



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:54 pm BST

PDB ID : 1KV3
Title : HUMAN TISSUE TRANSGLUTAMINASE IN GDP BOUND FORM
Authors : Liu, S.; Cerione, R.A.; Clardy, J.
Deposited on : 2002-01-24
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

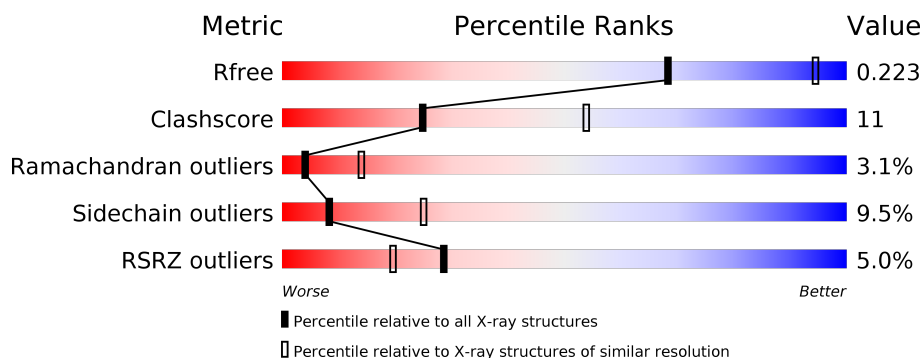
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	687	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>20%</div> <div>5%</div> <div>5%</div> </div> </div>
1	B	687	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>22%</div> <div>5%</div> <div>5%</div> </div> </div>
1	C	687	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>22%</div> <div>5%</div> <div>5%</div> </div> </div>
1	D	687	<div> <div>5%</div> <div> <div></div> <div>65%</div> <div>24%</div> <div>5%</div> <div>5%</div> </div> </div>
1	E	687	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>22%</div> <div>5%</div> <div>5%</div> </div> </div>
1	F	687	<div> <div>6%</div> <div> <div></div> <div>67%</div> <div>23%</div> <div>5%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31466 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 Protein-glutamine gamma-glutamyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	651	Total	C	N	O	S	0	0	0
			5145	3251	889	976	29			
1	B	651	Total	C	N	O	S	0	0	0
			5145	3251	889	976	29			
1	C	651	Total	C	N	O	S	0	0	0
			5145	3251	889	976	29			
1	D	651	Total	C	N	O	S	0	0	0
			5145	3251	889	976	29			
1	E	651	Total	C	N	O	S	0	0	0
			5145	3251	889	976	29			
1	F	651	Total	C	N	O	S	0	0	0
			5145	3251	889	976	29			

There are 30 discrepancies between the modelled and reference sequences:

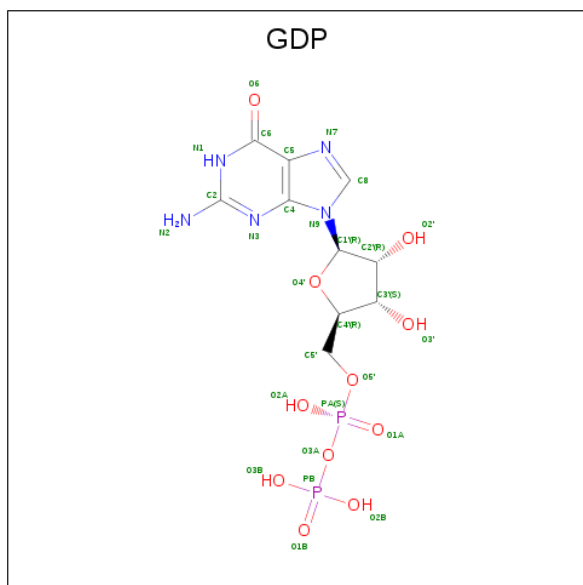
Chain	Residue	Modelled	Actual	Comment	Reference
A	51	GLN	GLU	SEE REMARK 999	UNP P21980
A	186	GLN	GLU	SEE REMARK 999	UNP P21980
A	224	GLY	VAL	SEE REMARK 999	UNP P21980
A	533	THR	ASN	SEE REMARK 999	UNP P21980
A	655	VAL	LEU	SEE REMARK 999	UNP P21980
B	51	GLN	GLU	SEE REMARK 999	UNP P21980
B	186	GLN	GLU	SEE REMARK 999	UNP P21980
B	224	GLY	VAL	SEE REMARK 999	UNP P21980
B	533	THR	ASN	SEE REMARK 999	UNP P21980
B	655	VAL	LEU	SEE REMARK 999	UNP P21980
C	51	GLN	GLU	SEE REMARK 999	UNP P21980
C	186	GLN	GLU	SEE REMARK 999	UNP P21980
C	224	GLY	VAL	SEE REMARK 999	UNP P21980
C	533	THR	ASN	SEE REMARK 999	UNP P21980
C	655	VAL	LEU	SEE REMARK 999	UNP P21980
D	51	GLN	GLU	SEE REMARK 999	UNP P21980
D	186	GLN	GLU	SEE REMARK 999	UNP P21980

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Chain	Residue	Modelled	Actual	Comment	Reference
D	224	GLY	VAL	SEE REMARK 999	UNP P21980
D	533	THR	ASN	SEE REMARK 999	UNP P21980
D	655	VAL	LEU	SEE REMARK 999	UNP P21980
E	51	GLN	GLU	SEE REMARK 999	UNP P21980
E	186	GLN	GLU	SEE REMARK 999	UNP P21980
E	224	GLY	VAL	SEE REMARK 999	UNP P21980
E	533	THR	ASN	SEE REMARK 999	UNP P21980
E	655	VAL	LEU	SEE REMARK 999	UNP P21980
F	51	GLN	GLU	SEE REMARK 999	UNP P21980
F	186	GLN	GLU	SEE REMARK 999	UNP P21980
F	224	GLY	VAL	SEE REMARK 999	UNP P21980
F	533	THR	ASN	SEE REMARK 999	UNP P21980
F	655	VAL	LEU	SEE REMARK 999	UNP P21980

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	F	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

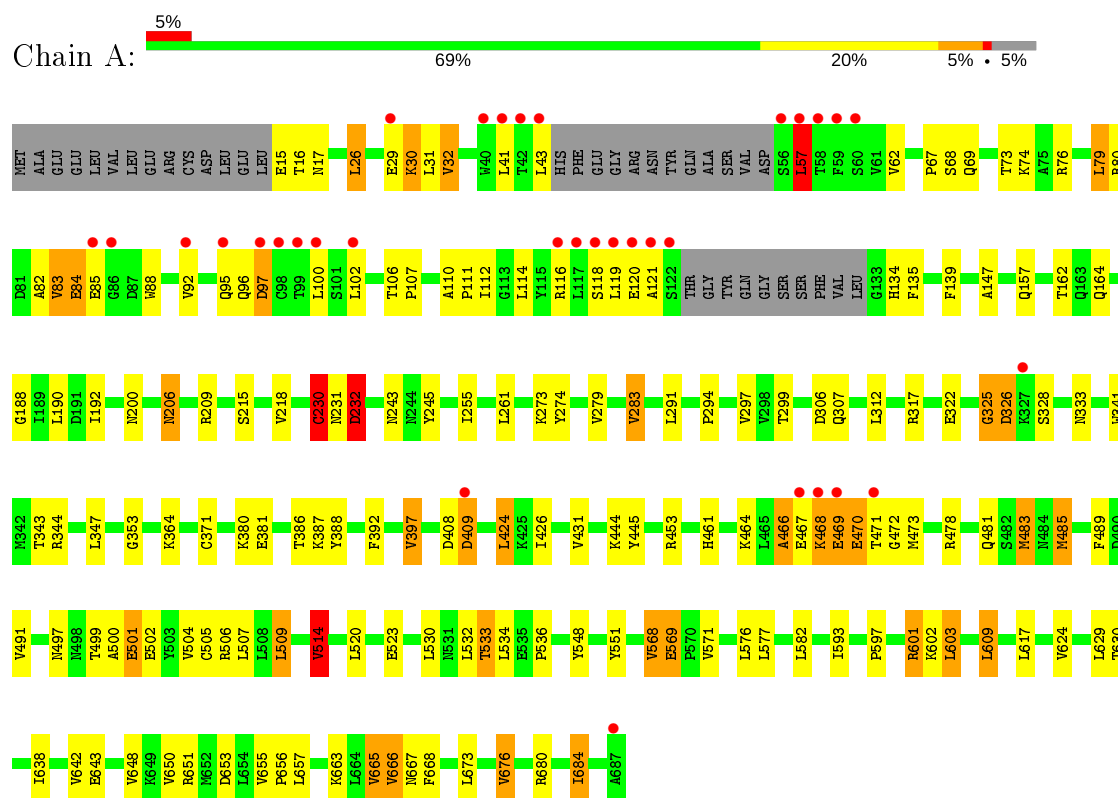
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	64	Total	O	0	0
			64	64		
3	B	68	Total	O	0	0
			68	68		
3	C	104	Total	O	0	0
			104	104		
3	D	66	Total	O	0	0
			66	66		
3	E	72	Total	O	0	0
			72	72		
3	F	54	Total	O	0	0
			54	54		

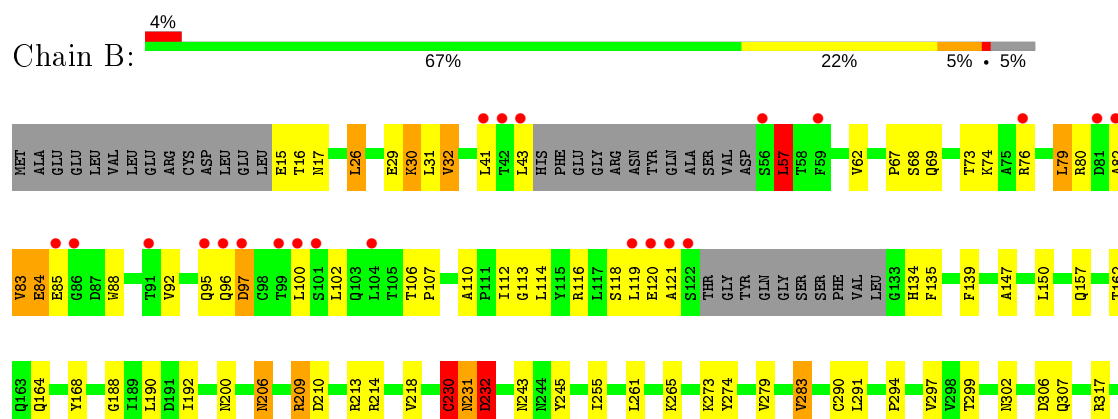
3 Residue-property plots

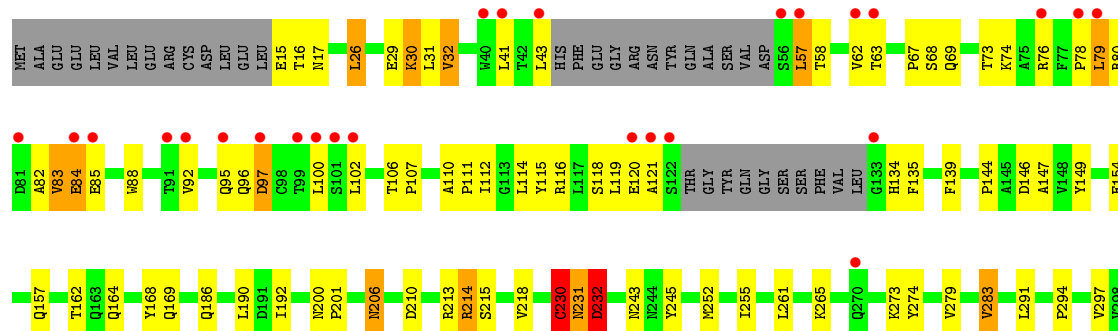
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

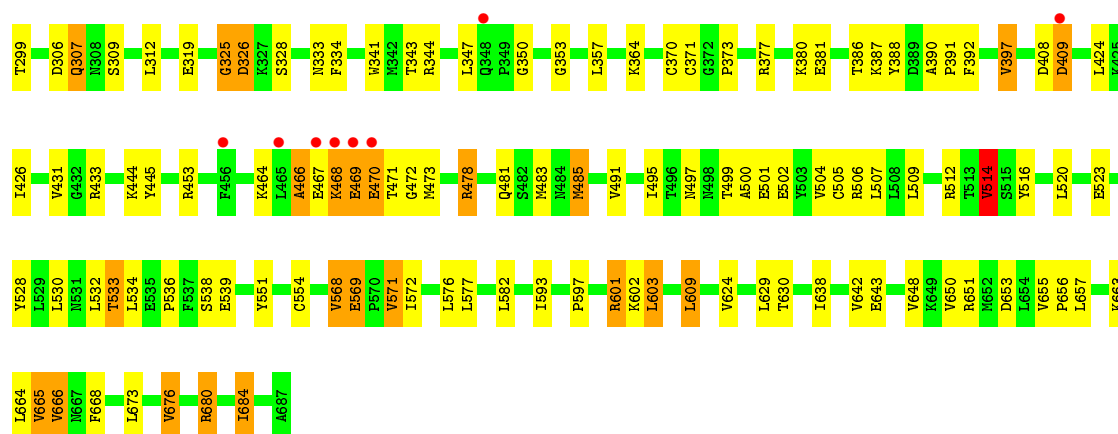
- Molecule 1: Protein-glutamine gamma-glutamyltransferase



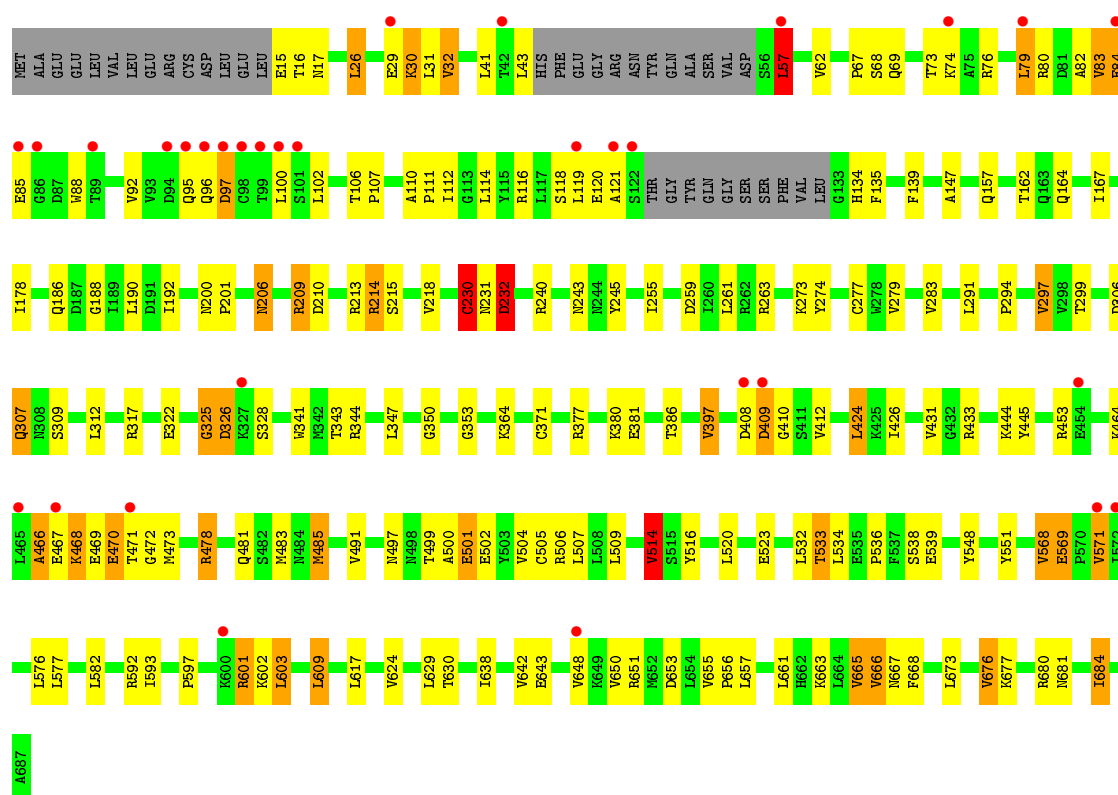
- Molecule 1: Protein-glutamine gamma-glutamyltransferase





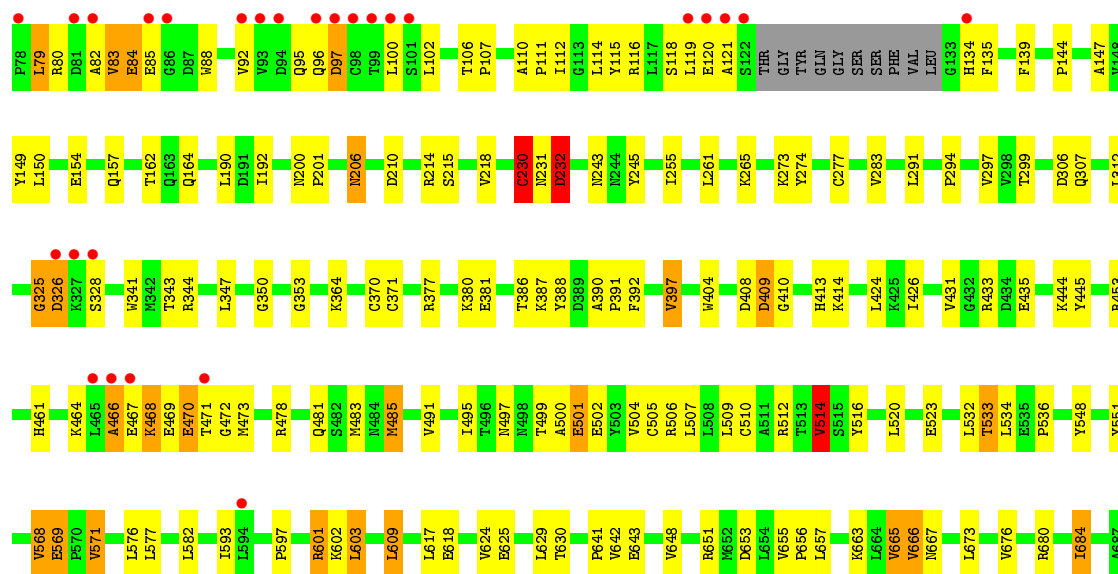


• Molecule 1: Protein-glutamine gamma-glutamyltransferase



• Molecule 1: Protein-glutamine gamma-glutamyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.48 Å 168.80 Å 238.57 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.79 – 2.80 51.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.6 (51.79-2.80) 94.7 (51.79-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 2.81 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.272 0.224 , 0.223	Depositor DCC
R_{free} test set	6274 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31466	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP

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	0.63	0/5256	0.80	5/7131 (0.1%)
1	B	0.65	1/5256 (0.0%)	0.80	5/7131 (0.1%)
1	C	0.69	4/5256 (0.1%)	0.82	4/7131 (0.1%)
1	D	0.66	2/5256 (0.0%)	0.81	4/7131 (0.1%)
1	E	0.63	0/5256	0.80	5/7131 (0.1%)
1	F	0.64	2/5256 (0.0%)	0.81	4/7131 (0.1%)
All	All	0.65	9/31536 (0.0%)	0.81	27/42786 (0.1%)

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

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	290	CYS	CB-SG	-8.31	1.68	1.82
1	C	370	CYS	CB-SG	-7.34	1.69	1.82
1	D	554	CYS	CB-SG	-6.28	1.71	1.82
1	C	277	CYS	CB-SG	-5.95	1.72	1.81
1	F	510	CYS	CB-SG	-5.90	1.72	1.81
1	C	290	CYS	CB-SG	-5.63	1.72	1.81
1	F	370	CYS	CB-SG	-5.37	1.73	1.81
1	C	554	CYS	CB-SG	-5.18	1.73	1.81
1	D	370	CYS	CB-SG	-5.14	1.73	1.81

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	307	GLN	N-CA-C	-6.58	93.22	111.00
1	A	307	GLN	N-CA-C	-6.55	93.31	111.00
1	B	514	VAL	CB-CA-C	-6.43	99.18	111.40
1	E	307	GLN	N-CA-C	-6.28	94.05	111.00
1	B	307	GLN	N-CA-C	-6.27	94.07	111.00
1	C	307	GLN	N-CA-C	-6.26	94.09	111.00
1	C	514	VAL	CB-CA-C	-6.22	99.58	111.40
1	A	514	VAL	CB-CA-C	-6.08	99.86	111.40
1	D	307	GLN	N-CA-C	-6.06	94.64	111.00
1	D	424	LEU	N-CA-C	6.04	127.31	111.00
1	D	514	VAL	CB-CA-C	-5.90	100.19	111.40
1	E	514	VAL	CB-CA-C	-5.88	100.22	111.40
1	C	424	LEU	N-CA-C	5.87	126.84	111.00
1	E	424	LEU	N-CA-C	5.71	126.43	111.00
1	B	424	LEU	N-CA-C	5.56	126.00	111.00
1	A	424	LEU	N-CA-C	5.48	125.80	111.00
1	F	424	LEU	N-CA-C	5.46	125.75	111.00
1	E	232	ASP	N-CA-C	5.34	125.43	111.00
1	F	514	VAL	CB-CA-C	-5.30	101.33	111.40
1	F	232	ASP	N-CA-C	5.26	125.21	111.00
1	D	232	ASP	N-CA-C	5.26	125.19	111.00
1	A	232	ASP	N-CA-C	5.25	125.17	111.00
1	C	232	ASP	N-CA-C	5.21	125.08	111.00
1	B	232	ASP	N-CA-C	5.21	125.06	111.00
1	B	57	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	57	LEU	CA-CB-CG	5.03	126.86	115.30
1	E	57	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	168	TYR	Sidechain
1	C	168	TYR	Sidechain
1	D	168	TYR	Sidechain

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	5145	0	5060	104	0
1	B	5145	0	5060	116	0
1	C	5145	0	5060	110	0
1	D	5145	0	5060	122	0
1	E	5145	0	5060	117	0
1	F	5145	0	5060	105	0
2	A	28	0	12	0	0
2	B	28	0	12	0	0
2	C	28	0	12	0	0
2	D	28	0	12	0	0
2	E	28	0	12	0	0
2	F	28	0	12	0	0
3	A	64	0	0	1	0
3	B	68	0	0	6	0
3	C	104	0	0	4	0
3	D	66	0	0	5	0
3	E	72	0	0	4	0
3	F	54	0	0	1	0
All	All	31466	0	30432	665	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 11.

All (665) 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:D:83:VAL:HG13	1:D:84:GLU:H	1.32	0.95
1:F:83:VAL:HG13	1:F:84:GLU:H	1.31	0.94
1:E:83:VAL:HG13	1:E:84:GLU:H	1.32	0.94
1:B:83:VAL:HG13	1:B:84:GLU:H	1.31	0.94
1:C:83:VAL:HG13	1:C:84:GLU:H	1.33	0.93
1:A:83:VAL:HG13	1:A:84:GLU:H	1.31	0.93
1:C:499:THR:HG22	1:C:501:GLU:H	1.35	0.92
1:D:499:THR:HG22	1:D:501:GLU:H	1.36	0.88
1:D:397:VAL:HG13	1:D:444:LYS:HD2	1.55	0.86
1:B:397:VAL:HG13	1:B:444:LYS:HD2	1.58	0.85
1:A:397:VAL:HG13	1:A:444:LYS:HD2	1.58	0.85
1:E:499:THR:HG22	1:E:501:GLU:H	1.37	0.85
1:A:499:THR:HG22	1:A:501:GLU:H	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:THR:HG22	1:B:501:GLU:H	1.42	0.83
1:B:514:VAL:HG13	1:B:520:LEU:HD23	1.58	0.82
1:F:397:VAL:HG13	1:F:444:LYS:HD2	1.59	0.82
1:F:499:THR:HG22	1:F:501:GLU:H	1.42	0.81
1:C:514:VAL:HG13	1:C:520:LEU:HD23	1.62	0.80
1:A:491:VAL:HG11	1:A:582:LEU:HD21	1.63	0.80
1:E:514:VAL:HG13	1:E:520:LEU:HD23	1.61	0.80
1:B:491:VAL:HG11	1:B:582:LEU:HD21	1.61	0.80
1:F:514:VAL:HG13	1:F:520:LEU:HD23	1.64	0.80
1:F:491:VAL:HG11	1:F:582:LEU:HD21	1.64	0.80
1:D:491:VAL:HG11	1:D:582:LEU:HD21	1.65	0.79
1:E:491:VAL:HG11	1:E:582:LEU:HD21	1.64	0.78
1:E:397:VAL:HG13	1:E:444:LYS:HD2	1.65	0.78
1:C:397:VAL:HG13	1:C:444:LYS:HD2	1.65	0.78
1:C:157:GLN:O	1:C:162:THR:HG23	1.84	0.77
1:C:491:VAL:HG11	1:C:582:LEU:HD21	1.66	0.77
1:E:408:ASP:HA	3:E:711:HOH:O	1.85	0.77
1:D:162:THR:HG21	3:D:730:HOH:O	1.85	0.76
1:B:31:LEU:HD23	1:B:135:PHE:HB3	1.66	0.76
1:D:514:VAL:HG13	1:D:520:LEU:HD23	1.67	0.75
1:A:530:LEU:HD22	1:D:530:LEU:HD21	1.69	0.75
1:A:31:LEU:HD23	1:A:135:PHE:HB3	1.69	0.75
1:E:506:ARG:HG3	1:E:568:VAL:HG13	1.67	0.74
1:C:112:ILE:HG13	1:C:139:PHE:CE2	2.22	0.74
1:C:31:LEU:HD23	1:C:135:PHE:HB3	1.69	0.74
1:E:601:ARG:HG2	1:E:601:ARG:HH11	1.53	0.74
1:A:506:ARG:HG3	1:A:568:VAL:HG13	1.68	0.74
1:C:601:ARG:HG2	1:C:601:ARG:HH11	1.53	0.73
1:A:601:ARG:HG2	1:A:601:ARG:HH11	1.51	0.73
1:B:231:ASN:HB3	3:B:713:HOH:O	1.88	0.73
1:C:147:ALA:HB1	1:C:343:THR:HG22	1.69	0.72
1:A:26:LEU:HB3	1:A:32:VAL:HG11	1.70	0.72
1:A:514:VAL:HG13	1:A:520:LEU:HD23	1.70	0.72
1:B:601:ARG:HG2	1:B:601:ARG:HH11	1.56	0.71
1:C:473:MET:HE3	1:C:534:LEU:HD13	1.71	0.71
1:D:601:ARG:HH11	1:D:601:ARG:HG2	1.55	0.71
1:A:116:ARG:HG2	1:A:134:HIS:CE1	2.27	0.70
1:E:157:GLN:O	1:E:162:THR:HG23	1.91	0.70
1:F:601:ARG:HG2	1:F:601:ARG:HH11	1.55	0.69
1:E:31:LEU:HD23	1:E:135:PHE:HB3	1.74	0.69
1:B:147:ALA:HB1	1:B:343:THR:HG22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ILE:HG13	1:A:139:PHE:CE2	2.27	0.69
1:B:157:GLN:O	1:B:162:THR:HG23	1.92	0.69
1:D:602:LYS:NZ	1:D:653:ASP:HB3	2.08	0.69
1:C:580:ARG:NH1	3:C:751:HOH:O	2.27	0.68
1:A:602:LYS:NZ	1:A:653:ASP:HB3	2.09	0.68
1:E:112:ILE:HG13	1:E:139:PHE:CE2	2.27	0.68
1:E:602:LYS:NZ	1:E:653:ASP:HB3	2.09	0.68
1:F:602:LYS:NZ	1:F:653:ASP:HB3	2.07	0.68
1:B:602:LYS:NZ	1:B:653:ASP:HB3	2.08	0.68
1:F:43:LEU:HD12	1:F:100:LEU:HD23	1.76	0.68
1:D:31:LEU:HD23	1:D:135:PHE:HB3	1.75	0.68
1:B:112:ILE:HG13	1:B:139:PHE:CE2	2.29	0.68
1:D:112:ILE:HG13	1:D:139:PHE:CE2	2.29	0.68
1:C:43:LEU:HD12	1:C:100:LEU:HD23	1.76	0.67
1:C:164:GLN:HB2	3:C:757:HOH:O	1.93	0.67
1:C:602:LYS:NZ	1:C:653:ASP:HB3	2.09	0.67
1:F:31:LEU:HD23	1:F:135:PHE:HB3	1.76	0.67
1:F:147:ALA:HB1	1:F:343:THR:HG22	1.76	0.67
1:C:602:LYS:HZ1	1:C:653:ASP:HB3	1.58	0.67
1:D:147:ALA:HB1	1:D:343:THR:HG22	1.77	0.67
1:A:157:GLN:O	1:A:162:THR:HG23	1.93	0.67
1:F:497:ASN:OD1	1:F:499:THR:HB	1.95	0.67
1:A:147:ALA:HB1	1:A:343:THR:HG22	1.76	0.67
1:B:497:ASN:OD1	1:B:499:THR:HB	1.95	0.67
1:C:506:ARG:HG3	1:C:568:VAL:HG13	1.77	0.67
1:F:506:ARG:HG3	1:F:568:VAL:HG13	1.77	0.67
1:D:157:GLN:O	1:D:162:THR:HG23	1.95	0.66
1:E:485:MET:CE	1:E:551:TYR:HE1	2.08	0.66
1:D:206:ASN:C	1:D:206:ASN:HD22	1.99	0.66
1:C:499:THR:HG22	1:C:501:GLU:N	2.09	0.66
1:D:499:THR:HG22	1:D:501:GLU:N	2.09	0.66
1:F:157:GLN:O	1:F:162:THR:HG23	1.95	0.66
1:E:43:LEU:HD12	1:E:100:LEU:HD23	1.76	0.66
1:E:147:ALA:HB1	1:E:343:THR:HG22	1.77	0.66
1:B:107:PRO:HG2	1:B:110:ALA:HB2	1.78	0.66
1:E:497:ASN:OD1	1:E:499:THR:HB	1.96	0.66
1:E:26:LEU:HB3	1:E:32:VAL:HG11	1.77	0.65
1:F:116:ARG:HG2	1:F:134:HIS:CE1	2.32	0.65
1:C:497:ASN:OD1	1:C:499:THR:HB	1.97	0.65
1:B:506:ARG:HG3	1:B:568:VAL:HG13	1.76	0.65
1:D:497:ASN:OD1	1:D:499:THR:HB	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:GLU:C	1:C:472:GLY:H	2.01	0.65
1:B:116:ARG:HG2	1:B:134:HIS:CE1	2.33	0.64
1:D:502:GLU:HB3	1:D:536:PRO:HD3	1.79	0.64
1:F:26:LEU:HB3	1:F:32:VAL:HG11	1.78	0.64
1:F:112:ILE:HG13	1:F:139:PHE:CE2	2.32	0.64
1:A:206:ASN:HD22	1:A:206:ASN:C	2.00	0.64
1:D:538:SER:HB3	1:E:538:SER:HB3	1.80	0.64
1:B:206:ASN:C	1:B:206:ASN:HD22	2.01	0.64
1:A:502:GLU:HB3	1:A:536:PRO:HD3	1.79	0.63
1:D:506:ARG:HG3	1:D:568:VAL:HG13	1.80	0.63
1:A:41:LEU:O	1:A:102:LEU:HD23	1.99	0.63
1:C:502:GLU:HB3	1:C:536:PRO:HD3	1.79	0.63
1:E:206:ASN:C	1:E:206:ASN:HD22	2.02	0.63
1:F:624:VAL:HG22	1:F:666:VAL:HB	1.81	0.63
1:A:497:ASN:OD1	1:A:499:THR:HB	1.98	0.63
1:E:502:GLU:HB3	1:E:536:PRO:HD3	1.79	0.62
1:E:116:ARG:HG2	1:E:134:HIS:CE1	2.34	0.62
1:A:333:ASN:HB3	3:A:711:HOH:O	1.98	0.62
1:B:43:LEU:HD12	1:B:100:LEU:HD23	1.80	0.62
1:B:26:LEU:HB3	1:B:32:VAL:HG11	1.82	0.62
1:E:499:THR:HG22	1:E:501:GLU:N	2.11	0.62
1:C:116:ARG:HG2	1:C:134:HIS:CE1	2.34	0.62
1:D:26:LEU:HB3	1:D:32:VAL:HG11	1.82	0.62
1:E:603:LEU:HD23	3:E:721:HOH:O	2.00	0.61
1:C:107:PRO:HG2	1:C:110:ALA:HB2	1.82	0.61
1:B:209:ARG:HD2	1:B:213:ARG:CZ	2.31	0.61
1:D:478:ARG:NH2	1:E:478:ARG:NH2	2.48	0.61
1:F:499:THR:HG22	1:F:501:GLU:N	2.14	0.61
1:D:107:PRO:HG2	1:D:110:ALA:HB2	1.83	0.61
1:F:433:ARG:NH1	1:F:435:GLU:HB2	2.16	0.61
1:B:502:GLU:HB3	1:B:536:PRO:HD3	1.82	0.60
1:C:26:LEU:HB3	1:C:32:VAL:HG11	1.82	0.60
1:C:569:GLU:OE2	1:C:571:VAL:HB	2.01	0.60
1:E:624:VAL:HG22	1:E:666:VAL:HB	1.83	0.60
1:C:88:TRP:CZ3	1:C:106:THR:HG22	2.37	0.60
1:D:213:ARG:C	1:D:215:SER:H	2.05	0.60
1:D:116:ARG:HG2	1:D:134:HIS:CE1	2.36	0.60
1:D:43:LEU:HD12	1:D:100:LEU:HD23	1.82	0.60
1:E:41:LEU:O	1:E:102:LEU:HD23	2.01	0.60
1:E:470:GLU:C	1:E:472:GLY:H	2.04	0.60
1:D:470:GLU:C	1:D:472:GLY:H	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:680:ARG:HD3	1:E:433:ARG:HH11	1.66	0.60
1:A:107:PRO:HG2	1:A:110:ALA:HB2	1.84	0.59
1:A:209:ARG:HH11	1:A:209:ARG:HG3	1.66	0.59
1:B:485:MET:CE	1:B:551:TYR:HE1	2.15	0.59
1:E:88:TRP:CZ3	1:E:106:THR:HG22	2.37	0.59
1:B:624:VAL:HG22	1:B:666:VAL:HB	1.83	0.59
1:C:485:MET:CE	1:C:551:TYR:HE1	2.16	0.59
1:F:206:ASN:C	1:F:206:ASN:HD22	2.06	0.59
1:F:569:GLU:OE2	1:F:571:VAL:HB	2.02	0.59
1:A:43:LEU:HD12	1:A:100:LEU:HD23	1.82	0.59
1:E:107:PRO:HG2	1:E:110:ALA:HB2	1.85	0.59
1:F:470:GLU:C	1:F:472:GLY:H	2.05	0.59
1:C:41:LEU:O	1:C:102:LEU:HD23	2.03	0.59
1:D:485:MET:CE	1:D:551:TYR:HE1	2.16	0.59
1:B:88:TRP:CZ3	1:B:106:THR:HG22	2.37	0.59
1:B:470:GLU:C	1:B:472:GLY:H	2.06	0.59
1:A:470:GLU:C	1:A:472:GLY:H	2.05	0.58
1:C:473:MET:CE	1:C:534:LEU:HD13	2.33	0.58
1:D:597:PRO:HA	1:D:603:LEU:HD21	1.85	0.58
1:E:642:VAL:HG21	1:E:648:VAL:HG22	1.84	0.58
1:A:88:TRP:CZ3	1:A:106:THR:HG22	2.38	0.58
1:D:380:LYS:HE2	1:D:445:TYR:CE1	2.38	0.58
1:E:602:LYS:HZ1	1:E:653:ASP:HB3	1.66	0.58
1:D:624:VAL:HG22	1:D:666:VAL:HB	1.86	0.58
1:E:569:GLU:OE2	1:E:571:VAL:HB	2.04	0.58
1:E:68:SER:H	1:E:73:THR:HG23	1.69	0.58
1:F:485:MET:CE	1:F:551:TYR:HE1	2.15	0.58
1:B:597:PRO:HA	1:B:603:LEU:HD21	1.85	0.58
1:B:499:THR:HG22	1:B:501:GLU:N	2.14	0.58
1:D:473:MET:HE3	1:D:534:LEU:HD13	1.86	0.58
1:B:380:LYS:HE2	1:B:445:TYR:CE1	2.38	0.58
1:D:569:GLU:OE2	1:D:571:VAL:HB	2.04	0.58
1:F:107:PRO:HG2	1:F:110:ALA:HB2	1.86	0.58
1:F:602:LYS:HZ1	1:F:653:ASP:HB3	1.69	0.58
1:B:41:LEU:O	1:B:102:LEU:HD23	2.04	0.57
1:E:164:GLN:HG3	1:E:663:LYS:H	1.68	0.57
1:F:473:MET:HE3	1:F:534:LEU:HD13	1.86	0.57
1:A:642:VAL:HG21	1:A:648:VAL:HG22	1.87	0.57
1:C:597:PRO:HA	1:C:603:LEU:HD21	1.85	0.57
1:A:380:LYS:HE2	1:A:445:TYR:CE1	2.39	0.57
1:A:485:MET:CE	1:A:551:TYR:HE1	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:VAL:HG21	1:C:648:VAL:HG22	1.85	0.57
1:F:164:GLN:HG3	1:F:663:LYS:H	1.70	0.57
1:C:231:ASN:HB3	3:C:743:HOH:O	2.04	0.57
1:F:502:GLU:HB3	1:F:536:PRO:HD3	1.86	0.57
1:A:601:ARG:NH1	1:A:601:ARG:HG2	2.20	0.57
1:B:83:VAL:HG13	1:B:84:GLU:N	2.13	0.57
1:B:466:ALA:HB3	1:B:468:LYS:HE3	1.87	0.56
1:B:602:LYS:HZ3	1:B:653:ASP:HB3	1.70	0.56
1:E:597:PRO:HA	1:E:603:LEU:HD21	1.85	0.56
1:D:499:THR:CG2	1:D:501:GLU:H	2.15	0.56
1:F:597:PRO:HA	1:F:603:LEU:HD21	1.88	0.56
1:D:364:LYS:HE3	1:D:371:CYS:SG	2.45	0.56
1:E:466:ALA:HB3	1:E:468:LYS:HE3	1.87	0.56
1:F:88:TRP:CZ3	1:F:106:THR:HG22	2.40	0.56
1:C:68:SER:H	1:C:73:THR:HG23	1.70	0.56
1:D:656:PRO:HB2	1:D:684:ILE:HD13	1.87	0.56
1:F:380:LYS:HE2	1:F:445:TYR:CE1	2.40	0.56
1:C:95:GLN:O	1:C:97:ASP:N	2.38	0.56
1:C:499:THR:CG2	1:C:501:GLU:H	2.14	0.56
1:E:601:ARG:NH1	1:E:601:ARG:HG2	2.20	0.56
1:A:624:VAL:HG22	1:A:666:VAL:HB	1.88	0.56
1:D:642:VAL:HG21	1:D:648:VAL:HG22	1.88	0.56
1:A:164:GLN:HG3	1:A:663:LYS:H	1.71	0.56
1:C:601:ARG:HG2	1:C:601:ARG:NH1	2.20	0.56
1:E:213:ARG:C	1:E:215:SER:H	2.09	0.56
1:C:624:VAL:HG22	1:C:666:VAL:HB	1.88	0.56
1:D:41:LEU:O	1:D:102:LEU:HD23	2.06	0.55
1:A:656:PRO:HB2	1:A:684:ILE:HD13	1.88	0.55
1:F:41:LEU:O	1:F:102:LEU:HD23	2.06	0.55
1:A:499:THR:HG22	1:A:501:GLU:N	2.15	0.55
1:A:569:GLU:OE2	1:A:571:VAL:HB	2.07	0.55
1:C:206:ASN:C	1:C:206:ASN:HD22	2.10	0.55
1:D:164:GLN:HG3	1:D:663:LYS:H	1.71	0.55
1:E:95:GLN:O	1:E:97:ASP:N	2.38	0.55
1:A:116:ARG:HG2	1:A:134:HIS:ND1	2.21	0.55
1:B:642:VAL:HG21	1:B:648:VAL:HG22	1.88	0.55
1:F:243:ASN:HA	1:F:245:TYR:CE2	2.41	0.55
1:B:473:MET:HE3	1:B:534:LEU:HD13	1.89	0.55
1:B:569:GLU:OE2	1:B:571:VAL:HB	2.07	0.55
1:F:68:SER:H	1:F:73:THR:HG23	1.71	0.55
1:A:505:CYS:HB3	1:A:568:VAL:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:ALA:HB3	1:C:468:LYS:HE3	1.87	0.55
1:D:602:LYS:HZ2	1:D:653:ASP:HB3	1.71	0.54
1:C:294:PRO:HB2	1:C:341:TRP:HB3	1.89	0.54
1:D:255:ILE:HB	1:D:665:VAL:CG2	2.37	0.54
1:B:656:PRO:HB2	1:B:684:ILE:HD13	1.88	0.54
1:B:68:SER:H	1:B:73:THR:HG23	1.73	0.54
1:F:294:PRO:HB2	1:F:341:TRP:HB3	1.88	0.54
1:A:597:PRO:HA	1:A:603:LEU:HD21	1.88	0.54
1:D:243:ASN:HA	1:D:245:TYR:CE2	2.42	0.54
1:D:95:GLN:O	1:D:97:ASP:N	2.39	0.54
1:D:68:SER:H	1:D:73:THR:HG23	1.72	0.54
1:C:322:GLU:OE1	1:C:512:ARG:NH1	2.41	0.54
1:D:83:VAL:CG1	1:D:84:GLU:H	2.12	0.54
1:A:317:ARG:HA	1:A:322:GLU:O	2.07	0.53
1:C:243:ASN:HA	1:C:245:TYR:CE2	2.43	0.53
1:E:299:THR:O	1:E:426:ILE:HA	2.07	0.53
1:A:83:VAL:HG13	1:A:84:GLU:N	2.13	0.53
1:F:499:THR:CG2	1:F:501:GLU:H	2.18	0.53
1:D:83:VAL:HG13	1:D:84:GLU:N	2.14	0.53
1:D:325:GLY:O	1:D:326:ASP:HB3	2.09	0.53
1:D:507:LEU:HG	1:D:509:LEU:HD13	1.90	0.53
1:C:116:ARG:HG2	1:C:134:HIS:ND1	2.24	0.53
1:C:656:PRO:HB2	1:C:684:ILE:HD13	1.89	0.53
1:A:68:SER:H	1:A:73:THR:HG23	1.74	0.53
1:A:83:VAL:CG1	1:A:84:GLU:H	2.12	0.53
1:D:466:ALA:HB3	1:D:468:LYS:HE3	1.91	0.53
1:D:88:TRP:CZ3	1:D:106:THR:HG22	2.43	0.52
1:F:83:VAL:HG13	1:F:84:GLU:N	2.13	0.52
1:E:656:PRO:HB2	1:E:684:ILE:HD13	1.91	0.52
1:E:255:ILE:HB	1:E:665:VAL:CG2	2.39	0.52
1:F:57:LEU:H	1:F:57:LEU:HD13	1.74	0.52
1:A:243:ASN:HA	1:A:245:TYR:CE2	2.44	0.52
1:F:255:ILE:HB	1:F:665:VAL:CG2	2.39	0.52
1:F:642:VAL:HG21	1:F:648:VAL:HG22	1.90	0.52
1:E:294:PRO:HB2	1:E:341:TRP:HB3	1.91	0.52
1:E:507:LEU:HG	1:E:509:LEU:HD13	1.92	0.52
1:F:116:ARG:HG2	1:F:134:HIS:ND1	2.24	0.52
1:B:507:LEU:HG	1:B:509:LEU:HD13	1.92	0.52
1:F:507:LEU:HG	1:F:509:LEU:HD13	1.91	0.52
1:A:294:PRO:HB2	1:A:341:TRP:HB3	1.91	0.52
1:B:347:LEU:HD22	1:B:386:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:364:LYS:HG2	1:F:392:PHE:CZ	2.44	0.52
1:A:466:ALA:HB3	1:A:468:LYS:HE3	1.91	0.52
1:D:572:ILE:HD12	3:D:752:HOH:O	2.08	0.52
1:B:255:ILE:HB	1:B:665:VAL:CG2	2.40	0.52
1:C:471:THR:C	1:C:473:MET:H	2.13	0.52
1:F:601:ARG:NH1	1:F:601:ARG:HG2	2.22	0.52
1:A:655:VAL:O	1:A:657:LEU:HD13	2.10	0.51
1:B:601:ARG:HG2	1:B:601:ARG:NH1	2.23	0.51
1:E:116:ARG:HG2	1:E:134:HIS:ND1	2.24	0.51
1:E:213:ARG:O	1:E:215:SER:N	2.43	0.51
1:E:317:ARG:HA	1:E:322:GLU:O	2.10	0.51
1:D:57:LEU:HB2	1:D:120:GLU:O	2.10	0.51
1:F:656:PRO:HB2	1:F:684:ILE:HD13	1.91	0.51
1:B:243:ASN:HA	1:B:245:TYR:CE2	2.46	0.51
1:A:506:ARG:NH1	1:D:528:TYR:OH	2.43	0.51
1:C:507:LEU:HG	1:C:509:LEU:HD13	1.91	0.51
1:D:601:ARG:HG2	1:D:601:ARG:NH1	2.21	0.51
1:E:364:LYS:HE3	1:E:371:CYS:SG	2.50	0.51
1:F:408:ASP:O	1:F:409:ASP:HB3	2.11	0.51
1:B:668:PHE:HB3	1:B:676:VAL:HG13	1.92	0.51
1:A:467:GLU:O	1:A:469:GLU:N	2.43	0.51
1:B:162:THR:HG21	3:B:727:HOH:O	2.10	0.51
1:D:57:LEU:HD13	1:D:57:LEU:H	1.76	0.51
1:E:467:GLU:O	1:E:469:GLU:N	2.44	0.51
1:F:466:ALA:HB3	1:F:468:LYS:HE3	1.90	0.51
1:A:57:LEU:HD13	1:A:57:LEU:H	1.76	0.51
1:B:255:ILE:HG21	1:B:667:ASN:HB2	1.93	0.51
1:E:470:GLU:HG2	1:E:472:GLY:H	1.76	0.51
1:A:548:TYR:HA	1:A:551:TYR:CE2	2.46	0.51
1:C:655:VAL:O	1:C:657:LEU:HD13	2.11	0.51
1:D:473:MET:CE	1:D:534:LEU:HD13	2.40	0.51
1:B:116:ARG:HG2	1:B:134:HIS:ND1	2.25	0.51
1:B:206:ASN:ND2	1:B:209:ARG:H	2.09	0.51
1:E:408:ASP:O	1:E:409:ASP:HB3	2.11	0.51
1:A:668:PHE:HB3	1:A:676:VAL:HG13	1.93	0.50
1:D:344:ARG:HB3	1:D:347:LEU:HD12	1.92	0.50
1:C:277:CYS:SG	1:C:516:TYR:OH	2.67	0.50
1:F:473:MET:CE	1:F:534:LEU:HD13	2.41	0.50
1:A:408:ASP:O	1:A:409:ASP:HB3	2.11	0.50
1:A:602:LYS:HZ1	1:A:653:ASP:HB3	1.74	0.50
1:C:364:LYS:HE3	1:C:371:CYS:SG	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:LEU:HB2	1:F:120:GLU:O	2.11	0.50
1:D:252:MET:HB2	3:D:731:HOH:O	2.11	0.50
1:A:523:GLU:OE2	1:D:523:GLU:HG3	2.12	0.50
1:F:325:GLY:O	1:F:326:ASP:HB3	2.12	0.50
1:A:344:ARG:HB3	1:A:347:LEU:HD12	1.94	0.50
1:F:344:ARG:HB3	1:F:347:LEU:HD12	1.93	0.50
1:F:299:THR:O	1:F:426:ILE:HA	2.12	0.50
1:B:83:VAL:CG1	1:B:84:GLU:H	2.11	0.50
1:F:655:VAL:O	1:F:657:LEU:HD13	2.12	0.50
1:A:279:VAL:O	1:A:283:VAL:HG13	2.12	0.50
1:C:255:ILE:HB	1:C:665:VAL:CG2	2.41	0.50
1:D:471:THR:C	1:D:473:MET:H	2.15	0.50
1:E:57:LEU:HB2	1:E:120:GLU:O	2.12	0.50
1:F:471:THR:C	1:F:473:MET:H	2.15	0.50
1:A:299:THR:O	1:A:426:ILE:HA	2.12	0.49
1:A:602:LYS:HZ2	1:A:653:ASP:HB3	1.74	0.49
1:D:154:GLU:OE2	1:E:592:ARG:HG2	2.12	0.49
1:F:470:GLU:HG2	1:F:472:GLY:H	1.77	0.49
1:A:609:LEU:C	1:A:609:LEU:HD12	2.32	0.49
1:D:408:ASP:O	1:D:409:ASP:HB3	2.11	0.49
1:D:299:THR:O	1:D:426:ILE:HA	2.11	0.49
1:E:467:GLU:C	1:E:469:GLU:H	2.15	0.49
1:E:277:CYS:SG	1:E:516:TYR:OH	2.64	0.49
1:F:273:LYS:HG3	1:F:274:TYR:CE1	2.47	0.49
1:F:347:LEU:HD22	1:F:386:THR:HG23	1.93	0.49
1:C:470:GLU:C	1:C:472:GLY:N	2.65	0.49
1:C:83:VAL:HG13	1:C:84:GLU:N	2.14	0.49
1:D:57:LEU:HD21	1:D:79:LEU:HD12	1.94	0.49
1:E:243:ASN:HA	1:E:245:TYR:CE2	2.47	0.49
1:F:512:ARG:HG2	1:F:523:GLU:HA	1.94	0.49
1:B:113:GLY:CA	3:B:739:HOH:O	2.60	0.49
1:B:230:CYS:O	1:B:232:ASP:N	2.45	0.49
1:D:116:ARG:HG2	1:D:134:HIS:ND1	2.27	0.49
1:E:380:LYS:HE2	1:E:445:TYR:CE1	2.46	0.49
1:E:609:LEU:HD12	1:E:609:LEU:C	2.33	0.49
1:C:57:LEU:HB2	1:C:120:GLU:O	2.12	0.49
1:C:325:GLY:O	1:C:326:ASP:HB3	2.13	0.49
1:D:609:LEU:C	1:D:609:LEU:HD12	2.33	0.49
1:A:255:ILE:HB	1:A:665:VAL:CG2	2.42	0.49
1:A:467:GLU:C	1:A:469:GLU:H	2.14	0.49
1:B:471:THR:C	1:B:473:MET:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:LYS:HG3	1:C:274:TYR:CE1	2.47	0.49
1:D:29:GLU:O	1:D:30:LYS:HB2	2.13	0.49
1:A:57:LEU:HB2	1:A:120:GLU:O	2.12	0.49
1:A:470:GLU:HG2	1:A:472:GLY:H	1.78	0.49
1:B:325:GLY:O	1:B:326:ASP:HB3	2.12	0.49
1:C:467:GLU:HB3	1:C:469:GLU:HG3	1.95	0.49
1:D:655:VAL:O	1:D:657:LEU:HD13	2.13	0.49
1:E:470:GLU:C	1:E:472:GLY:N	2.66	0.49
1:B:294:PRO:HB2	1:B:341:TRP:HB3	1.95	0.49
1:C:609:LEU:C	1:C:609:LEU:HD12	2.33	0.49
1:D:668:PHE:HB3	1:D:676:VAL:HG13	1.94	0.49
1:E:505:CYS:HB3	1:E:568:VAL:O	2.12	0.49
1:E:83:VAL:HG13	1:E:84:GLU:N	2.14	0.49
1:C:350:GLY:O	1:C:377:ARG:NH1	2.46	0.48
1:C:408:ASP:O	1:C:409:ASP:HB3	2.13	0.48
1:C:380:LYS:HE2	1:C:445:TYR:CE1	2.48	0.48
1:C:624:VAL:CG1	1:C:664:LEU:HD11	2.43	0.48
1:D:364:LYS:HG2	1:D:392:PHE:CZ	2.48	0.48
1:D:467:GLU:C	1:D:469:GLU:H	2.16	0.48
1:E:467:GLU:HB3	1:E:469:GLU:HG3	1.95	0.48
1:F:467:GLU:HB3	1:F:469:GLU:HG3	1.95	0.48
1:A:325:GLY:O	1:A:326:ASP:HB3	2.12	0.48
1:C:467:GLU:C	1:C:469:GLU:H	2.17	0.48
1:D:294:PRO:HB2	1:D:341:TRP:HB3	1.93	0.48
1:E:471:THR:C	1:E:473:MET:H	2.16	0.48
1:B:57:LEU:HB2	1:B:120:GLU:O	2.12	0.48
1:B:491:VAL:CG1	1:B:582:LEU:HD21	2.40	0.48
1:D:169:GLN:HG2	1:D:334:PHE:CZ	2.49	0.48
1:D:470:GLU:HG2	1:D:472:GLY:H	1.78	0.48
1:F:15:GLU:C	1:F:17:ASN:H	2.15	0.48
1:B:279:VAL:O	1:B:283:VAL:HG13	2.12	0.48
1:C:467:GLU:O	1:C:469:GLU:N	2.46	0.48
1:C:57:LEU:HD13	1:C:57:LEU:H	1.77	0.48
1:E:279:VAL:O	1:E:283:VAL:HG13	2.13	0.48
1:F:504:VAL:HG22	1:F:533:THR:HG23	1.95	0.48
1:A:507:LEU:HG	1:A:509:LEU:HD13	1.94	0.48
1:C:506:ARG:NH1	3:C:768:HOH:O	2.46	0.48
1:D:279:VAL:O	1:D:283:VAL:HG13	2.12	0.48
1:D:467:GLU:O	1:D:469:GLU:N	2.47	0.48
1:E:83:VAL:CG1	1:E:84:GLU:H	2.13	0.48
1:F:467:GLU:C	1:F:469:GLU:H	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:GLU:O	1:B:469:GLU:N	2.46	0.48
1:D:79:LEU:HD21	1:D:92:VAL:HB	1.95	0.48
1:E:15:GLU:C	1:E:17:ASN:H	2.16	0.48
1:E:344:ARG:HB3	1:E:347:LEU:HD12	1.95	0.48
1:F:602:LYS:HZ3	1:F:653:ASP:HB3	1.78	0.48
1:B:470:GLU:HG2	1:B:472:GLY:H	1.79	0.48
1:C:642:VAL:HG11	1:C:648:VAL:HG22	1.95	0.48
1:F:467:GLU:O	1:F:469:GLU:N	2.46	0.48
1:F:79:LEU:HD21	1:F:92:VAL:HB	1.96	0.48
1:B:67:PRO:HB2	1:B:74:LYS:HB2	1.96	0.48
1:C:164:GLN:HG3	1:C:663:LYS:H	1.77	0.48
1:B:344:ARG:HB3	1:B:347:LEU:HD12	1.95	0.48
1:B:473:MET:CE	1:B:534:LEU:HD13	2.44	0.48
1:B:499:THR:CG2	1:B:501:GLU:H	2.19	0.48
1:B:504:VAL:HG22	1:B:533:THR:HG23	1.95	0.48
1:D:593:ILE:HG23	1:D:603:LEU:HD11	1.96	0.48
1:E:307:GLN:O	1:E:309:SER:N	2.42	0.48
1:A:470:GLU:C	1:A:472:GLY:N	2.67	0.48
1:D:601:ARG:HB3	3:D:759:HOH:O	2.14	0.47
1:C:82:ALA:O	1:C:83:VAL:HB	2.14	0.47
1:E:499:THR:CG2	1:E:501:GLU:H	2.17	0.47
1:A:473:MET:CE	1:A:534:LEU:HD13	2.43	0.47
1:B:467:GLU:C	1:B:469:GLU:H	2.17	0.47
1:D:15:GLU:C	1:D:17:ASN:H	2.16	0.47
1:D:470:GLU:C	1:D:472:GLY:N	2.67	0.47
1:F:67:PRO:HB2	1:F:74:LYS:HB2	1.97	0.47
1:D:67:PRO:HB2	1:D:74:LYS:HB2	1.96	0.47
1:B:164:GLN:HG3	1:B:663:LYS:H	1.78	0.47
1:C:299:THR:O	1:C:426:ILE:HA	2.14	0.47
1:F:548:TYR:HA	1:F:551:TYR:CE2	2.49	0.47
1:A:473:MET:HE3	1:A:534:LEU:HD13	1.95	0.47
1:D:273:LYS:HG3	1:D:274:TYR:CE1	2.49	0.47
1:D:307:GLN:O	1:D:309:SER:N	2.44	0.47
1:A:273:LYS:HG3	1:A:274:TYR:CE1	2.49	0.47
1:B:29:GLU:O	1:B:30:LYS:HB2	2.14	0.47
1:D:347:LEU:HD22	1:D:386:THR:HG23	1.96	0.47
1:E:230:CYS:O	1:E:232:ASP:N	2.47	0.47
1:E:504:VAL:HG22	1:E:533:THR:HG23	1.95	0.47
1:E:57:LEU:HD13	1:E:57:LEU:H	1.79	0.47
1:F:255:ILE:HG21	1:F:667:ASN:HB2	1.95	0.47
1:A:467:GLU:HB3	1:A:469:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:GLY:O	1:B:377:ARG:NH1	2.48	0.47
1:B:467:GLU:HB3	1:B:469:GLU:HG3	1.96	0.47
1:C:504:VAL:HG22	1:C:533:THR:HG23	1.97	0.47
1:D:231:ASN:HB3	3:D:724:HOH:O	2.15	0.47
1:A:347:LEU:HD22	1:A:386:THR:HG23	1.96	0.47
1:A:471:THR:C	1:A:473:MET:H	2.17	0.47
1:A:483:MET:HG2	1:A:489:PHE:CD1	2.49	0.47
1:E:347:LEU:HD22	1:E:386:THR:HG23	1.96	0.47
1:E:593:ILE:HG23	1:E:603:LEU:HD11	1.96	0.47
1:B:602:LYS:HZ1	1:B:653:ASP:HB3	1.79	0.47
1:E:473:MET:CE	1:E:534:LEU:HD13	2.45	0.47
1:F:470:GLU:C	1:F:472:GLY:N	2.68	0.47
1:A:504:VAL:HG22	1:A:533:THR:HG23	1.96	0.47
1:C:505:CYS:HB3	1:C:568:VAL:O	2.15	0.46
1:D:602:LYS:HZ1	1:D:653:ASP:HB3	1.78	0.46
1:B:408:ASP:O	1:B:409:ASP:HB3	2.16	0.46
1:C:255:ILE:HG21	1:C:667:ASN:HB2	1.97	0.46
1:E:188:GLY:O	1:E:192:ILE:HG13	2.15	0.46
1:E:255:ILE:HG21	1:E:667:ASN:HB2	1.97	0.46
1:F:230:CYS:O	1:F:232:ASP:N	2.47	0.46
1:A:499:THR:CG2	1:A:501:GLU:H	2.20	0.46
1:D:144:PRO:HA	1:D:149:TYR:CG	2.51	0.46
1:D:504:VAL:HG22	1:D:533:THR:HG23	1.98	0.46
1:E:79:LEU:HD21	1:E:92:VAL:HB	1.97	0.46
1:E:29:GLU:O	1:E:30:LYS:HB2	2.15	0.46
1:B:113:GLY:HA3	3:B:739:HOH:O	2.14	0.46
1:B:15:GLU:C	1:B:17:ASN:H	2.18	0.46
1:D:333:ASN:HB2	1:D:516:TYR:O	2.14	0.46
1:A:364:LYS:HE3	1:A:371:CYS:SG	2.55	0.46
1:F:29:GLU:O	1:F:30:LYS:HB2	2.15	0.46
1:C:470:GLU:HG2	1:C:472:GLY:H	1.79	0.46
1:C:83:VAL:CG1	1:C:84:GLU:H	2.14	0.46
1:F:505:CYS:HB3	1:F:568:VAL:O	2.15	0.46
1:F:57:LEU:HD21	1:F:79:LEU:HD12	1.97	0.46
1:F:609:LEU:HD12	1:F:609:LEU:C	2.37	0.46
1:F:95:GLN:O	1:F:97:ASP:N	2.43	0.46
1:B:470:GLU:C	1:B:472:GLY:N	2.68	0.46
1:B:57:LEU:HD13	1:B:57:LEU:H	1.79	0.46
1:C:15:GLU:C	1:C:17:ASN:H	2.17	0.46
1:C:347:LEU:HD22	1:C:386:THR:HG23	1.98	0.46
1:D:230:CYS:O	1:D:232:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:467:GLU:HB3	1:D:469:GLU:HG3	1.96	0.46
1:E:325:GLY:O	1:E:326:ASP:HB3	2.15	0.46
1:D:539:GLU:HB2	1:E:539:GLU:HB2	1.98	0.46
1:A:15:GLU:C	1:A:17:ASN:H	2.19	0.45
1:A:29:GLU:O	1:A:30:LYS:HB2	2.15	0.45
1:D:210:ASP:O	1:D:214:ARG:HG3	2.17	0.45
1:F:390:ALA:N	1:F:391:PRO:HD2	2.31	0.45
1:B:82:ALA:O	1:B:83:VAL:HB	2.16	0.45
1:C:29:GLU:O	1:C:30:LYS:HB2	2.17	0.45
1:A:230:CYS:O	1:A:232:ASP:N	2.49	0.45
1:B:505:CYS:HB3	1:B:568:VAL:O	2.16	0.45
1:A:79:LEU:HD21	1:A:92:VAL:HB	1.98	0.45
1:D:380:LYS:HE2	1:D:445:TYR:CZ	2.52	0.45
1:F:413:HIS:HB3	3:F:722:HOH:O	2.17	0.45
1:A:67:PRO:HB2	1:A:74:LYS:HB2	1.97	0.45
1:C:210:ASP:O	1:C:214:ARG:HG3	2.15	0.45
1:C:642:VAL:HG21	1:C:648:VAL:CG2	2.47	0.45
1:B:273:LYS:HG3	1:B:274:TYR:CE1	2.51	0.45
1:B:409:ASP:HB3	3:B:729:HOH:O	2.15	0.45
1:B:655:VAL:O	1:B:657:LEU:HD13	2.17	0.45
1:E:424:LEU:HA	1:E:424:LEU:HD23	1.74	0.45
1:F:364:LYS:HE3	1:F:371:CYS:SG	2.57	0.45
1:B:387:LYS:HA	1:B:388:TYR:HA	1.82	0.45
1:B:408:ASP:HA	3:B:734:HOH:O	2.17	0.45
1:D:213:ARG:O	1:D:215:SER:N	2.48	0.45
1:C:230:CYS:O	1:C:232:ASP:N	2.50	0.45
1:C:67:PRO:HB2	1:C:74:LYS:HB2	1.98	0.45
1:D:499:THR:CG2	1:D:500:ALA:N	2.80	0.45
1:A:387:LYS:HA	1:A:388:TYR:HA	1.86	0.45
1:D:473:MET:HE1	1:D:495:ILE:CG2	2.47	0.45
1:F:404:TRP:CZ3	1:F:414:LYS:HB2	2.52	0.45
1:A:82:ALA:O	1:A:83:VAL:HB	2.17	0.45
1:E:206:ASN:ND2	1:E:209:ARG:H	2.14	0.45
1:C:79:LEU:HD21	1:C:92:VAL:HB	1.99	0.44
1:D:642:VAL:HG11	1:D:648:VAL:HG22	1.98	0.44
1:E:499:THR:CG2	1:E:500:ALA:N	2.79	0.44
1:A:593:ILE:HG23	1:A:603:LEU:HD11	1.99	0.44
1:B:210:ASP:O	1:B:214:ARG:HG3	2.16	0.44
1:C:512:ARG:NH1	1:C:523:GLU:HG2	2.32	0.44
1:D:387:LYS:HG2	1:D:388:TYR:CD2	2.53	0.44
1:E:642:VAL:HG11	1:E:648:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:PRO:HB2	1:E:74:LYS:HB2	1.98	0.44
1:A:188:GLY:O	1:A:192:ILE:HG13	2.18	0.44
1:A:364:LYS:HG2	1:A:392:PHE:CZ	2.52	0.44
1:C:364:LYS:HG2	1:C:392:PHE:CZ	2.53	0.44
1:A:206:ASN:ND2	1:A:209:ARG:H	2.16	0.44
1:E:209:ARG:HD3	1:E:209:ARG:HA	1.47	0.44
1:A:642:VAL:HG11	1:A:648:VAL:HG22	1.98	0.44
1:F:192:ILE:HG12	1:F:265:LYS:HD2	1.99	0.44
1:D:624:VAL:CG1	1:D:664:LEU:HD11	2.48	0.44
1:E:350:GLY:O	1:E:377:ARG:NH1	2.50	0.44
1:F:408:ASP:O	1:F:409:ASP:CB	2.65	0.44
1:F:82:ALA:O	1:F:83:VAL:HB	2.17	0.44
1:B:638:ILE:CD1	1:B:650:VAL:HG11	2.48	0.44
1:B:95:GLN:O	1:B:97:ASP:N	2.47	0.44
1:C:344:ARG:HB3	1:C:347:LEU:HD12	2.00	0.44
1:F:624:VAL:CG1	1:F:625:GLU:N	2.81	0.44
1:C:307:GLN:O	1:C:309:SER:N	2.47	0.44
1:D:390:ALA:N	1:D:391:PRO:HD2	2.33	0.44
1:E:548:TYR:HA	1:E:551:TYR:CE2	2.53	0.44
1:E:668:PHE:HB3	1:E:676:VAL:HG13	2.00	0.44
1:C:638:ILE:CD1	1:C:650:VAL:HG11	2.48	0.44
1:D:213:ARG:C	1:D:215:SER:N	2.70	0.44
1:E:473:MET:HE3	1:E:534:LEU:HD13	2.00	0.44
1:C:548:TYR:HA	1:C:551:TYR:CE2	2.53	0.43
1:E:167:ILE:HD12	1:E:297:VAL:HG21	1.99	0.43
1:C:473:MET:HE1	1:C:495:ILE:CG2	2.48	0.43
1:D:505:CYS:HB3	1:D:568:VAL:O	2.17	0.43
1:D:656:PRO:CB	1:D:684:ILE:HD13	2.48	0.43
1:A:408:ASP:O	1:A:409:ASP:CB	2.66	0.43
1:A:95:GLN:O	1:A:97:ASP:N	2.46	0.43
1:E:68:SER:N	1:E:73:THR:HG23	2.33	0.43
1:F:150:LEU:HA	1:F:150:LEU:HD23	1.84	0.43
1:A:642:VAL:HG21	1:A:648:VAL:CG2	2.49	0.43
1:B:357:LEU:HD21	1:B:373:PRO:HD3	2.01	0.43
1:B:461:HIS:O	1:B:461:HIS:CG	2.71	0.43
1:C:147:ALA:CB	1:C:343:THR:HG22	2.45	0.43
1:C:57:LEU:HD21	1:C:79:LEU:HD12	2.01	0.43
1:D:408:ASP:O	1:D:409:ASP:CB	2.67	0.43
1:E:408:ASP:O	1:E:409:ASP:CB	2.66	0.43
1:A:341:TRP:CZ3	1:A:353:GLY:HA2	2.54	0.43
1:A:638:ILE:CD1	1:A:650:VAL:HG11	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ARG:HA	1:B:322:GLU:O	2.19	0.43
1:B:255:ILE:CG2	1:B:667:ASN:HB2	2.48	0.43
1:B:642:VAL:HG21	1:B:648:VAL:CG2	2.48	0.43
1:C:461:HIS:CG	1:C:461:HIS:O	2.72	0.43
1:C:499:THR:CG2	1:C:500:ALA:N	2.81	0.43
1:D:111:PRO:HA	1:D:215:SER:HA	2.01	0.43
1:E:240:ARG:HD2	1:E:274:TYR:CE1	2.54	0.43
1:D:206:ASN:C	1:D:206:ASN:ND2	2.71	0.43
1:E:642:VAL:HG21	1:E:648:VAL:CG2	2.49	0.43
1:F:210:ASP:O	1:F:214:ARG:HG3	2.19	0.43
1:B:150:LEU:HD23	1:B:150:LEU:HA	1.86	0.42
1:B:642:VAL:HG11	1:B:648:VAL:HG22	2.00	0.42
1:B:656:PRO:CB	1:B:684:ILE:HD13	2.49	0.42
1:D:82:ALA:O	1:D:83:VAL:HB	2.18	0.42
1:E:178:ILE:N	1:E:178:ILE:CD1	2.82	0.42
1:B:79:LEU:HD21	1:B:92:VAL:HB	2.00	0.42
1:F:277:CYS:SG	1:F:516:TYR:OH	2.69	0.42
1:B:57:LEU:HD21	1:B:79:LEU:HD12	1.99	0.42
1:D:186:GLN:HE21	1:D:186:GLN:HB3	1.65	0.42
1:E:655:VAL:O	1:E:657:LEU:HD13	2.19	0.42
1:F:341:TRP:CZ3	1:F:353:GLY:HA2	2.54	0.42
1:A:506:ARG:CG	1:A:568:VAL:HG13	2.45	0.42
1:B:404:TRP:CZ3	1:B:414:LYS:HB2	2.54	0.42
1:B:473:MET:HE1	1:B:495:ILE:CG2	2.49	0.42
1:C:668:PHE:HB3	1:C:676:VAL:HG13	2.00	0.42
1:D:638:ILE:HD11	1:D:650:VAL:HG11	2.01	0.42
1:E:82:ALA:O	1:E:83:VAL:HB	2.19	0.42
1:A:57:LEU:HD21	1:A:79:LEU:HD12	2.01	0.42
1:B:302:ASN:O	1:B:422:VAL:HG13	2.19	0.42
1:B:609:LEU:HD12	1:B:609:LEU:C	2.40	0.42
1:C:390:ALA:N	1:C:391:PRO:HD2	2.34	0.42
1:F:473:MET:HE1	1:F:495:ILE:CG2	2.50	0.42
1:B:512:ARG:HH11	1:B:520:LEU:HB3	1.83	0.42
1:C:506:ARG:HA	1:C:529:LEU:O	2.19	0.42
1:F:350:GLY:O	1:F:377:ARG:NH1	2.53	0.42
1:B:326:ASP:CG	1:B:327:LYS:H	2.21	0.42
1:B:317:ARG:CZ	1:B:577:LEU:HD11	2.50	0.42
1:D:350:GLY:O	1:D:377:ARG:NH1	2.51	0.42
1:E:57:LEU:HD21	1:E:79:LEU:HD12	2.01	0.42
1:E:661:LEU:HD11	1:E:681:ASN:HB3	2.02	0.42
1:B:299:THR:O	1:B:426:ILE:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:ASP:O	1:E:263:ARG:HG3	2.19	0.42
1:B:592:ARG:HG2	1:F:154:GLU:OE2	2.20	0.42
1:F:576:LEU:HA	1:F:576:LEU:HD12	1.77	0.42
1:A:461:HIS:CG	1:A:461:HIS:O	2.73	0.42
1:B:147:ALA:CB	1:B:343:THR:HG22	2.48	0.42
1:D:638:ILE:CD1	1:D:650:VAL:HG11	2.50	0.42
1:F:499:THR:CG2	1:F:500:ALA:N	2.82	0.42
1:B:454:GLU:O	1:B:458:ARG:HG3	2.20	0.42
1:C:341:TRP:CZ3	1:C:353:GLY:HA2	2.54	0.42
1:D:192:ILE:HG12	1:D:265:LYS:HD2	2.01	0.42
1:A:206:ASN:ND2	1:A:206:ASN:C	2.71	0.41
1:A:255:ILE:HG21	1:A:667:ASN:HB2	2.01	0.41
1:B:341:TRP:CZ3	1:B:353:GLY:HA2	2.55	0.41
1:B:569:GLU:HA	1:B:570:PRO:HD2	1.86	0.41
1:E:213:ARG:C	1:E:215:SER:N	2.72	0.41
1:F:15:GLU:C	1:F:17:ASN:N	2.73	0.41
1:F:461:HIS:O	1:F:461:HIS:CG	2.73	0.41
1:A:209:ARG:NH1	1:A:209:ARG:HG3	2.34	0.41
1:A:656:PRO:CB	1:A:684:ILE:HD13	2.49	0.41
1:D:63:THR:HB	1:D:115:TYR:CD2	2.55	0.41
1:F:111:PRO:HA	1:F:215:SER:HA	2.02	0.41
1:F:593:ILE:HG23	1:F:603:LEU:HD11	2.01	0.41
1:C:638:ILE:HD11	1:C:650:VAL:HG11	2.03	0.41
1:E:210:ASP:O	1:E:214:ARG:HG3	2.21	0.41
1:C:279:VAL:O	1:C:283:VAL:HG13	2.21	0.41
1:D:576:LEU:HA	1:D:576:LEU:HD12	1.76	0.41
1:E:273:LYS:HG3	1:E:274:TYR:CE1	2.56	0.41
1:E:164:GLN:HB3	1:E:663:LYS:HB2	2.02	0.41
1:F:602:LYS:HB3	1:F:602:LYS:HE3	1.90	0.41
1:F:642:VAL:HG11	1:F:648:VAL:HG22	2.01	0.41
1:A:111:PRO:HA	1:A:215:SER:HA	2.03	0.41
1:C:150:LEU:HD23	1:C:150:LEU:HA	1.86	0.41
1:C:656:PRO:CB	1:C:684:ILE:HD13	2.49	0.41
1:D:15:GLU:C	1:D:17:ASN:N	2.74	0.41
1:D:341:TRP:CZ3	1:D:353:GLY:HA2	2.55	0.41
1:E:576:LEU:HA	1:E:576:LEU:HD12	1.85	0.41
1:F:144:PRO:HA	1:F:149:TYR:CG	2.56	0.41
1:E:15:GLU:C	1:E:17:ASN:N	2.74	0.41
1:A:424:LEU:HA	1:A:424:LEU:HD23	1.72	0.41
1:A:499:THR:CG2	1:A:500:ALA:N	2.83	0.41
1:B:576:LEU:HD12	1:B:576:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:ARG:NH1	1:C:601:ARG:CG	2.84	0.41
1:D:58:THR:HG22	1:D:78:PRO:HA	2.03	0.41
1:B:514:VAL:CG1	1:B:520:LEU:HD23	2.40	0.41
1:C:602:LYS:HE3	1:C:602:LYS:HB3	1.87	0.41
1:D:146:ASP:OD1	1:D:147:ALA:N	2.54	0.41
1:E:186:GLN:HE21	1:E:186:GLN:HB3	1.69	0.41
1:E:677:LYS:NZ	3:E:740:HOH:O	2.53	0.41
1:B:326:ASP:CG	1:B:327:LYS:N	2.73	0.41
1:E:111:PRO:HA	1:E:215:SER:HA	2.02	0.41
1:B:206:ASN:ND2	1:B:206:ASN:C	2.72	0.40
1:B:499:THR:CG2	1:B:500:ALA:N	2.85	0.40
1:C:41:LEU:HD23	1:C:104:LEU:HD11	2.03	0.40
1:C:436:ARG:HH11	1:C:436:ARG:HD3	1.68	0.40
1:C:660:GLY:O	1:C:683:ILE:O	2.38	0.40
1:C:68:SER:N	1:C:73:THR:HG23	2.35	0.40
1:D:485:MET:HE1	1:D:551:TYR:HE1	1.86	0.40
1:E:15:GLU:N	3:E:706:HOH:O	2.54	0.40
1:E:638:ILE:CD1	1:E:650:VAL:HG11	2.51	0.40
1:F:387:LYS:HA	1:F:388:TYR:HA	1.94	0.40
1:A:387:LYS:HG2	1:A:388:TYR:CD1	2.55	0.40
1:C:192:ILE:HG12	1:C:265:LYS:HD2	2.04	0.40
1:F:102:LEU:N	1:F:102:LEU:HD23	2.37	0.40
1:B:364:LYS:HG2	1:B:392:PHE:CZ	2.57	0.40
1:C:408:ASP:O	1:C:409:ASP:CB	2.69	0.40
1:E:178:ILE:HD12	1:E:178:ILE:N	2.36	0.40
1:E:341:TRP:CZ3	1:E:353:GLY:HA2	2.57	0.40
1:F:147:ALA:CB	1:F:343:THR:HG22	2.49	0.40
1:F:656:PRO:CB	1:F:684:ILE:HD13	2.52	0.40
1:A:576:LEU:HD12	1:A:576:LEU:HA	1.85	0.40
1:B:188:GLY:O	1:B:192:ILE:HG13	2.22	0.40
1:B:192:ILE:HG12	1:B:265:LYS:HD2	2.03	0.40
1:B:593:ILE:HG23	1:B:603:LEU:HD11	2.03	0.40
1:C:15:GLU:C	1:C:17:ASN:N	2.75	0.40
1:D:357:LEU:HD21	1:D:373:PRO:HD3	2.03	0.40
1:E:485:MET:HE3	1:E:551:TYR:HE1	1.85	0.40
1:F:618:GLU:HG2	1:F:641:PRO:HB3	2.04	0.40
1:F:63:THR:HB	1:F:115:TYR:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	645/687 (94%)	584 (90%)	42 (6%)	19 (3%)	4	15
1	B	645/687 (94%)	587 (91%)	38 (6%)	20 (3%)	4	14
1	C	645/687 (94%)	588 (91%)	37 (6%)	20 (3%)	4	14
1	D	645/687 (94%)	585 (91%)	39 (6%)	21 (3%)	4	13
1	E	645/687 (94%)	587 (91%)	37 (6%)	21 (3%)	4	13
1	F	645/687 (94%)	587 (91%)	38 (6%)	20 (3%)	4	14
All	All	3870/4122 (94%)	3518 (91%)	231 (6%)	121 (3%)	4	14

All (121) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	VAL
1	A	85	GLU
1	A	96	GLN
1	A	121	ALA
1	A	231	ASN
1	A	326	ASP
1	A	464	LYS
1	A	468	LYS
1	B	83	VAL
1	B	85	GLU
1	B	96	GLN
1	B	121	ALA
1	B	231	ASN
1	B	326	ASP
1	B	464	LYS
1	B	468	LYS
1	C	83	VAL
1	C	85	GLU
1	C	96	GLN
1	C	121	ALA

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Mol	Chain	Res	Type
1	C	231	ASN
1	C	326	ASP
1	C	464	LYS
1	C	468	LYS
1	D	83	VAL
1	D	85	GLU
1	D	96	GLN
1	D	121	ALA
1	D	230	CYS
1	D	231	ASN
1	D	326	ASP
1	D	464	LYS
1	D	468	LYS
1	E	83	VAL
1	E	85	GLU
1	E	96	GLN
1	E	121	ALA
1	E	231	ASN
1	E	326	ASP
1	E	464	LYS
1	E	468	LYS
1	F	83	VAL
1	F	85	GLU
1	F	96	GLN
1	F	121	ALA
1	F	231	ASN
1	F	326	ASP
1	F	464	LYS
1	F	468	LYS
1	F	470	GLU
1	A	30	LYS
1	A	230	CYS
1	A	232	ASP
1	A	466	ALA
1	A	470	GLU
1	B	30	LYS
1	B	230	CYS
1	B	232	ASP
1	B	466	ALA
1	B	470	GLU
1	C	30	LYS
1	C	80	ARG

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Mol	Chain	Res	Type
1	C	230	CYS
1	C	466	ALA
1	C	470	GLU
1	D	30	LYS
1	D	80	ARG
1	D	214	ARG
1	D	325	GLY
1	D	466	ALA
1	D	470	GLU
1	E	30	LYS
1	E	214	ARG
1	E	230	CYS
1	E	232	ASP
1	E	466	ALA
1	E	470	GLU
1	F	30	LYS
1	F	230	CYS
1	F	232	ASP
1	F	466	ALA
1	A	80	ARG
1	B	80	ARG
1	B	325	GLY
1	C	97	ASP
1	C	232	ASP
1	D	232	ASP
1	E	80	ARG
1	E	97	ASP
1	F	80	ARG
1	F	409	ASP
1	A	97	ASP
1	A	325	GLY
1	A	409	ASP
1	B	97	ASP
1	B	409	ASP
1	C	409	ASP
1	D	97	ASP
1	D	409	ASP
1	E	409	ASP
1	F	97	ASP
1	F	325	GLY
1	F	684	ILE
1	A	684	ILE

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Mol	Chain	Res	Type
1	B	644	ALA
1	B	684	ILE
1	C	684	ILE
1	D	684	ILE
1	E	325	GLY
1	E	684	ILE
1	A	469	GLU
1	C	644	ALA
1	D	469	GLU
1	E	571	VAL
1	B	571	VAL
1	C	571	VAL
1	E	410	GLY
1	F	410	GLY
1	F	571	VAL
1	C	325	GLY
1	D	571	VAL

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	565/596 (95%)	512 (91%)	53 (9%)	8	26
1	B	565/596 (95%)	510 (90%)	55 (10%)	8	24
1	C	565/596 (95%)	512 (91%)	53 (9%)	8	26
1	D	565/596 (95%)	511 (90%)	54 (10%)	8	24
1	E	565/596 (95%)	510 (90%)	55 (10%)	8	24
1	F	565/596 (95%)	512 (91%)	53 (9%)	8	26
All	All	3390/3576 (95%)	3067 (90%)	323 (10%)	8	25

All (323) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR

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Mol	Chain	Res	Type
1	A	26	LEU
1	A	32	VAL
1	A	57	LEU
1	A	62	VAL
1	A	69	GLN
1	A	76	ARG
1	A	79	LEU
1	A	84	GLU
1	A	114	LEU
1	A	118	SER
1	A	119	LEU
1	A	190	LEU
1	A	200	ASN
1	A	206	ASN
1	A	218	VAL
1	A	230	CYS
1	A	261	LEU
1	A	283	VAL
1	A	291	LEU
1	A	297	VAL
1	A	306	ASP
1	A	312	LEU
1	A	328	SER
1	A	381	GLU
1	A	397	VAL
1	A	431	VAL
1	A	453	ARG
1	A	478	ARG
1	A	481	GLN
1	A	483	MET
1	A	485	MET
1	A	501	GLU
1	A	509	LEU
1	A	514	VAL
1	A	532	LEU
1	A	533	THR
1	A	568	VAL
1	A	569	GLU
1	A	577	LEU
1	A	601	ARG
1	A	603	LEU
1	A	609	LEU

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Mol	Chain	Res	Type
1	A	617	LEU
1	A	629	LEU
1	A	630	THR
1	A	643	GLU
1	A	651	ARG
1	A	665	VAL
1	A	666	VAL
1	A	673	LEU
1	A	676	VAL
1	A	680	ARG
1	B	16	THR
1	B	26	LEU
1	B	32	VAL
1	B	57	LEU
1	B	62	VAL
1	B	69	GLN
1	B	76	ARG
1	B	79	LEU
1	B	84	GLU
1	B	114	LEU
1	B	118	SER
1	B	119	LEU
1	B	190	LEU
1	B	200	ASN
1	B	206	ASN
1	B	209	ARG
1	B	218	VAL
1	B	230	CYS
1	B	261	LEU
1	B	283	VAL
1	B	291	LEU
1	B	297	VAL
1	B	306	ASP
1	B	328	SER
1	B	381	GLU
1	B	397	VAL
1	B	431	VAL
1	B	436	ARG
1	B	453	ARG
1	B	478	ARG
1	B	481	GLN
1	B	483	MET

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Mol	Chain	Res	Type
1	B	485	MET
1	B	501	GLU
1	B	509	LEU
1	B	512	ARG
1	B	514	VAL
1	B	532	LEU
1	B	533	THR
1	B	568	VAL
1	B	569	GLU
1	B	577	LEU
1	B	601	ARG
1	B	603	LEU
1	B	609	LEU
1	B	617	LEU
1	B	629	LEU
1	B	630	THR
1	B	643	GLU
1	B	651	ARG
1	B	665	VAL
1	B	666	VAL
1	B	673	LEU
1	B	676	VAL
1	B	680	ARG
1	C	16	THR
1	C	26	LEU
1	C	32	VAL
1	C	57	LEU
1	C	62	VAL
1	C	69	GLN
1	C	76	ARG
1	C	79	LEU
1	C	84	GLU
1	C	114	LEU
1	C	118	SER
1	C	119	LEU
1	C	190	LEU
1	C	200	ASN
1	C	206	ASN
1	C	218	VAL
1	C	230	CYS
1	C	261	LEU
1	C	291	LEU

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Mol	Chain	Res	Type
1	C	297	VAL
1	C	306	ASP
1	C	328	SER
1	C	381	GLU
1	C	397	VAL
1	C	412	VAL
1	C	431	VAL
1	C	453	ARG
1	C	478	ARG
1	C	481	GLN
1	C	483	MET
1	C	485	MET
1	C	501	GLU
1	C	514	VAL
1	C	532	LEU
1	C	533	THR
1	C	562	LYS
1	C	568	VAL
1	C	569	GLU
1	C	577	LEU
1	C	601	ARG
1	C	603	LEU
1	C	609	LEU
1	C	617	LEU
1	C	629	LEU
1	C	630	THR
1	C	643	GLU
1	C	651	ARG
1	C	657	LEU
1	C	665	VAL
1	C	666	VAL
1	C	673	LEU
1	C	676	VAL
1	C	680	ARG
1	D	16	THR
1	D	26	LEU
1	D	32	VAL
1	D	57	LEU
1	D	62	VAL
1	D	69	GLN
1	D	76	ARG
1	D	79	LEU

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Mol	Chain	Res	Type
1	D	84	GLU
1	D	114	LEU
1	D	118	SER
1	D	119	LEU
1	D	190	LEU
1	D	200	ASN
1	D	201	PRO
1	D	206	ASN
1	D	218	VAL
1	D	230	CYS
1	D	261	LEU
1	D	283	VAL
1	D	291	LEU
1	D	297	VAL
1	D	306	ASP
1	D	312	LEU
1	D	319	GLU
1	D	328	SER
1	D	381	GLU
1	D	397	VAL
1	D	431	VAL
1	D	433	ARG
1	D	453	ARG
1	D	478	ARG
1	D	481	GLN
1	D	483	MET
1	D	485	MET
1	D	512	ARG
1	D	514	VAL
1	D	532	LEU
1	D	533	THR
1	D	568	VAL
1	D	569	GLU
1	D	577	LEU
1	D	601	ARG
1	D	603	LEU
1	D	609	LEU
1	D	629	LEU
1	D	630	THR
1	D	643	GLU
1	D	651	ARG
1	D	665	VAL

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Mol	Chain	Res	Type
1	D	666	VAL
1	D	673	LEU
1	D	676	VAL
1	D	680	ARG
1	E	16	THR
1	E	26	LEU
1	E	32	VAL
1	E	57	LEU
1	E	62	VAL
1	E	69	GLN
1	E	76	ARG
1	E	79	LEU
1	E	84	GLU
1	E	114	LEU
1	E	118	SER
1	E	119	LEU
1	E	190	LEU
1	E	200	ASN
1	E	201	PRO
1	E	206	ASN
1	E	209	ARG
1	E	218	VAL
1	E	230	CYS
1	E	261	LEU
1	E	291	LEU
1	E	297	VAL
1	E	306	ASP
1	E	312	LEU
1	E	328	SER
1	E	381	GLU
1	E	397	VAL
1	E	412	VAL
1	E	431	VAL
1	E	453	ARG
1	E	478	ARG
1	E	481	GLN
1	E	483	MET
1	E	485	MET
1	E	501	GLU
1	E	514	VAL
1	E	523	GLU
1	E	532	LEU

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Mol	Chain	Res	Type
1	E	533	THR
1	E	568	VAL
1	E	569	GLU
1	E	577	LEU
1	E	601	ARG
1	E	603	LEU
1	E	609	LEU
1	E	617	LEU
1	E	629	LEU
1	E	630	THR
1	E	643	GLU
1	E	651	ARG
1	E	665	VAL
1	E	666	VAL
1	E	673	LEU
1	E	676	VAL
1	E	680	ARG
1	F	16	THR
1	F	26	LEU
1	F	32	VAL
1	F	57	LEU
1	F	62	VAL
1	F	69	GLN
1	F	76	ARG
1	F	79	LEU
1	F	84	GLU
1	F	114	LEU
1	F	118	SER
1	F	119	LEU
1	F	190	LEU
1	F	200	ASN
1	F	201	PRO
1	F	206	ASN
1	F	218	VAL
1	F	230	CYS
1	F	261	LEU
1	F	283	VAL
1	F	291	LEU
1	F	297	VAL
1	F	306	ASP
1	F	312	LEU
1	F	328	SER

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Mol	Chain	Res	Type
1	F	381	GLU
1	F	397	VAL
1	F	431	VAL
1	F	453	ARG
1	F	478	ARG
1	F	481	GLN
1	F	483	MET
1	F	485	MET
1	F	501	GLU
1	F	514	VAL
1	F	532	LEU
1	F	533	THR
1	F	568	VAL
1	F	569	GLU
1	F	577	LEU
1	F	601	ARG
1	F	603	LEU
1	F	609	LEU
1	F	617	LEU
1	F	629	LEU
1	F	630	THR
1	F	643	GLU
1	F	651	ARG
1	F	665	VAL
1	F	666	VAL
1	F	673	LEU
1	F	676	VAL
1	F	680	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	69	GLN
1	A	103	GLN
1	A	169	GLN
1	A	186	GLN
1	A	206	ASN
1	A	234	GLN
1	A	266	ASN
1	A	333	ASN
1	A	348	GLN

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Mol	Chain	Res	Type
1	A	481	GLN
1	B	37	GLN
1	B	69	GLN
1	B	103	GLN
1	B	169	GLN
1	B	186	GLN
1	B	206	ASN
1	B	234	GLN
1	B	266	ASN
1	B	333	ASN
1	B	348	GLN
1	B	481	GLN
1	C	37	GLN
1	C	69	GLN
1	C	103	GLN
1	C	169	GLN
1	C	186	GLN
1	C	206	ASN
1	C	234	GLN
1	C	266	ASN
1	C	348	GLN
1	C	481	GLN
1	D	37	GLN
1	D	69	GLN
1	D	103	GLN
1	D	169	GLN
1	D	186	GLN
1	D	206	ASN
1	D	234	GLN
1	D	266	ASN
1	D	276	GLN
1	D	333	ASN
1	D	348	GLN
1	D	481	GLN
1	E	37	GLN
1	E	69	GLN
1	E	103	GLN
1	E	169	GLN
1	E	186	GLN
1	E	206	ASN
1	E	234	GLN
1	E	266	ASN

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Mol	Chain	Res	Type
1	E	348	GLN
1	E	481	GLN
1	F	37	GLN
1	F	69	GLN
1	F	103	GLN
1	F	169	GLN
1	F	186	GLN
1	F	206	ASN
1	F	234	GLN
1	F	266	ASN
1	F	333	ASN
1	F	348	GLN
1	F	481	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 carbohydrates 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	GDP	C	702	-	24,30,30	1.69	4 (16%)	31,47,47	2.12	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GDP	D	703	-	24,30,30	1.58	4 (16%)	31,47,47	2.10	5 (16%)
2	GDP	E	704	-	24,30,30	1.59	4 (16%)	31,47,47	2.05	4 (12%)
2	GDP	F	705	-	24,30,30	1.69	3 (12%)	31,47,47	2.12	4 (12%)
2	GDP	A	700	-	24,30,30	1.64	4 (16%)	31,47,47	2.10	5 (16%)
2	GDP	B	701	-	24,30,30	1.47	4 (16%)	31,47,47	2.09	5 (16%)

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	GDP	C	702	-	-	3/12/32/32	0/3/3/3
2	GDP	D	703	-	-	4/12/32/32	0/3/3/3
2	GDP	E	704	-	-	3/12/32/32	0/3/3/3
2	GDP	F	705	-	-	4/12/32/32	0/3/3/3
2	GDP	A	700	-	-	3/12/32/32	0/3/3/3
2	GDP	B	701	-	-	3/12/32/32	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	705	GDP	C6-N1	5.18	1.42	1.33
2	A	700	GDP	C6-N1	4.79	1.41	1.33
2	C	702	GDP	C6-N1	4.55	1.41	1.33
2	D	703	GDP	C6-N1	4.30	1.40	1.33
2	E	704	GDP	C6-N1	4.18	1.40	1.33
2	B	701	GDP	C8-N7	-3.80	1.27	1.34
2	C	702	GDP	C8-N7	-3.80	1.27	1.34
2	E	704	GDP	C8-N7	-3.77	1.28	1.34
2	A	700	GDP	C8-N7	-3.52	1.28	1.34
2	F	705	GDP	C8-N7	-3.35	1.28	1.34
2	D	703	GDP	C8-N7	-3.18	1.29	1.34
2	B	701	GDP	C6-N1	3.09	1.38	1.33
2	F	705	GDP	PB-O2B	-2.91	1.43	1.54
2	A	700	GDP	PB-O2B	-2.64	1.44	1.54
2	D	703	GDP	PB-O2B	-2.43	1.45	1.54
2	C	702	GDP	PB-O2B	-2.40	1.45	1.54
2	C	702	GDP	O4'-C1'	2.35	1.44	1.41
2	D	703	GDP	O4'-C1'	2.30	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	GDP	PB-O2B	-2.25	1.46	1.54
2	A	700	GDP	PA-O2A	-2.09	1.45	1.55
2	B	701	GDP	C5-C4	-2.09	1.35	1.40
2	E	704	GDP	C2-N1	2.08	1.39	1.35
2	E	704	GDP	PA-O2A	-2.02	1.45	1.55

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	703	GDP	C5-C6-N1	-8.86	111.31	123.43
2	F	705	GDP	C5-C6-N1	-8.58	111.69	123.43
2	C	702	GDP	C5-C6-N1	-8.42	111.92	123.43
2	B	701	GDP	C5-C6-N1	-8.32	112.05	123.43
2	A	700	GDP	C5-C6-N1	-8.26	112.13	123.43
2	E	704	GDP	C5-C6-N1	-8.17	112.25	123.43
2	A	700	GDP	C6-N1-C2	5.54	124.73	115.93
2	F	705	GDP	C6-N1-C2	5.44	124.57	115.93
2	C	702	GDP	C6-N1-C2	5.40	124.51	115.93
2	B	701	GDP	C6-N1-C2	5.37	124.46	115.93
2	D	703	GDP	C6-N1-C2	5.36	124.45	115.93
2	E	704	GDP	C6-N1-C2	5.23	124.24	115.93
2	A	700	GDP	N3-C2-N1	-3.20	122.95	127.22
2	E	704	GDP	N3-C2-N1	-3.11	123.08	127.22
2	B	701	GDP	N3-C2-N1	-3.08	123.11	127.22
2	C	702	GDP	N3-C2-N1	-3.08	123.11	127.22
2	F	705	GDP	N3-C2-N1	-2.93	123.31	127.22
2	D	703	GDP	N3-C2-N1	-2.50	123.89	127.22
2	E	704	GDP	O2B-PB-O1B	2.29	119.63	110.68
2	A	700	GDP	O2B-PB-O1B	2.27	119.56	110.68
2	D	703	GDP	O2B-PB-O1B	2.25	119.51	110.68
2	B	701	GDP	C2-N3-C4	-2.22	112.82	115.36
2	C	702	GDP	O2B-PB-O1B	2.20	119.28	110.68
2	A	700	GDP	C2-N3-C4	-2.19	112.86	115.36
2	B	701	GDP	O2B-PB-O1B	2.14	119.04	110.68
2	F	705	GDP	C2-N3-C4	-2.12	112.93	115.36
2	D	703	GDP	C2-N3-C4	-2.11	112.95	115.36
2	C	702	GDP	C2-N3-C4	-2.03	113.03	115.36

There are no chirality outliers.

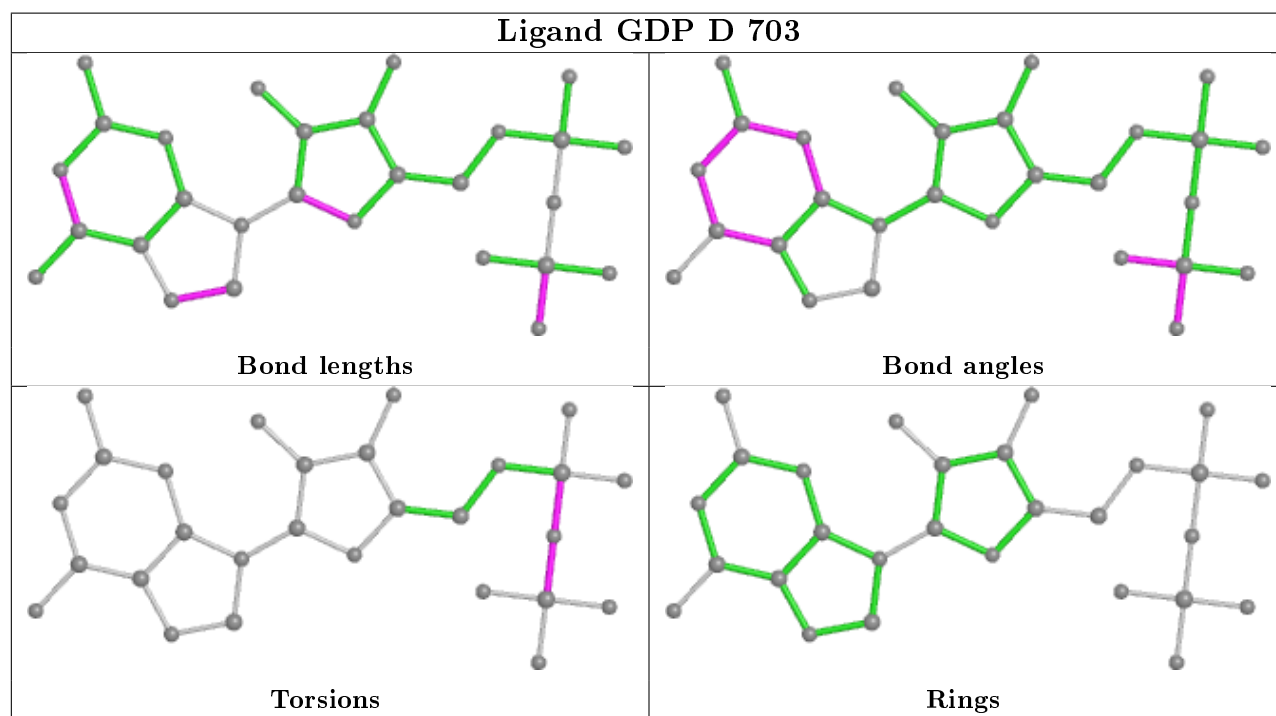
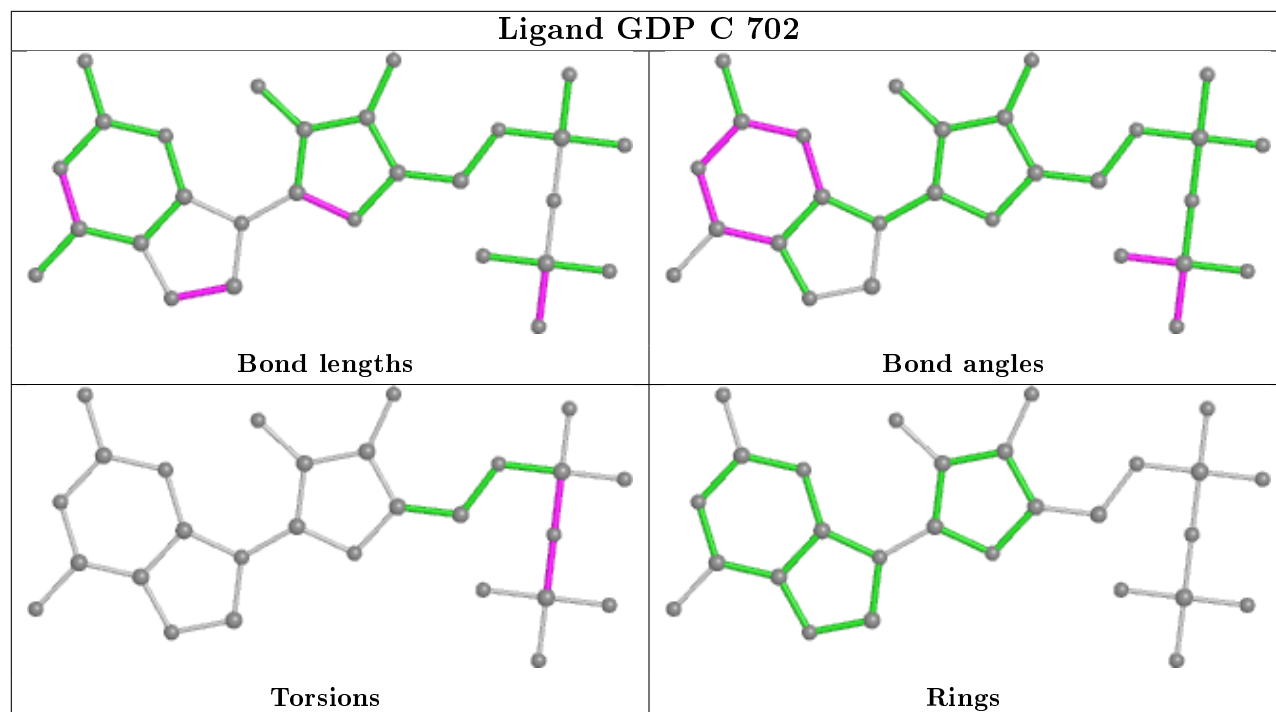
All (20) torsion outliers are listed below:

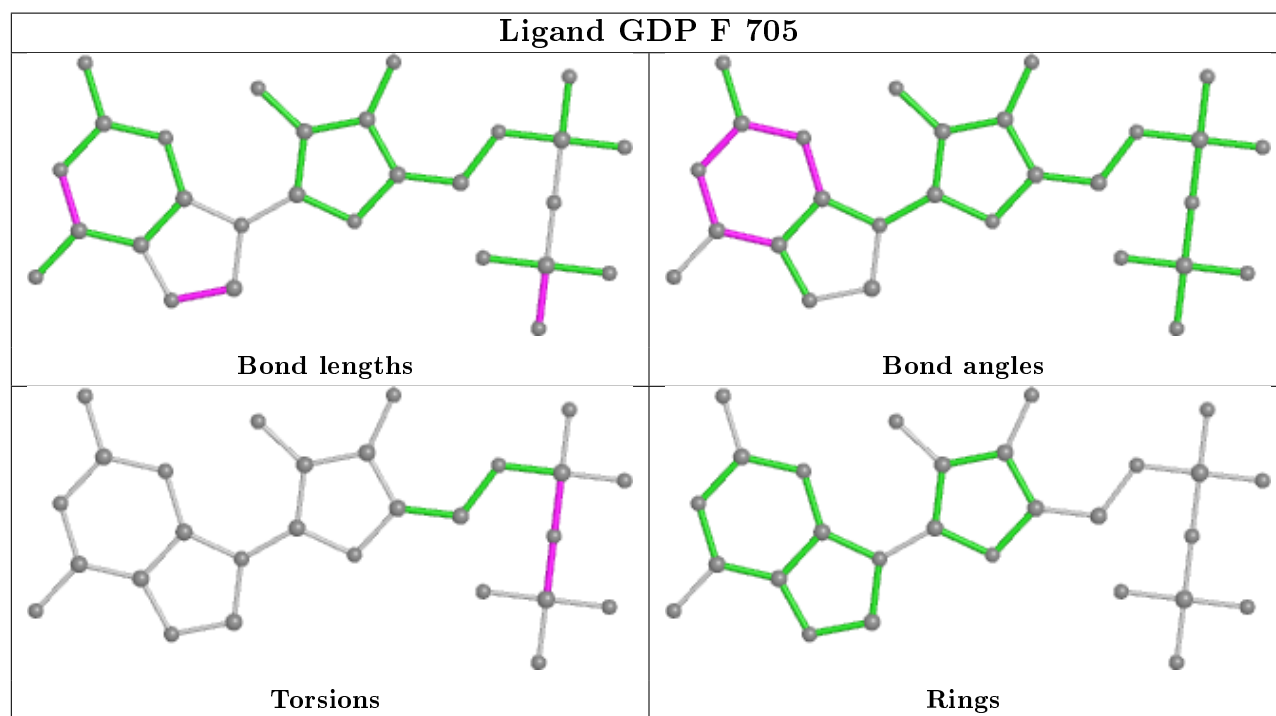
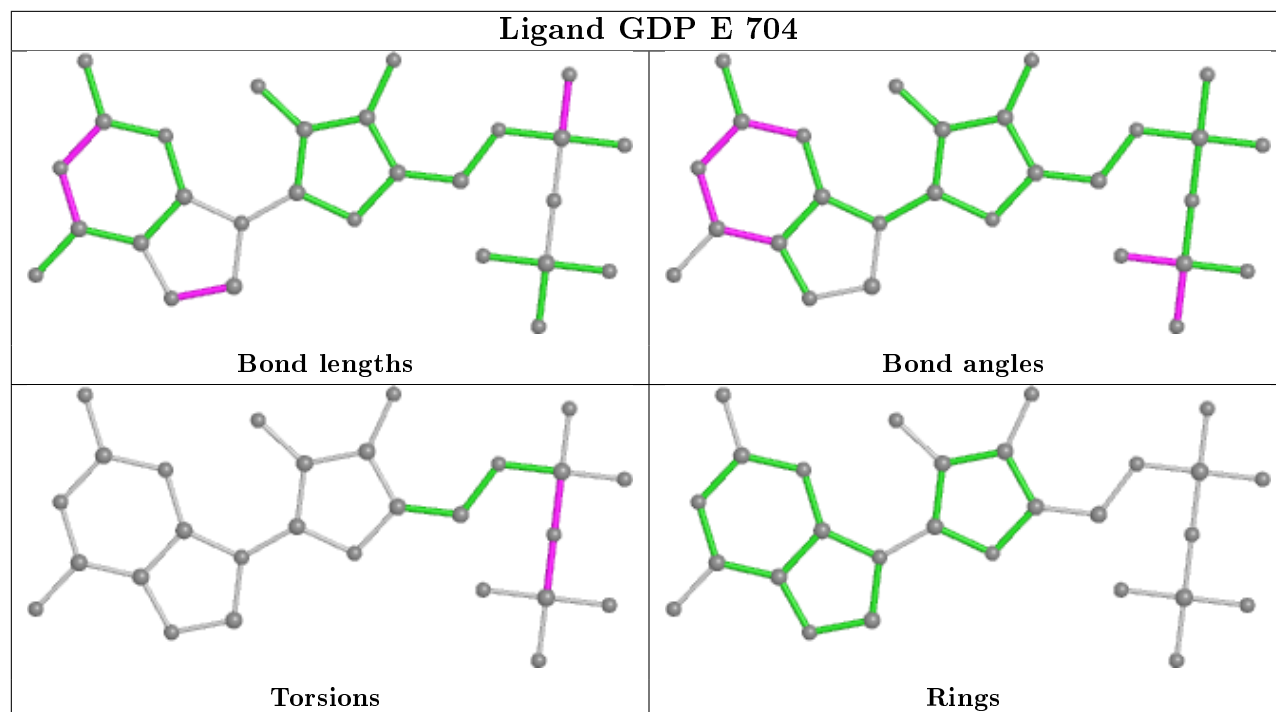
Mol	Chain	Res	Type	Atoms
2	C	702	GDP	PA-O3A-PB-O2B
2	D	703	GDP	PA-O3A-PB-O2B
2	D	703	GDP	PB-O3A-PA-O5'
2	E	704	GDP	PA-O3A-PB-O2B
2	F	705	GDP	PA-O3A-PB-O2B
2	F	705	GDP	PB-O3A-PA-O5'
2	A	700	GDP	PA-O3A-PB-O2B
2	B	701	GDP	PA-O3A-PB-O2B
2	C	702	GDP	PB-O3A-PA-O5'
2	E	704	GDP	PB-O3A-PA-O5'
2	A	700	GDP	PB-O3A-PA-O5'
2	B	701	GDP	PB-O3A-PA-O5'
2	D	703	GDP	PA-O3A-PB-O3B
2	F	705	GDP	PA-O3A-PB-O3B
2	C	702	GDP	PA-O3A-PB-O3B
2	E	704	GDP	PA-O3A-PB-O3B
2	A	700	GDP	PA-O3A-PB-O3B
2	B	701	GDP	PA-O3A-PB-O3B
2	D	703	GDP	PA-O3A-PB-O1B
2	F	705	GDP	PA-O3A-PB-O1B

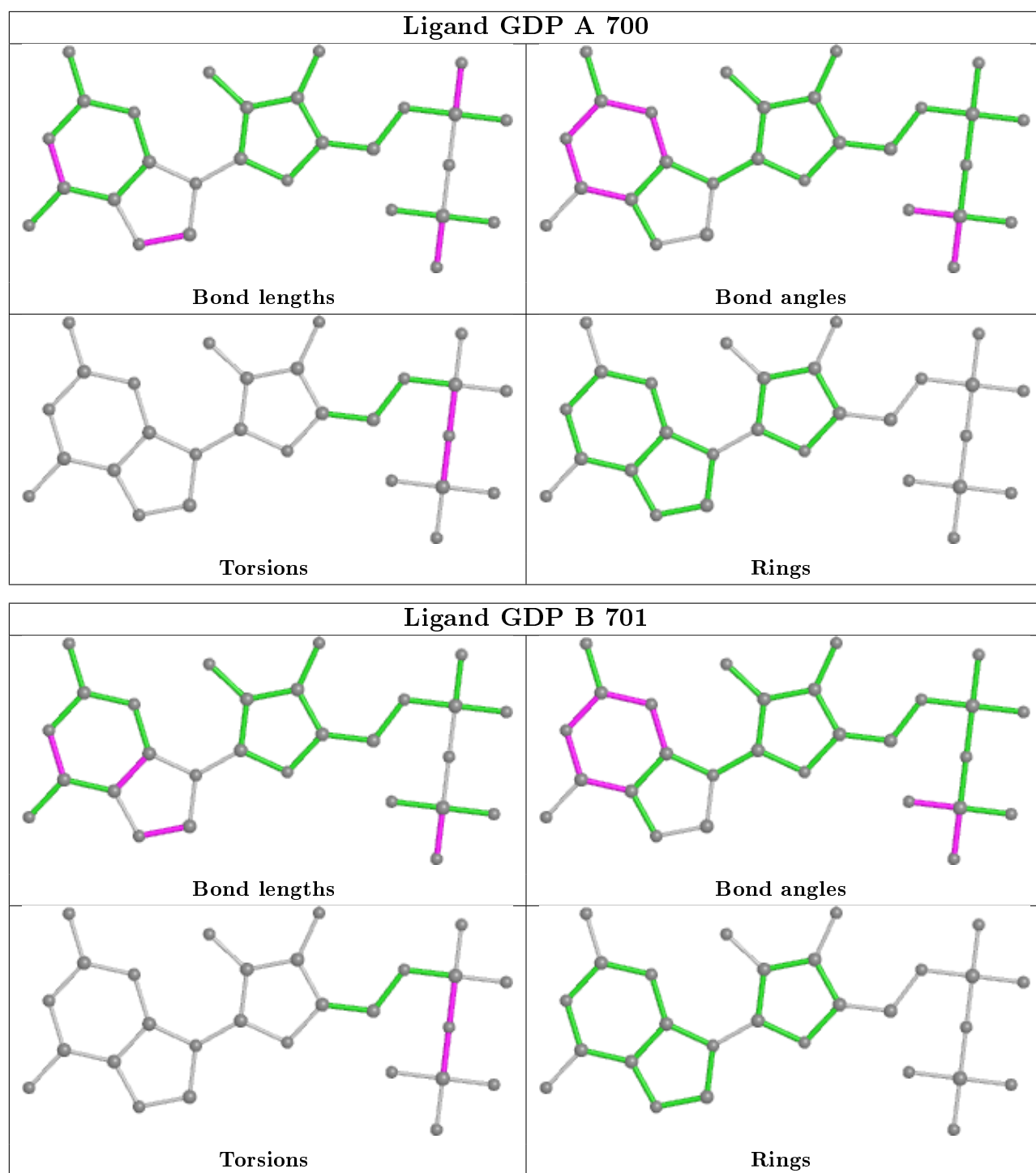
There are no ring outliers.

No monomer is involved in short contacts.

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	651/687 (94%)	-0.03	33 (5%)	28	19	22, 53, 108, 141	0
1	B	651/687 (94%)	0.05	30 (4%)	32	22	23, 52, 107, 140	0
1	C	651/687 (94%)	-0.05	29 (4%)	33	23	21, 48, 106, 140	0
1	D	651/687 (94%)	0.05	34 (5%)	27	18	22, 52, 107, 142	0
1	E	651/687 (94%)	0.01	31 (4%)	30	21	28, 53, 106, 141	0
1	F	651/687 (94%)	0.05	38 (5%)	23	15	21, 52, 107, 142	0
All	All	3906/4122 (94%)	0.01	195 (4%)	28	19	21, 52, 107, 142	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	467	GLU	7.0
1	C	85	GLU	6.7
1	B	86	GLY	6.2
1	F	327	LYS	5.4
1	D	467	GLU	5.4
1	D	97	ASP	5.3
1	D	121	ALA	5.2
1	D	85	GLU	5.2
1	F	467	GLU	5.2
1	B	119	LEU	5.1
1	F	100	LEU	5.0
1	F	97	ASP	4.9
1	A	41	LEU	4.8
1	F	85	GLU	4.8
1	D	57	LEU	4.7
1	E	100	LEU	4.6
1	F	57	LEU	4.6
1	D	465	LEU	4.5
1	A	119	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	96	GLN	4.3
1	E	85	GLU	4.2
1	F	98	CYS	4.2
1	B	81	ASP	4.2
1	C	86	GLY	4.2
1	D	101	SER	4.1
1	B	97	ASP	4.1
1	A	121	ALA	4.1
1	B	121	ALA	4.1
1	F	121	ALA	4.1
1	D	133	GLY	4.0
1	B	409	ASP	4.0
1	A	120	GLU	4.0
1	C	57	LEU	4.0
1	B	469	GLU	3.9
1	A	100	LEU	3.9
1	A	57	LEU	3.9
1	D	56	SER	3.8
1	D	102	LEU	3.8
1	E	99	THR	3.8
1	B	327	LYS	3.8
1	F	466	ALA	3.8
1	A	122	SER	3.7
1	D	409	ASP	3.7
1	A	98	CYS	3.7
1	E	57	LEU	3.7
1	E	98	CYS	3.7
1	B	467	GLU	3.6
1	E	86	GLY	3.6
1	B	85	GLU	3.6
1	C	466	ALA	3.6
1	A	43	LEU	3.6
1	F	56	SER	3.6
1	F	43	LEU	3.6
1	F	96	GLN	3.6
1	E	471	THR	3.6
1	F	92	VAL	3.6
1	C	100	LEU	3.5
1	E	95	GLN	3.5
1	B	100	LEU	3.5
1	D	120	GLU	3.5
1	D	469	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	471	THR	3.4
1	F	94	ASP	3.4
1	A	29	GLU	3.4
1	E	96	GLN	3.4
1	F	101	SER	3.4
1	C	468	LYS	3.3
1	B	101	SER	3.3
1	A	327	LYS	3.3
1	E	467	GLU	3.2
1	A	97	ASP	3.2
1	E	571	VAL	3.2
1	B	82	ALA	3.2
1	F	58	THR	3.2
1	F	59	PHE	3.2
1	D	81	ASP	3.2
1	F	42	THR	3.2
1	E	465	LEU	3.2
1	F	119	LEU	3.2
1	C	41	LEU	3.1
1	E	79	LEU	3.1
1	B	56	SER	3.1
1	C	56	SER	3.1
1	B	120	GLU	3.1
1	D	40	TRP	3.0
1	E	42	THR	3.0
1	D	95	GLN	3.0
1	E	572	ILE	3.0
1	F	93	VAL	3.0
1	A	60	SER	3.0
1	D	470	GLU	3.0
1	E	101	SER	2.9
1	C	470	GLU	2.9
1	D	99	THR	2.9
1	F	122	SER	2.9
1	A	468	LYS	2.9
1	E	327	LYS	2.9
1	C	43	LEU	2.9
1	A	118	SER	2.8
1	A	471	THR	2.8
1	E	89	THR	2.8
1	D	43	LEU	2.8
1	A	102	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	409	ASP	2.8
1	D	79	LEU	2.8
1	A	687	ALA	2.8
1	D	270	GLN	2.8
1	F	78	PRO	2.7
1	F	70	GLU	2.6
1	B	531	ASN	2.6
1	A	59	PHE	2.6
1	E	122	SER	2.6
1	F	86	GLY	2.6
1	C	69	GLN	2.6
1	E	648	VAL	2.6
1	F	99	THR	2.6
1	C	119	LEU	2.6
1	A	40	TRP	2.5
1	D	63	THR	2.5
1	B	122	SER	2.5
1	D	62	VAL	2.5
1	B	95	GLN	2.5
1	A	409	ASP	2.5
1	F	41	LEU	2.5
1	A	58	THR	2.5
1	C	469	GLU	2.5
1	A	85	GLU	2.4
1	F	82	ALA	2.4
1	B	76	ARG	2.4
1	A	95	GLN	2.4
1	B	468	LYS	2.4
1	C	530	LEU	2.4
1	B	59	PHE	2.4
1	C	77	PHE	2.4
1	C	349	PRO	2.4
1	F	40	TRP	2.4
1	C	95	GLN	2.4
1	F	81	ASP	2.4
1	A	469	GLU	2.4
1	C	96	GLN	2.4
1	B	43	LEU	2.3
1	F	120	GLU	2.3
1	C	407	GLN	2.3
1	E	119	LEU	2.3
1	F	465	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	77	PHE	2.3
1	E	94	ASP	2.3
1	D	100	LEU	2.3
1	E	600	LYS	2.3
1	D	92	VAL	2.3
1	B	470	GLU	2.3
1	D	84	GLU	2.3
1	C	102	LEU	2.3
1	E	409	ASP	2.2
1	F	326	ASP	2.2
1	C	467	GLU	2.2
1	E	97	ASP	2.2
1	C	465	LEU	2.2
1	C	122	SER	2.2
1	A	92	VAL	2.2
1	D	456	PHE	2.2
1	D	468	LYS	2.2
1	A	42	THR	2.2
1	A	86	GLY	2.2
1	C	42	THR	2.2
1	F	328	SER	2.2
1	F	471	THR	2.2
1	B	42	THR	2.2
1	F	594	LEU	2.1
1	F	134	HIS	2.1
1	B	99	THR	2.1
1	F	61	VAL	2.1
1	B	104	LEU	2.1
1	D	122	SER	2.1
1	A	116	ARG	2.1
1	D	41	LEU	2.1
1	E	29	GLU	2.1
1	A	56	SER	2.1
1	D	76	ARG	2.1
1	B	41	LEU	2.1
1	C	79	LEU	2.1
1	C	94	ASP	2.1
1	E	454	GLU	2.1
1	D	78	PRO	2.1
1	A	117	LEU	2.0
1	E	74	LYS	2.0
1	C	104	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	348	GLN	2.0
1	E	408	ASP	2.0
1	B	91	THR	2.0
1	E	84	GLU	2.0
1	E	121	ALA	2.0
1	A	99	THR	2.0
1	C	76	ARG	2.0
1	D	91	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 carbohydrates in this entry.

6.4 Ligands [i](#)

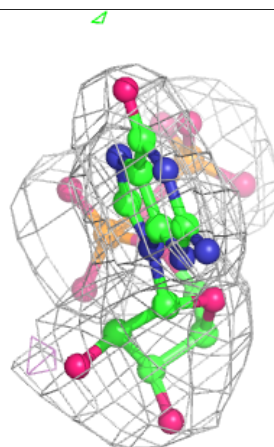
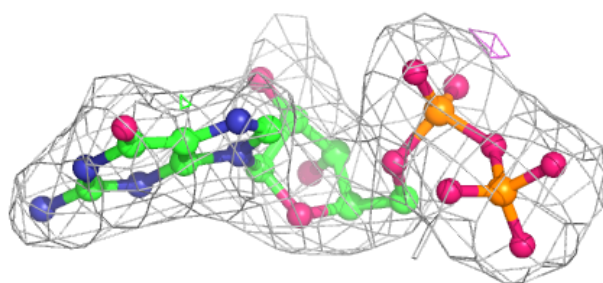
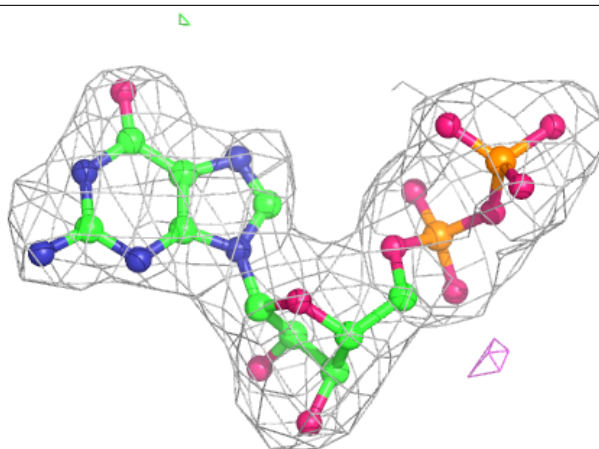
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GDP	E	704	28/28	0.97	0.14	32,42,51,58	0
2	GDP	D	703	28/28	0.98	0.14	25,34,51,57	0
2	GDP	C	702	28/28	0.98	0.15	27,37,50,53	0
2	GDP	F	705	28/28	0.98	0.14	33,38,45,57	0
2	GDP	A	700	28/28	0.98	0.15	29,36,54,55	0
2	GDP	B	701	28/28	0.98	0.14	20,36,48,53	0

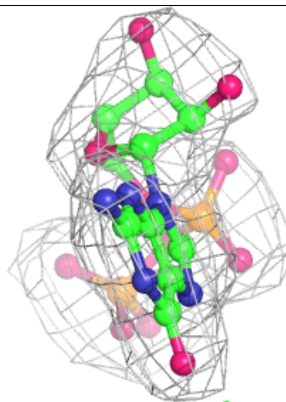
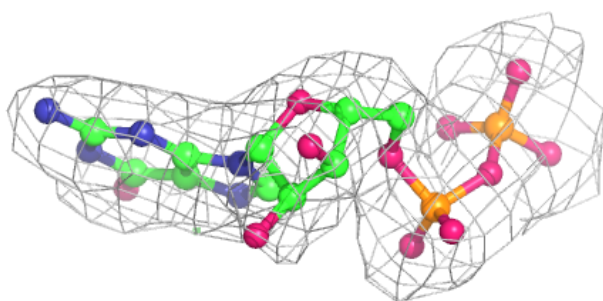
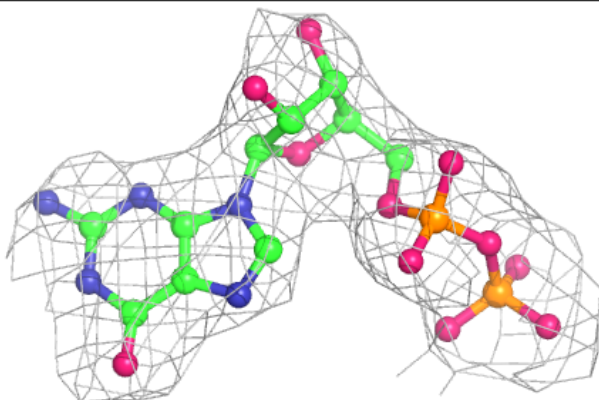
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GDP E 704:

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

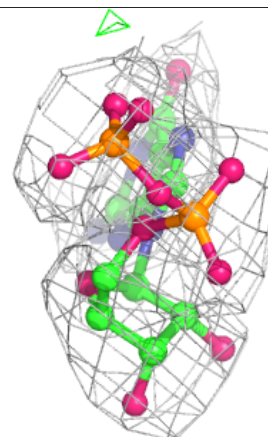
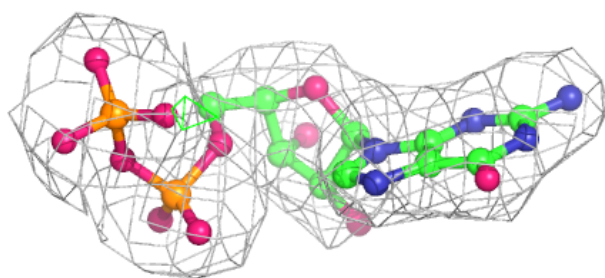
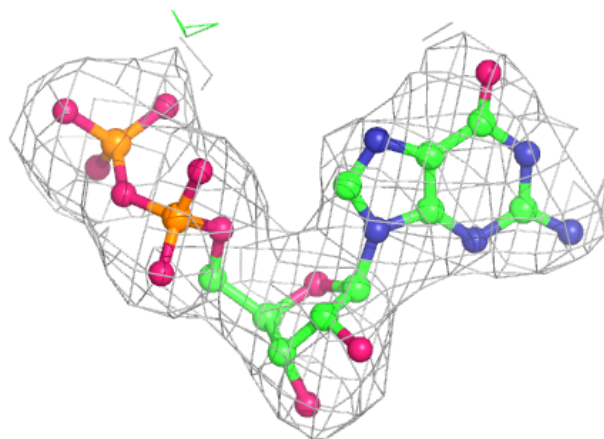
**Electron density around GDP D 703:**

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

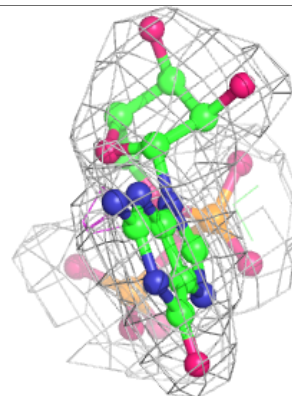
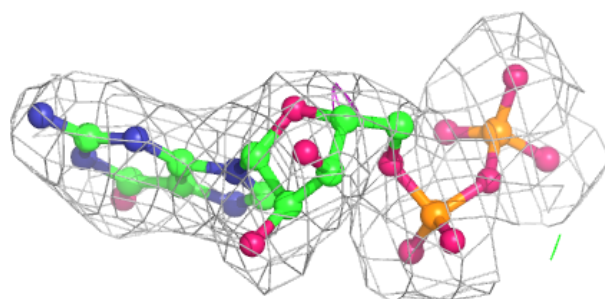
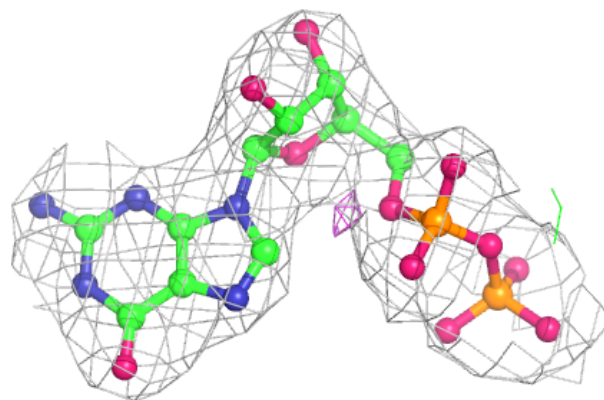


Electron density around GDP C 702:

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

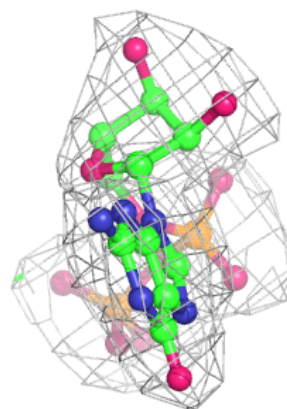
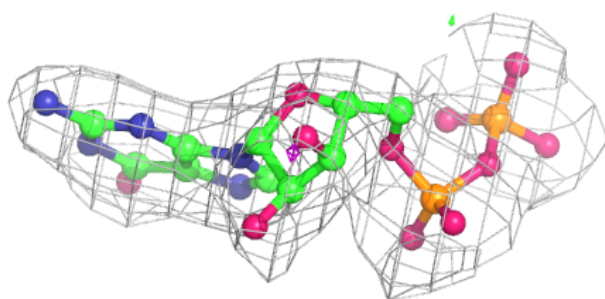
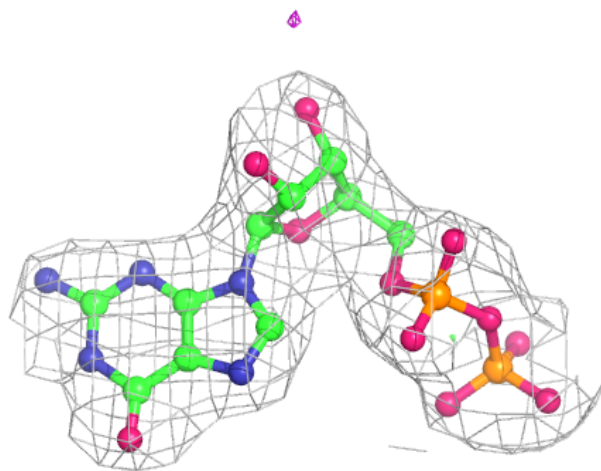
**Electron density around GDP F 705:**

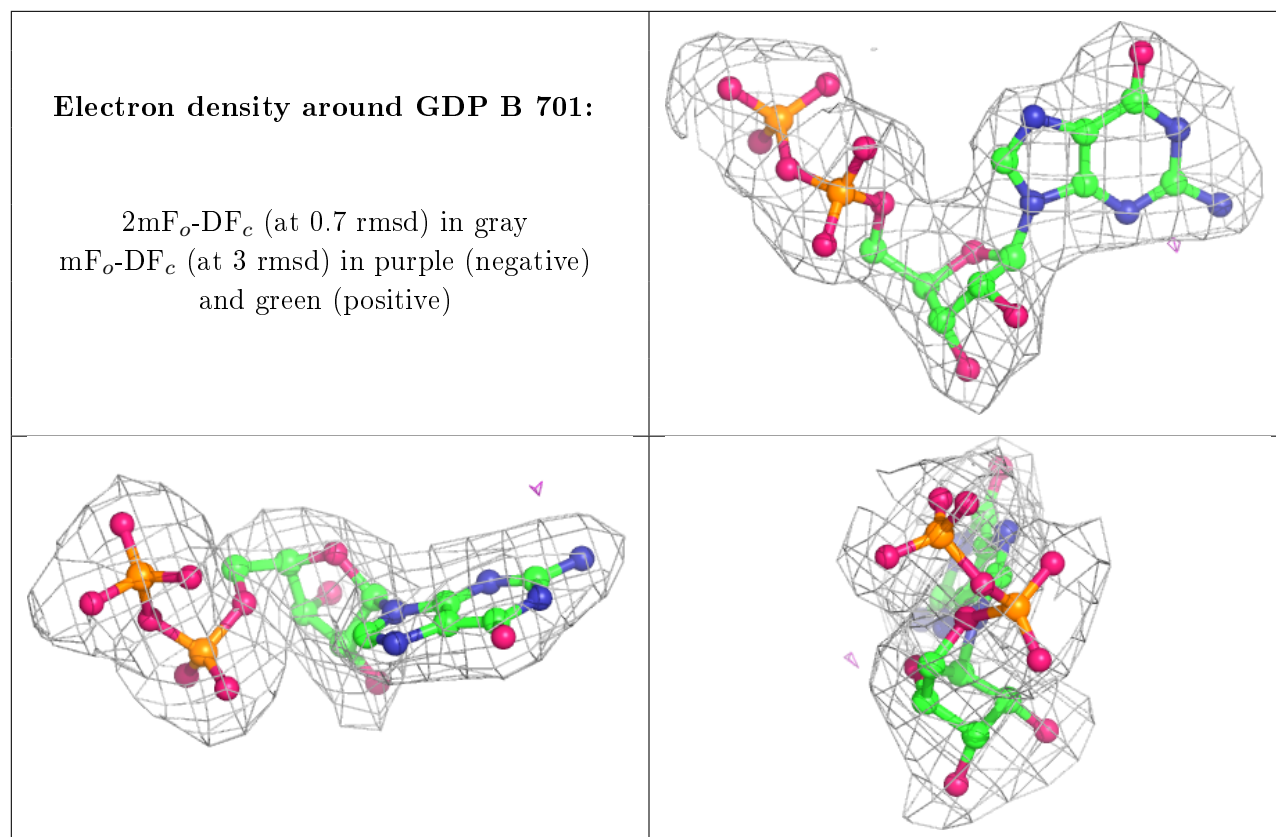
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP A 700:

$2mF_o-DF_c$ (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.