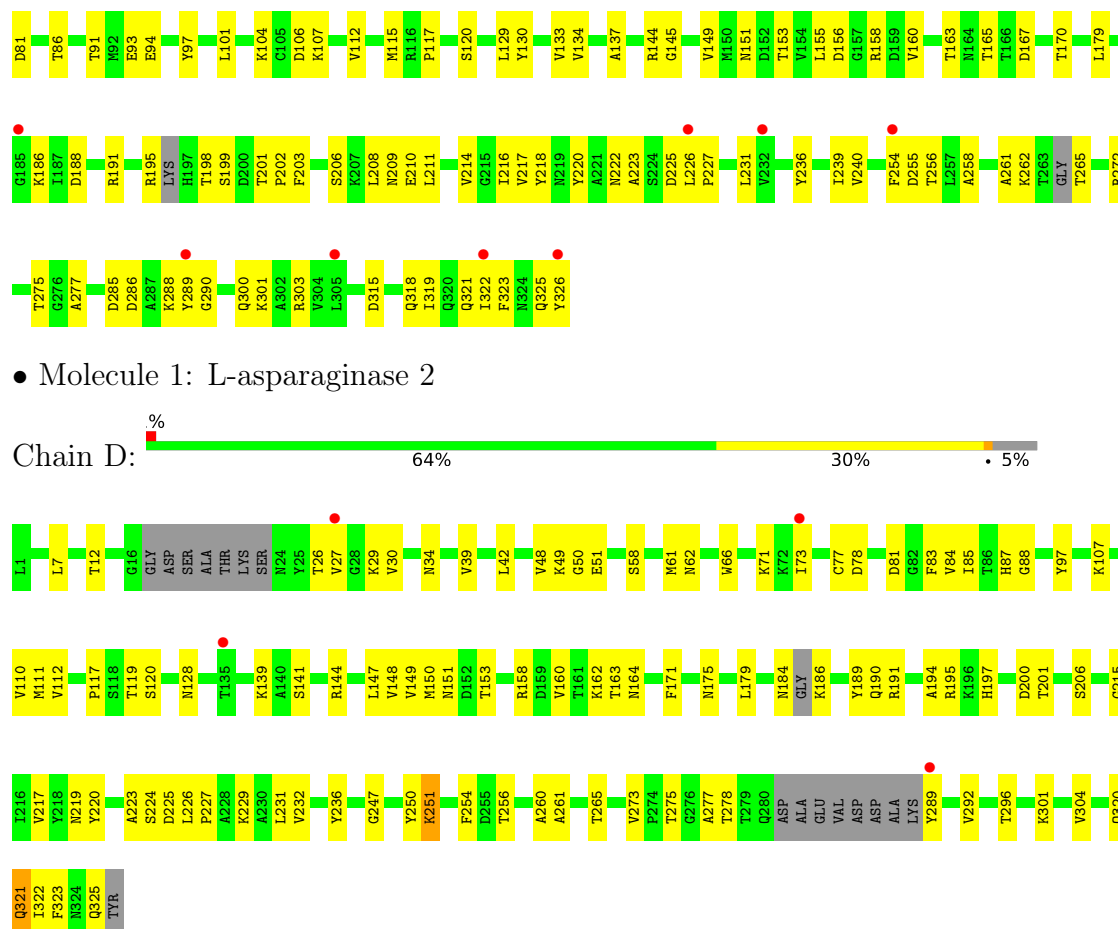
- Molecule 3 is SUCCINIC ACID (CCD ID: SIN) (formula: $C_4H_6O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			8	4	4		
3	C	1	Total	C	O	0	0
			8	4	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	62	Total	O	0	0
			62	62		
4	C	48	Total	O	0	0
			48	48		
4	D	60	Total	O	0	0
			60	60		



• Molecule 1: L-asparaginase 2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.92Å 125.44Å 68.82Å 90.00° 106.94° 90.00°	Depositor
Resolution (Å)	33.37 – 2.10 33.37 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.7 (33.37-2.10) 93.7 (33.37-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.230 , 0.298 0.231 , 0.297	Depositor DCC
R_{free} test set	2000 reflections (3.67%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9423	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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: SIN

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	0.55	0/2438	0.81	1/3317 (0.0%)
1	B	0.60	3/2289 (0.1%)	0.77	1/3117 (0.0%)
1	C	0.53	1/2242 (0.0%)	0.79	0/3052
1	D	0.55	0/2343	0.79	1/3189 (0.0%)
All	All	0.56	4/9312 (0.0%)	0.79	3/12675 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	256	THR	C-O	-5.46	1.17	1.24
1	C	255	ASP	C-O	-5.34	1.18	1.24
1	B	139	LYS	C-O	-5.07	1.17	1.24
1	B	282	ALA	CA-C	-5.01	1.50	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	50	GLY	N-CA-C	6.13	120.29	110.90
1	B	321	GLN	N-CA-C	-5.38	105.10	110.97
1	A	321	GLN	CB-CG-CD	-5.01	104.09	112.60

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	2404	0	2396	138	3
1	B	2255	0	2253	76	1
1	C	2210	0	2197	95	3
1	D	2310	0	2317	78	1
2	A	9	0	3	4	0
2	D	9	0	3	7	0
3	B	8	0	4	1	0
3	C	8	0	4	0	0
4	A	40	0	0	6	0
4	B	62	0	0	11	0
4	C	48	0	0	13	0
4	D	60	0	0	6	0
All	All	9423	0	9177	349	4

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 19.

All (349) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:VAL:O	1:A:42:LEU:CD1	1.92	1.15
1:C:262:LYS:NZ	1:C:289:TYR:HA	1.64	1.11
1:A:112:VAL:HG21	1:A:132:ALA:HB2	1.37	1.02
1:B:275:THR:HG22	1:D:164:ASN:HD22	1.26	0.98
1:C:262:LYS:HZ1	1:C:289:TYR:HA	1.34	0.90
1:C:117:PRO:HG2	1:C:120:SER:HB2	1.53	0.90
1:B:77:CYS:O	1:B:107:LYS:NZ	2.06	0.87
1:A:13:ILE:CD1	1:A:86:THR:HB	2.07	0.85
1:A:39:VAL:HB	1:A:42:LEU:HD11	1.56	0.85
1:A:106:ASP:OD2	1:A:142:ALA:HB1	1.76	0.85
1:A:11:GLY:C	1:A:27:VAL:HG22	2.02	0.84
1:A:39:VAL:O	1:A:42:LEU:HD13	1.78	0.83
1:C:286:ASP:OD2	4:C:501:HOH:O	1.96	0.82
1:D:144:ARG:NH1	1:D:191:ARG:O	2.12	0.82
1:A:11:GLY:C	1:A:27:VAL:CG2	2.52	0.82
1:A:300:GLN:HG2	1:C:272:ARG:NH1	1.95	0.81
1:A:13:ILE:HG13	1:A:14:ALA:N	1.94	0.80
1:A:141:SER:HA	1:A:144:ARG:HD2	1.63	0.80
1:D:12:THR:H	2:D:401:ASP:HB3	1.46	0.80
1:A:63:ASP:H	1:C:222:ASN:HD22	1.29	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:LYS:HZ2	1:C:289:TYR:HA	1.45	0.79
1:D:321:GLN:HE21	1:D:321:GLN:HA	1.47	0.78
1:A:82:GLY:HA2	1:A:107:LYS:HB3	1.65	0.77
1:C:321:GLN:HG3	1:C:325:GLN:HE22	1.50	0.77
1:A:112:VAL:HG22	1:A:149:VAL:O	1.86	0.76
1:C:61:MET:HE2	1:C:66:TRP:CD1	2.20	0.75
1:A:39:VAL:O	1:A:42:LEU:HD11	1.85	0.74
1:B:171:PHE:C	1:B:172:LYS:HG2	2.13	0.73
1:C:261:ALA:HA	1:C:265:THR:O	1.90	0.72
1:A:269:ARG:CZ	1:A:284:VAL:HG21	2.20	0.71
1:B:5:THR:OG1	1:B:80:THR:HG21	1.90	0.71
1:D:58:SER:H	2:D:401:ASP:N	1.89	0.71
1:A:64:ASN:ND2	4:A:505:HOH:O	2.17	0.71
1:A:11:GLY:O	1:A:27:VAL:HG22	1.90	0.71
1:C:120:SER:OG	4:C:502:HOH:O	2.09	0.70
1:A:187:ILE:O	4:A:503:HOH:O	2.09	0.70
1:A:188:ASP:O	4:A:502:HOH:O	2.09	0.70
1:A:108:PRO:HB2	1:A:136:ALA:HA	1.72	0.70
1:A:39:VAL:O	1:A:42:LEU:HD12	1.90	0.69
1:A:112:VAL:CG2	1:A:132:ALA:HB2	2.20	0.69
1:C:101:LEU:O	1:C:201:THR:HG21	1.93	0.69
1:A:82:GLY:HA2	1:A:107:LYS:CB	2.23	0.68
1:B:281:ASP:OD2	4:B:501:HOH:O	2.11	0.68
1:B:36:VAL:HG23	1:B:38:ALA:H	1.57	0.68
1:D:61:MET:HE3	1:D:87:HIS:NE2	2.08	0.68
1:A:315:ASP:HB3	1:A:318:GLN:HB2	1.76	0.68
1:B:79:LYS:N	4:B:509:HOH:O	2.26	0.68
1:A:144:ARG:HG2	1:A:144:ARG:HH11	1.57	0.67
1:D:48:VAL:C	1:D:49:LYS:HD3	2.19	0.67
1:B:272:ARG:NH2	4:B:505:HOH:O	2.21	0.67
1:A:12:THR:HA	1:A:27:VAL:HG23	1.77	0.66
1:A:39:VAL:CB	1:A:42:LEU:HD11	2.25	0.66
1:B:252:SER:O	4:B:502:HOH:O	2.12	0.66
1:D:7:LEU:HD11	1:D:83:PHE:HD2	1.59	0.66
1:A:13:ILE:HD13	1:A:86:THR:HB	1.78	0.66
1:B:58:SER:HB3	1:B:88:GLY:HA3	1.78	0.66
1:C:117:PRO:HG2	1:C:120:SER:CB	2.25	0.65
1:A:80:THR:O	1:A:107:LYS:HD2	1.96	0.65
1:B:256:THR:OG1	4:B:502:HOH:O	2.14	0.65
1:C:240:VAL:O	4:C:503:HOH:O	2.15	0.65
1:B:227:PRO:HB3	1:D:227:PRO:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ASP:OD1	1:C:106:ASP:N	2.30	0.64
1:B:204:ASP:OD1	4:B:503:HOH:O	2.14	0.64
1:A:198:THR:OG1	1:A:199:SER:N	2.30	0.64
1:A:27:VAL:CG1	1:A:57:GLY:CA	2.75	0.64
1:C:286:ASP:O	1:C:290:GLY:N	2.31	0.64
1:A:27:VAL:HG11	1:A:57:GLY:HA2	1.80	0.63
1:A:135:THR:OG1	1:A:149:VAL:HG21	1.99	0.63
1:C:13:ILE:HG21	1:C:86:THR:HB	1.81	0.63
1:A:234:ALA:CB	1:C:226:LEU:HD11	2.29	0.62
1:B:61:MET:HE3	1:B:87:HIS:NE2	2.13	0.62
1:A:27:VAL:HG11	1:A:57:GLY:CA	2.30	0.62
1:A:58:SER:OG	2:A:401:ASP:O	2.16	0.62
1:A:300:GLN:HG2	1:C:272:ARG:CZ	2.30	0.61
1:B:171:PHE:O	1:B:172:LYS:HG2	2.00	0.61
1:A:269:ARG:NE	1:A:284:VAL:HG21	2.16	0.61
1:C:94:GLU:HG2	1:C:300:GLN:HB3	1.83	0.61
1:B:38:ALA:O	1:B:40:PRO:HD3	2.01	0.60
1:C:3:ASN:O	1:C:81:ASP:HB2	2.01	0.60
1:A:105:CYS:SG	1:A:107:LYS:HG3	2.40	0.60
1:A:224:SER:HB2	1:C:236:TYR:OH	2.01	0.60
1:C:144:ARG:O	4:C:504:HOH:O	2.16	0.60
1:C:285:ASP:OD2	1:C:288:LYS:HB2	2.02	0.60
1:D:144:ARG:HH22	1:D:189:TYR:HB3	1.66	0.60
1:A:21:THR:HG23	1:A:22:LYS:H	1.67	0.60
1:B:56:ILE:HD11	1:B:61:MET:HE1	1.82	0.60
1:A:12:THR:N	1:A:27:VAL:CG2	2.65	0.59
1:D:195:ARG:HD2	1:D:325:GLN:HB3	1.82	0.59
1:D:111:MET:HB2	1:D:148:VAL:HG22	1.83	0.59
1:B:275:THR:HG22	1:D:164:ASN:ND2	2.08	0.59
1:D:48:VAL:O	1:D:49:LYS:HD3	2.02	0.59
1:A:83:PHE:N	1:A:83:PHE:HD1	1.99	0.59
1:B:292:VAL:HG13	1:B:320:GLN:HA	1.83	0.59
1:B:88:GLY:HA3	3:B:401:SIN:O3	2.02	0.58
1:D:195:ARG:NH2	1:D:323:PHE:O	2.27	0.58
1:A:227:PRO:HB3	1:C:227:PRO:HB3	1.85	0.58
1:D:81:ASP:O	4:D:502:HOH:O	2.17	0.58
1:A:101:LEU:HA	1:A:201:THR:HG21	1.84	0.58
1:A:300:GLN:NE2	1:C:218:TYR:OH	2.36	0.58
1:A:115:MET:HG3	1:A:167:ASP:O	2.03	0.58
1:C:209:ASN:O	4:C:505:HOH:O	2.17	0.58
1:A:27:VAL:CG1	1:A:57:GLY:HA2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:PHE:N	1:A:83:PHE:CD1	2.72	0.58
1:A:80:THR:O	1:A:107:LYS:CD	2.51	0.57
1:B:73:ILE:HD11	1:B:85:ILE:HD11	1.85	0.57
1:A:160:VAL:O	1:A:301:LYS:NZ	2.22	0.57
1:A:21:THR:OG1	4:A:504:HOH:O	2.17	0.57
1:D:88:GLY:HA3	2:D:401:ASP:N	2.20	0.57
1:C:115:MET:HG3	1:C:167:ASP:O	2.05	0.57
1:A:81:ASP:C	1:A:107:LYS:HD3	2.30	0.56
1:C:220:TYR:CE2	1:C:223:ALA:HA	2.41	0.56
1:C:201:THR:HG23	1:C:203:PHE:H	1.71	0.56
1:A:144:ARG:HG2	1:A:144:ARG:NH1	2.18	0.56
1:B:218:TYR:OH	1:B:272:ARG:HD3	2.05	0.56
1:B:197:HIS:ND1	1:B:198:THR:OG1	2.32	0.56
1:C:156:ASP:HB3	1:C:179:LEU:HD11	1.88	0.56
1:A:13:ILE:HG13	1:A:14:ALA:H	1.70	0.55
1:A:82:GLY:CA	1:A:107:LYS:HB3	2.36	0.55
1:D:88:GLY:HA2	2:D:401:ASP:HB2	1.89	0.55
1:D:150:MET:HG3	1:D:171:PHE:CD2	2.41	0.55
1:C:202:PRO:HD3	1:C:326:TYR:OH	2.06	0.55
1:A:36:VAL:CG2	1:A:48:VAL:HG11	2.36	0.55
1:A:117:PRO:HD2	1:A:120:SER:HB2	1.88	0.55
1:C:86:THR:HA	1:C:112:VAL:O	2.07	0.54
1:B:162:LYS:O	1:D:273:VAL:HG13	2.07	0.54
1:A:191:ARG:HD2	1:D:191:ARG:HD2	1.90	0.54
1:B:89:THR:HA	1:B:92:MET:HE3	1.89	0.54
1:B:222:ASN:OD1	1:D:62:ASN:HB2	2.08	0.54
1:B:254:PHE:C	1:B:254:PHE:HD1	2.15	0.54
1:D:27:VAL:HG11	2:D:401:ASP:O	2.07	0.54
1:A:244:VAL:HG12	1:A:272:ARG:CZ	2.38	0.53
1:A:149:VAL:HG22	1:A:154:VAL:HG22	1.89	0.53
1:B:254:PHE:C	1:B:254:PHE:CD1	2.87	0.53
1:B:224:SER:HB2	1:D:236:TYR:OH	2.09	0.53
1:A:62:ASN:HA	1:C:222:ASN:HB2	1.91	0.53
1:B:182:ILE:HG12	1:B:187:ILE:HG12	1.90	0.53
1:A:61:MET:HE3	1:A:87:HIS:NE2	2.23	0.53
1:B:105:CYS:SG	1:B:107:LYS:HG3	2.48	0.53
1:B:254:PHE:HD1	1:B:254:PHE:O	1.92	0.53
1:C:151:ASN:OD1	4:C:506:HOH:O	2.18	0.53
1:C:225:ASP:OD2	1:C:256:THR:CB	2.57	0.53
1:A:220:TYR:CE2	1:A:223:ALA:HA	2.44	0.52
1:C:210:GLU:HA	4:C:505:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:GLY:HA3	4:B:504:HOH:O	2.09	0.52
1:B:218:TYR:CZ	1:B:272:ARG:HD3	2.44	0.52
1:A:272:ARG:NH1	1:C:300:GLN:HG2	2.25	0.52
1:C:254:PHE:CD1	1:C:254:PHE:C	2.86	0.52
1:A:63:ASP:H	1:C:222:ASN:ND2	2.04	0.51
1:A:202:PRO:HD3	1:A:326:TYR:OH	2.09	0.51
1:D:66:TRP:CH2	1:D:304:VAL:HG12	2.46	0.51
1:B:66:TRP:HB3	1:B:98:PHE:CE2	2.46	0.51
1:D:117:PRO:HB2	1:D:119:THR:HG22	1.91	0.51
1:B:41:GLN:OE1	1:B:41:GLN:N	2.36	0.51
1:C:93:GLU:HB2	1:C:301:LYS:NZ	2.25	0.51
1:A:167:ASP:O	1:A:170:THR:HB	2.10	0.51
1:D:225:ASP:O	1:D:229:LYS:HG3	2.11	0.51
1:A:58:SER:HB3	1:A:88:GLY:HA3	1.93	0.51
1:D:144:ARG:HB2	1:D:147:LEU:HD21	1.93	0.51
1:A:222:ASN:HA	1:A:250:TYR:CZ	2.45	0.50
1:C:225:ASP:OD2	1:C:256:THR:HB	2.10	0.50
1:D:179:LEU:HA	1:D:191:ARG:HB2	1.93	0.50
1:C:12:THR:HG22	1:C:117:PRO:HA	1.94	0.50
1:A:165:THR:OG1	1:C:277:ALA:O	2.26	0.50
1:B:258:ALA:O	1:B:262:LYS:HG3	2.12	0.50
1:D:97:TYR:CE1	1:D:158:ARG:HG3	2.47	0.50
1:D:322:ILE:O	1:D:325:GLN:HB2	2.11	0.50
1:A:12:THR:CA	1:A:27:VAL:HG23	2.40	0.50
1:A:80:THR:O	1:A:107:LYS:NZ	2.40	0.50
1:A:227:PRO:HG3	1:C:231:LEU:HD21	1.93	0.50
1:D:184:ASN:O	1:D:186:LYS:HD3	2.11	0.50
1:D:220:TYR:CE2	1:D:223:ALA:HA	2.47	0.50
1:A:10:GLY:HA2	1:A:55:ASN:OD1	2.12	0.50
1:A:59:GLN:OE1	2:A:401:ASP:N	2.45	0.49
1:B:249:LEU:HD23	1:B:253:VAL:HG12	1.93	0.49
1:C:285:ASP:O	1:C:289:TYR:HD2	1.96	0.49
1:D:232:VAL:HG22	1:D:260:ALA:HB2	1.94	0.49
1:A:228:ALA:O	1:A:232:VAL:HG23	2.13	0.49
1:A:158:ARG:NH1	1:D:190:GLN:HE22	2.10	0.49
1:A:269:ARG:CZ	1:A:284:VAL:CG2	2.90	0.49
1:C:321:GLN:HG3	1:C:325:GLN:NE2	2.23	0.48
1:C:254:PHE:C	1:C:254:PHE:HD1	2.21	0.48
1:A:13:ILE:HD11	4:A:513:HOH:O	2.12	0.48
1:B:275:THR:HB	1:D:163:THR:O	2.12	0.48
1:C:300:GLN:CD	1:C:300:GLN:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ILE:O	1:A:35:LEU:HD21	2.13	0.48
1:A:108:PRO:HG2	1:A:136:ALA:O	2.14	0.48
1:A:130:TYR:CD1	1:B:121:MET:HE1	2.48	0.48
1:C:4:ILE:HD11	1:C:137:ALA:HA	1.95	0.48
1:A:214:VAL:HG12	1:A:303:ARG:HG3	1.96	0.48
1:B:275:THR:HG23	4:B:528:HOH:O	2.13	0.48
1:C:315:ASP:OD2	1:C:318:GLN:HG3	2.13	0.48
1:C:5:THR:HG22	1:C:7:LEU:HD12	1.96	0.48
1:D:117:PRO:HG2	1:D:120:SER:HB2	1.95	0.48
1:A:292:VAL:HG13	1:A:320:GLN:HA	1.96	0.48
1:D:261:ALA:HA	1:D:265:THR:O	2.13	0.48
1:A:151:ASN:HD21	1:B:168:VAL:HG22	1.78	0.48
1:B:214:VAL:HA	1:B:238:GLY:O	2.14	0.48
1:C:225:ASP:OD2	1:C:256:THR:OG1	2.31	0.48
1:C:315:ASP:HB3	1:C:318:GLN:HG3	1.96	0.48
1:A:39:VAL:CG1	1:A:42:LEU:HD11	2.44	0.47
1:A:214:VAL:HA	1:A:238:GLY:O	2.14	0.47
1:B:255:ASP:O	1:B:259:THR:HG23	2.14	0.47
1:B:289:TYR:O	4:B:504:HOH:O	2.20	0.47
1:C:97:TYR:CE1	1:C:158:ARG:HG3	2.49	0.47
1:B:254:PHE:HZ	1:B:289:TYR:CE2	2.32	0.47
1:C:58:SER:HB2	1:C:91:THR:OG1	2.14	0.47
1:D:254:PHE:HE2	1:D:289:TYR:HE1	1.62	0.47
1:C:61:MET:HE1	1:C:65:VAL:CG1	2.44	0.47
1:A:89:THR:OG1	2:A:401:ASP:OD1	2.32	0.47
1:B:260:ALA:O	1:B:263:THR:HG22	2.14	0.47
1:C:145:GLY:HA2	1:C:198:THR:HG21	1.96	0.47
1:C:239:ILE:HG23	4:C:503:HOH:O	2.14	0.47
1:B:6:ILE:HG12	1:B:84:VAL:HB	1.96	0.47
1:B:115:MET:HG3	1:B:167:ASP:O	2.13	0.47
1:C:130:TYR:O	1:C:134:VAL:HG23	2.14	0.47
1:A:216:ILE:HA	1:A:240:VAL:O	2.14	0.47
1:C:191:ARG:NE	4:C:513:HOH:O	2.37	0.47
1:A:3:ASN:O	1:A:81:ASP:HB2	2.15	0.47
1:B:142:ALA:O	1:B:143:ASN:CG	2.57	0.47
1:D:151:ASN:O	1:D:153:THR:HG23	2.14	0.47
1:A:90:ASP:OD1	2:A:401:ASP:HB3	2.14	0.47
1:A:155:LEU:HD13	1:A:160:VAL:HG23	1.97	0.46
1:B:56:ILE:HD11	1:B:61:MET:CE	2.44	0.46
1:B:169:ALA:HB1	4:B:531:HOH:O	2.14	0.46
1:C:145:GLY:HA3	4:C:504:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:SER:HB3	1:D:88:GLY:HA3	1.97	0.46
1:D:141:SER:O	4:D:503:HOH:O	2.20	0.46
1:D:229:LYS:HE2	1:D:256:THR:OG1	2.15	0.46
1:A:115:MET:HE1	1:A:162:LYS:NZ	2.30	0.46
1:A:8:ALA:HA	1:A:86:THR:OG1	2.16	0.46
1:A:63:ASP:HB3	1:A:211:LEU:HG	1.97	0.46
1:D:12:THR:N	2:D:401:ASP:HB3	2.23	0.46
1:A:97:TYR:OH	1:A:326:TYR:O	2.29	0.46
1:A:105:CYS:SG	1:A:107:LYS:CG	3.03	0.46
1:A:259:THR:O	1:A:263:THR:HG22	2.16	0.46
1:A:127:PHE:HB2	1:B:121:MET:HB2	1.98	0.46
1:B:58:SER:HB3	1:B:88:GLY:CA	2.43	0.46
1:B:220:TYR:CE2	1:B:223:ALA:HA	2.51	0.46
1:B:164:ASN:ND2	1:D:275:THR:HG22	2.31	0.46
1:D:195:ARG:HH21	1:D:325:GLN:HB3	1.80	0.45
1:A:101:LEU:HD13	1:A:308:LEU:HD12	1.98	0.45
1:B:164:ASN:HD22	1:D:275:THR:HG22	1.82	0.45
1:C:80:THR:OG1	1:C:81:ASP:N	2.49	0.45
1:A:36:VAL:HG22	1:A:48:VAL:HG11	1.98	0.45
1:B:170:THR:HG23	1:B:171:PHE:CD1	2.51	0.45
1:C:319:ILE:HA	1:C:322:ILE:HD12	1.98	0.45
1:D:12:THR:H	2:D:401:ASP:CB	2.20	0.45
1:D:39:VAL:HG13	1:D:42:LEU:HG	1.99	0.45
1:A:182:ILE:HG12	1:A:187:ILE:HG12	1.99	0.45
1:A:270:SER:OG	1:A:271:SER:N	2.46	0.45
1:B:277:ALA:HA	1:B:296:THR:HA	1.98	0.45
1:C:61:MET:HE3	1:C:65:VAL:HB	1.99	0.45
1:D:7:LEU:HD12	1:D:7:LEU:N	2.32	0.45
1:A:130:TYR:CG	1:B:121:MET:HE1	2.52	0.45
1:A:156:ASP:HB3	1:A:179:LEU:HD11	1.98	0.45
1:B:148:VAL:HG21	1:B:160:VAL:HG11	1.98	0.45
1:D:42:LEU:HD13	1:D:48:VAL:HG21	1.97	0.45
1:A:163:THR:O	1:C:275:THR:HB	2.16	0.45
1:C:160:VAL:O	1:C:301:LYS:NZ	2.39	0.45
1:C:214:VAL:CG1	1:C:303:ARG:HG3	2.48	0.44
1:C:163:THR:OG1	1:C:170:THR:O	2.16	0.44
1:D:151:ASN:ND2	4:D:506:HOH:O	2.31	0.44
1:D:277:ALA:HA	1:D:296:THR:HA	1.99	0.44
1:A:6:ILE:HA	1:A:84:VAL:O	2.18	0.44
1:A:228:ALA:HB1	1:A:257:LEU:HD21	2.00	0.44
1:A:234:ALA:CB	1:C:226:LEU:CD1	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:TYR:CZ	1:D:223:ALA:HA	2.53	0.44
1:A:275:THR:O	1:C:165:THR:HG23	2.17	0.44
1:A:268:VAL:HG22	1:A:292:VAL:HB	2.00	0.44
1:B:195:ARG:HH21	1:C:188:ASP:CG	2.25	0.44
1:B:249:LEU:HD23	1:B:253:VAL:CG1	2.48	0.44
1:D:77:CYS:O	1:D:107:LYS:NZ	2.43	0.44
1:C:315:ASP:O	1:C:319:ILE:HG13	2.18	0.44
1:D:325:GLN:HG3	1:D:325:GLN:O	2.18	0.44
1:A:321:GLN:HA	1:A:324:ASN:HB2	1.99	0.43
1:A:30:VAL:HG13	1:A:34:ASN:HB2	2.00	0.43
1:A:165:THR:HG23	1:C:275:THR:O	2.18	0.43
1:A:237:ASP:HB3	1:A:310:LEU:HD13	2.00	0.43
1:C:61:MET:HE2	1:C:66:TRP:HD1	1.78	0.43
1:D:112:VAL:CG2	1:D:128:ASN:HB3	2.47	0.43
1:A:214:VAL:HG22	1:A:238:GLY:HA3	2.00	0.43
1:D:112:VAL:HG23	1:D:149:VAL:O	2.18	0.43
1:A:107:LYS:H	1:A:107:LYS:HG2	1.56	0.43
1:B:96:ALA:O	1:B:100:ASP:HB2	2.18	0.43
1:B:254:PHE:CZ	1:B:289:TYR:CE2	3.07	0.43
1:C:153:THR:HG22	1:C:155:LEU:HG	2.01	0.43
1:C:216:ILE:HA	4:C:503:HOH:O	2.19	0.43
1:D:71:LYS:HE2	1:D:206:SER:O	2.19	0.43
1:A:164:ASN:HD22	1:C:275:THR:HG22	1.84	0.43
1:C:112:VAL:HG23	1:C:149:VAL:O	2.19	0.43
1:D:219:ASN:HD22	1:D:250:TYR:H	1.66	0.43
1:D:197:HIS:O	1:D:200:ASP:HB2	2.19	0.43
1:A:190:GLN:HA	1:D:194:ALA:HB3	2.00	0.43
1:B:7:LEU:HB3	1:B:53:VAL:CG2	2.49	0.43
1:C:71:LYS:NZ	1:C:208:LEU:O	2.41	0.43
1:C:217:VAL:N	4:C:503:HOH:O	2.51	0.42
1:D:175:ASN:ND2	4:D:514:HOH:O	2.38	0.42
1:D:226:LEU:HD23	1:D:226:LEU:HA	1.84	0.42
1:B:116:ARG:HB2	1:B:124:ASP:OD1	2.20	0.42
1:C:211:LEU:HD23	1:C:211:LEU:HA	1.75	0.42
1:D:73:ILE:HD11	1:D:85:ILE:HD11	2.00	0.42
1:D:292:VAL:HG13	1:D:320:GLN:HA	2.01	0.42
1:B:108:PRO:HD3	1:B:142:ALA:HB2	2.01	0.42
1:D:144:ARG:NH2	1:D:189:TYR:HB3	2.32	0.42
1:C:104:LYS:HA	1:C:104:LYS:HD3	1.91	0.42
1:D:215:GLY:HA3	1:D:231:LEU:CD1	2.50	0.42
1:A:63:ASP:CG	1:C:222:ASN:HD22	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:THR:O	4:A:506:HOH:O	2.21	0.42
1:A:305:LEU:HD12	1:A:305:LEU:HA	1.76	0.42
1:D:84:VAL:HA	1:D:110:VAL:O	2.20	0.42
1:B:222:ASN:HB2	4:D:511:HOH:O	2.19	0.42
1:C:71:LYS:HD3	1:C:206:SER:O	2.20	0.42
1:C:158:ARG:NE	1:C:326:TYR:O	2.40	0.42
1:C:195:ARG:NH1	1:C:323:PHE:O	2.52	0.42
1:C:10:GLY:HA2	1:C:55:ASN:OD1	2.20	0.42
1:A:91:THR:O	1:A:94:GLU:N	2.48	0.42
1:C:179:LEU:HA	1:C:191:ARG:HB2	2.02	0.42
1:B:67:LEU:HB3	1:B:71:LYS:NZ	2.35	0.41
1:B:273:VAL:HG13	1:D:162:LYS:O	2.20	0.41
1:C:77:CYS:SG	1:C:107:LYS:HD2	2.61	0.41
1:D:30:VAL:HG13	1:D:34:ASN:HB2	2.02	0.41
1:D:49:LYS:HD3	1:D:49:LYS:N	2.32	0.41
1:A:80:THR:HG22	1:A:81:ASP:N	2.35	0.41
1:A:202:PRO:HD3	1:A:326:TYR:CZ	2.55	0.41
1:D:26:THR:CG2	1:D:29:LYS:HD3	2.50	0.41
1:A:14:ALA:HB1	1:A:30:VAL:O	2.20	0.41
1:A:106:ASP:O	1:A:107:LYS:C	2.63	0.41
1:C:199:SER:HB2	4:C:507:HOH:O	2.20	0.41
1:D:247:GLY:HA3	1:D:278:THR:HG23	2.02	0.41
1:A:100:ASP:O	1:A:198:THR:N	2.21	0.41
1:A:106:ASP:OD2	1:A:142:ALA:CB	2.58	0.41
1:A:43:LYS:H	1:A:43:LYS:HG2	1.71	0.41
1:A:108:PRO:CB	1:A:136:ALA:HA	2.45	0.41
1:A:222:ASN:HB2	1:C:62:ASN:HA	2.02	0.41
1:A:27:VAL:CG1	1:A:57:GLY:HA3	2.51	0.41
1:C:258:ALA:O	1:C:262:LYS:HG3	2.21	0.41
1:A:11:GLY:O	1:A:27:VAL:CG2	2.60	0.41
1:A:72:LYS:HE2	1:A:72:LYS:CA	2.51	0.41
1:B:76:ASP:O	1:B:79:LYS:HA	2.20	0.41
1:B:172:LYS:HB3	4:B:553:HOH:O	2.20	0.41
1:D:160:VAL:O	1:D:301:LYS:NZ	2.47	0.41
1:B:236:TYR:OH	1:D:224:SER:HB2	2.21	0.41
1:B:259:THR:O	1:B:262:LYS:HB2	2.21	0.41
1:A:42:LEU:HD12	1:A:42:LEU:N	2.36	0.40
1:B:211:LEU:HD23	1:B:211:LEU:HA	1.77	0.40
1:D:251:LYS:HE3	1:D:251:LYS:HB3	1.47	0.40
1:C:129:LEU:HD23	1:C:133:VAL:HG23	2.02	0.40
1:C:129:LEU:HD23	1:C:129:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:VAL:HG13	4:D:524:HOH:O	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:SER:OG	1:C:325:GLN:OE1[1_455]	1.94	0.26
1:A:204:ASP:OD2	1:C:318:GLN:NE2[1_455]	2.03	0.17
1:B:325:GLN:NE2	1:D:201:THR:O[1_655]	2.10	0.10
1:A:204:ASP:OD2	1:C:318:GLN:OE1[1_455]	2.12	0.08

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	315/326 (97%)	302 (96%)	13 (4%)	0	100	100
1	B	294/326 (90%)	287 (98%)	7 (2%)	0	100	100
1	C	287/326 (88%)	281 (98%)	6 (2%)	0	100	100
1	D	301/326 (92%)	295 (98%)	6 (2%)	0	100	100
All	All	1197/1304 (92%)	1165 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	263/266 (99%)	257 (98%)	6 (2%)	44	51
1	B	248/266 (93%)	242 (98%)	6 (2%)	43	49
1	C	242/266 (91%)	241 (100%)	1 (0%)	84	89
1	D	254/266 (96%)	249 (98%)	5 (2%)	48	56
All	All	1007/1064 (95%)	989 (98%)	18 (2%)	51	60

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	48	VAL
1	A	83	PHE
1	A	106	ASP
1	A	107	LYS
1	A	210	GLU
1	B	139	LYS
1	B	172	LYS
1	B	186	LYS
1	B	207	LYS
1	B	254	PHE
1	B	314	LYS
1	C	186	LYS
1	D	51	GLU
1	D	78	ASP
1	D	139	LYS
1	D	251	LYS
1	D	321	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	37	ASN
1	A	64	ASN
1	A	151	ASN
1	A	190	GLN
1	A	300	GLN
1	A	307	GLN
1	B	55	ASN
1	B	143	ASN

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Mol	Chain	Res	Type
1	B	151	ASN
1	B	209	ASN
1	B	321	GLN
1	C	222	ASN
1	C	280	GLN
1	C	321	GLN
1	C	324	ASN
1	C	325	GLN
1	D	34	ASN
1	D	190	GLN
1	D	321	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	ASP	D	401	-	7,8,8	1.49	2 (28%)	6,10,10	1.59	1 (16%)
2	ASP	A	401	-	7,8,8	1.20	1 (14%)	6,10,10	1.61	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SIN	B	401	-	7,7,7	1.01	0	8,8,8	1.94	3 (37%)
3	SIN	C	401	-	7,7,7	1.14	0	8,8,8	1.57	2 (25%)

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	ASP	D	401	-	-	0/8/8/8	-
2	ASP	A	401	-	-	5/8/8/8	-
3	SIN	B	401	-	-	5/5/5/5	-
3	SIN	C	401	-	-	2/5/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	ASP	OXT-C	-3.07	1.20	1.30
2	D	401	ASP	OD2-CG	-2.16	1.23	1.30
2	A	401	ASP	OXT-C	-2.03	1.24	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	SIN	O4-C4-C3	3.02	123.53	114.00
2	D	401	ASP	OXT-C-O	-2.91	117.48	124.08
2	A	401	ASP	OD2-CG-CB	2.46	121.66	114.00
3	B	401	SIN	O2-C1-C2	2.43	121.69	114.00
3	C	401	SIN	C2-C3-C4	-2.40	107.29	113.67
3	B	401	SIN	O4-C4-O3	-2.39	117.18	123.33
3	C	401	SIN	O2-C1-O1	-2.30	117.42	123.33
2	A	401	ASP	OD1-CG-CB	-2.19	116.12	122.84
2	A	401	ASP	OXT-C-O	-2.06	119.40	124.08

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ASP	O-C-CA-N
3	B	401	SIN	C1-C2-C3-C4

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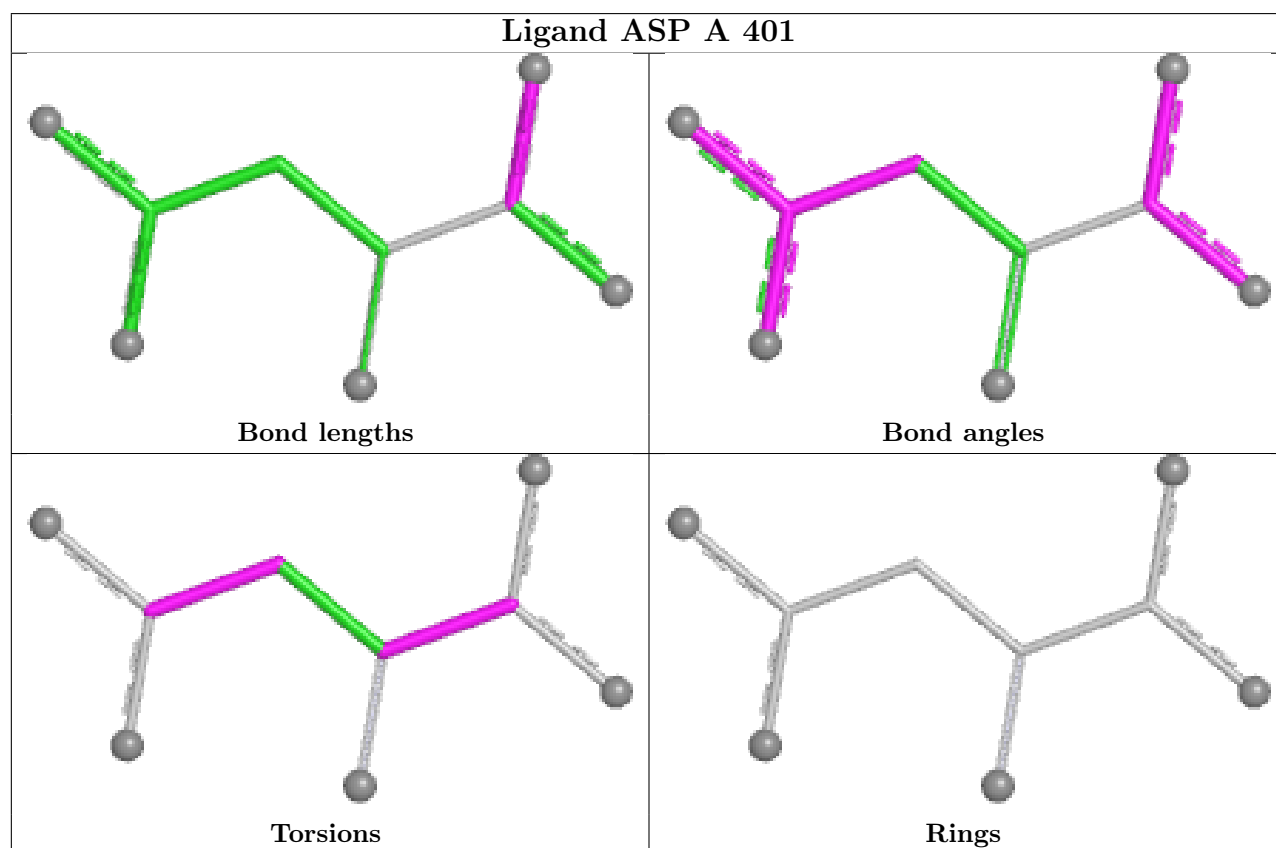
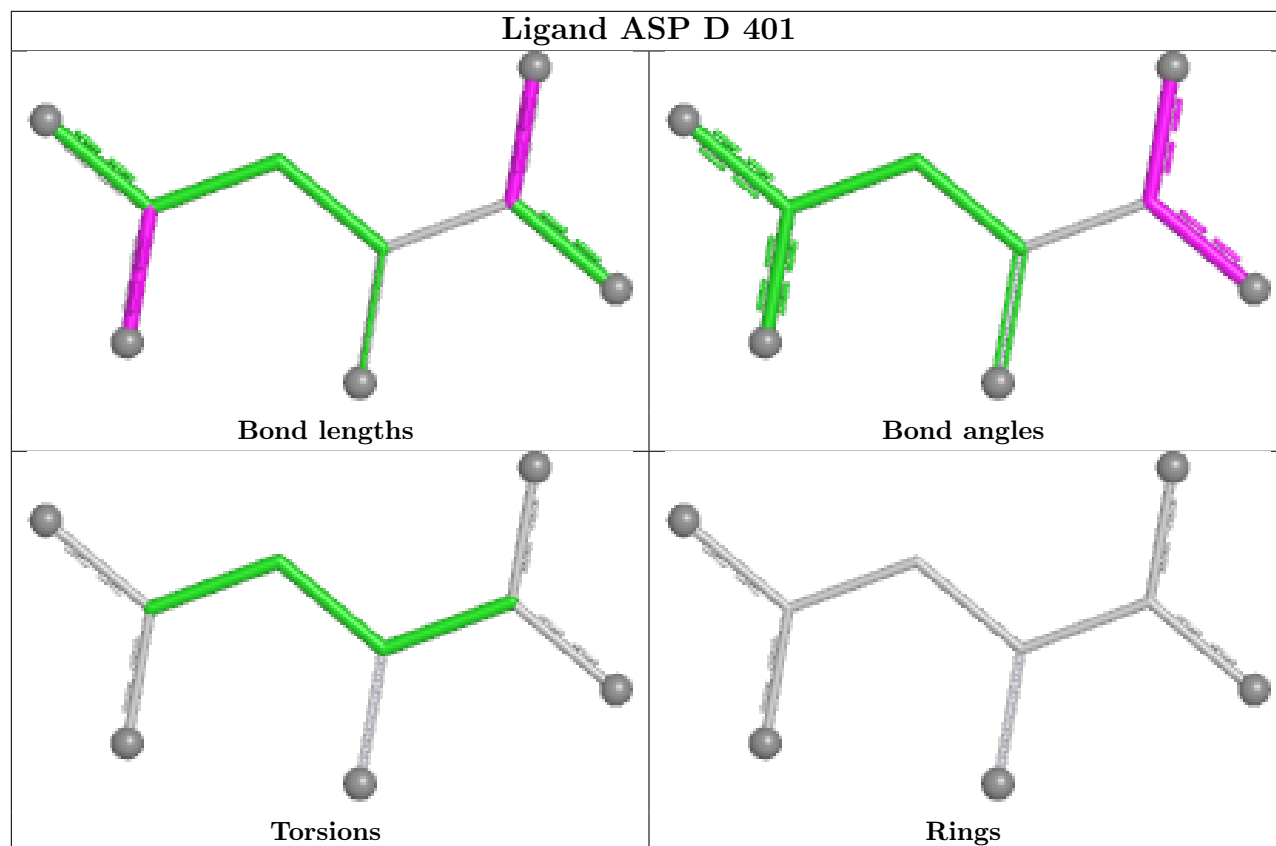
Mol	Chain	Res	Type	Atoms
2	A	401	ASP	OXT-C-CA-N
2	A	401	ASP	OXT-C-CA-CB
2	A	401	ASP	O-C-CA-CB
3	B	401	SIN	C2-C3-C4-O3
3	B	401	SIN	C2-C3-C4-O4
3	B	401	SIN	O2-C1-C2-C3
3	B	401	SIN	O1-C1-C2-C3
2	A	401	ASP	CA-CB-CG-OD2
3	C	401	SIN	C2-C3-C4-O3
3	C	401	SIN	C2-C3-C4-O4

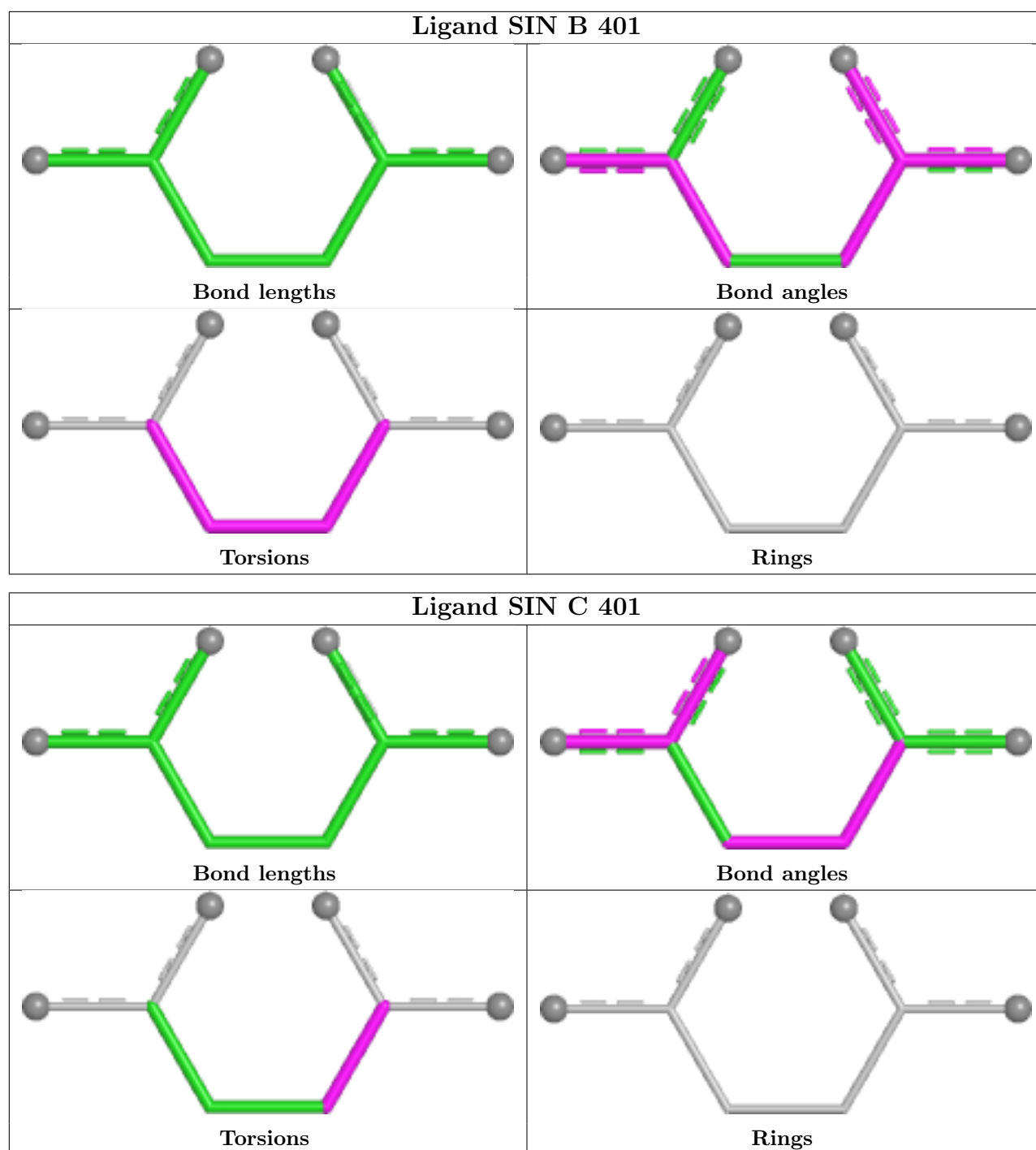
There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	ASP	7	0
2	A	401	ASP	4	0
3	B	401	SIN	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	323/326 (99%)	0.69	13 (4%) 42 44	22, 45, 58, 69	12 (3%)
1	B	300/326 (92%)	0.38	3 (1%) 79 81	21, 40, 53, 68	4 (1%)
1	C	295/326 (90%)	0.58	8 (2%) 56 59	27, 43, 56, 70	5 (1%)
1	D	309/326 (94%)	0.43	4 (1%) 75 77	23, 40, 53, 63	3 (0%)
All	All	1227/1304 (94%)	0.52	28 (2%) 61 64	21, 42, 56, 70	24 (1%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	VAL	3.2
1	D	289	TYR	3.0
1	A	107	LYS	2.9
1	B	172	LYS	2.9
1	B	36	VAL	2.8
1	C	254	PHE	2.8
1	C	226	LEU	2.8
1	A	103	VAL	2.8
1	D	27	VAL	2.7
1	A	13	ILE	2.7
1	A	204	ASP	2.5
1	C	185	GLY	2.5
1	A	192	THR	2.4
1	D	135	THR	2.3
1	C	232	VAL	2.3
1	C	322	ILE	2.2
1	A	232	VAL	2.2
1	A	257	LEU	2.2
1	C	289	TYR	2.2
1	A	265	THR	2.2
1	A	205	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	305	LEU	2.1
1	C	326	TYR	2.1
1	A	21	THR	2.1
1	D	73	ILE	2.1
1	A	108	PRO	2.1
1	A	23	SER	2.1
1	B	193	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

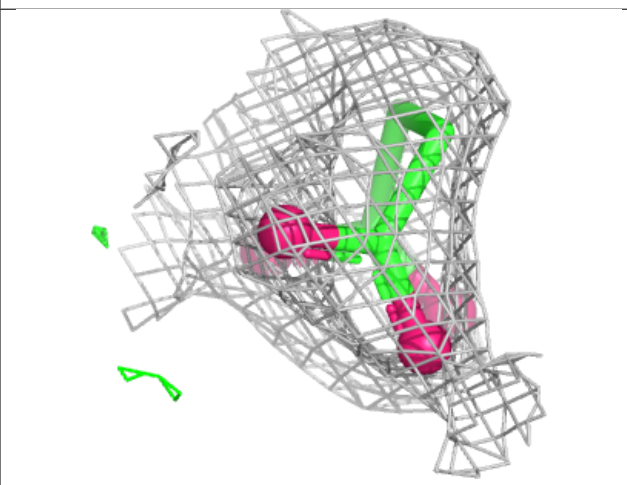
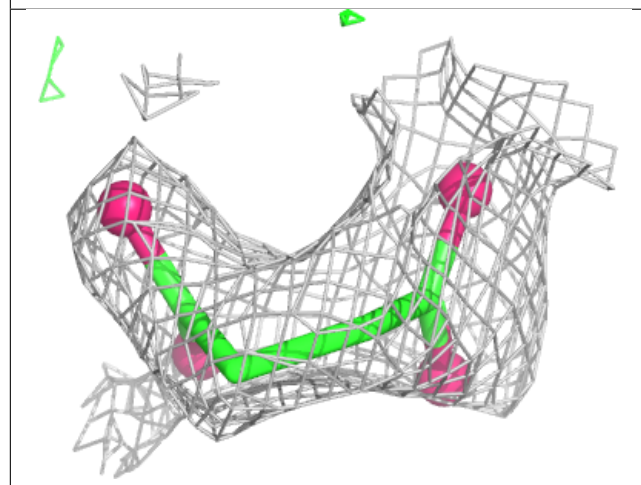
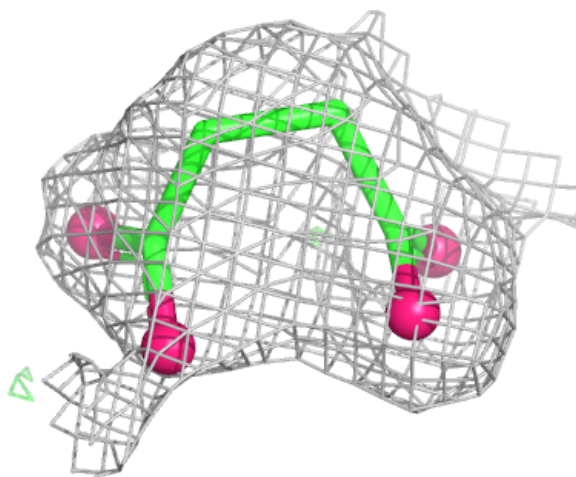
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SIN	B	401	8/8	0.59	0.11	44,54,58,61	0
2	ASP	D	401	9/9	0.80	0.14	35,38,45,52	0
2	ASP	A	401	9/9	0.84	0.08	39,42,47,49	0
3	SIN	C	401	8/8	0.88	0.08	38,42,45,46	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.

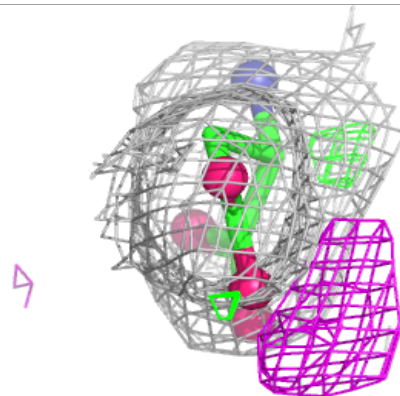
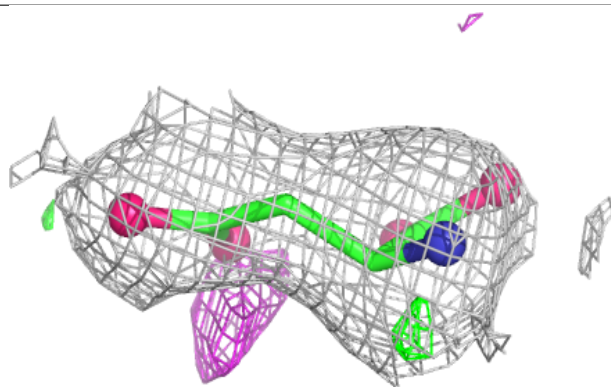
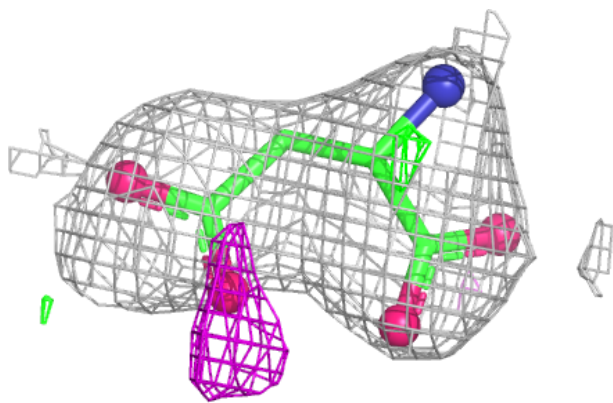
Electron density around SIN B 401:

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



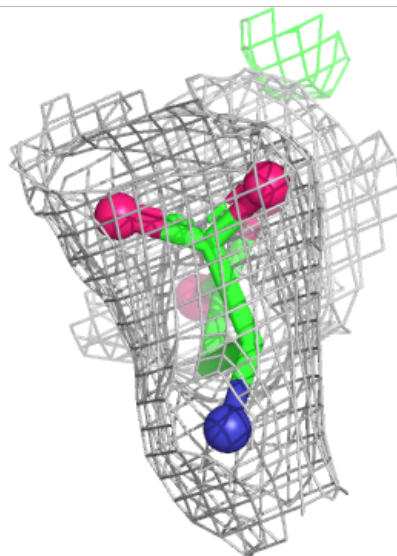
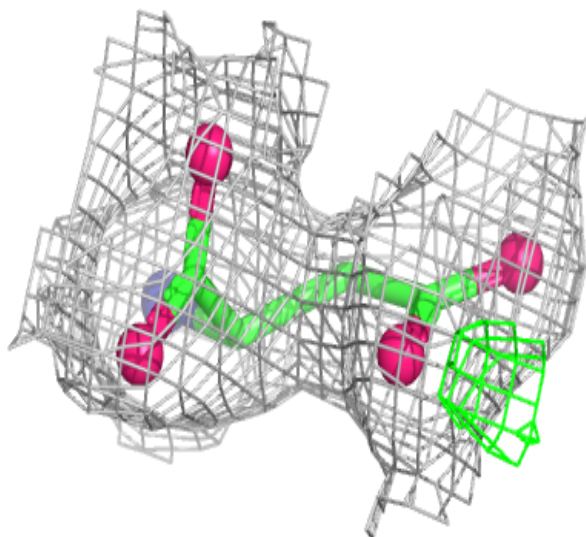
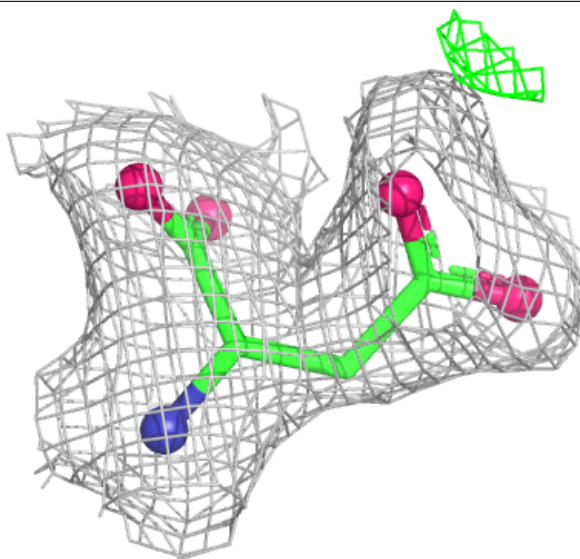
Electron density around ASP D 401:

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



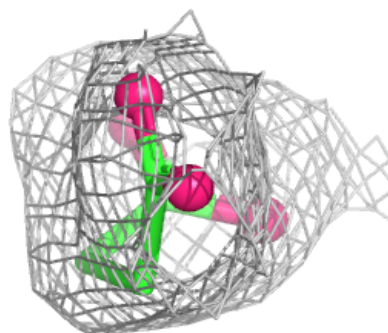
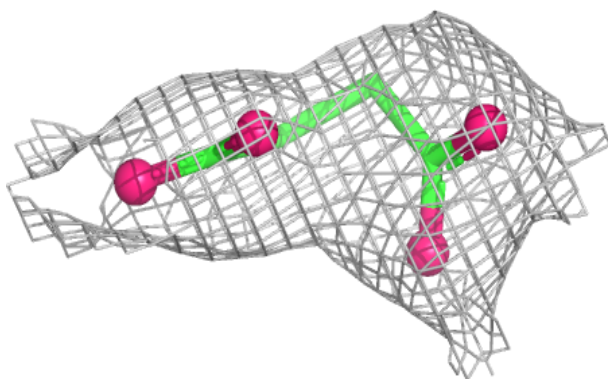
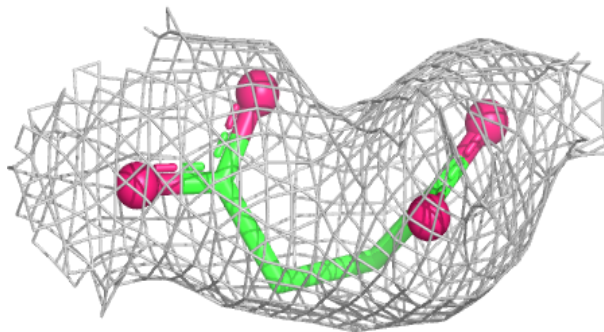
Electron density around ASP A 401:

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



Electron density around SIN C 401:

$2mF_o-DF_c$ (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.