



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:25 PM UTC

PDB ID : 1QA7 / pdb_00001qa7
Title : CRYSTAL COMPLEX OF THE 3C PROTEINASE FROM HEPATITIS
A VIRUS WITH ITS INHIBITOR AND IMPLICATIONS FOR THE
POLYPROTEIN PROCESSING IN HAV
Authors : Bergmann, E.M.; Cherney, M.M.; Mckendrick, J.; Vederas, J.C.; James,
M.N.G.
Deposited on : 1999-04-15
Resolution : 1.90 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 ①](#)) were used in the production of this report:

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

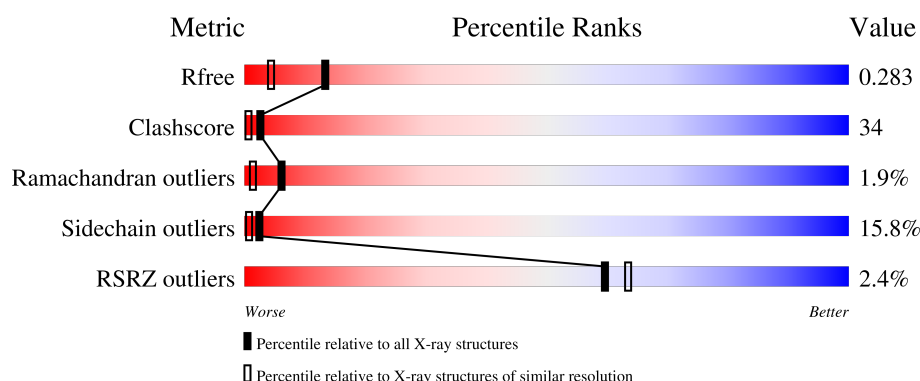
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	217	2% 49% 35% 11% • •
1	B	217	2% 54% 35% 9% •
1	C	217	4% 41% 44% 10% • •
1	D	217	% 59% 32% 8% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7228 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.

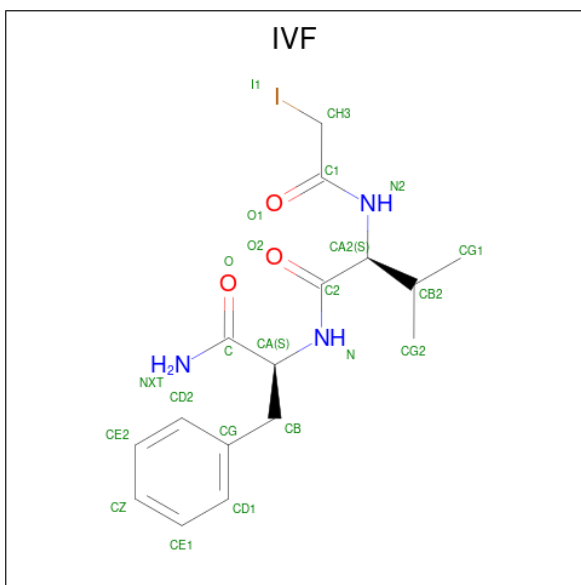
- Molecule 1 is a protein called HAV 3C PROTEINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1636	1040	281	306	9			
1	B	217	Total	C	N	O	S	0	0	0
			1672	1063	287	313	9			
1	C	213	Total	C	N	O	S	0	0	0
			1636	1040	281	306	9			
1	D	217	Total	C	N	O	S	0	0	0
			1672	1063	287	313	9			

There are 12 discrepancies between the modelled and reference sequences:

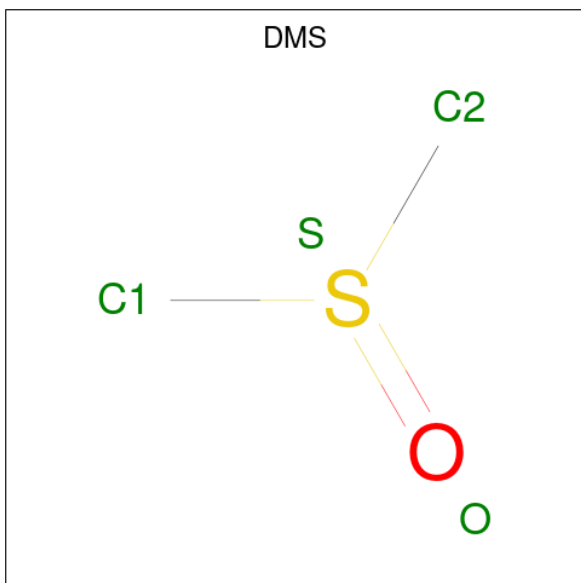
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	SER	CYS	engineered mutation	UNP P26582
A	82	ALA	PHE	engineered mutation	UNP P26582
A	101	GLN	GLU	conflict	UNP P26582
B	24	SER	CYS	engineered mutation	UNP P26582
B	82	ALA	PHE	engineered mutation	UNP P26582
B	101	GLN	GLU	conflict	UNP P26582
C	24	SER	CYS	engineered mutation	UNP P26582
C	82	ALA	PHE	engineered mutation	UNP P26582
C	101	GLN	GLU	conflict	UNP P26582
D	24	SER	CYS	engineered mutation	UNP P26582
D	82	ALA	PHE	engineered mutation	UNP P26582
D	101	GLN	GLU	conflict	UNP P26582

- Molecule 2 is N-(iodoacetyl)-L-valyl-L-phenylalaninamide (CCD ID: IVF) (formula: $C_{16}H_{22}IN_3O_3$).



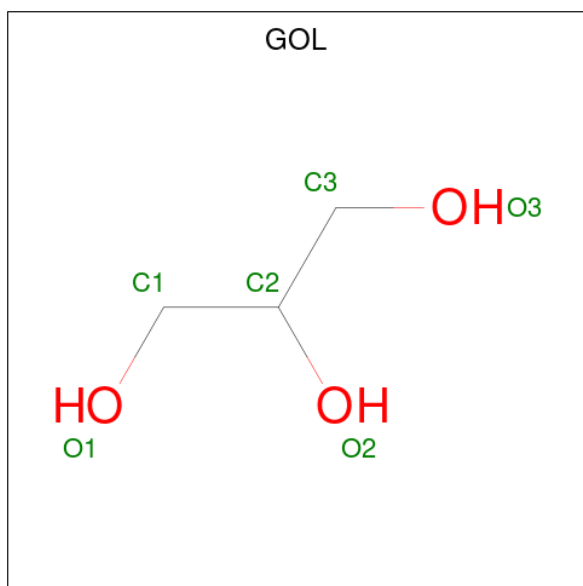
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			22	16	3	3		
2	B	1	Total	C	N	O	0	0
			22	16	3	3		
2	C	1	Total	C	N	O	0	0
			22	16	3	3		
2	D	1	Total	C	N	O	0	0
			22	16	3	3		

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		

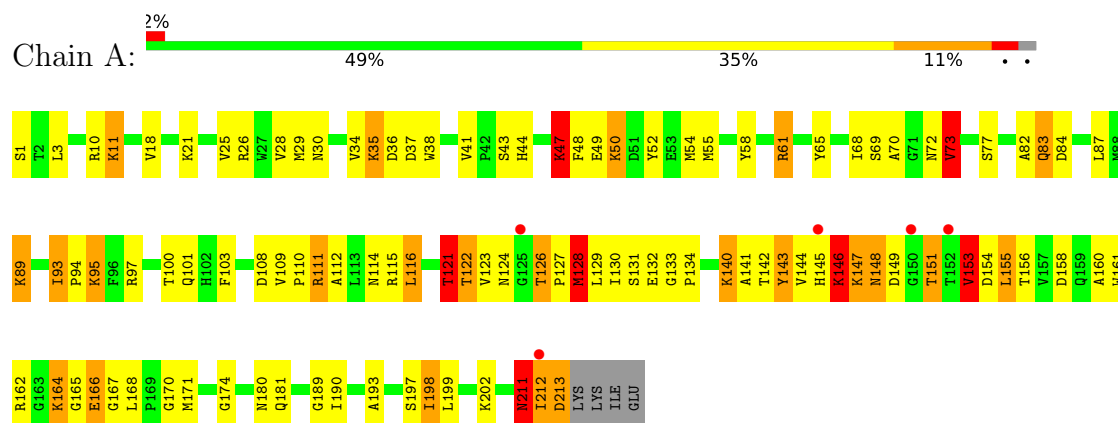
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	131	Total	O	0	0
			131	131		
5	B	129	Total	O	0	0
			129	129		
5	C	121	Total	O	0	0
			121	121		
5	D	133	Total	O	0	0
			133	133		

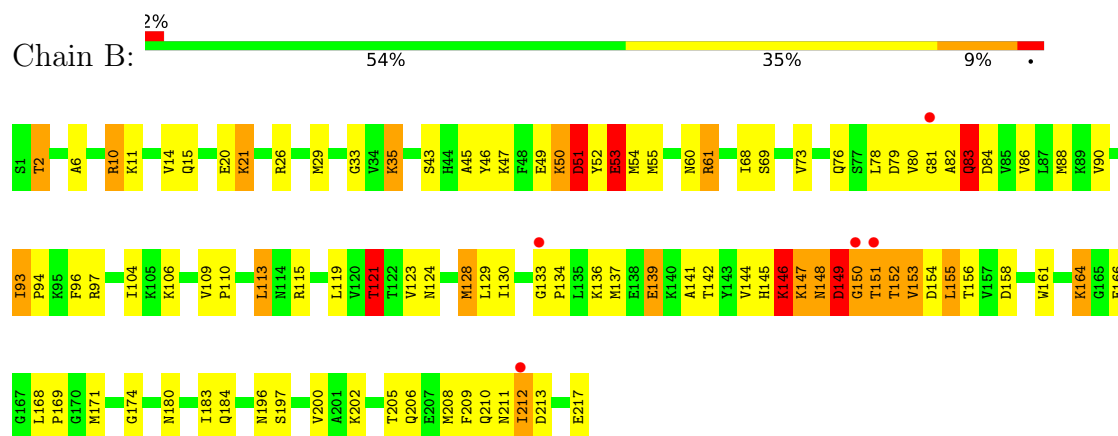
3 Residue-property plots

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.

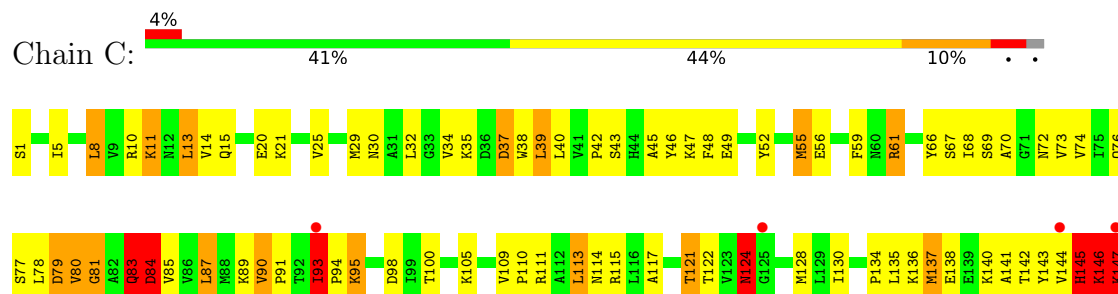
• Molecule 1: HAV 3C PROTEINASE

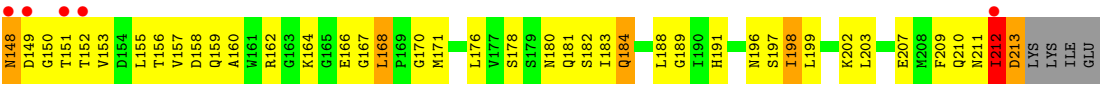


• Molecule 1: HAV 3C PROTEINASE

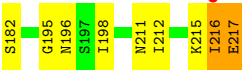
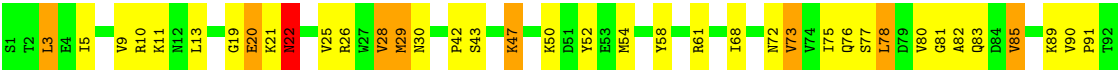


• Molecule 1: HAV 3C PROTEINASE





● Molecule 1: HAV 3C PROTEINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.56Å 78.36Å 105.29Å 90.00° 97.50° 90.00°	Depositor
Resolution (Å)	15.00 – 1.90 15.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.3 (15.00-1.90) 92.3 (15.00-1.90)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.90Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.204 , 0.298 0.198 , 0.283	Depositor DCC
R_{free} test set	3902 reflections (6.57%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.48 , 146.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7228	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.73% 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: GOL, DMS, IVF

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	0.97	2/1665 (0.1%)	1.23	13/2252 (0.6%)
1	B	3.30	4/1701 (0.2%)	1.27	16/2297 (0.7%)
1	C	0.92	1/1665 (0.1%)	1.33	14/2252 (0.6%)
1	D	4.70	2/1701 (0.1%)	1.25	13/2297 (0.6%)
All	All	2.96	9/6732 (0.1%)	1.27	56/9098 (0.6%)

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	A	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	217	GLU	C-OXT	189.31	5.02	1.23
1	B	217	GLU	C-OXT	129.62	3.82	1.23
1	A	128	MET	SD-CE	-8.13	1.59	1.79
1	B	212	ILE	CA-CB	6.08	1.61	1.54
1	A	41	VAL	CA-CB	5.81	1.61	1.54
1	B	51	ASP	N-CA	-5.66	1.40	1.46
1	B	151	THR	CA-CB	5.59	1.62	1.53
1	D	29	MET	SD-CE	-5.24	1.66	1.79
1	C	145	HIS	CA-C	-5.05	1.49	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	ASN	N-CA-C	14.40	128.28	111.71
1	C	212	ILE	N-CA-C	-12.97	100.82	113.53
1	D	125	GLY	N-CA-C	-9.41	103.49	114.69
1	C	93	ILE	N-CA-C	9.29	118.05	108.95
1	D	78	LEU	N-CA-C	-9.14	102.64	113.88
1	C	84	ASP	N-CA-C	-8.54	103.46	114.04
1	B	146	LYS	N-CA-C	8.29	124.41	113.30
1	C	144	VAL	CA-C-N	-8.21	112.67	122.44
1	C	144	VAL	C-N-CA	-8.21	112.67	122.44
1	B	150	GLY	N-CA-C	-8.04	94.11	113.18
1	C	95	LYS	N-CA-C	7.73	121.62	110.10
1	A	148	ASN	N-CA-C	7.71	122.82	112.88
1	A	153	VAL	N-CA-C	7.56	118.74	106.72
1	A	146	LYS	N-CA-C	7.49	121.11	108.90
1	D	122	THR	CB-CA-C	-6.92	102.85	111.43
1	D	72	ASN	CA-C-N	-6.74	115.06	122.27
1	D	72	ASN	C-N-CA	-6.74	115.06	122.27
1	A	73	VAL	CB-CA-C	-6.62	101.20	111.26
1	C	90	VAL	CA-C-N	6.55	126.32	119.05
1	C	90	VAL	C-N-CA	6.55	126.32	119.05
1	D	135	LEU	N-CA-C	6.37	119.70	110.28
1	B	51	ASP	CB-CA-C	6.28	120.83	111.17
1	A	95	LYS	N-CA-C	6.26	118.86	110.35
1	C	147	LYS	N-CA-C	-5.85	98.34	110.80
1	B	200	VAL	N-CA-C	5.79	116.21	107.75
1	D	121	THR	CB-CA-C	-5.67	101.36	114.41
1	B	97	ARG	N-CA-C	-5.64	102.54	110.50
1	B	129	LEU	N-CA-C	-5.61	100.55	109.76
1	B	210	GLN	N-CA-C	5.60	118.10	111.33
1	D	82	ALA	CA-C-N	-5.58	114.32	122.19
1	D	82	ALA	C-N-CA	-5.58	114.32	122.19
1	C	83	GLN	N-CA-C	5.58	118.91	109.76
1	D	149	ASP	N-CA-C	-5.52	106.43	112.72
1	B	153	VAL	CB-CA-C	-5.37	103.17	110.90
1	C	211	ASN	N-CA-C	5.37	118.05	111.82
1	A	160	ALA	N-CA-C	5.36	117.63	108.90
1	C	144	VAL	N-CA-C	-5.36	101.92	109.63
1	D	28	VAL	N-CA-C	5.35	116.23	111.90
1	A	121	THR	CB-CA-C	-5.34	101.08	114.11
1	D	93	ILE	N-CA-C	5.32	113.20	108.63
1	A	47	LYS	N-CA-C	5.28	119.21	112.87
1	B	10	ARG	N-CA-C	5.26	116.70	111.07
1	B	152	THR	N-CA-C	5.24	116.80	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	THR	N-CA-C	5.23	121.38	109.81
1	A	143	TYR	N-CA-C	5.21	117.98	109.59
1	C	55	MET	N-CA-C	5.16	117.86	109.86
1	B	50	LYS	CA-C-O	5.16	125.72	119.38
1	D	212	ILE	N-CA-C	5.16	117.50	111.05
1	B	2	THR	N-CA-C	-5.15	105.67	111.28
1	B	121	THR	CB-CA-C	-5.11	100.25	110.42
1	A	144	VAL	CB-CA-C	-5.10	104.60	111.63
1	A	211	ASN	N-CA-C	5.08	119.13	111.81
1	B	6	ALA	N-CA-C	-5.07	105.75	111.28
1	A	116	LEU	N-CA-C	-5.02	104.06	110.53
1	C	25	VAL	N-CA-CB	5.02	117.01	110.99
1	B	139	GLU	N-CA-C	-5.01	106.01	111.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	GLU	Mainchain

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	1636	0	1661	117	0
1	B	1672	0	1704	94	0
1	C	1636	0	1661	162	0
1	D	1672	0	1704	93	0
2	A	22	0	20	7	0
2	B	22	0	20	0	0
2	C	22	0	20	3	0
2	D	22	0	20	4	0
3	D	4	0	6	1	0
4	D	6	0	8	0	0
5	A	131	0	0	8	0
5	B	129	0	0	19	0
5	C	121	0	0	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	133	0	0	15	0
All	All	7228	0	6824	460	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 34.

All (460) 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:138:GLU:HG3	1:C:162:ARG:HD2	1.36	1.06
1:D:76:GLN:HE22	1:D:211:ASN:HB2	1.14	1.04
1:C:128:MET:HE1	1:C:168:LEU:HG	1.38	1.03
1:B:144:VAL:HG21	1:B:196:ASN:ND2	1.86	0.91
1:D:144:VAL:HG11	1:D:152:THR:HG22	1.51	0.91
1:C:146:LYS:HD2	1:C:147:LYS:HE2	1.53	0.89
1:A:10:ARG:CZ	1:A:127:PRO:HB3	2.03	0.88
1:C:20:GLU:HG2	1:C:21:LYS:H	1.36	0.87
1:D:121:THR:HG23	1:D:174:GLY:HA3	1.54	0.87
1:D:76:GLN:NE2	1:D:211:ASN:HB2	1.90	0.87
1:D:147:LYS:HD2	1:D:148:ASN:H	1.37	0.87
1:C:83:GLN:HE21	1:C:84:ASP:H	1.24	0.86
1:C:147:LYS:HD2	1:C:148:ASN:ND2	1.91	0.85
1:C:90:VAL:HG23	1:C:93:ILE:HG13	1.57	0.85
1:C:90:VAL:CG2	1:C:93:ILE:HG13	2.07	0.85
1:B:93:ILE:HG13	1:B:94:PRO:HD2	1.58	0.85
1:C:128:MET:HE1	1:C:168:LEU:CG	2.08	0.83
1:D:78:LEU:HD11	1:D:85:VAL:HG22	1.59	0.83
1:D:147:LYS:NZ	5:D:4100:HOH:O	2.11	0.82
1:B:14:VAL:HG13	5:B:2122:HOH:O	1.79	0.82
1:A:50:LYS:HD3	1:A:50:LYS:N	1.95	0.81
1:C:147:LYS:HB2	1:C:148:ASN:OD1	1.81	0.80
1:B:78:LEU:HD22	1:B:208:MET:HB3	1.64	0.80
1:C:100:THR:HG22	1:C:209:PHE:CE1	2.17	0.80
1:C:142:THR:HG22	1:C:156:THR:HG22	1.65	0.79
1:D:144:VAL:CG1	1:D:152:THR:HG22	2.12	0.79
1:D:170:GLY:HA3	2:D:301:IVF:H17	1.66	0.78
1:A:167:GLY:HA3	1:A:171:MET:HE1	1.64	0.78
1:A:128:MET:HB2	1:A:130:ILE:CD1	2.12	0.78
1:A:43:SER:O	1:A:47:LYS:HB3	1.83	0.77
1:B:52:TYR:HD1	1:B:55:MET:HE1	1.48	0.77
1:B:121:THR:HG23	1:B:174:GLY:HA3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:LEU:HD23	1:C:212:ILE:CG2	2.15	0.77
1:A:131:SER:HB2	1:B:83:GLN:OE1	1.85	0.76
1:A:131:SER:HB3	1:B:81:GLY:O	1.85	0.76
1:D:26:ARG:HD2	5:D:4084:HOH:O	1.86	0.76
1:D:170:GLY:CA	2:D:301:IVF:H17	2.15	0.76
1:C:52:TYR:HA	1:C:55:MET:SD	2.26	0.75
1:A:123:VAL:HB	1:A:128:MET:HE2	1.68	0.75
1:C:147:LYS:HD2	1:C:148:ASN:CG	2.11	0.75
1:A:121:THR:HG23	1:A:174:GLY:HA3	1.67	0.75
1:D:136:LYS:HD3	5:D:4081:HOH:O	1.86	0.75
1:C:5:ILE:HA	1:C:8:LEU:HD12	1.68	0.75
1:B:209:PHE:O	1:B:212:ILE:HG22	1.87	0.75
1:C:5:ILE:HD13	1:C:8:LEU:HD11	1.68	0.74
1:D:130:ILE:HD12	1:D:168:LEU:HD12	1.69	0.74
1:A:143:TYR:HA	5:A:1071:HOH:O	1.88	0.74
1:B:123:VAL:HG13	1:B:169:PRO:O	1.88	0.74
1:D:138:GLU:HG3	1:D:162:ARG:CD	2.16	0.74
1:B:128:MET:HE2	1:B:130:ILE:CD1	2.19	0.73
1:B:20:GLU:OE2	1:B:26:ARG:HD3	1.89	0.73
1:B:35:LYS:HG2	1:B:212:ILE:HD11	1.68	0.72
1:A:155:LEU:CD1	1:A:193:ALA:HB2	2.19	0.72
1:C:138:GLU:HG3	1:C:162:ARG:CD	2.18	0.72
1:A:128:MET:HB2	1:A:130:ILE:HD11	1.71	0.72
1:C:61:ARG:HG2	1:C:94:PRO:HG2	1.70	0.72
1:A:155:LEU:HD12	1:A:193:ALA:HB2	1.70	0.71
1:D:122:THR:HG22	1:D:125:GLY:H	1.56	0.71
1:A:170:GLY:H	2:A:301:IVF:C1	2.04	0.70
1:C:146:LYS:HB2	5:C:3045:HOH:O	1.91	0.70
1:D:90:VAL:O	1:D:93:ILE:HG22	1.90	0.70
1:D:145:HIS:O	1:D:153:VAL:HG22	1.91	0.70
1:D:68:ILE:HD13	1:D:73:VAL:HG13	1.73	0.70
1:A:93:ILE:HG13	1:A:94:PRO:HD2	1.73	0.70
1:B:49:GLU:HG3	1:B:55:MET:SD	2.32	0.70
1:B:158:ASP:O	1:B:202:LYS:HE2	1.91	0.70
1:A:167:GLY:HA3	1:A:171:MET:CE	2.21	0.70
1:C:209:PHE:O	1:C:213:ASP:HB3	1.89	0.70
1:C:21:LYS:HG2	1:C:56:GLU:HG3	1.72	0.69
1:D:147:LYS:HD2	1:D:148:ASN:N	2.06	0.69
1:C:151:THR:HG23	5:C:3036:HOH:O	1.93	0.69
1:C:153:VAL:HG11	1:C:155:LEU:HD21	1.73	0.69
1:A:47:LYS:HG2	1:A:48:PHE:CE2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:LYS:CD	1:D:148:ASN:H	2.07	0.68
1:A:128:MET:HE1	1:A:168:LEU:HD12	1.74	0.68
1:C:37:ASP:HB2	5:C:3032:HOH:O	1.93	0.68
1:D:138:GLU:HG3	1:D:162:ARG:HD2	1.76	0.67
1:C:105:LYS:NZ	5:C:3106:HOH:O	2.27	0.67
1:B:90:VAL:O	1:B:93:ILE:HG22	1.94	0.67
1:D:78:LEU:CD1	1:D:85:VAL:HG22	2.26	0.66
1:D:115:ARG:NH1	5:D:4063:HOH:O	2.27	0.66
1:C:20:GLU:HG2	1:C:21:LYS:N	2.08	0.66
1:D:3:LEU:HB2	5:D:4117:HOH:O	1.95	0.66
1:A:123:VAL:HB	1:A:128:MET:CE	2.26	0.66
1:C:52:TYR:HB2	5:C:3076:HOH:O	1.95	0.66
1:A:115:ARG:O	1:A:134:PRO:HA	1.96	0.65
1:C:83:GLN:HA	1:C:83:GLN:NE2	2.10	0.65
1:C:183:ILE:O	1:C:184:GLN:HG2	1.96	0.65
1:A:146:LYS:O	1:A:147:LYS:HG2	1.95	0.65
1:C:114:ASN:OD1	1:C:136:LYS:NZ	2.29	0.65
1:C:124:ASN:O	1:C:124:ASN:ND2	2.29	0.65
1:C:147:LYS:CG	1:C:148:ASN:H	2.07	0.65
1:A:146:LYS:NZ	1:A:148:ASN:OD1	2.29	0.65
1:B:11:LYS:O	1:B:61:ARG:NH2	2.29	0.65
1:C:78:LEU:HB2	1:C:83:GLN:OE1	1.96	0.65
1:B:73:VAL:CG1	1:B:88:MET:HG3	2.27	0.64
1:D:73:VAL:HG12	1:D:89:LYS:O	1.97	0.64
1:C:43:SER:CB	1:C:47:LYS:HE3	2.27	0.64
1:C:90:VAL:O	1:C:93:ILE:HB	1.97	0.64
1:C:146:LYS:CD	1:C:147:LYS:HE2	2.24	0.64
1:A:164:LYS:NZ	1:A:166:GLU:OE2	2.31	0.64
1:A:123:VAL:CB	1:A:128:MET:HE2	2.28	0.64
1:B:202:LYS:NZ	5:B:2095:HOH:O	2.30	0.64
1:C:37:ASP:OD2	1:C:95:LYS:NZ	2.30	0.64
1:C:34:VAL:HB	1:C:209:PHE:CE1	2.33	0.64
1:B:128:MET:HG3	5:B:2107:HOH:O	1.98	0.63
1:B:76:GLN:HE22	1:B:211:ASN:HB2	1.62	0.63
1:C:148:ASN:O	1:C:150:GLY:N	2.31	0.63
1:C:43:SER:OG	1:C:47:LYS:HE3	1.97	0.63
1:C:83:GLN:NE2	1:C:84:ASP:OD1	2.32	0.63
1:D:215:LYS:O	1:D:216:ILE:HG22	1.98	0.63
1:B:141:ALA:O	1:B:156:THR:HA	1.99	0.63
1:D:130:ILE:CD1	1:D:168:LEU:HD12	2.27	0.63
1:D:21:LYS:NZ	5:D:4048:HOH:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:LYS:HE2	5:B:2041:HOH:O	1.98	0.63
1:C:47:LYS:HD2	5:C:3041:HOH:O	1.99	0.63
1:C:79:ASP:OD1	1:C:79:ASP:N	2.32	0.62
1:C:167:GLY:HA3	1:C:171:MET:CE	2.29	0.62
1:C:153:VAL:CG1	1:C:155:LEU:HD21	2.29	0.62
1:A:72:ASN:ND2	5:A:1081:HOH:O	2.32	0.62
1:C:146:LYS:NZ	5:C:3109:HOH:O	2.32	0.61
1:D:76:GLN:NE2	5:D:4108:HOH:O	2.33	0.61
1:A:141:ALA:O	1:A:156:THR:HA	2.00	0.61
1:D:147:LYS:HA	5:D:4044:HOH:O	2.00	0.61
1:A:52:TYR:CD1	1:A:55:MET:HE2	2.35	0.61
1:D:101:GLN:NE2	5:D:4091:HOH:O	2.27	0.61
1:C:114:ASN:C	1:C:134:PRO:HB3	2.25	0.61
1:A:49:GLU:HG3	1:A:55:MET:SD	2.41	0.61
1:C:168:LEU:HD23	1:C:168:LEU:N	2.15	0.61
1:A:54:MET:HE2	5:A:1078:HOH:O	2.01	0.61
1:C:167:GLY:HA3	1:C:171:MET:HE1	1.83	0.61
1:A:28:VAL:HG13	2:A:301:IVF:H8	1.83	0.61
1:A:145:HIS:CG	1:A:146:LYS:H	2.19	0.61
1:A:47:LYS:HG2	1:A:48:PHE:CD2	2.36	0.60
1:D:20:GLU:HG2	1:D:21:LYS:N	2.16	0.60
1:B:83:GLN:HG3	1:B:86:VAL:CG1	2.32	0.60
1:B:128:MET:HE2	1:B:130:ILE:HD11	1.83	0.60
1:B:153:VAL:HG12	1:B:154:ASP:N	2.16	0.60
1:C:168:LEU:O	1:C:171:MET:HG3	2.01	0.60
5:C:3058:HOH:O	1:D:81:GLY:HA2	2.02	0.60
1:B:68:ILE:HG21	1:B:73:VAL:CG2	2.31	0.60
1:B:52:TYR:CD1	1:B:55:MET:HE1	2.34	0.60
1:C:87:LEU:HD23	1:C:212:ILE:HG21	1.85	0.59
1:A:170:GLY:HA3	2:A:301:IVF:CD1	2.32	0.59
1:C:5:ILE:HA	1:C:8:LEU:CD1	2.33	0.59
1:A:143:TYR:O	1:A:154:ASP:HA	2.01	0.59
1:D:76:GLN:HE22	1:D:211:ASN:CB	2.04	0.59
1:A:181:GLN:HG3	5:A:1105:HOH:O	2.03	0.59
1:C:49:GLU:HB2	5:C:3076:HOH:O	2.03	0.58
1:A:170:GLY:HA3	2:A:301:IVF:H17	1.83	0.58
1:B:79:ASP:HB2	5:B:2098:HOH:O	2.03	0.58
1:B:121:THR:CG2	1:B:174:GLY:HA3	2.32	0.58
1:C:140:LYS:HD2	1:C:158:ASP:OD1	2.03	0.58
1:C:43:SER:HB2	1:C:47:LYS:HE3	1.85	0.58
1:A:155:LEU:HD12	1:A:193:ALA:CB	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:PRO:HG3	5:B:2126:HOH:O	2.02	0.58
1:A:143:TYR:O	1:A:155:LEU:N	2.32	0.58
1:C:198:ILE:HG13	1:C:199:LEU:N	2.17	0.58
1:C:83:GLN:HE21	1:C:84:ASP:N	1.97	0.58
1:D:21:LYS:HE3	1:D:54:MET:CE	2.33	0.57
1:B:43:SER:O	1:B:47:LYS:HB2	2.05	0.57
1:D:215:LYS:HD2	1:D:216:ILE:H	1.68	0.57
1:D:11:LYS:HD2	5:D:4125:HOH:O	2.03	0.57
1:D:42:PRO:HD3	5:D:4016:HOH:O	2.05	0.57
1:C:11:LYS:HE2	5:D:4043:HOH:O	2.05	0.57
1:C:128:MET:HE1	1:C:168:LEU:CD1	2.34	0.57
1:B:121:THR:HG21	1:B:171:MET:O	2.04	0.57
1:C:183:ILE:C	1:C:184:GLN:HG2	2.30	0.57
1:B:130:ILE:HD11	5:B:2093:HOH:O	2.03	0.57
1:C:115:ARG:NH2	5:C:3025:HOH:O	2.38	0.57
1:C:143:TYR:HE2	1:C:157:VAL:CG2	2.18	0.57
1:A:130:ILE:N	1:A:130:ILE:HD12	2.20	0.56
1:C:117:ALA:CB	1:C:176:LEU:HD11	2.35	0.56
1:D:21:LYS:HE3	1:D:54:MET:HE3	1.86	0.56
1:B:154:ASP:C	1:B:155:LEU:HD23	2.29	0.56
1:B:51:ASP:HA	5:B:2033:HOH:O	2.05	0.56
1:A:34:VAL:O	1:A:35:LYS:HB3	2.06	0.56
1:A:44:HIS:HE1	1:A:84:ASP:HB3	1.71	0.56
1:C:68:ILE:CD1	1:C:91:PRO:HD2	2.35	0.56
1:C:117:ALA:HB3	1:C:176:LEU:HD11	1.87	0.56
1:C:170:GLY:N	2:C:301:IVF:O2	2.38	0.56
1:D:151:THR:HG21	5:D:4041:HOH:O	2.04	0.56
1:C:15:GLN:OE1	1:C:15:GLN:N	2.37	0.56
1:B:49:GLU:OE1	1:B:49:GLU:HA	2.06	0.56
1:A:142:THR:HA	1:A:156:THR:HA	1.88	0.56
1:B:115:ARG:HD3	1:B:180:ASN:HB2	1.87	0.56
1:D:83:GLN:HA	1:D:83:GLN:NE2	2.21	0.56
1:C:84:ASP:OD1	1:C:84:ASP:N	2.38	0.55
1:C:207:GLU:O	1:C:210:GLN:HG3	2.06	0.55
1:A:128:MET:O	1:A:129:LEU:HD23	2.06	0.55
1:C:189:GLY:HA3	1:C:202:LYS:O	2.06	0.55
1:C:212:ILE:HG12	1:C:213:ASP:N	2.20	0.55
1:A:87:LEU:HD13	1:A:212:ILE:HG21	1.87	0.55
1:A:121:THR:HG21	1:A:171:MET:O	2.07	0.55
1:A:116:LEU:HA	1:A:133:GLY:HA3	1.89	0.55
1:A:167:GLY:C	1:A:168:LEU:HG	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ARG:CB	1:A:26:ARG:HH11	2.21	0.54
1:D:30:ASN:OD1	1:D:122:THR:HB	2.06	0.54
1:A:109:VAL:N	1:A:110:PRO:HD2	2.23	0.54
1:B:145:HIS:CG	1:B:146:LYS:H	2.25	0.54
1:B:205:THR:H	1:B:208:MET:HG3	1.71	0.54
1:C:90:VAL:HG23	1:C:93:ILE:CG1	2.34	0.54
1:C:90:VAL:HG21	1:C:93:ILE:HG13	1.85	0.54
1:C:43:SER:O	1:C:47:LYS:HG3	2.08	0.54
1:B:2:THR:HG21	5:B:2062:HOH:O	2.08	0.54
1:A:168:LEU:O	1:A:171:MET:HG3	2.08	0.54
1:C:49:GLU:O	1:C:52:TYR:HB3	2.07	0.54
1:D:123:VAL:HG23	1:D:128:MET:HG3	1.90	0.54
1:A:21:LYS:HD3	5:A:1080:HOH:O	2.08	0.54
1:B:149:ASP:HB3	5:B:2087:HOH:O	2.07	0.54
1:C:61:ARG:HB3	1:C:66:TYR:CE2	2.43	0.53
1:B:133:GLY:HA2	1:B:134:PRO:C	2.33	0.53
1:D:121:THR:HG21	1:D:171:MET:O	2.08	0.53
1:A:213:ASP:HB2	5:A:1058:HOH:O	2.07	0.53
1:B:151:THR:C	1:B:152:THR:HG23	2.34	0.53
1:C:100:THR:HG22	1:C:209:PHE:CZ	2.44	0.53
1:D:136:LYS:HB2	3:D:302:DMS:H12	1.91	0.53
1:B:155:LEU:HD23	1:B:155:LEU:N	2.24	0.53
1:D:21:LYS:HE3	1:D:54:MET:SD	2.49	0.53
1:A:30:ASN:OD1	1:A:122:THR:HB	2.09	0.52
1:B:164:LYS:NZ	5:B:2018:HOH:O	2.37	0.52
1:A:49:GLU:CB	1:A:55:MET:HE1	2.39	0.52
1:C:39:LEU:HD11	1:C:90:VAL:HG21	1.91	0.52
1:B:110:PRO:HA	1:B:113:LEU:HD11	1.92	0.52
1:B:146:LYS:O	1:B:146:LYS:HD3	2.09	0.52
1:B:149:ASP:HB2	1:B:152:THR:O	2.10	0.52
1:C:83:GLN:NE2	1:C:84:ASP:H	2.01	0.52
1:D:43:SER:OG	1:D:47:LYS:HE2	2.10	0.52
1:A:44:HIS:ND1	1:A:44:HIS:N	2.56	0.52
1:A:70:ALA:HA	1:A:73:VAL:CG2	2.39	0.52
1:A:26:ARG:HH11	1:A:26:ARG:HB2	1.74	0.52
1:A:77:SER:HB3	1:A:83:GLN:HE22	1.75	0.52
1:A:123:VAL:CG2	1:A:128:MET:HE2	2.41	0.51
1:C:34:VAL:HB	1:C:209:PHE:HE1	1.73	0.51
1:C:39:LEU:HD13	1:C:59:PHE:CE2	2.45	0.51
1:A:47:LYS:HD3	1:A:48:PHE:CE2	2.46	0.51
1:B:184:GLN:HG3	5:B:2077:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:HIS:CG	1:C:146:LYS:N	2.79	0.51
1:C:145:HIS:O	1:C:146:LYS:O	2.28	0.51
1:D:157:VAL:CG1	1:D:160:ALA:HB2	2.40	0.51
1:C:143:TYR:CZ	1:C:155:LEU:HB2	2.46	0.51
1:C:158:ASP:O	1:C:159:GLN:HB2	2.11	0.51
1:D:115:ARG:HD3	1:D:180:ASN:HB2	1.92	0.51
1:A:38:TRP:CZ2	1:A:89:LYS:HE2	2.45	0.51
1:C:39:LEU:HD11	1:C:90:VAL:CG2	2.41	0.51
1:B:81:GLY:C	1:B:83:GLN:H	2.19	0.51
1:B:82:ALA:O	1:B:83:GLN:O	2.29	0.51
1:D:198:ILE:HB	5:D:4103:HOH:O	2.11	0.50
1:A:146:LYS:HD3	1:A:146:LYS:C	2.36	0.50
1:A:198:ILE:O	1:A:199:LEU:HD23	2.10	0.50
1:A:87:LEU:HD13	1:A:212:ILE:CG2	2.41	0.50
1:A:93:ILE:HG13	1:A:94:PRO:CD	2.41	0.50
1:A:116:LEU:HD23	1:A:133:GLY:C	2.36	0.50
1:B:96:PHE:HE1	5:B:2122:HOH:O	1.93	0.50
1:B:147:LYS:NZ	5:B:2038:HOH:O	2.40	0.50
1:C:48:PHE:CE1	1:C:153:VAL:HG21	2.46	0.50
1:A:166:GLU:OE2	1:B:81:GLY:HA2	2.12	0.50
1:B:47:LYS:O	1:B:52:TYR:OH	2.30	0.50
1:A:170:GLY:HA2	2:A:301:IVF:N	2.26	0.50
1:C:10:ARG:NH1	1:D:52:TYR:CE1	2.79	0.50
1:C:20:GLU:HB2	5:C:3094:HOH:O	2.11	0.50
1:D:10:ARG:CZ	1:D:127:PRO:HB3	2.41	0.50
1:B:10:ARG:NH1	5:B:2006:HOH:O	2.31	0.49
1:B:146:LYS:HA	1:B:146:LYS:CE	2.43	0.49
1:C:5:ILE:HD13	1:C:8:LEU:CD1	2.41	0.49
1:B:110:PRO:HA	1:B:113:LEU:CD1	2.43	0.49
1:C:72:ASN:ND2	5:C:3010:HOH:O	2.46	0.49
1:C:43:SER:HA	1:C:46:TYR:CE2	2.47	0.49
1:C:90:VAL:HG23	1:C:90:VAL:O	2.12	0.49
1:C:34:VAL:CB	1:C:209:PHE:HE1	2.25	0.49
1:C:80:VAL:HG12	1:C:81:GLY:N	2.27	0.49
1:D:76:GLN:HG3	1:D:77:SER:N	2.27	0.49
1:D:123:VAL:O	1:D:126:THR:N	2.42	0.49
1:D:138:GLU:HG3	1:D:162:ARG:HD3	1.92	0.49
1:A:151:THR:O	1:A:151:THR:OG1	2.29	0.49
1:C:40:LEU:HD23	1:C:87:LEU:CD1	2.42	0.48
1:C:68:ILE:HD12	1:C:91:PRO:HD2	1.94	0.48
1:C:121:THR:HG22	1:C:122:THR:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:GLU:OE2	1:B:197:SER:OG	2.29	0.48
1:C:180:ASN:HB3	1:C:183:ILE:HD11	1.95	0.48
1:B:35:LYS:HE2	1:B:213:ASP:OD1	2.14	0.48
1:C:79:ASP:HA	5:C:3050:HOH:O	2.13	0.48
1:D:157:VAL:HG11	1:D:160:ALA:HB2	1.94	0.48
1:A:70:ALA:HA	1:A:73:VAL:HG22	1.96	0.48
1:D:180:ASN:OD1	1:D:182:SER:HB2	2.14	0.48
1:B:110:PRO:O	1:B:113:LEU:HD12	2.12	0.48
1:C:30:ASN:ND2	1:C:121:THR:CG2	2.76	0.48
1:C:42:PRO:HA	1:C:85:VAL:HA	1.95	0.48
1:C:164:LYS:HG2	1:D:80:VAL:HG21	1.94	0.48
1:D:68:ILE:HD12	1:D:91:PRO:HD2	1.96	0.48
1:C:13:LEU:HD13	1:C:32:LEU:HD13	1.95	0.48
1:B:180:ASN:HB3	1:B:183:ILE:HG12	1.95	0.47
1:D:19:GLY:HA3	1:D:58:TYR:HE1	1.78	0.47
1:A:141:ALA:HB3	1:A:143:TYR:CE2	2.49	0.47
1:C:109:VAL:O	1:C:113:LEU:HD23	2.14	0.47
1:D:216:ILE:O	1:D:216:ILE:HG23	2.14	0.47
1:A:44:HIS:CE1	1:A:84:ASP:HB3	2.48	0.47
1:A:211:ASN:OD1	1:A:211:ASN:N	2.47	0.47
1:B:106:LYS:HD3	1:B:205:THR:HG21	1.95	0.47
1:C:87:LEU:HD23	1:C:212:ILE:HG23	1.96	0.47
1:A:165:GLY:O	1:A:197:SER:HA	2.14	0.47
5:B:2080:HOH:O	1:C:80:VAL:HA	2.13	0.47
1:C:70:ALA:O	1:C:73:VAL:HG22	2.15	0.47
1:A:28:VAL:HG12	1:A:29:MET:HG2	1.97	0.47
1:C:40:LEU:HD23	1:C:87:LEU:HD12	1.97	0.47
1:C:83:GLN:NE2	1:C:83:GLN:CA	2.78	0.47
1:C:162:ARG:HB3	1:C:198:ILE:HD12	1.97	0.47
1:D:76:GLN:NE2	1:D:211:ASN:HD22	2.12	0.47
1:A:133:GLY:HA2	1:A:134:PRO:C	2.40	0.47
1:C:191:HIS:HE1	1:C:199:LEU:HB3	1.78	0.47
1:C:29:MET:SD	1:C:45:ALA:HB2	2.55	0.47
1:C:140:LYS:HA	1:C:157:VAL:O	2.14	0.47
1:A:108:ASP:C	1:A:110:PRO:HD2	2.39	0.47
1:B:164:LYS:HA	1:B:197:SER:O	2.14	0.46
1:C:30:ASN:ND2	1:C:121:THR:HG22	2.30	0.46
1:B:115:ARG:CD	1:B:180:ASN:HB2	2.44	0.46
1:C:83:GLN:HE21	1:C:83:GLN:HA	1.81	0.46
1:C:147:LYS:HD3	2:C:301:IVF:CG2	2.46	0.46
1:D:5:ILE:O	1:D:9:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:LYS:HA	1:D:21:LYS:HD3	1.66	0.46
1:D:136:LYS:HD2	1:D:138:GLU:OE2	2.15	0.46
1:A:61:ARG:NH1	1:A:94:PRO:O	2.39	0.46
1:A:140:LYS:NZ	1:A:158:ASP:OD1	2.30	0.46
1:B:164:LYS:HG3	1:B:164:LYS:O	2.16	0.46
1:D:128:MET:CE	5:D:4003:HOH:O	2.63	0.46
1:D:153:VAL:O	1:D:153:VAL:HG23	2.15	0.46
1:B:33:GLY:HA3	1:B:96:PHE:CD1	2.50	0.46
1:C:143:TYR:CE2	1:C:157:VAL:HG23	2.50	0.46
1:A:145:HIS:N	1:A:153:VAL:O	2.49	0.46
1:A:213:ASP:N	1:A:213:ASP:OD1	2.49	0.46
1:C:20:GLU:HG3	5:C:3094:HOH:O	2.15	0.46
1:C:141:ALA:O	1:C:156:THR:HA	2.17	0.45
1:B:20:GLU:CD	1:B:26:ARG:HH11	2.25	0.45
1:A:114:ASN:HA	1:A:134:PRO:HB2	1.98	0.45
1:D:122:THR:HG22	1:D:125:GLY:N	2.29	0.45
1:A:11:LYS:HZ1	1:B:51:ASP:HB2	1.81	0.45
1:B:113:LEU:HD21	1:B:137:MET:HB2	1.98	0.45
1:C:137:MET:HG3	1:C:138:GLU:N	2.30	0.45
1:C:148:ASN:OD1	1:C:148:ASN:N	2.50	0.45
1:A:10:ARG:NH1	1:A:127:PRO:HB3	2.29	0.45
1:A:49:GLU:HB2	1:A:55:MET:HE1	1.98	0.45
1:A:166:GLU:HB2	5:A:1126:HOH:O	2.16	0.45
1:D:137:MET:HE2	1:D:137:MET:HB2	1.84	0.45
1:B:15:GLN:NE2	5:B:2108:HOH:O	2.29	0.45
1:B:35:LYS:HG2	1:B:212:ILE:CD1	2.41	0.45
1:C:143:TYR:CE2	1:C:157:VAL:CG2	3.00	0.45
1:D:215:LYS:CD	1:D:216:ILE:H	2.30	0.45
1:B:146:LYS:HA	1:B:146:LYS:HE2	1.99	0.45
1:A:26:ARG:CB	1:A:26:ARG:NH1	2.80	0.45
1:B:29:MET:HE3	1:B:45:ALA:HA	1.99	0.45
1:B:33:GLY:HA3	1:B:96:PHE:CE1	2.52	0.45
1:B:83:GLN:O	1:B:83:GLN:HG2	2.17	0.45
1:A:49:GLU:OE1	1:A:49:GLU:HA	2.16	0.45
1:D:149:ASP:C	1:D:151:THR:H	2.23	0.45
1:D:215:LYS:CG	1:D:216:ILE:N	2.79	0.45
1:C:84:ASP:OD2	1:C:157:VAL:HA	2.17	0.45
1:A:145:HIS:CG	1:A:146:LYS:N	2.85	0.44
1:A:3:LEU:HD23	1:A:3:LEU:HA	1.82	0.44
1:A:170:GLY:N	2:A:301:IVF:C2	2.80	0.44
1:A:189:GLY:HA3	1:A:202:LYS:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:MET:HE2	1:C:159:GLN:HA	2.00	0.44
1:A:69:SER:HB3	1:A:72:ASN:HB2	2.00	0.44
1:C:167:GLY:HA3	1:C:171:MET:SD	2.58	0.44
1:D:170:GLY:O	2:D:301:IVF:H19	2.17	0.44
1:D:195:GLY:O	1:D:196:ASN:HB2	2.18	0.44
1:B:146:LYS:HE2	1:B:146:LYS:CA	2.48	0.44
1:C:83:GLN:HE21	1:C:83:GLN:CA	2.30	0.44
1:D:123:VAL:N	1:D:126:THR:O	2.50	0.44
1:C:59:PHE:CD1	1:C:59:PHE:N	2.86	0.44
1:C:146:LYS:HD2	1:C:147:LYS:HG3	1.99	0.44
1:C:171:MET:HE3	1:C:191:HIS:NE2	2.33	0.44
1:A:141:ALA:HB3	1:A:143:TYR:CZ	2.52	0.43
1:B:84:ASP:OD2	1:B:202:LYS:HE3	2.18	0.43
1:C:143:TYR:HE2	1:C:157:VAL:HG23	1.80	0.43
1:C:167:GLY:N	5:C:3100:HOH:O	2.39	0.43
1:D:21:LYS:HE2	1:D:54:MET:HB3	2.00	0.43
1:D:68:ILE:CD1	1:D:91:PRO:HD2	2.48	0.43
1:A:212:ILE:HG13	1:A:213:ASP:OD1	2.18	0.43
1:C:168:LEU:N	1:C:168:LEU:CD2	2.79	0.43
1:A:26:ARG:NH1	1:A:26:ARG:HB3	2.33	0.43
1:B:14:VAL:HG12	1:B:60:ASN:O	2.18	0.43
1:C:5:ILE:CD1	1:C:8:LEU:HD11	2.43	0.43
1:C:76:GLN:HG3	5:C:3042:HOH:O	2.18	0.43
1:C:146:LYS:HD2	1:C:147:LYS:CG	2.48	0.43
1:A:65:TYR:N	1:A:65:TYR:CD1	2.85	0.43
1:C:147:LYS:HD3	2:C:301:IVF:H11	2.00	0.43
1:C:157:VAL:CG1	1:C:160:ALA:HB2	2.49	0.43
1:B:73:VAL:HG11	1:B:88:MET:HG3	1.99	0.43
1:B:109:VAL:N	1:B:110:PRO:CD	2.82	0.43
1:D:20:GLU:CG	1:D:21:LYS:N	2.80	0.43
1:A:21:LYS:NZ	5:A:1038:HOH:O	2.52	0.43
1:D:21:LYS:O	1:D:22:ASN:HB2	2.19	0.43
1:D:138:GLU:CG	1:D:162:ARG:HD3	2.49	0.43
1:D:139:GLU:OE1	1:D:159:GLN:NE2	2.52	0.43
1:A:168:LEU:H	1:A:171:MET:HE2	1.83	0.43
1:C:38:TRP:CZ2	1:C:89:LYS:HB2	2.53	0.43
1:D:89:LYS:HE3	1:D:217:GLU:HB2	2.00	0.43
1:A:25:VAL:HG22	1:A:58:TYR:CD2	2.53	0.43
1:C:38:TRP:CH2	1:C:89:LYS:HB2	2.54	0.43
1:A:145:HIS:HB3	1:A:153:VAL:O	2.19	0.42
1:C:48:PHE:CZ	1:C:153:VAL:HG11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:VAL:HB	1:C:89:LYS:HB3	2.01	0.42
1:D:168:LEU:HA	1:D:169:PRO:HD3	1.74	0.42
1:C:109:VAL:N	1:C:110:PRO:CD	2.82	0.42
1:C:178:SER:HB2	1:C:188:LEU:HD21	2.00	0.42
1:D:122:THR:HG23	1:D:125:GLY:C	2.45	0.42
1:A:149:ASP:OD1	1:A:149:ASP:N	2.52	0.42
1:B:29:MET:SD	1:B:45:ALA:HB2	2.59	0.42
1:C:115:ARG:O	1:C:134:PRO:HA	2.20	0.42
1:C:152:THR:HA	5:C:3045:HOH:O	2.19	0.42
1:C:152:THR:HG22	1:C:152:THR:O	2.19	0.42
1:D:215:LYS:CD	1:D:216:ILE:N	2.82	0.42
1:C:145:HIS:CD2	1:C:145:HIS:C	2.98	0.42
1:C:191:HIS:CE1	1:C:199:LEU:HB3	2.55	0.42
1:A:10:ARG:HD2	5:B:2034:HOH:O	2.19	0.42
1:A:37:ASP:OD1	1:A:37:ASP:N	2.48	0.42
1:B:119:LEU:HB3	1:B:130:ILE:HB	2.01	0.42
1:A:52:TYR:CE1	1:A:55:MET:CE	3.03	0.42
1:B:136:LYS:O	1:B:161:TRP:HA	2.20	0.42
1:B:168:LEU:HB3	1:B:169:PRO:CD	2.50	0.42
1:B:153:VAL:CG1	1:B:154:ASP:N	2.80	0.42
1:B:144:VAL:HG23	5:B:2088:HOH:O	2.19	0.41
1:A:170:GLY:CA	2:A:301:IVF:N	2.83	0.41
1:C:115:ARG:O	1:C:135:LEU:N	2.47	0.41
1:C:40:LEU:CD2	1:C:87:LEU:CD1	2.99	0.41
1:C:93:ILE:HG23	1:C:94:PRO:HD2	2.02	0.41
1:D:3:LEU:HD12	1:D:3:LEU:HA	1.68	0.41
1:D:78:LEU:HD11	1:D:85:VAL:CG2	2.40	0.41
1:D:122:THR:CG2	1:D:125:GLY:CA	2.98	0.41
1:A:116:LEU:HD23	1:A:133:GLY:HA3	2.03	0.41
1:B:46:TYR:CD1	1:B:46:TYR:C	2.99	0.41
1:C:37:ASP:CG	1:C:95:LYS:NZ	2.79	0.41
1:C:93:ILE:HA	1:C:94:PRO:HD3	1.91	0.41
1:A:100:THR:O	1:A:103:PHE:HB2	2.21	0.41
1:B:81:GLY:C	1:B:83:GLN:N	2.79	0.41
1:C:20:GLU:CG	1:C:21:LYS:N	2.78	0.41
1:D:28:VAL:HG12	1:D:29:MET:HG2	2.03	0.41
1:A:25:VAL:HG22	1:A:58:TYR:CE2	2.56	0.41
1:A:36:ASP:C	1:A:95:LYS:HG2	2.45	0.41
1:A:47:LYS:HD3	1:A:48:PHE:CZ	2.56	0.41
1:C:98:ASP:OD1	1:C:100:THR:OG1	2.32	0.41
1:C:153:VAL:CG1	1:C:155:LEU:CD2	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:THR:HG22	1:D:122:THR:O	2.18	0.41
1:A:189:GLY:O	1:A:190:ILE:HD13	2.21	0.41
1:B:113:LEU:CD2	1:B:137:MET:HB2	2.51	0.41
1:B:33:GLY:HA3	1:B:96:PHE:CG	2.55	0.40
1:B:145:HIS:CG	1:B:146:LYS:N	2.89	0.40
1:C:52:TYR:C	1:C:52:TYR:CD1	2.99	0.40
1:C:153:VAL:HG12	1:C:155:LEU:CD2	2.51	0.40
1:A:11:LYS:HZ2	1:A:11:LYS:HG2	1.67	0.40
1:C:90:VAL:HG23	1:C:93:ILE:HB	2.03	0.40
1:C:167:GLY:CA	1:C:171:MET:SD	3.09	0.40
1:A:111:ARG:O	1:A:180:ASN:ND2	2.45	0.40
1:A:112:ALA:HB3	1:A:161:TRP:CH2	2.56	0.40
1:B:53:GLU:HB3	1:B:54:MET:H	1.49	0.40
1:D:29:MET:HB2	1:D:30:ASN:H	1.70	0.40
1:D:149:ASP:C	1:D:151:THR:N	2.80	0.40
1:A:52:TYR:CE1	1:A:55:MET:HE2	2.56	0.40
1:A:198:ILE:HA	1:A:198:ILE:HD13	1.78	0.40
1:D:170:GLY:HA2	2:D:301:IVF:H17	1.98	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	211/217 (97%)	193 (92%)	14 (7%)	4 (2%)	6	1
1	B	215/217 (99%)	195 (91%)	16 (7%)	4 (2%)	6	1
1	C	211/217 (97%)	195 (92%)	10 (5%)	6 (3%)	4	0
1	D	215/217 (99%)	196 (91%)	17 (8%)	2 (1%)	14	6
All	All	852/868 (98%)	779 (91%)	57 (7%)	16 (2%)	6	1

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ALA
1	B	53	GLU
1	B	83	GLN
1	C	146	LYS
1	C	149	ASP
1	A	83	GLN
1	A	124	ASN
1	C	80	VAL
1	D	22	ASN
1	A	147	LYS
1	B	150	GLY
1	C	81	GLY
1	C	124	ASN
1	D	20	GLU
1	B	149	ASP
1	C	147	LYS

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	178/182 (98%)	148 (83%)	30 (17%)	2	0
1	B	182/182 (100%)	158 (87%)	24 (13%)	4	1
1	C	178/182 (98%)	140 (79%)	38 (21%)	1	0
1	D	182/182 (100%)	160 (88%)	22 (12%)	5	2
All	All	720/728 (99%)	606 (84%)	114 (16%)	2	1

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	11	LYS
1	A	18	VAL
1	A	35	LYS
1	A	47	LYS
1	A	50	LYS

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Mol	Chain	Res	Type
1	A	61	ARG
1	A	68	ILE
1	A	73	VAL
1	A	89	LYS
1	A	93	ILE
1	A	97	ARG
1	A	101	GLN
1	A	111	ARG
1	A	121	THR
1	A	122	THR
1	A	126	THR
1	A	128	MET
1	A	140	LYS
1	A	146	LYS
1	A	151	THR
1	A	153	VAL
1	A	155	LEU
1	A	162	ARG
1	A	164	LYS
1	A	166	GLU
1	A	198	ILE
1	A	211	ASN
1	A	212	ILE
1	A	213	ASP
1	B	21	LYS
1	B	35	LYS
1	B	50	LYS
1	B	51	ASP
1	B	53	GLU
1	B	61	ARG
1	B	69	SER
1	B	80	VAL
1	B	83	GLN
1	B	93	ILE
1	B	104	ILE
1	B	113	LEU
1	B	121	THR
1	B	124	ASN
1	B	128	MET
1	B	139	GLU
1	B	142	THR
1	B	146	LYS

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Mol	Chain	Res	Type
1	B	147	LYS
1	B	148	ASN
1	B	149	ASP
1	B	155	LEU
1	B	164	LYS
1	B	206	GLN
1	C	1	SER
1	C	8	LEU
1	C	11	LYS
1	C	13	LEU
1	C	14	VAL
1	C	35	LYS
1	C	37	ASP
1	C	39	LEU
1	C	61	ARG
1	C	67	SER
1	C	69	SER
1	C	77	SER
1	C	79	ASP
1	C	83	GLN
1	C	84	ASP
1	C	87	LEU
1	C	93	ILE
1	C	111	ARG
1	C	113	LEU
1	C	121	THR
1	C	124	ASN
1	C	130	ILE
1	C	137	MET
1	C	145	HIS
1	C	146	LYS
1	C	147	LYS
1	C	148	ASN
1	C	166	GLU
1	C	168	LEU
1	C	181	GLN
1	C	182	SER
1	C	184	GLN
1	C	196	ASN
1	C	197	SER
1	C	198	ILE
1	C	203	LEU

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Mol	Chain	Res	Type
1	C	212	ILE
1	C	213	ASP
1	D	3	LEU
1	D	13	LEU
1	D	22	ASN
1	D	25	VAL
1	D	47	LYS
1	D	50	LYS
1	D	61	ARG
1	D	73	VAL
1	D	75	ILE
1	D	85	VAL
1	D	106	LYS
1	D	121	THR
1	D	123	VAL
1	D	132	GLU
1	D	146	LYS
1	D	151	THR
1	D	152	THR
1	D	154	ASP
1	D	158	ASP
1	D	164	LYS
1	D	166	GLU
1	D	216	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	60	ASN
1	A	72	ASN
1	A	76	GLN
1	A	185	ASN
1	A	210	GLN
1	B	72	ASN
1	B	76	GLN
1	B	124	ASN
1	B	148	ASN
1	B	206	GLN
1	B	210	GLN
1	C	30	ASN
1	C	44	HIS

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Mol	Chain	Res	Type
1	C	72	ASN
1	C	76	GLN
1	C	83	GLN
1	C	124	ASN
1	C	185	ASN
1	D	72	ASN
1	D	76	GLN
1	D	102	HIS
1	D	159	GLN
1	D	185	ASN
1	D	210	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](#)

6 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	IVF	B	301	1	22,22,23	1.19	1 (4%)	29,29,30	0.67	0
2	IVF	A	301	1	22,22,23	1.23	1 (4%)	29,29,30	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	IVF	C	301	1	22,22,23	1.36	1 (4%)	29,29,30	0.93	1 (3%)
4	GOL	D	303	-	5,5,5	0.65	0	5,5,5	1.31	1 (20%)
2	IVF	D	301	1	22,22,23	1.39	2 (9%)	29,29,30	1.06	3 (10%)
3	DMS	D	302	-	3,3,3	0.12	0	3,3,3	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IVF	B	301	1	-	4/24/24/26	0/1/1/1
2	IVF	A	301	1	-	3/24/24/26	0/1/1/1
2	IVF	C	301	1	-	6/24/24/26	0/1/1/1
4	GOL	D	303	-	-	2/4/4/4	-
2	IVF	D	301	1	-	2/24/24/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	IVF	C-NXT	5.72	1.46	1.32
2	D	301	IVF	C-NXT	5.30	1.45	1.32
2	A	301	IVF	C-NXT	5.11	1.44	1.32
2	B	301	IVF	C-NXT	4.92	1.44	1.32
2	D	301	IVF	CE1-CD1	2.28	1.42	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	IVF	C2-CA2-N2	3.66	120.26	110.32
2	D	301	IVF	CH3-C1-N2	3.32	121.63	116.12
2	D	301	IVF	C-CA-N	-2.30	104.67	110.30
2	D	301	IVF	C2-CA2-N2	2.19	116.27	110.32
4	D	303	GOL	O2-C2-C3	-2.01	100.87	109.18

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	303	GOL	C1-C2-C3-O3
4	D	303	GOL	O2-C2-C3-O3
2	A	301	IVF	C-CA-N-C2
2	B	301	IVF	O-C-CA-N
2	C	301	IVF	O-C-CA-N
2	C	301	IVF	NXT-C-CA-N
2	D	301	IVF	CA-CB-CG-CD1
2	D	301	IVF	CA-CB-CG-CD2
2	C	301	IVF	O-C-CA-CB
2	C	301	IVF	CA-CB-CG-CD2
2	C	301	IVF	CA-CB-CG-CD1
2	B	301	IVF	NXT-C-CA-N
2	B	301	IVF	O-C-CA-CB
2	A	301	IVF	CA-CB-CG-CD2
2	C	301	IVF	O2-C2-CA2-CB2
2	A	301	IVF	CA-CB-CG-CD1
2	B	301	IVF	CA-CB-CG-CD2

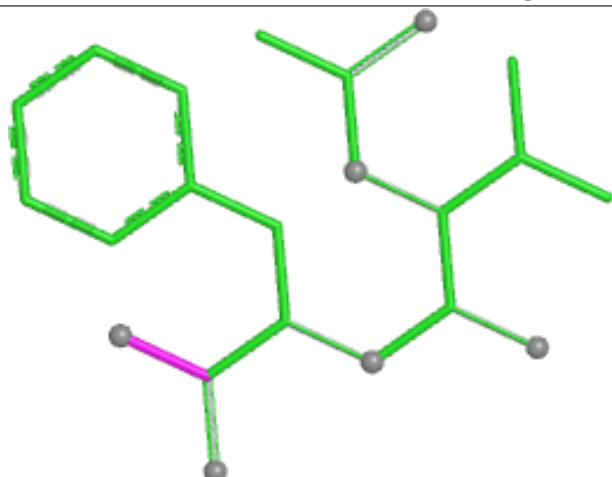
There are no ring outliers.

4 monomers are involved in 15 short contacts:

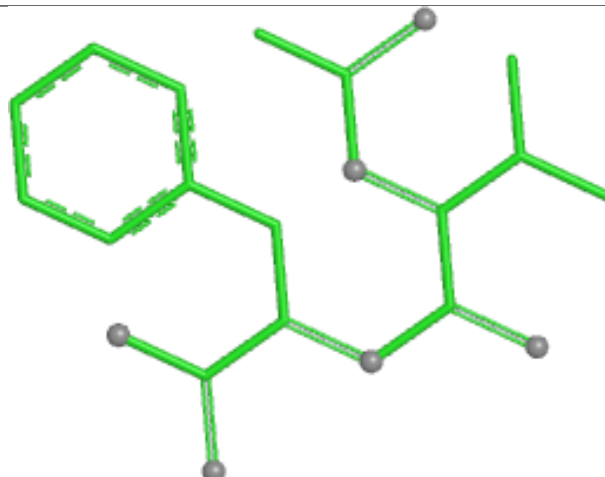
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	IVF	7	0
2	C	301	IVF	3	0
2	D	301	IVF	4	0
3	D	302	DMS	1	0

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.

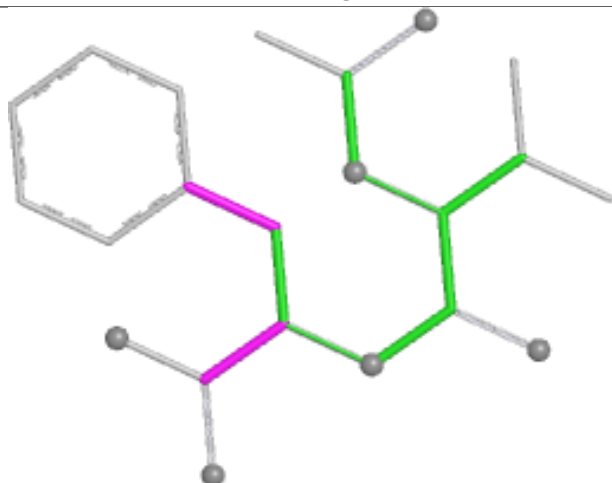
Ligand IVF B 301



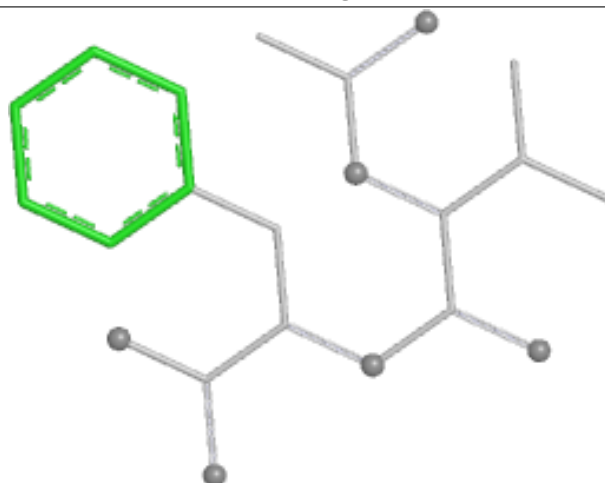
Bond lengths



Bond angles

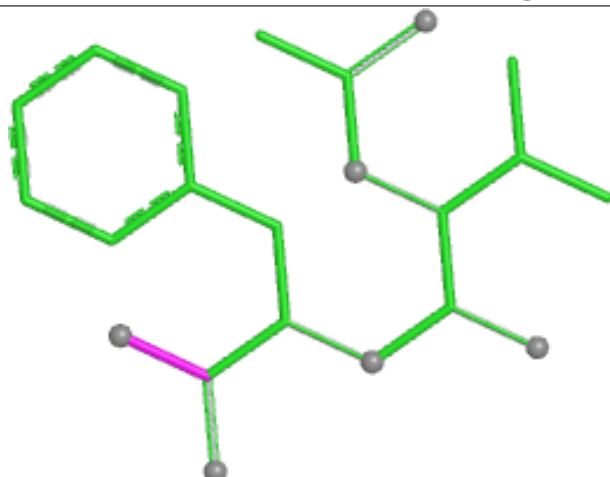


Torsions

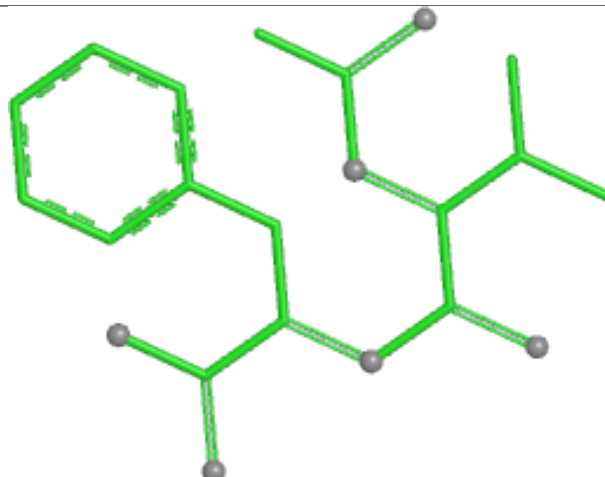


Rings

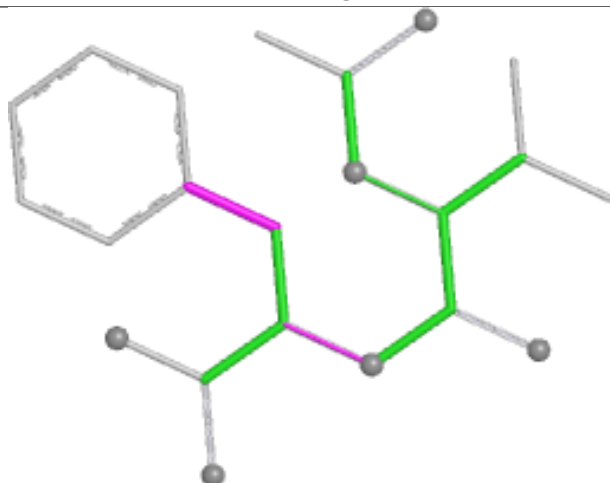
Ligand IVF A 301



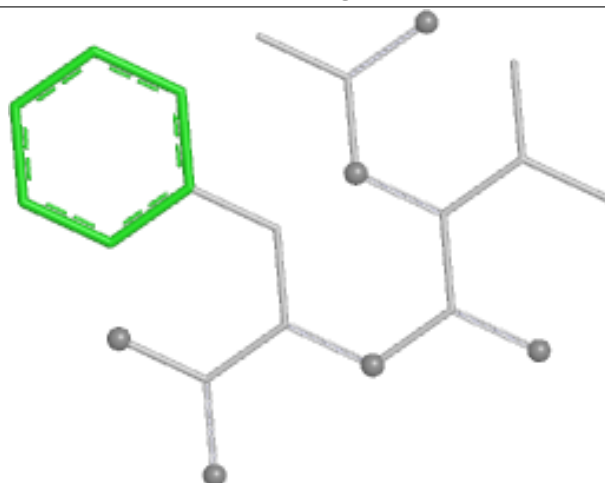
Bond lengths



Bond angles

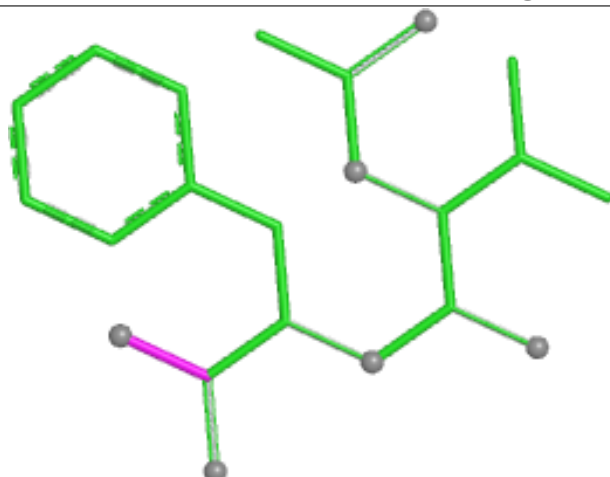


Torsions

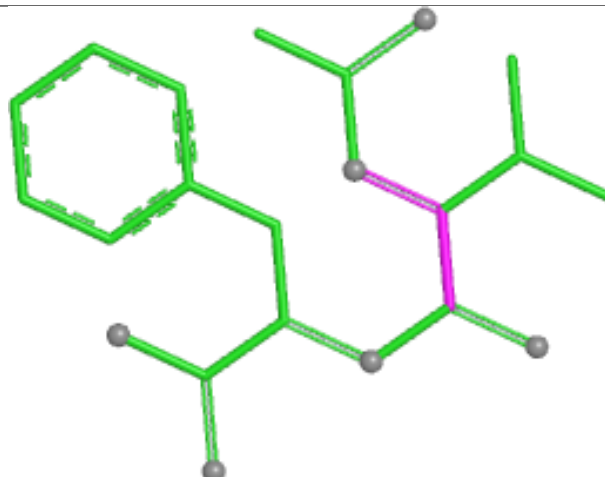


Rings

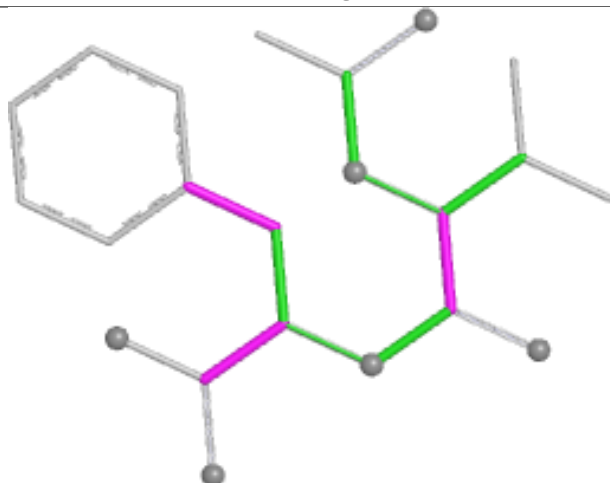
Ligand IVF C 301



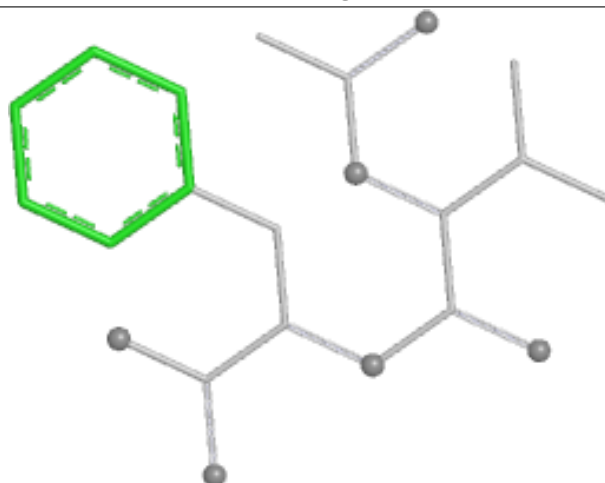
Bond lengths



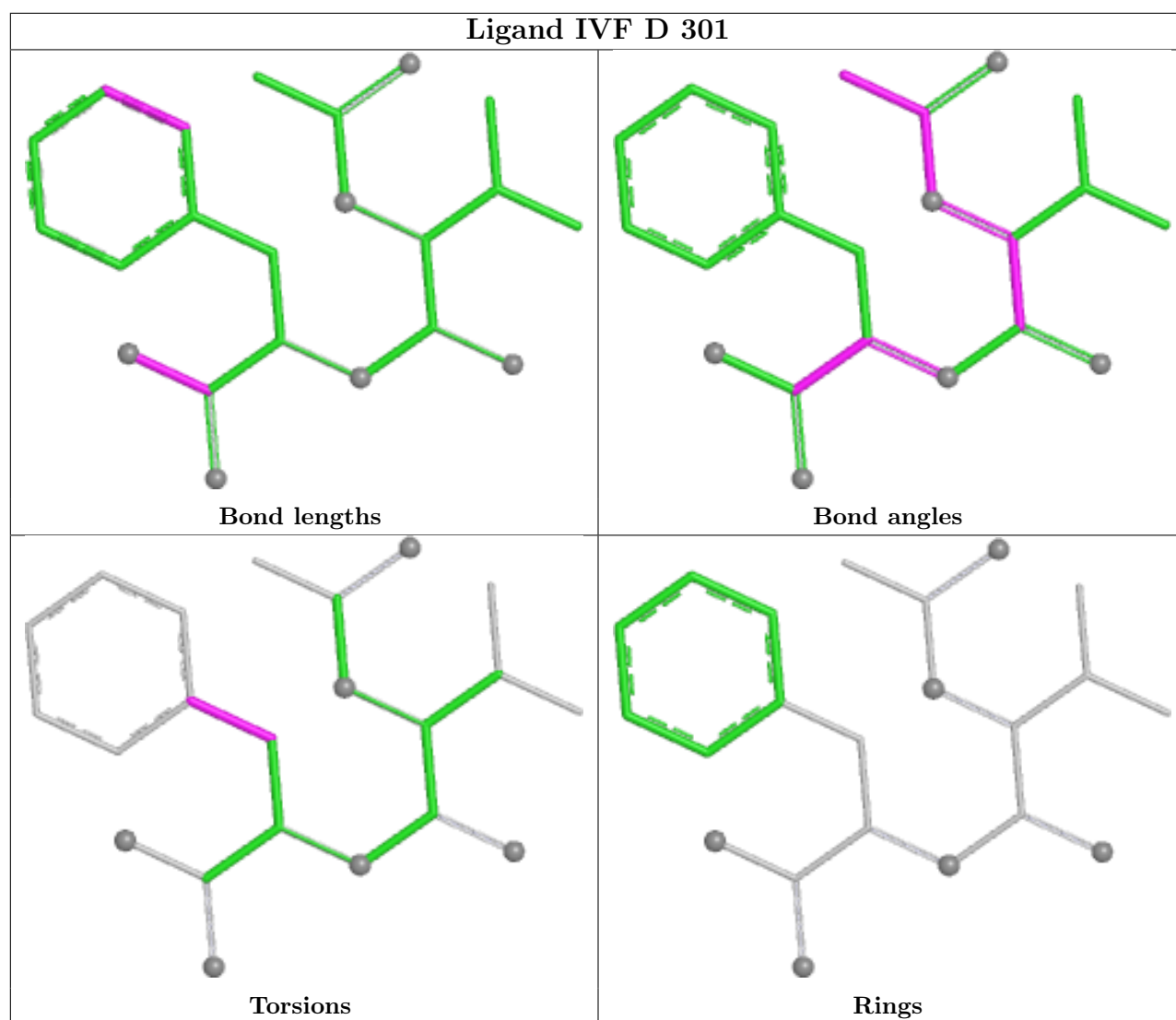
Bond angles



Torsions



Rings



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	213/217 (98%)	-0.05	5 (2%) 61 65	13, 27, 53, 71	0
1	B	217/217 (100%)	-0.07	5 (2%) 61 65	14, 26, 50, 63	0
1	C	213/217 (98%)	0.19	9 (4%) 40 43	16, 31, 55, 67	0
1	D	217/217 (100%)	-0.20	2 (0%) 81 83	11, 23, 47, 55	0
All	All	860/868 (99%)	-0.03	21 (2%) 59 63	11, 27, 52, 71	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	148	ASN	4.0
1	C	149	ASP	3.8
1	B	81	GLY	3.3
1	D	216	ILE	3.1
1	C	147	LYS	3.0
1	B	150	GLY	3.0
1	A	150	GLY	3.0
1	C	152	THR	2.8
1	A	125	GLY	2.6
1	C	93	ILE	2.6
1	C	144	VAL	2.5
1	C	212	ILE	2.5
1	A	152	THR	2.4
1	A	145	HIS	2.4
1	B	133	GLY	2.4
1	C	125	GLY	2.3
1	B	212	ILE	2.2
1	C	151	THR	2.2
1	A	212	ILE	2.1
1	B	151	THR	2.0
1	D	156	THR	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](#)

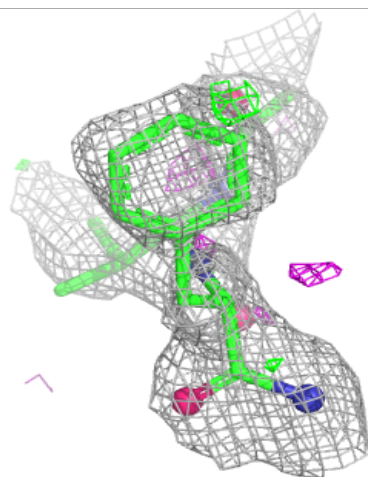
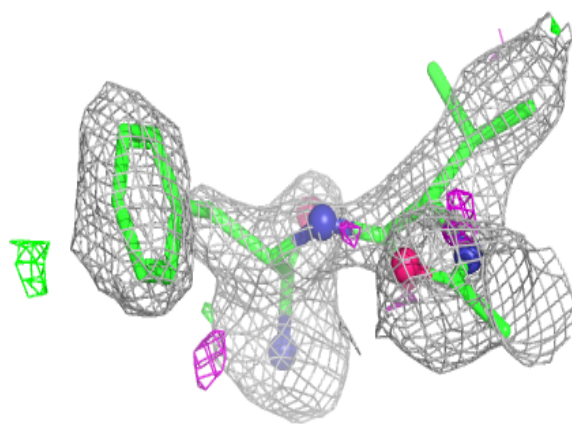
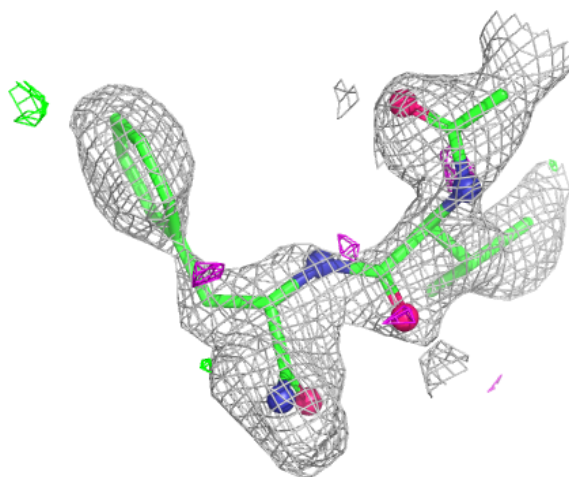
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	IVF	A	301	22/23	0.76	0.13	29,41,49,55	0
2	IVF	C	301	22/23	0.87	0.08	21,33,40,43	0
2	IVF	D	301	22/23	0.88	0.09	18,28,38,43	0
4	GOL	D	303	6/6	0.92	0.07	33,36,38,44	0
2	IVF	B	301	22/23	0.94	0.06	19,26,30,32	0
3	DMS	D	302	4/4	0.96	0.08	22,25,28,32	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.

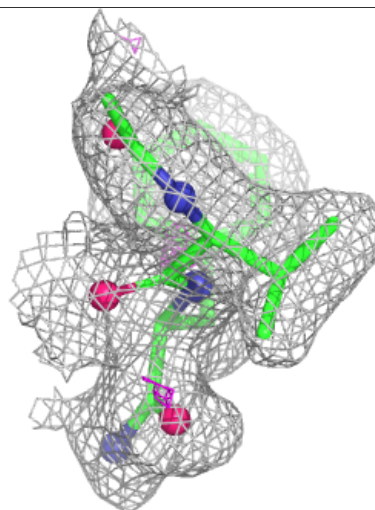
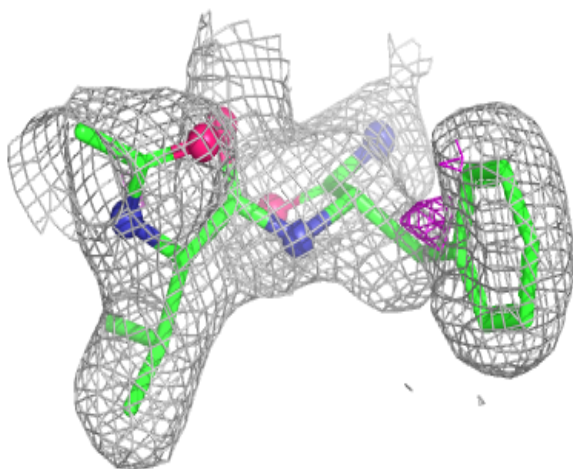
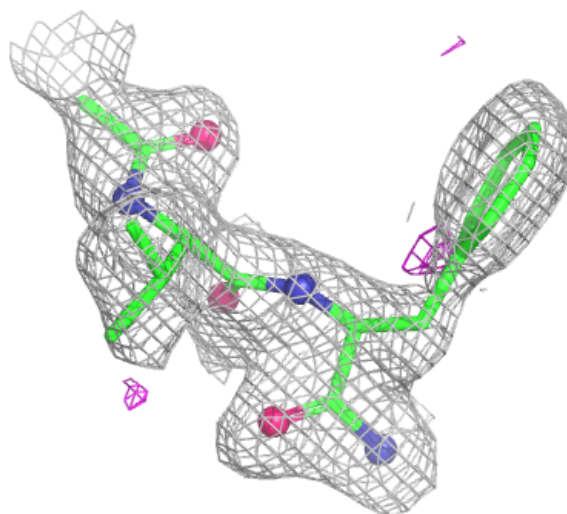
Electron density around IVF A 301:

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



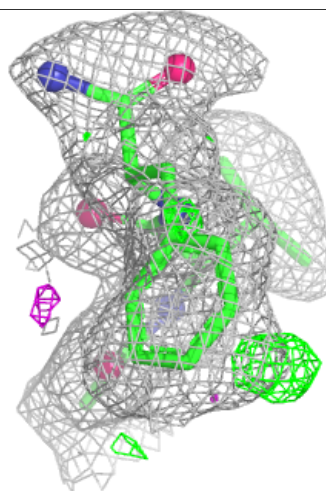
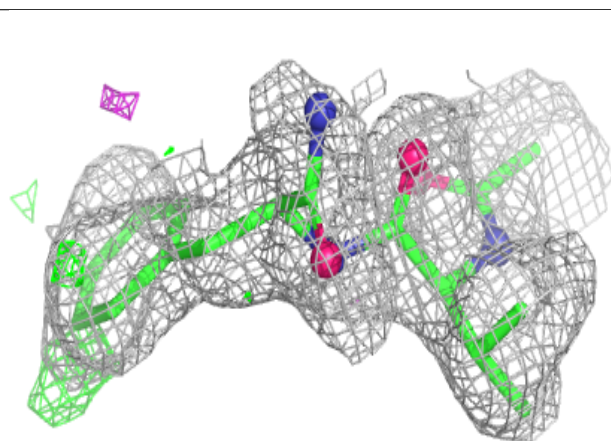
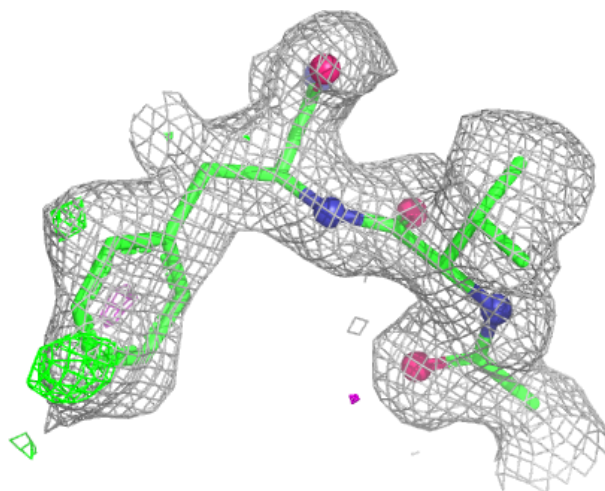
Electron density around IVF C 301:

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



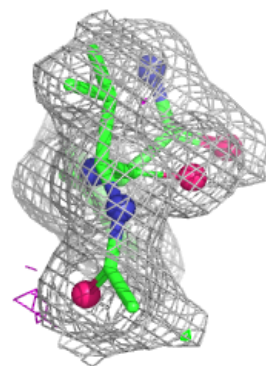
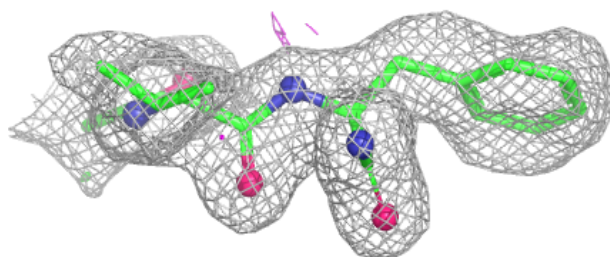
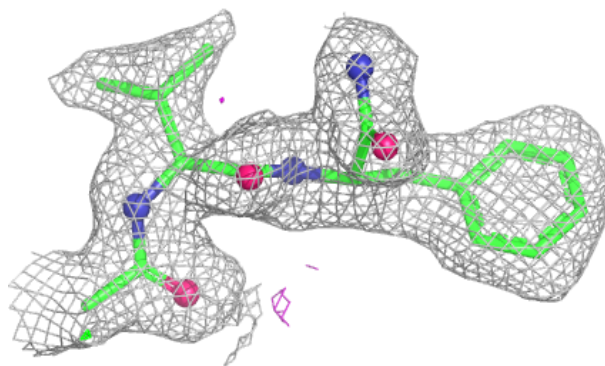
Electron density around IVF D 301:

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



Electron density around IVF B 301:

$2mF_o-DF_c$ (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.