



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:24 PM UTC

PDB ID : 6UT3 / pdb_00006ut3
Title : X-ray structure of Thermococcus gammatolerans McrB AAA+ domain hexamer in P21 symmetry
Authors : Niu, Y.; Hosford, C.J.; Chappie, J.S.
Deposited on : 2019-10-29
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

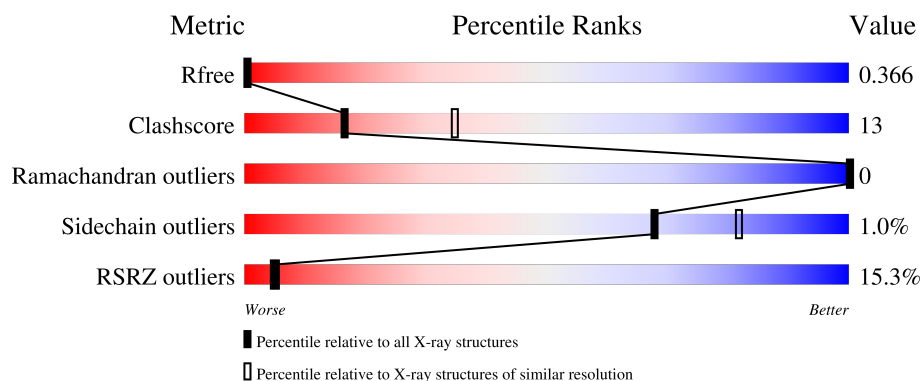
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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.



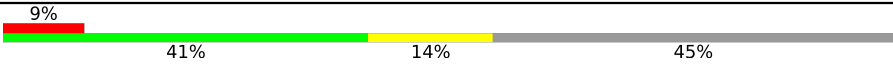
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	428	30% 61% 13% • 25%
1	B	428	11% 68% 16% • 15%
1	C	428	8% 67% 19% • 12%
1	D	428	6% 69% 19% • 11%
1	E	428	11% 54% 33% • 10%

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Mol	Chain	Length	Quality of chain
1	F	428	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GSP	C	701	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15959 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.

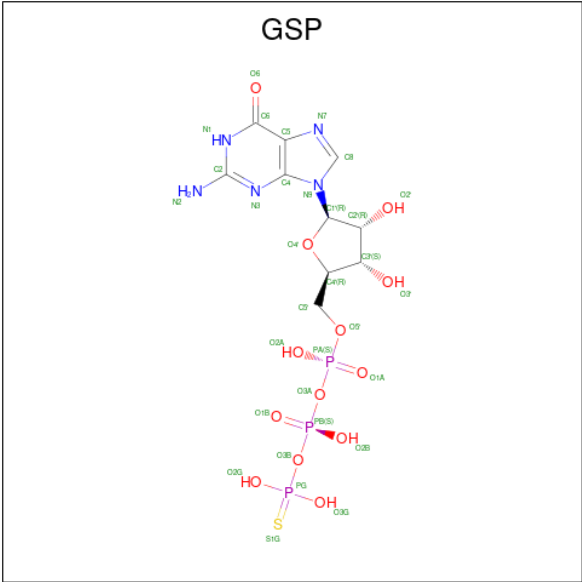
- Molecule 1 is a protein called GTPase subunit of restriction endonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2453	1575	425	451	2			
1	B	365	Total	C	N	O	S	0	0	0
			2667	1722	455	487	3			
1	C	375	Total	C	N	O	S	0	0	0
			2981	1938	507	533	3			
1	D	381	Total	C	N	O	S	0	0	0
			3016	1959	516	538	3			
1	E	384	Total	C	N	O	S	0	0	0
			2952	1919	495	535	3			
1	F	235	Total	C	N	O	S	0	0	0
			1758	1139	294	323	2			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S) (labeled as "Ligand of Interest" by depositor).

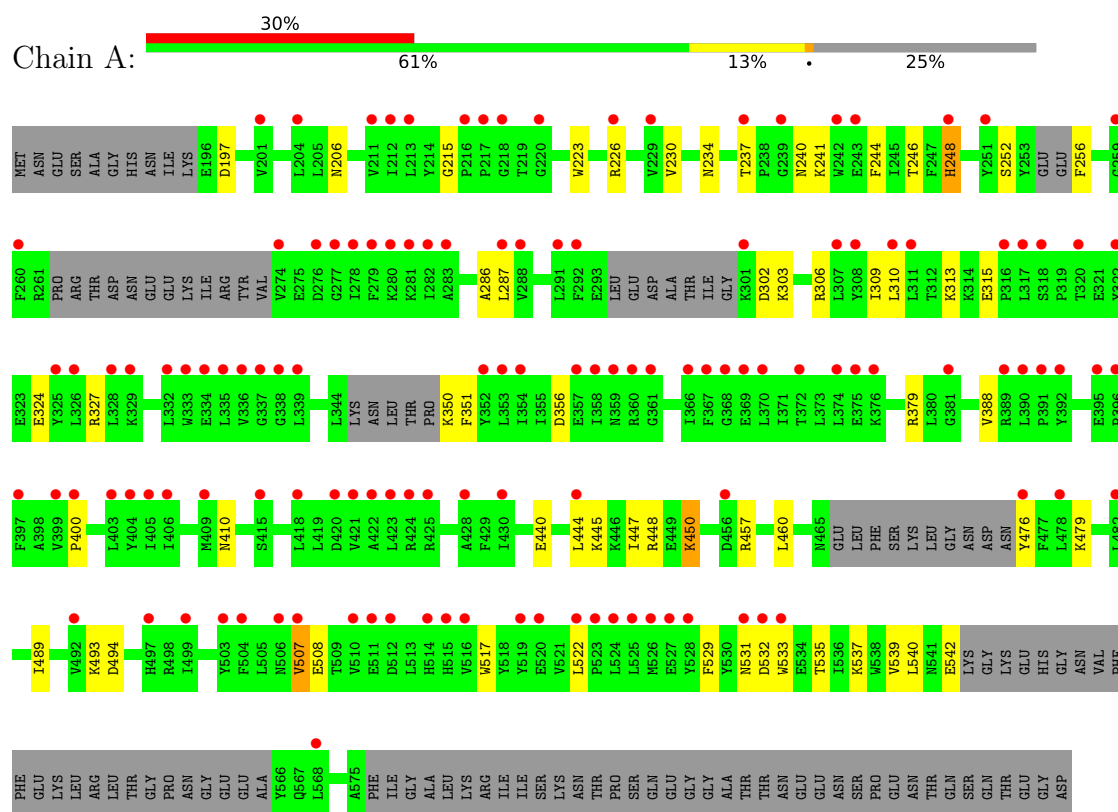


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
3	E	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		

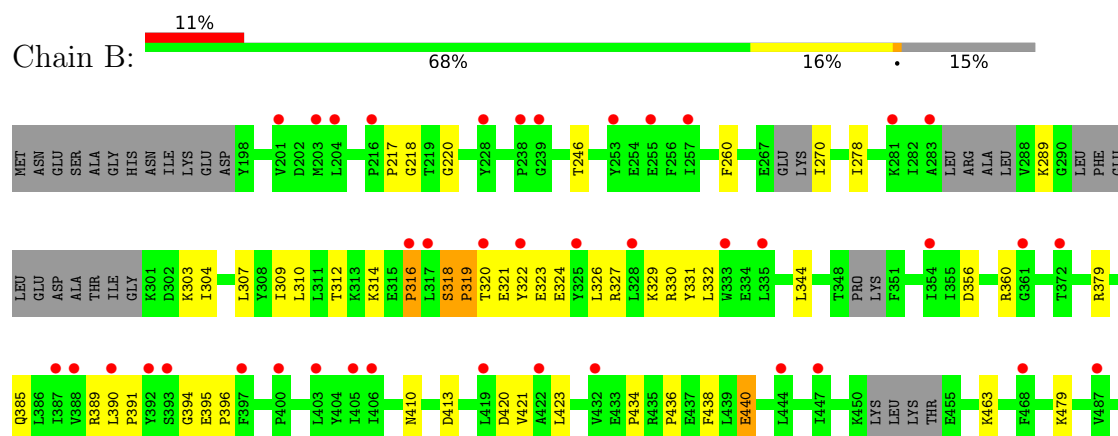
3 Residue-property plots

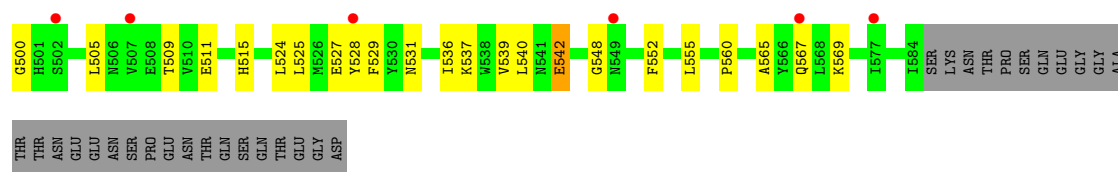
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

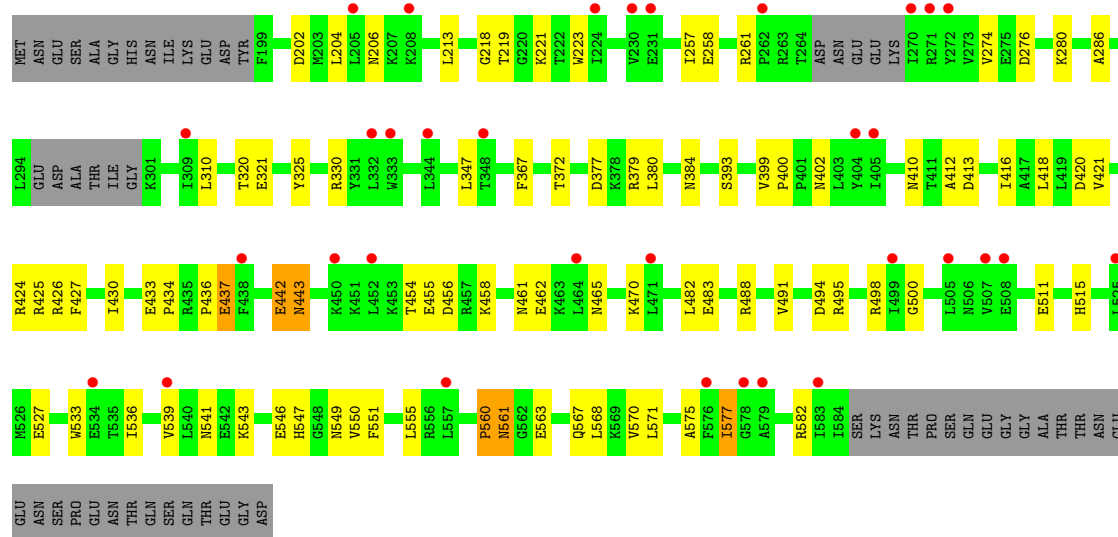


- Molecule 1: GTPase subunit of restriction endonuclease

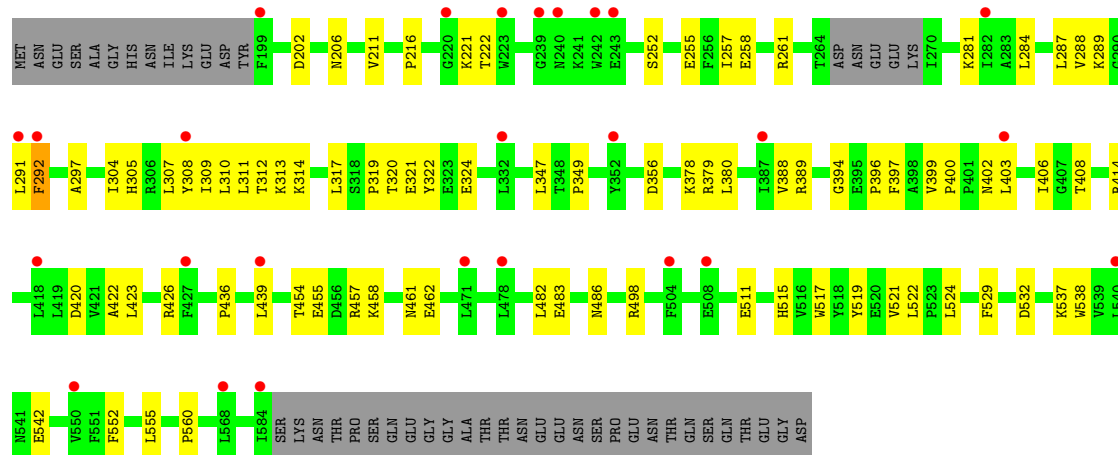




- Molecule 1: GTPase subunit of restriction endonuclease

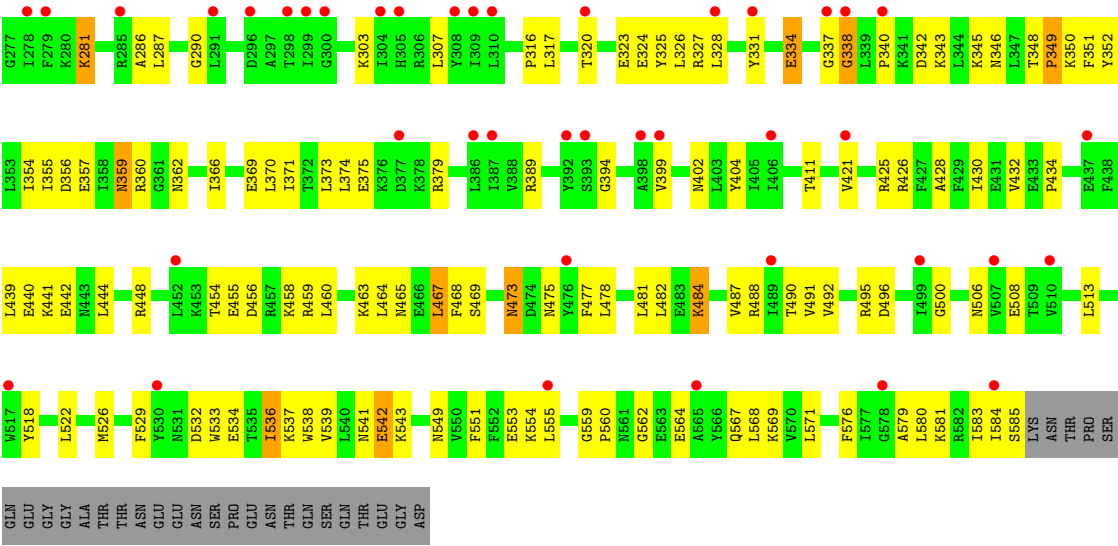


- Molecule 1: GTPase subunit of restriction endonuclease

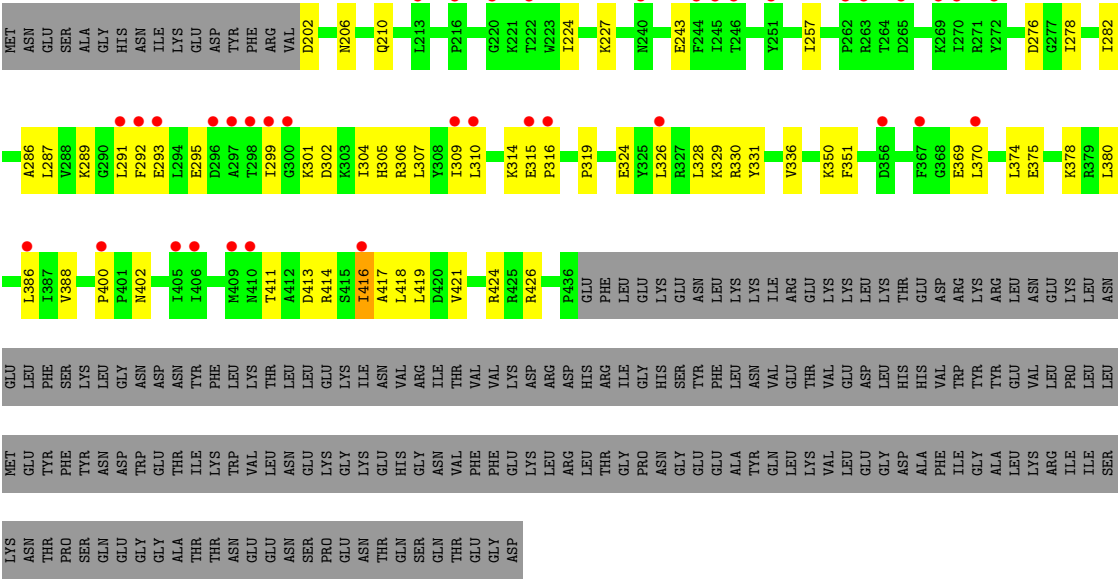
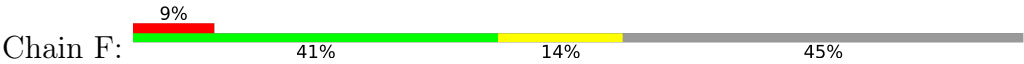


- Molecule 1: GTPase subunit of restriction endonuclease





● Molecule 1: GTPase subunit of restriction endonuclease



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.47Å 109.62Å 120.78Å 90.00° 108.33° 90.00°	Depositor
Resolution (Å)	114.65 – 2.95 114.65 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.5 (114.65-2.95) 99.5 (114.65-2.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.345 , 0.363 0.350 , 0.366	Depositor DCC
R_{free} test set	2000 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å ²)	109.1	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 121.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	15959	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: GSP, MG

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	0.41	0/2492	0.76	4/3369 (0.1%)
1	B	0.46	0/2714	0.84	7/3688 (0.2%)
1	C	0.42	0/3045	0.74	4/4125 (0.1%)
1	D	0.38	0/3081	0.76	6/4173 (0.1%)
1	E	0.65	0/3015	1.17	13/4096 (0.3%)
1	F	0.51	1/1792 (0.1%)	0.89	2/2439 (0.1%)
All	All	0.48	1/16139 (0.0%)	0.88	36/21890 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	301	LYS	C-O	-5.08	1.17	1.24

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	319	PRO	N-CA-C	-8.44	101.79	113.53
1	E	560	PRO	N-CA-C	-8.23	102.53	113.65
1	F	319	PRO	N-CA-C	-8.00	102.41	113.53
1	E	338	GLY	N-CA-C	-7.35	106.59	114.67
1	B	319	PRO	N-CA-C	-7.17	103.06	113.75
1	A	252	SER	N-CA-C	-7.15	104.43	113.01
1	B	316	PRO	N-CA-C	-7.08	105.50	114.35
1	B	542	GLU	N-CA-C	-6.86	103.03	111.33
1	D	322	TYR	N-CA-C	-6.79	103.81	111.07
1	C	560	PRO	CB-CA-C	-6.27	102.27	112.62
1	E	542	GLU	N-CA-C	-5.97	101.36	109.54
1	F	331	TYR	N-CA-C	-5.96	104.78	111.28
1	E	484	LYS	N-CA-C	-5.96	104.79	111.28
1	E	337	GLY	N-CA-C	-5.91	106.33	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	455	GLU	N-CA-C	-5.86	104.89	111.28
1	E	239	GLY	CA-C-O	-5.83	118.21	122.23
1	E	349	PRO	CB-CA-C	-5.75	103.56	111.21
1	A	248	HIS	CB-CA-C	5.64	120.24	110.94
1	B	318	SER	N-CA-C	-5.58	101.91	110.01
1	E	334	GLU	N-CA-C	-5.57	105.20	111.28
1	D	297	ALA	N-CA-C	-5.57	106.07	112.86
1	D	292	PHE	CB-CA-C	-5.54	102.19	110.88
1	A	450	LYS	CB-CA-C	-5.44	101.77	110.79
1	E	369	GLU	N-CA-C	-5.43	106.50	113.01
1	E	373	LEU	N-CA-C	5.42	117.00	111.14
1	B	324	GLU	N-CA-C	-5.37	105.43	111.28
1	C	434	PRO	N-CA-C	-5.36	102.70	110.80
1	B	309	ILE	N-CA-C	-5.34	105.17	110.62
1	C	541	ASN	CB-CA-C	5.34	119.60	111.80
1	C	561	ASN	N-CA-C	-5.26	106.63	113.16
1	E	281	LYS	N-CA-C	-5.20	105.61	111.28
1	D	314	LYS	N-CA-C	-5.19	106.94	113.28
1	A	531	ASN	N-CA-C	-5.15	105.65	112.24
1	E	350	LYS	N-CA-C	5.06	117.21	110.53
1	B	303	LYS	N-CA-C	-5.04	105.79	111.28
1	E	473	ASN	CB-CA-C	5.03	119.15	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2453	0	2337	49	0
1	B	2667	0	2432	65	0
1	C	2981	0	2910	76	0
1	D	3016	0	2938	67	0
1	E	2952	0	2808	119	0
1	F	1758	0	1679	46	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	C	64	0	24	17	0
3	D	32	0	12	1	0
3	E	32	0	12	1	0
All	All	15959	0	15152	400	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 13.

All (400) 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:E:240:ASN:O	1:E:241:LYS:HG2	1.29	1.29
1:E:342:ASP:HA	1:E:345:LYS:HD2	1.38	1.04
1:A:529:PHE:CB	1:A:532:ASP:HB3	1.90	1.00
1:B:390:LEU:HD12	1:B:391:PRO:HD2	1.41	0.98
1:E:240:ASN:O	1:E:241:LYS:CG	2.15	0.94
3:C:701:GSP:C5'	3:C:701:GSP:C8	2.53	0.91
1:E:229:VAL:HG21	1:E:354:ILE:HD11	1.54	0.90
1:E:529:PHE:HB3	1:E:532:ASP:HB3	1.55	0.88
1:D:288:VAL:HG21	1:D:307:LEU:HD22	1.57	0.87
1:B:390:LEU:HD12	1:B:391:PRO:CD	2.08	0.84
1:B:389:ARG:HA	1:B:396:PRO:HA	1.59	0.84
3:C:701:GSP:C8	3:C:701:GSP:H5'2	2.15	0.82
1:C:560:PRO:HB3	1:D:538:TRP:CD1	2.15	0.82
1:B:323:GLU:N	1:B:323:GLU:OE2	2.14	0.81
1:B:389:ARG:HA	1:B:396:PRO:CA	2.10	0.81
1:E:490:THR:HG22	1:E:495:ARG:HA	1.61	0.81
1:A:241:LYS:O	1:A:241:LYS:HG2	1.82	0.80
1:A:522:LEU:HA	1:A:539:VAL:CB	2.11	0.80
1:E:440:GLU:HG3	1:E:442:GLU:HG2	1.64	0.80
1:E:456:ASP:HB3	1:E:459:ARG:HE	1.47	0.79
1:F:315:GLU:N	1:F:316:PRO:HD2	1.99	0.78
1:A:241:LYS:HB2	1:A:351:PHE:CD1	2.19	0.78
1:B:390:LEU:HD23	1:B:394:GLY:HA3	1.65	0.77
1:C:577:ILE:N	1:C:577:ILE:HD12	1.99	0.77
3:C:701:GSP:C8	3:C:701:GSP:H5'1	2.19	0.77
1:B:289:LYS:HE3	1:B:304:ILE:CB	2.16	0.76
1:B:379:ARG:O	1:B:385:GLN:HG3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:346:ASN:OD1	1:E:346:ASN:O	2.04	0.75
1:B:440:GLU:OE1	1:B:440:GLU:N	2.20	0.75
1:C:560:PRO:HB3	1:D:538:TRP:CG	2.22	0.74
1:C:550:VAL:HA	1:C:582:ARG:HH22	1.52	0.74
1:C:555:LEU:HD21	1:C:567:GLN:HB2	1.68	0.74
1:B:505:LEU:HD12	3:C:701:GSP:H1'	1.69	0.74
1:C:570:VAL:O	1:C:570:VAL:HG23	1.88	0.74
1:F:418:LEU:C	1:F:418:LEU:HD23	2.13	0.73
1:A:241:LYS:HB2	1:A:351:PHE:HD1	1.54	0.72
1:E:254:GLU:N	1:E:254:GLU:OE1	2.23	0.71
1:F:287:LEU:HB2	1:F:400:PRO:HG3	1.71	0.71
1:A:246:THR:HA	1:A:356:ASP:HB2	1.74	0.69
1:A:315:GLU:HB3	1:B:389:ARG:HG3	1.74	0.68
1:B:548:GLY:O	1:B:569:LYS:NZ	2.26	0.68
1:C:367:PHE:HE2	1:C:427:PHE:HZ	1.40	0.68
1:A:529:PHE:CB	1:A:535:THR:HB	2.24	0.68
1:E:454:THR:O	1:E:454:THR:HG22	1.94	0.67
1:C:563:GLU:OE1	1:C:563:GLU:N	2.21	0.67
1:E:459:ARG:O	1:E:463:LYS:HG3	1.95	0.66
1:E:478:LEU:HD21	1:E:513:LEU:HD11	1.77	0.66
1:C:436:PRO:HG2	1:C:483:GLU:HG2	1.76	0.66
3:C:702:GSP:S1G	1:D:426:ARG:NH1	2.69	0.66
1:E:542:GLU:O	1:E:542:GLU:HG3	1.96	0.66
1:F:416:ILE:O	1:F:416:ILE:HG22	1.94	0.66
1:A:537:LYS:O	1:A:537:LYS:HG3	1.96	0.66
1:E:456:ASP:O	1:E:459:ARG:HG3	1.95	0.66
1:C:413:ASP:HB3	1:C:416:ILE:HG12	1.77	0.65
1:E:334:GLU:O	1:E:338:GLY:N	2.30	0.65
1:C:577:ILE:HD12	1:C:577:ILE:H	1.58	0.64
1:B:278:ILE:HD11	1:B:310:LEU:O	1.97	0.64
1:C:442:GLU:N	1:C:442:GLU:OE1	2.29	0.64
1:D:458:LYS:HA	1:D:461:ASN:ND2	2.12	0.64
1:E:323:GLU:HA	1:E:326:LEU:HD12	1.79	0.63
1:E:441:LYS:HZ3	1:E:465:ASN:HA	1.63	0.63
1:E:229:VAL:CG2	1:E:354:ILE:HD11	2.27	0.63
1:B:524:LEU:HD13	1:C:424:ARG:HD2	1.78	0.63
1:D:305:HIS:O	1:D:309:ILE:HG12	1.98	0.63
1:F:287:LEU:C	1:F:287:LEU:HD13	2.23	0.63
1:E:238:PRO:HA	1:E:242:TRP:CE3	2.33	0.63
1:B:220:GLY:HA2	3:C:701:GSP:PA	2.39	0.63
1:E:534:GLU:HB3	1:E:543:LYS:HE2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:488:ARG:O	1:E:491:VAL:HG22	1.99	0.63
1:B:389:ARG:CA	1:B:396:PRO:HA	2.29	0.62
1:F:289:LYS:O	1:F:292:PHE:HB2	1.99	0.62
1:B:314:LYS:HD3	1:C:330:ARG:HD2	1.80	0.62
1:B:537:LYS:HD2	1:B:542:GLU:CB	2.29	0.62
1:C:223:TRP:CD1	3:C:702:GSP:HO2'	2.18	0.62
3:C:701:GSP:H5'2	3:C:701:GSP:H8	1.64	0.62
1:E:362:ASN:O	1:E:366:ILE:HG12	2.00	0.62
1:E:455:GLU:HA	1:E:458:LYS:CE	2.30	0.62
1:F:306:ARG:O	1:F:309:ILE:HG12	1.99	0.62
1:D:281:LYS:HZ3	1:D:311:LEU:HA	1.64	0.61
1:E:477:PHE:HE1	1:E:581:LYS:HG2	1.65	0.61
1:B:555:LEU:HD21	1:B:567:GLN:HB2	1.81	0.61
1:B:217:PRO:HG2	1:C:421:VAL:HG22	1.82	0.61
1:D:308:TYR:CE2	1:D:312:THR:HG21	2.36	0.61
1:E:338:GLY:C	1:E:340:PRO:HD3	2.25	0.61
1:E:439:LEU:HD11	1:E:482:LEU:HD22	1.82	0.60
1:E:568:LEU:HD23	1:E:568:LEU:C	2.26	0.60
1:B:390:LEU:CD1	1:B:391:PRO:HD2	2.26	0.60
1:E:441:LYS:HZ2	1:E:468:PHE:HD2	1.49	0.60
1:B:318:SER:O	1:B:319:PRO:C	2.43	0.60
1:E:491:VAL:HG23	1:E:492:VAL:HG13	1.83	0.60
1:E:440:GLU:CG	1:E:442:GLU:HG2	2.32	0.59
1:F:302:ASP:O	1:F:306:ARG:HG2	2.02	0.59
1:E:238:PRO:HA	1:E:242:TRP:HE3	1.68	0.59
1:B:217:PRO:HG2	1:C:421:VAL:CG2	2.33	0.59
1:C:560:PRO:HD3	1:D:538:TRP:CD2	2.38	0.59
1:E:342:ASP:O	1:E:345:LYS:HB2	2.02	0.59
1:D:380:LEU:HB2	1:D:400:PRO:HA	1.84	0.59
3:C:702:GSP:O1A	1:D:378:LYS:NZ	2.34	0.58
1:D:292:PHE:CZ	1:D:305:HIS:HA	2.38	0.58
1:A:533:TRP:O	1:A:537:LYS:N	2.26	0.58
1:A:246:THR:CA	1:A:356:ASP:HB2	2.32	0.58
1:F:224:ILE:HA	1:F:227:LYS:HB2	1.85	0.58
1:F:306:ARG:O	1:F:310:LEU:HG	2.04	0.58
1:B:312:THR:CB	1:B:316:PRO:HB3	2.34	0.58
1:E:327:ARG:NE	1:E:331:TYR:OH	2.37	0.57
1:A:444:LEU:HG	1:A:445:LYS:HG3	1.86	0.57
1:B:260:PHE:O	1:B:270:ILE:N	2.37	0.57
1:B:390:LEU:HG	1:B:391:PRO:O	2.04	0.57
1:B:511:GLU:O	1:B:515:HIS:ND1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:ARG:NH2	1:D:403:LEU:O	2.37	0.57
1:C:511:GLU:O	1:C:515:HIS:ND1	2.37	0.57
1:E:458:LYS:HE2	1:E:458:LYS:H	1.68	0.57
1:B:389:ARG:HA	1:B:396:PRO:CB	2.34	0.57
1:F:306:ARG:HB2	1:F:328:LEU:CD1	2.34	0.57
1:A:445:LYS:HG2	1:A:448:ARG:CB	2.35	0.57
1:D:289:LYS:HG3	1:D:349:PRO:HG3	1.86	0.57
1:F:287:LEU:HD23	1:F:400:PRO:HB3	1.86	0.56
1:C:577:ILE:N	1:C:577:ILE:CD1	2.68	0.56
1:D:289:LYS:CG	1:D:349:PRO:HG3	2.36	0.56
1:A:457:ARG:HG2	1:A:457:ARG:HH11	1.70	0.56
1:A:447:ILE:O	1:A:450:LYS:HE3	2.06	0.56
1:C:577:ILE:H	1:C:577:ILE:CD1	2.19	0.56
1:E:441:LYS:NZ	1:E:465:ASN:HA	2.21	0.56
1:B:326:LEU:O	1:B:329:LYS:HB2	2.05	0.55
1:E:352:TYR:CD1	1:E:404:TYR:HB2	2.41	0.55
1:A:445:LYS:NZ	1:A:507:VAL:O	2.40	0.55
1:B:536:ILE:O	1:B:539:VAL:HG22	2.06	0.55
1:C:442:GLU:CD	1:C:442:GLU:H	2.09	0.55
1:B:314:LYS:HD3	1:C:330:ARG:CD	2.36	0.55
1:E:233:THR:O	1:E:234:ASN:HB2	2.07	0.55
1:D:537:LYS:NZ	1:D:542:GLU:OE2	2.37	0.55
1:C:527:GLU:OE2	1:D:414:ARG:NH2	2.39	0.55
1:F:315:GLU:N	1:F:316:PRO:CD	2.68	0.55
1:E:455:GLU:O	1:E:455:GLU:HG2	2.06	0.55
1:B:307:LEU:HD12	1:B:307:LEU:O	2.07	0.55
1:C:377:ASP:OD2	3:C:701:GSP:O3'	2.24	0.55
1:F:210:GLN:NE2	1:F:374:LEU:O	2.38	0.55
1:E:477:PHE:CE1	1:E:581:LYS:HG2	2.41	0.54
1:E:290:GLY:HA2	1:E:349:PRO:HD2	1.89	0.54
1:E:357:GLU:HB3	1:E:360:ARG:HG3	1.90	0.54
1:A:215:GLY:O	1:A:410:ASN:ND2	2.40	0.54
1:C:570:VAL:O	1:C:570:VAL:CG2	2.56	0.54
1:E:320:THR:O	1:E:324:GLU:N	2.40	0.54
1:B:360:ARG:NH2	1:C:420:ASP:OD2	2.41	0.54
1:D:321:GLU:HA	1:D:324:GLU:CB	2.38	0.54
1:D:457:ARG:HG2	1:D:458:LYS:N	2.21	0.54
1:C:379:ARG:HG2	1:C:399:VAL:HG13	1.89	0.54
1:E:240:ASN:C	1:E:241:LYS:HG2	2.24	0.54
1:D:202:ASP:O	1:D:206:ASN:ND2	2.40	0.53
1:E:371:ILE:O	1:E:426:ARG:NE	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:291:LEU:HD21	1:F:336:VAL:HG12	1.89	0.53
1:A:230:VAL:O	1:A:234:ASN:ND2	2.41	0.53
1:A:517:TRP:CD1	1:A:542:GLU:HG2	2.42	0.53
1:D:511:GLU:O	1:D:515:HIS:ND1	2.41	0.53
1:E:389:ARG:NH1	1:E:394:GLY:O	2.39	0.53
1:E:469:SER:HA	1:E:473:ASN:CG	2.33	0.53
1:E:568:LEU:HD23	1:E:569:LYS:N	2.24	0.53
1:D:255:GLU:OE2	1:D:261:ARG:NH2	2.42	0.53
1:D:347:LEU:HD12	1:D:402:ASN:HB2	1.89	0.53
1:E:286:ALA:HB1	1:E:402:ASN:CG	2.33	0.53
1:F:324:GLU:O	1:F:328:LEU:HG	2.07	0.53
1:A:460:LEU:HD21	1:A:508:GLU:HG2	1.91	0.53
1:E:448:ARG:NH1	1:E:506:ASN:HA	2.23	0.53
1:A:197:ASP:OD1	1:A:197:ASP:N	2.42	0.53
1:E:481:LEU:HD12	1:E:583:ILE:HD11	1.91	0.53
1:B:218:GLY:HA3	1:B:500:GLY:HA3	1.90	0.53
1:C:458:LYS:HA	1:C:461:ASN:HD22	1.73	0.53
1:C:258:GLU:OE1	1:C:280:LYS:NZ	2.41	0.52
1:B:560:PRO:HB3	1:C:543:LYS:HE3	1.92	0.52
1:E:488:ARG:HD3	1:E:539:VAL:HA	1.91	0.52
1:D:281:LYS:NZ	1:D:311:LEU:HA	2.23	0.52
1:E:221:LYS:O	1:E:224:ILE:HG22	2.09	0.52
1:D:517:TRP:HA	1:D:521:VAL:HG22	1.92	0.52
1:E:541:ASN:ND2	1:E:585:SER:O	2.42	0.52
1:D:389:ARG:NH1	1:D:394:GLY:O	2.43	0.52
1:A:248:HIS:CD2	1:B:421:VAL:HG21	2.45	0.52
1:C:426:ARG:NH1	3:C:701:GSP:S1G	2.78	0.52
1:D:529:PHE:HB3	1:D:532:ASP:HB3	1.92	0.52
1:F:307:LEU:O	1:F:310:LEU:HB2	2.10	0.52
1:F:421:VAL:HA	1:F:424:ARG:HD3	1.91	0.52
1:B:220:GLY:HA2	3:C:701:GSP:O3A	2.10	0.52
1:D:389:ARG:HA	1:D:396:PRO:HA	1.91	0.52
1:F:413:ASP:O	1:F:417:ALA:HB2	2.09	0.52
1:F:417:ALA:O	1:F:419:LEU:HG	2.10	0.52
1:C:204:LEU:HD12	1:C:430:ILE:HD11	1.91	0.52
1:D:307:LEU:C	1:D:307:LEU:HD23	2.35	0.52
1:B:327:ARG:HA	1:B:330:ARG:CG	2.40	0.51
1:C:560:PRO:HD3	1:D:538:TRP:CE3	2.45	0.51
1:E:316:PRO:HA	1:F:330:ARG:HD2	1.92	0.51
1:E:464:LEU:HA	1:E:467:LEU:HB2	1.91	0.51
1:D:555:LEU:HD13	1:E:487:VAL:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:GLN:C	1:B:385:GLN:CD	2.78	0.51
1:C:494:ASP:N	1:C:494:ASP:OD1	2.44	0.51
1:D:257:ILE:HG22	1:D:258:GLU:HG2	1.91	0.51
1:A:457:ARG:HB3	1:A:457:ARG:CZ	2.39	0.51
1:C:551:PHE:O	1:C:568:LEU:HD12	2.11	0.51
1:F:202:ASP:O	1:F:206:ASN:ND2	2.41	0.51
1:F:326:LEU:HB3	1:F:330:ARG:HH21	1.76	0.51
1:D:313:LYS:NZ	1:D:317:LEU:HA	2.24	0.51
1:C:202:ASP:OD1	1:C:202:ASP:N	2.42	0.51
1:C:380:LEU:HB2	1:C:400:PRO:HA	1.93	0.51
1:B:540:LEU:HD12	1:B:552:PHE:CE2	2.46	0.51
1:E:379:ARG:HG2	1:E:399:VAL:HG23	1.93	0.51
1:E:464:LEU:HD21	1:E:508:GLU:HA	1.93	0.51
1:E:241:LYS:HA	1:E:351:PHE:CD2	2.47	0.50
1:E:554:LYS:NZ	1:E:555:LEU:O	2.44	0.50
1:F:314:LYS:C	1:F:316:PRO:HD2	2.36	0.50
1:D:307:LEU:HA	1:D:310:LEU:HD12	1.93	0.50
1:B:434:PRO:HB3	1:B:500:GLY:HA2	1.93	0.50
1:C:218:GLY:HA3	1:C:500:GLY:HA3	1.93	0.50
1:D:524:LEU:HD11	1:E:421:VAL:HG23	1.93	0.50
1:F:378:LYS:HD3	1:F:386:LEU:HD12	1.92	0.50
1:B:220:GLY:HA2	3:C:701:GSP:O5'	2.11	0.50
1:E:274:VAL:O	1:E:274:VAL:HG13	2.11	0.50
1:C:286:ALA:O	1:C:402:ASN:ND2	2.42	0.50
1:D:537:LYS:HZ2	1:D:552:PHE:HB2	1.76	0.50
1:C:219:THR:OG1	1:C:221:LYS:NZ	2.45	0.50
1:D:216:PRO:O	1:D:221:LYS:NZ	2.44	0.50
1:E:303:LYS:HA	1:E:307:LEU:HG	1.94	0.50
1:B:436:PRO:HB2	1:B:479:LYS:HG2	1.94	0.50
1:E:454:THR:O	1:E:455:GLU:HB3	2.11	0.50
1:F:416:ILE:O	1:F:416:ILE:CG2	2.59	0.50
1:B:565:ALA:HB2	1:C:491:VAL:HA	1.94	0.49
1:D:454:THR:O	1:D:457:ARG:NH2	2.38	0.49
1:F:293:GLU:N	1:F:293:GLU:OE1	2.44	0.49
1:D:436:PRO:HB3	1:D:482:LEU:HB3	1.93	0.49
1:A:479:LYS:O	1:A:479:LYS:NZ	2.45	0.49
1:C:202:ASP:O	1:C:206:ASN:ND2	2.45	0.49
1:E:533:TRP:O	1:E:537:LYS:HG3	2.11	0.49
1:D:560:PRO:HD3	1:E:538:TRP:CZ3	2.47	0.49
1:A:310:LEU:HD12	1:A:313:LYS:HD2	1.95	0.49
1:E:218:GLY:HA3	1:E:500:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:ALA:O	1:E:229:VAL:HG22	2.12	0.49
1:E:533:TRP:O	1:E:536:ILE:HG22	2.13	0.49
1:B:389:ARG:HA	1:B:396:PRO:CG	2.43	0.48
1:B:524:LEU:HB2	1:C:424:ARG:HD3	1.94	0.48
1:A:306:ARG:HD2	1:A:309:ILE:CG2	2.43	0.48
1:C:571:LEU:HD22	1:C:575:ALA:HB1	1.95	0.48
1:F:418:LEU:C	1:F:418:LEU:CD2	2.84	0.48
1:A:517:TRP:HZ2	1:A:540:LEU:HB3	1.78	0.48
1:B:331:TYR:O	1:B:332:LEU:C	2.57	0.48
1:E:439:LEU:N	1:E:439:LEU:HD23	2.28	0.48
1:A:256:PHE:HE2	1:A:388:VAL:HG21	1.79	0.47
1:B:318:SER:CB	1:B:321:GLU:CB	2.92	0.47
1:D:349:PRO:HG2	1:D:402:ASN:HD21	1.79	0.47
1:F:418:LEU:HD23	1:F:419:LEU:N	2.29	0.47
1:B:436:PRO:C	1:B:438:PHE:N	2.70	0.47
1:E:490:THR:HG22	1:E:495:ARG:CA	2.37	0.47
1:A:287:LEU:HB2	1:A:400:PRO:HB3	1.96	0.47
1:D:284:LEU:O	1:D:288:VAL:HG23	2.14	0.47
1:D:313:LYS:HZ3	1:D:317:LEU:HA	1.78	0.47
1:E:211:VAL:HG22	1:E:428:ALA:HB3	1.96	0.47
1:E:325:TYR:HA	1:E:328:LEU:HD12	1.97	0.47
1:E:359:ASN:OD1	1:E:359:ASN:N	2.45	0.47
1:E:536:ILE:O	1:E:539:VAL:HG22	2.15	0.47
1:A:537:LYS:O	1:A:537:LYS:CG	2.61	0.47
1:D:292:PHE:HD1	1:D:304:ILE:HD12	1.80	0.47
1:D:560:PRO:HD3	1:E:538:TRP:CE3	2.50	0.47
1:E:484:LYS:HE2	1:E:584:ILE:HG23	1.97	0.47
1:A:241:LYS:HE2	1:A:350:LYS:HG3	1.97	0.47
1:A:256:PHE:CE2	1:A:388:VAL:HG21	2.50	0.47
1:C:495:ARG:O	1:C:498:ARG:NE	2.47	0.47
1:C:462:GLU:HA	1:C:465:ASN:HB2	1.97	0.47
1:D:422:ALA:O	1:D:426:ARG:NH1	2.46	0.47
1:E:370:LEU:HB3	1:E:374:LEU:HG	1.97	0.47
1:A:522:LEU:CA	1:A:539:VAL:CB	2.89	0.46
1:B:527:GLU:HG2	1:C:424:ARG:NH2	2.30	0.46
1:C:213:LEU:HA	1:C:430:ILE:O	2.15	0.46
1:B:525:LEU:HD23	1:B:528:TYR:HD2	1.80	0.46
1:C:443:ASN:OD1	1:C:443:ASN:N	2.48	0.46
3:C:701:GSP:C5'	3:C:701:GSP:N9	2.79	0.46
1:E:375:GLU:OE2	1:E:425:ARG:NH1	2.47	0.46
1:E:571:LEU:C	1:E:576:PHE:HB2	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:LEU:O	1:C:424:ARG:NH2	2.48	0.46
1:A:440:GLU:O	1:A:444:LEU:N	2.49	0.46
1:A:517:TRP:CZ2	1:A:540:LEU:HB3	2.51	0.45
1:F:411:THR:O	1:F:414:ARG:HG3	2.16	0.45
1:E:411:THR:HG23	1:E:496:ASP:HB3	1.98	0.45
1:E:468:PHE:CD1	1:E:475:ASN:HA	2.52	0.45
1:C:437:GLU:CD	1:C:437:GLU:H	2.24	0.45
1:D:261:ARG:HD3	1:D:261:ARG:HA	1.77	0.45
1:A:226:ARG:HH12	1:A:244:PHE:N	2.14	0.45
1:C:384:ASN:ND2	3:C:701:GSP:O3'	2.48	0.45
1:D:202:ASP:OD1	1:D:202:ASP:N	2.49	0.45
1:D:288:VAL:HG21	1:D:307:LEU:CD2	2.39	0.45
1:D:436:PRO:HG2	1:D:483:GLU:HG2	1.97	0.45
1:B:389:ARG:HA	1:B:396:PRO:HG3	1.99	0.45
1:F:287:LEU:HD11	1:F:291:LEU:HD22	1.99	0.45
1:C:425:ARG:NH1	3:C:701:GSP:O2A	2.50	0.45
1:E:522:LEU:HG	1:E:526:MET:HE2	1.99	0.45
1:F:375:GLU:HB2	1:F:378:LYS:HG2	1.99	0.45
1:D:287:LEU:O	1:D:291:LEU:HG	2.17	0.44
1:B:463:LYS:HD2	1:B:509:THR:HG22	2.00	0.44
1:C:320:THR:OG1	1:C:321:GLU:OE1	2.34	0.44
1:F:286:ALA:HA	1:F:351:PHE:CE1	2.52	0.44
1:E:286:ALA:O	1:E:287:LEU:C	2.61	0.44
1:E:580:LEU:O	1:E:583:ILE:HG12	2.17	0.44
1:A:517:TRP:CZ2	1:A:540:LEU:HD22	2.53	0.44
1:D:320:THR:HB	1:D:321:GLU:OE1	2.17	0.44
1:E:456:ASP:HA	1:E:459:ARG:HG3	2.00	0.44
1:F:276:ASP:OD2	1:F:329:LYS:NZ	2.50	0.44
1:F:291:LEU:HD21	1:F:336:VAL:CG1	2.47	0.44
1:B:436:PRO:C	1:B:438:PHE:H	2.26	0.44
1:D:519:TYR:HE1	1:E:430:ILE:HG23	1.82	0.44
1:E:455:GLU:HA	1:E:458:LYS:NZ	2.33	0.44
1:F:380:LEU:HB2	1:F:400:PRO:HA	1.99	0.44
1:A:241:LYS:HB2	1:A:351:PHE:CE1	2.53	0.43
1:B:320:THR:O	1:B:323:GLU:HB2	2.18	0.43
1:C:436:PRO:HB3	1:C:482:LEU:HB3	2.00	0.43
1:E:281:LYS:NZ	1:E:327:ARG:HH22	2.15	0.43
1:E:551:PHE:O	1:E:568:LEU:HA	2.18	0.43
1:E:559:GLY:C	1:E:562:GLY:H	2.26	0.43
1:D:486:ASN:HB3	1:D:498:ARG:HD2	2.00	0.43
1:E:348:THR:CB	1:E:349:PRO:HD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:THR:HG22	1:B:356:ASP:HB3	2.00	0.43
1:B:356:ASP:OD2	1:C:372:THR:OG1	2.34	0.43
1:E:276:ASP:OD1	1:E:276:ASP:N	2.50	0.43
1:B:531:ASN:HD21	1:C:494:ASP:HA	1.83	0.43
1:A:457:ARG:HH11	1:A:457:ARG:CG	2.31	0.43
1:D:461:ASN:OD1	1:D:462:GLU:N	2.51	0.43
1:E:248:HIS:CE1	1:E:250:SER:HB2	2.54	0.43
1:F:306:ARG:HB2	1:F:328:LEU:HD11	2.00	0.43
1:C:261:ARG:HA	1:C:261:ARG:HD3	1.75	0.43
1:C:563:GLU:H	1:C:563:GLU:CD	2.20	0.43
1:D:420:ASP:HB3	1:D:423:LEU:HB3	2.00	0.43
1:E:343:LYS:HE3	1:E:343:LYS:HB2	1.77	0.43
1:E:448:ARG:HD3	1:E:460:LEU:HD21	2.00	0.43
1:A:324:GLU:HG3	1:A:327:ARG:HE	1.84	0.43
1:C:549:ASN:CG	1:C:549:ASN:O	2.61	0.43
1:E:491:VAL:HG21	1:E:538:TRP:CZ3	2.53	0.43
1:A:302:ASP:OD1	1:A:303:LYS:N	2.51	0.43
1:E:221:LYS:HG2	1:E:432:VAL:HG21	2.01	0.43
1:E:245:ILE:CG2	1:E:355:ILE:HG12	2.49	0.43
1:E:581:LYS:HA	1:E:584:ILE:HD12	2.00	0.43
1:E:434:PRO:HB3	1:E:500:GLY:HA2	2.01	0.43
1:F:305:HIS:O	1:F:309:ILE:HG23	2.19	0.43
1:D:388:VAL:O	1:D:397:PHE:N	2.52	0.42
1:C:560:PRO:HD3	1:D:538:TRP:CE2	2.55	0.42
1:A:440:GLU:OE2	1:A:476:TYR:N	2.52	0.42
1:D:211:VAL:HG12	1:D:406:ILE:HG12	2.02	0.42
1:D:379:ARG:HG2	1:D:399:VAL:HG23	2.01	0.42
1:E:554:LYS:HE2	1:E:564:GLU:CB	2.49	0.42
1:B:525:LEU:HB3	1:B:536:ILE:CD1	2.48	0.42
1:C:276:ASP:OD2	1:C:325:TYR:OH	2.35	0.42
1:D:288:VAL:HG12	1:D:292:PHE:CE1	2.54	0.42
1:E:334:GLU:O	1:E:338:GLY:CA	2.67	0.42
1:E:491:VAL:CG2	1:E:538:TRP:HZ3	2.32	0.42
1:A:286:ALA:HA	1:A:351:PHE:HD2	1.84	0.42
1:E:252:SER:HB3	1:E:255:GLU:HG3	2.01	0.42
1:E:323:GLU:O	1:E:326:LEU:HB2	2.19	0.42
1:A:206:ASN:OD1	1:A:379:ARG:NH1	2.53	0.42
1:B:410:ASN:ND2	1:B:413:ASP:OD2	2.53	0.42
1:C:257:ILE:HG22	1:C:258:GLU:HG2	2.02	0.42
1:E:244:PHE:HD2	1:F:388:VAL:HG23	1.85	0.42
1:F:257:ILE:HD11	1:F:370:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:ILE:HD12	1:A:493:LYS:HG2	2.02	0.42
1:D:439:LEU:HD23	1:D:439:LEU:HA	1.91	0.42
1:E:454:THR:O	1:E:454:THR:CG2	2.63	0.42
1:E:518:TYR:OH	1:E:571:LEU:N	2.53	0.42
1:B:321:GLU:O	1:B:322:TYR:C	2.63	0.41
1:C:488:ARG:HD3	1:C:539:VAL:HA	2.02	0.41
1:A:223:TRP:CZ3	1:A:450:LYS:HE2	2.55	0.41
1:D:252:SER:OG	1:D:255:GLU:OE1	2.31	0.41
1:E:549:ASN:OD1	1:E:579:ALA:HB2	2.19	0.41
1:B:394:GLY:O	1:B:395:GLU:C	2.62	0.41
1:C:410:ASN:HD21	1:C:412:ALA:HB3	1.86	0.41
1:C:546:GLU:O	1:C:547:HIS:C	2.62	0.41
1:D:222:THR:OG1	3:D:700:GSP:O1B	2.38	0.41
1:E:448:ARG:HG2	1:E:448:ARG:O	2.20	0.41
1:C:274:VAL:HG11	1:C:393:SER:HB3	2.02	0.41
1:E:456:ASP:HB3	1:E:459:ARG:NE	2.25	0.41
1:B:327:ARG:O	1:B:330:ARG:HG3	2.20	0.41
3:C:701:GSP:H5'1	3:C:701:GSP:N9	2.35	0.41
1:C:347:LEU:HD12	1:C:402:ASN:HB2	2.02	0.41
1:C:560:PRO:HG2	1:C:561:ASN:H	1.86	0.41
1:F:243:GLU:HB2	1:F:282:ILE:HD12	2.03	0.41
1:E:317:LEU:HD12	1:E:317:LEU:HA	1.95	0.41
1:E:478:LEU:CD2	1:E:513:LEU:HD11	2.49	0.41
1:A:237:THR:HG23	1:A:240:ASN:OD1	2.20	0.41
1:C:310:LEU:HD13	1:C:325:TYR:HB2	2.01	0.41
1:D:356:ASP:OD1	1:D:408:THR:OG1	2.33	0.41
1:E:553:GLU:O	1:E:567:GLN:N	2.53	0.41
1:A:494:ASP:OD1	1:A:494:ASP:N	2.53	0.41
1:D:522:LEU:HD23	1:D:522:LEU:HA	1.89	0.41
1:B:327:ARG:O	1:B:330:ARG:N	2.54	0.40
1:C:454:THR:HG22	1:C:455:GLU:H	1.86	0.40
1:D:289:LYS:HE2	1:D:308:TYR:CE1	2.56	0.40
1:C:533:TRP:HA	1:C:536:ILE:HG22	2.02	0.40
1:E:440:GLU:O	1:E:444:LEU:N	2.48	0.40
1:A:302:ASP:OD1	1:A:302:ASP:C	2.64	0.40
1:B:420:ASP:OD2	1:B:423:LEU:N	2.54	0.40
1:C:456:ASP:OD1	1:C:456:ASP:N	2.48	0.40
1:F:292:PHE:CE1	1:F:304:ILE:HG22	2.56	0.40
1:F:350:LYS:HA	1:F:402:ASN:HB2	2.03	0.40
1:C:470:LYS:HD3	1:C:470:LYS:HA	1.89	0.40
1:F:295:GLU:O	1:F:299:ILE:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:GLU:OE2	1:C:495:ARG:NH2	2.54	0.40
1:E:246:THR:HB	1:F:369:GLU:HG3	2.03	0.40
1:E:323:GLU:HA	1:E:326:LEU:HB2	2.04	0.40
3:E:700:GSP:PG	1:F:426:ARG:HH12	2.44	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	307/428 (72%)	275 (90%)	32 (10%)	0	100	100
1	B	353/428 (82%)	338 (96%)	15 (4%)	0	100	100
1	C	369/428 (86%)	353 (96%)	16 (4%)	0	100	100
1	D	377/428 (88%)	358 (95%)	19 (5%)	0	100	100
1	E	382/428 (89%)	360 (94%)	22 (6%)	0	100	100
1	F	233/428 (54%)	224 (96%)	9 (4%)	0	100	100
All	All	2021/2568 (79%)	1908 (94%)	113 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	237/385 (62%)	236 (100%)	1 (0%)	84	92
1	B	237/385 (62%)	234 (99%)	3 (1%)	61	78
1	C	302/385 (78%)	298 (99%)	4 (1%)	61	78
1	D	302/385 (78%)	302 (100%)	0	100	100
1	E	285/385 (74%)	279 (98%)	6 (2%)	47	69
1	F	168/385 (44%)	166 (99%)	2 (1%)	63	79
All	All	1531/2310 (66%)	1515 (99%)	16 (1%)	68	82

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	507	VAL
1	B	344	LEU
1	B	440	GLU
1	B	529	PHE
1	C	437	GLU
1	C	442	GLU
1	C	443	ASN
1	C	577	ILE
1	E	229	VAL
1	E	257	ILE
1	E	356	ASP
1	E	359	ASN
1	E	467	LEU
1	E	536	ILE
1	F	278	ILE
1	F	416	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	A	359	ASN
1	A	501	HIS
1	B	384	ASN
1	B	486	ASN
1	C	248	HIS
1	C	384	ASN
1	C	461	ASN
1	C	465	ASN

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Mol	Chain	Res	Type
1	C	501	HIS
1	D	206	ASN
1	D	384	ASN
1	D	443	ASN
1	E	346	ASN
1	E	443	ASN
1	F	384	ASN

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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
3	GSP	D	700	2	33,34,34	0.60	0	47,54,54	0.64	1 (2%)
3	GSP	E	700	2	33,34,34	0.59	0	47,54,54	0.65	0
3	GSP	C	701	2	33,34,34	0.60	0	47,54,54	0.79	1 (2%)
3	GSP	C	702	2	33,34,34	0.61	0	47,54,54	0.74	1 (2%)

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
3	GSP	D	700	2	-	0/21/38/38	0/3/3/3
3	GSP	E	700	2	-	0/21/38/38	0/3/3/3
3	GSP	C	701	2	-	5/21/38/38	0/3/3/3
3	GSP	C	702	2	-	1/21/38/38	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	GSP	PB-O3B-PG	-3.33	120.97	133.17
3	C	702	GSP	PB-O3B-PG	-3.00	122.21	133.17
3	D	700	GSP	PB-O3B-PG	-2.07	125.59	133.17

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	701	GSP	C5'-O5'-PA-O3A
3	C	701	GSP	C3'-C4'-C5'-O5'
3	C	701	GSP	C4'-C5'-O5'-PA
3	C	701	GSP	O4'-C4'-C5'-O5'
3	C	701	GSP	C5'-O5'-PA-O1A
3	C	702	GSP	PB-O3B-PG-O2G

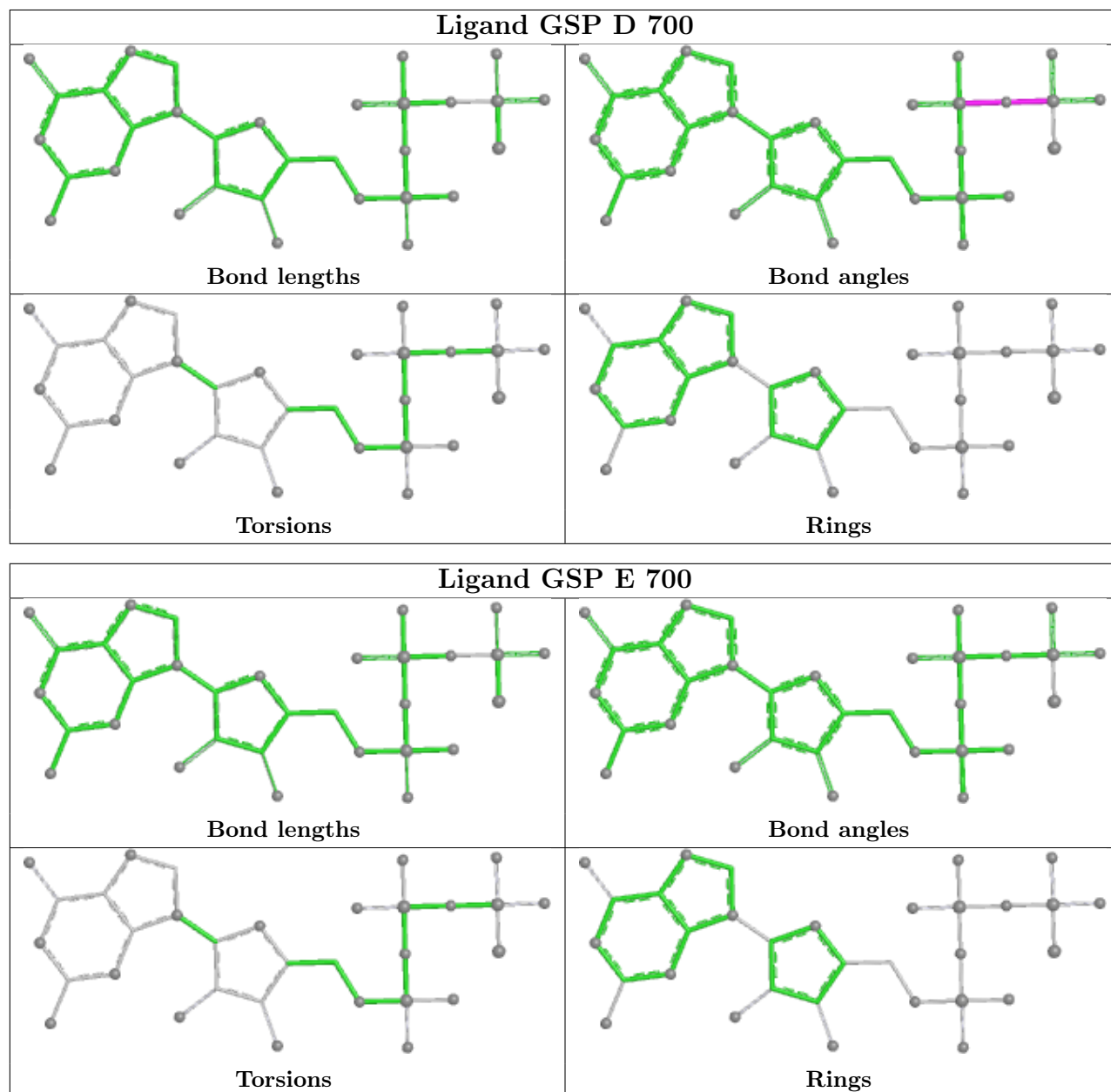
There are no ring outliers.

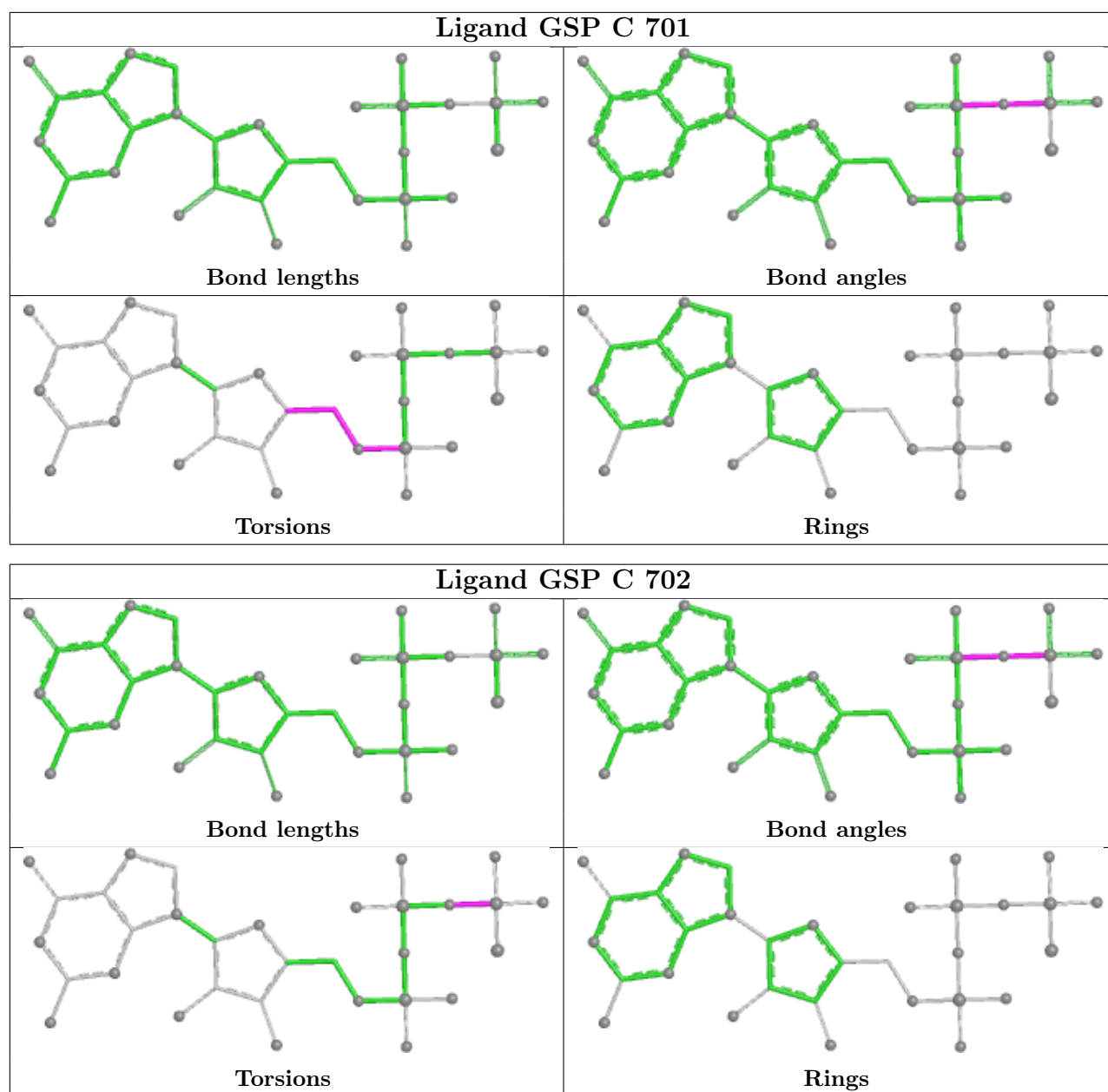
4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	700	GSP	1	0
3	E	700	GSP	1	0
3	C	701	GSP	14	0
3	C	702	GSP	3	0

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

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	321/428 (75%)	1.95	127 (39%) 1 0	70, 211, 232, 246	0
1	B	365/428 (85%)	0.99	46 (12%) 8 7	30, 119, 167, 186	0
1	C	375/428 (87%)	0.87	33 (8%) 15 14	46, 103, 140, 175	0
1	D	381/428 (89%)	0.77	26 (6%) 23 20	76, 108, 140, 155	0
1	E	384/428 (89%)	0.89	45 (11%) 9 8	30, 114, 151, 187	0
1	F	235/428 (54%)	1.11	38 (16%) 4 4	30, 119, 156, 170	0
All	All	2061/2568 (80%)	1.07	315 (15%) 5 5	30, 118, 219, 246	0

All (315) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	LYS	11.0
1	A	519	TYR	8.1
1	A	332	LEU	7.7
1	C	271	ARG	7.0
1	A	281	LYS	6.8
1	A	338	GLY	5.7
1	A	352	TYR	5.5
1	A	370	LEU	5.3
1	A	366	ILE	5.2
1	A	358	ILE	5.2
1	F	269	LYS	5.2
1	A	396	PRO	5.2
1	A	406	ILE	5.1
1	F	246	THR	5.0
1	A	405	ILE	5.0
1	A	278	ILE	4.9
1	A	277	GLY	4.9
1	B	361	GLY	4.8
1	A	353	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	F	220	GLY	4.8
1	A	318	SER	4.7
1	E	304	ILE	4.7
1	A	499	ILE	4.5
1	A	204	LEU	4.5
1	E	204	LEU	4.5
1	F	216	PRO	4.5
1	A	328	LEU	4.5
1	B	393	SER	4.4
1	A	390	LEU	4.3
1	F	405	ILE	4.2
1	A	399	VAL	4.2
1	B	316	PRO	4.2
1	F	310	LEU	4.2
1	F	300	GLY	4.1
1	D	240	ASN	4.1
1	A	423	LEU	4.1
1	F	299	ILE	4.1
1	F	213	LEU	4.1
1	A	528	TYR	4.1
1	A	368	GLY	4.0
1	A	372	THR	4.0
1	A	515	HIS	3.9
1	D	243	GLU	3.9
1	A	391	PRO	3.9
1	B	388	VAL	3.9
1	A	360	ARG	3.8
1	D	427	PHE	3.8
1	A	276	ASP	3.7
1	A	317	LEU	3.7
1	A	524	LEU	3.7
1	A	397	PHE	3.7
1	A	288	VAL	3.7
1	B	317	LEU	3.7
1	A	422	ALA	3.7
1	A	279	PHE	3.7
1	A	424	ARG	3.7
1	A	291	LEU	3.6
1	A	325	TYR	3.6
1	C	270	ILE	3.6
1	E	387	ILE	3.6
1	A	507	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	492	VAL	3.6
1	B	392	TYR	3.6
1	C	205	LEU	3.6
1	E	331	TYR	3.5
1	A	212	ILE	3.5
1	A	357	GLU	3.5
1	A	282	ILE	3.5
1	A	211	VAL	3.5
1	A	242	TRP	3.5
1	A	333	TRP	3.5
1	A	520	GLU	3.4
1	A	322	TYR	3.4
1	F	309	ILE	3.4
1	E	310	LEU	3.4
1	A	359	ASN	3.4
1	B	403	LEU	3.4
1	B	387	ILE	3.4
1	F	315	GLU	3.4
1	A	478	LEU	3.3
1	C	262	PRO	3.3
1	E	291	LEU	3.3
1	E	265	ASP	3.3
1	B	283	ALA	3.3
1	E	305	HIS	3.3
1	F	222	THR	3.3
1	B	257	ILE	3.3
1	A	229	VAL	3.3
1	D	220	GLY	3.3
1	A	527	GLU	3.2
1	A	418	LEU	3.2
1	B	406	ILE	3.2
1	E	584	ILE	3.2
1	D	223	TRP	3.2
1	E	392	TYR	3.2
1	F	409	MET	3.2
1	F	296	ASP	3.2
1	C	507	VAL	3.2
1	F	270	ILE	3.2
1	E	377	ASP	3.2
1	A	409	MET	3.2
1	B	372	THR	3.2
1	A	329	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	510	VAL	3.1
1	C	464	LEU	3.1
1	A	425	ARG	3.1
1	B	502	SER	3.1
1	A	361	GLY	3.1
1	E	229	VAL	3.0
1	E	393	SER	3.0
1	A	476	TYR	3.0
1	E	398	ALA	3.0
1	A	326	LEU	3.0
1	A	369	GLU	3.0
1	C	579	ALA	3.0
1	C	438	PHE	3.0
1	B	419	LEU	2.9
1	E	285	ARG	2.9
1	A	217	PRO	2.9
1	E	298	THR	2.9
1	E	309	ILE	2.9
1	A	403	LEU	2.9
1	B	444	LEU	2.9
1	F	326	LEU	2.9
1	A	283	ALA	2.9
1	A	421	VAL	2.9
1	A	292	PHE	2.9
1	C	471	LEU	2.9
1	A	334	GLU	2.8
1	D	352	TYR	2.8
1	A	506	ASN	2.8
1	A	307	LEU	2.8
1	E	300	GLY	2.8
1	B	328	LEU	2.8
1	B	390	LEU	2.8
1	A	420	ASP	2.8
1	F	356	ASP	2.8
1	F	262	PRO	2.8
1	C	231	GLU	2.8
1	B	228	TYR	2.8
1	A	339	LEU	2.8
1	F	386	LEU	2.8
1	D	308	TYR	2.7
1	F	251	TYR	2.7
1	E	299	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	251	TYR	2.7
1	A	392	TYR	2.7
1	E	320	THR	2.7
1	A	337	GLY	2.7
1	A	336	VAL	2.7
1	A	430	ILE	2.7
1	B	400	PRO	2.7
1	C	344	LEU	2.7
1	A	354	ILE	2.6
1	A	376	LYS	2.6
1	A	308	TYR	2.6
1	B	325	TYR	2.6
1	A	444	LEU	2.6
1	B	281	LYS	2.6
1	C	450	LYS	2.6
1	B	447	ILE	2.6
1	E	279	PHE	2.6
1	A	404	TYR	2.6
1	A	523	PRO	2.6
1	B	239	GLY	2.6
1	B	335	LEU	2.6
1	C	272	TYR	2.6
1	D	239	GLY	2.6
1	A	201	VAL	2.6
1	E	565	ALA	2.6
1	A	512	ASP	2.6
1	B	320	THR	2.5
1	B	397	PHE	2.5
1	A	381	GLY	2.5
1	B	322	TYR	2.5
1	A	511	GLU	2.5
1	F	410	ASN	2.5
1	A	400	PRO	2.5
1	D	291	LEU	2.5
1	F	406	ILE	2.5
1	E	399	VAL	2.5
1	F	298	THR	2.5
1	E	296	ASP	2.5
1	A	374	LEU	2.5
1	E	406	ILE	2.5
1	A	260	PHE	2.5
1	E	437	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	583	ILE	2.4
1	E	489	ILE	2.4
1	C	576	PHE	2.4
1	F	240	ASN	2.4
1	A	568	LEU	2.4
1	D	568	LEU	2.4
1	E	452	LEU	2.4
1	B	201	VAL	2.4
1	D	199	PHE	2.4
1	B	577	ILE	2.4
1	F	263	ARG	2.4
1	B	422	ALA	2.4
1	A	310	LEU	2.4
1	A	218	GLY	2.4
1	E	517	TRP	2.4
1	C	404	TYR	2.4
1	A	514	HIS	2.4
1	C	508	GLU	2.3
1	A	311	LEU	2.3
1	A	525	LEU	2.3
1	C	224	ILE	2.3
1	C	405	ILE	2.3
1	A	301	LYS	2.3
1	A	395	GLU	2.3
1	A	532	ASP	2.3
1	A	482	LEU	2.3
1	D	439	LEU	2.3
1	A	320	THR	2.3
1	F	245	ILE	2.3
1	C	578	GLY	2.3
1	A	243	GLU	2.3
1	A	375	GLU	2.3
1	A	316	PRO	2.3
1	B	487	VAL	2.3
1	E	338	GLY	2.3
1	A	335	LEU	2.3
1	A	497	HIS	2.3
1	D	584	ILE	2.3
1	B	333	TRP	2.3
1	C	348	THR	2.3
1	E	530	TYR	2.3
1	B	432	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	504	PHE	2.2
1	B	255	GLU	2.2
1	F	265	ASP	2.2
1	B	405	ILE	2.2
1	D	387	ILE	2.2
1	E	499	ILE	2.2
1	A	389	ARG	2.2
1	E	242	TRP	2.2
1	A	216	PRO	2.2
1	A	516	VAL	2.2
1	F	400	PRO	2.2
1	A	503	TYR	2.2
1	B	253	TYR	2.2
1	D	508	GLU	2.2
1	A	226	ARG	2.2
1	A	510	VAL	2.2
1	B	468	PHE	2.2
1	F	292	PHE	2.2
1	C	505	LEU	2.2
1	C	534	GLU	2.2
1	E	328	LEU	2.2
1	C	309	ILE	2.2
1	E	278	ILE	2.2
1	A	533	TRP	2.2
1	C	333	TRP	2.2
1	A	367	PHE	2.2
1	D	471	LEU	2.2
1	F	297	ALA	2.2
1	B	567	GLN	2.2
1	A	239	GLY	2.2
1	E	337	GLY	2.2
1	A	287	LEU	2.2
1	B	354	ILE	2.1
1	A	274	VAL	2.1
1	D	242	TRP	2.1
1	C	332	LEU	2.1
1	D	478	LEU	2.1
1	F	291	LEU	2.1
1	A	415	SER	2.1
1	A	248	HIS	2.1
1	B	549	ASN	2.1
1	E	340	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	452	LEU	2.1
1	C	557	LEU	2.1
1	D	540	LEU	2.1
1	E	386	LEU	2.1
1	F	367	PHE	2.1
1	F	370	LEU	2.1
1	E	308	TYR	2.1
1	F	272	TYR	2.1
1	F	293	GLU	2.1
1	C	230	VAL	2.1
1	D	550	VAL	2.1
1	E	507	VAL	2.1
1	A	213	LEU	2.1
1	A	259	GLY	2.1
1	B	204	LEU	2.1
1	A	237	THR	2.1
1	B	528	TYR	2.1
1	E	476	TYR	2.1
1	E	421	VAL	2.1
1	F	244	PHE	2.1
1	A	428	ALA	2.1
1	A	526	MET	2.0
1	B	216	PRO	2.0
1	F	316	PRO	2.0
1	A	522	LEU	2.0
1	D	403	LEU	2.0
1	E	555	LEU	2.0
1	D	292	PHE	2.0
1	D	504	PHE	2.0
1	C	499	ILE	2.0
1	D	282	ILE	2.0
1	B	238	PRO	2.0
1	C	525	LEU	2.0
1	D	332	LEU	2.0
1	D	418	LEU	2.0
1	A	531	ASN	2.0
1	A	220	GLY	2.0
1	E	578	GLY	2.0
1	F	416	ILE	2.0
1	A	456	ASP	2.0
1	C	208	LYS	2.0
1	B	203	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	507	VAL	2.0
1	C	539	VAL	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](#)

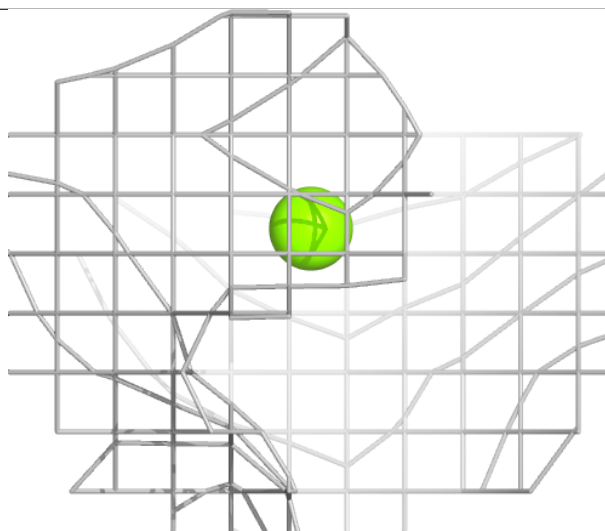
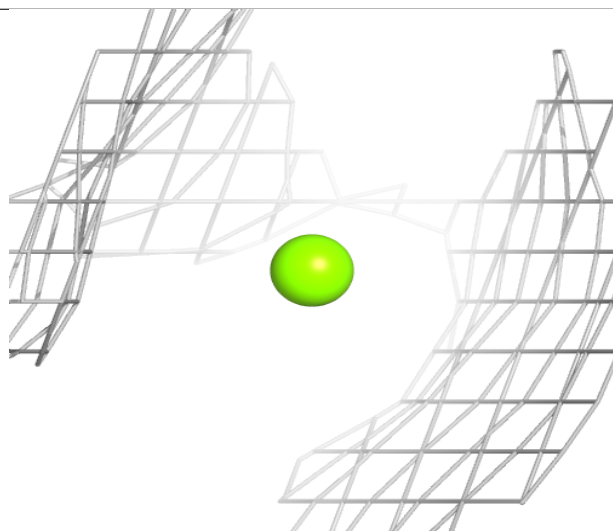
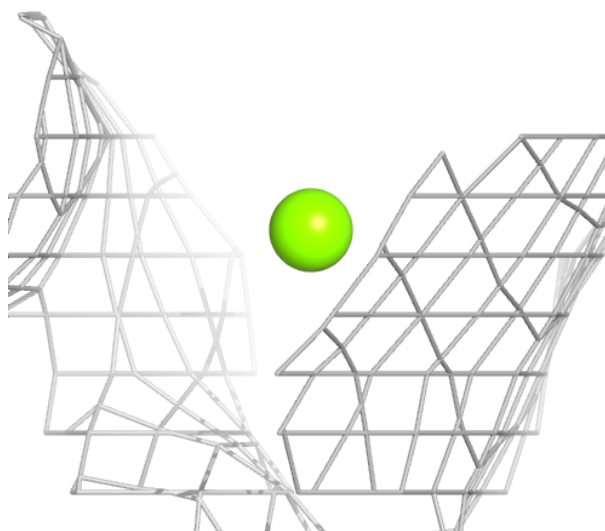
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	E	701	1/1	0.84	0.13	100,100,100,100	0
3	GSP	C	701	32/32	0.85	0.09	120,120,120,120	0
2	MG	B	701	1/1	0.87	0.09	115,115,115,115	0
3	GSP	C	702	32/32	0.89	0.09	101,101,101,101	0
3	GSP	D	700	32/32	0.90	0.09	107,107,107,107	0
3	GSP	E	700	32/32	0.90	0.09	113,113,113,113	0
2	MG	D	701	1/1	0.94	0.11	84,84,84,84	0
2	MG	C	703	1/1	0.94	0.11	80,80,80,80	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.

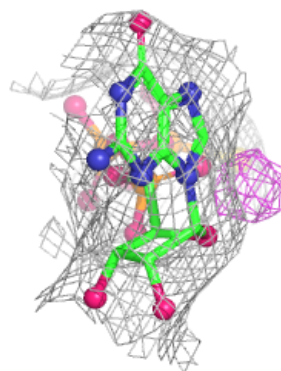
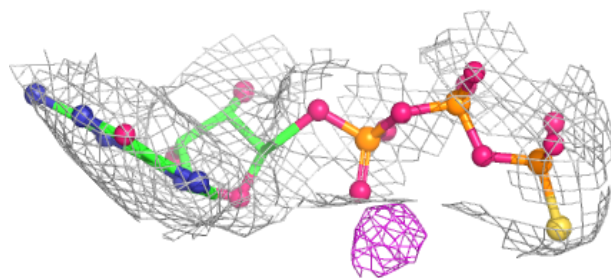
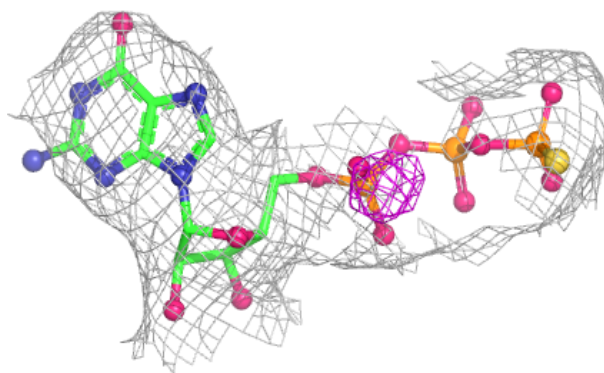
Electron density around MG E 701:

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



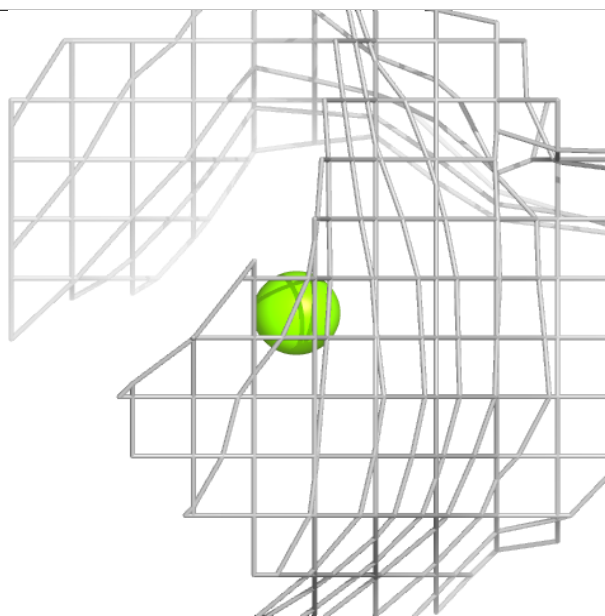
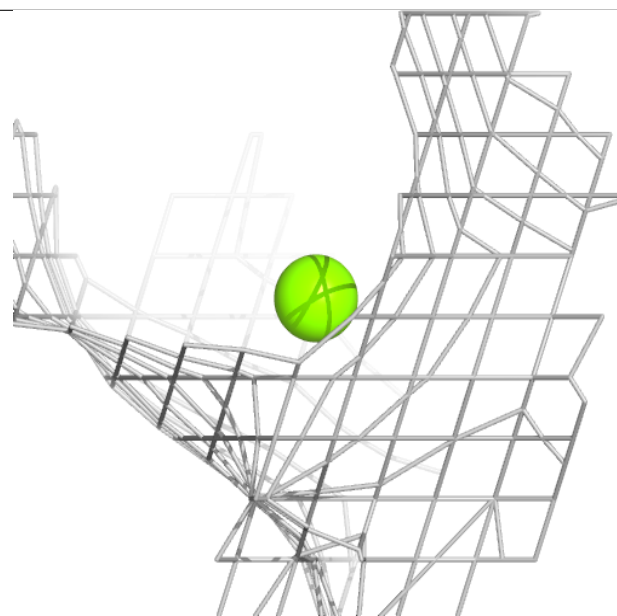
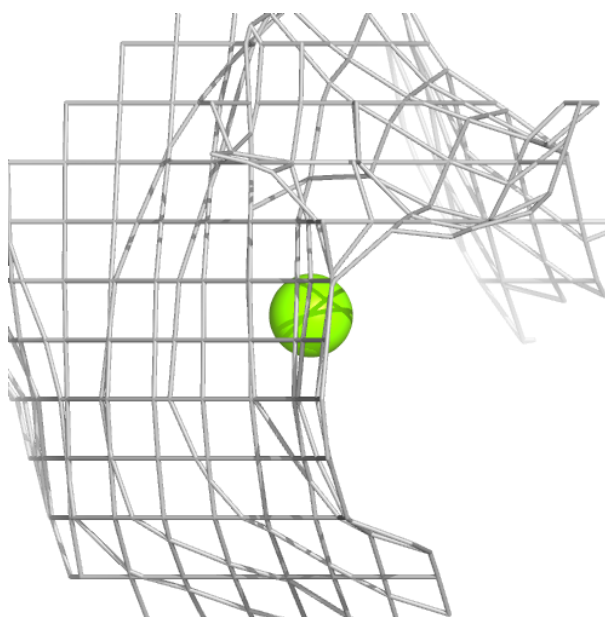
Electron density around GSP C 701:

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



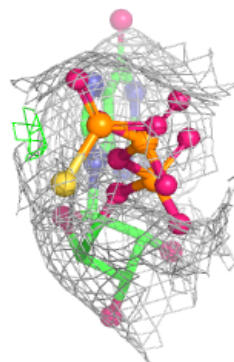
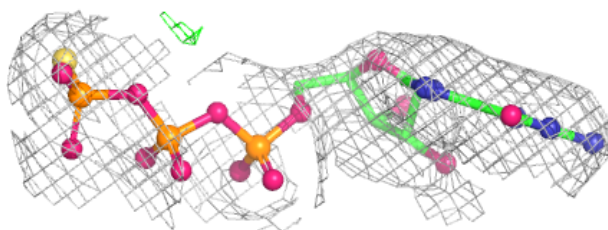
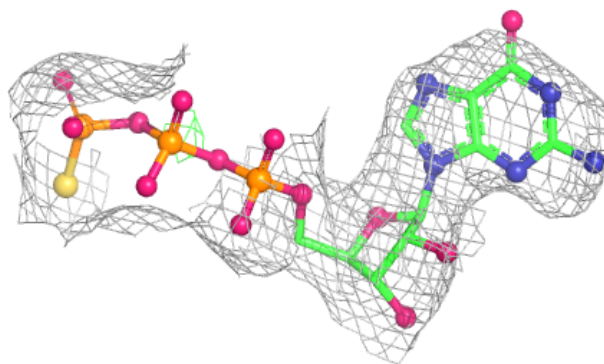
Electron density around MG B 701:

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

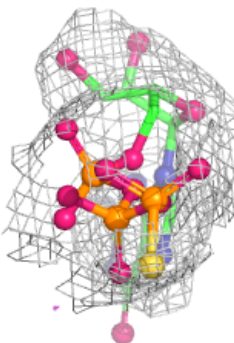
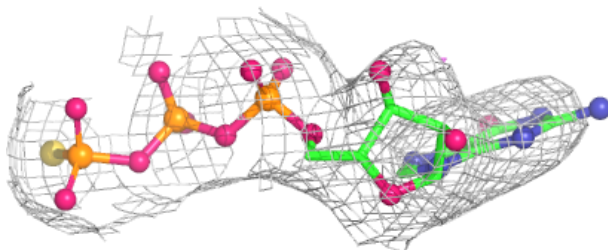
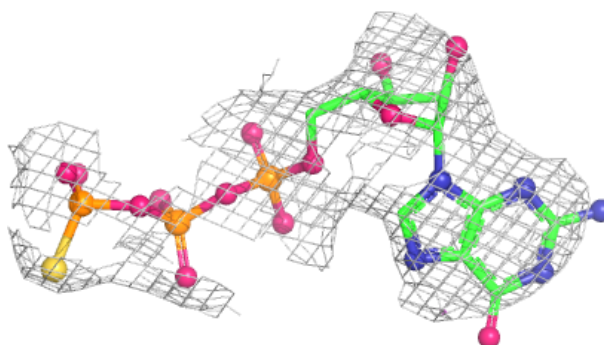


Electron density around GSP C 702:

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

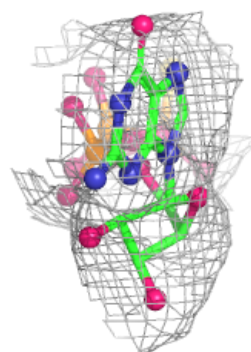
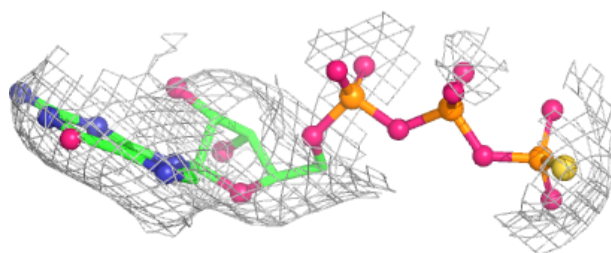
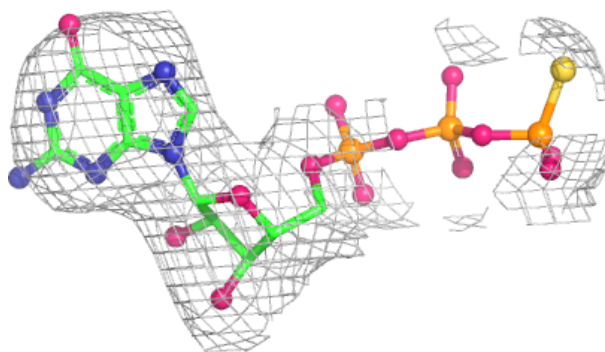
**Electron density around GSP D 700:**

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



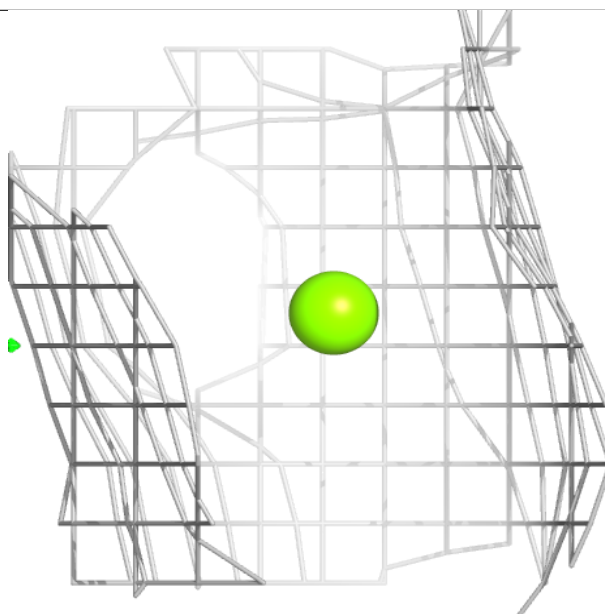
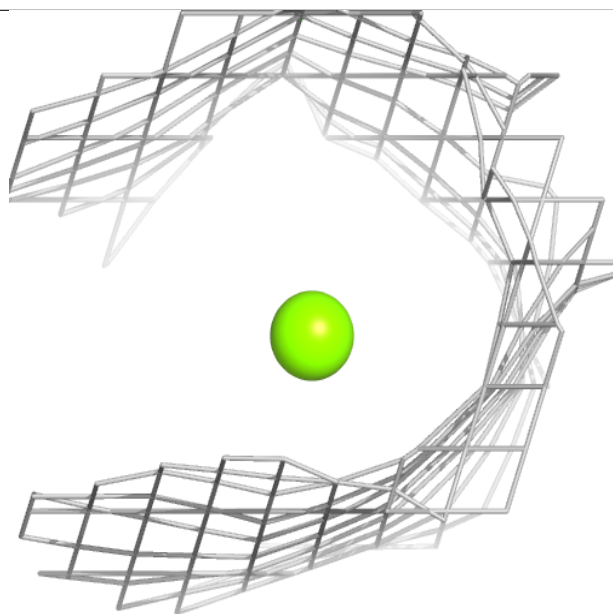
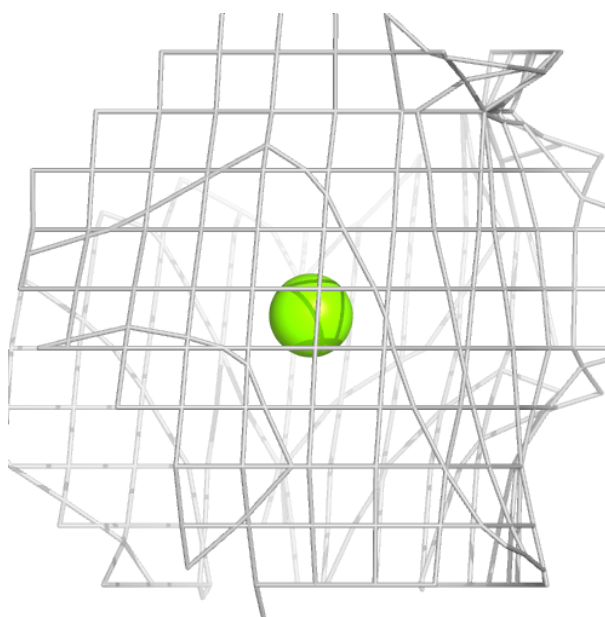
Electron density around GSP E 700:

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



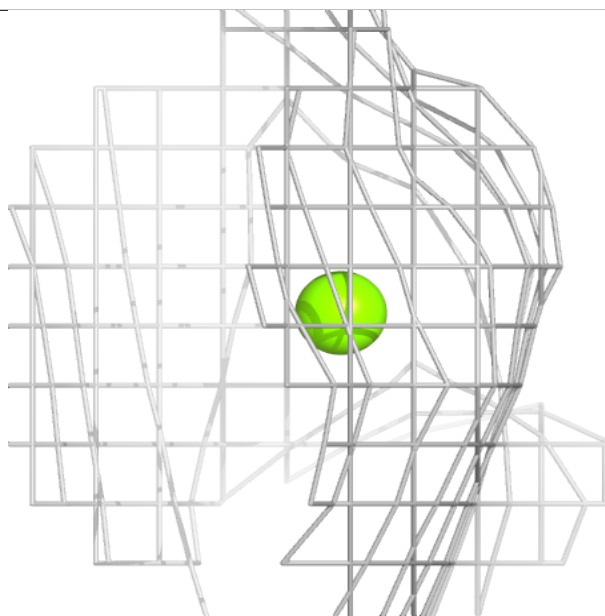
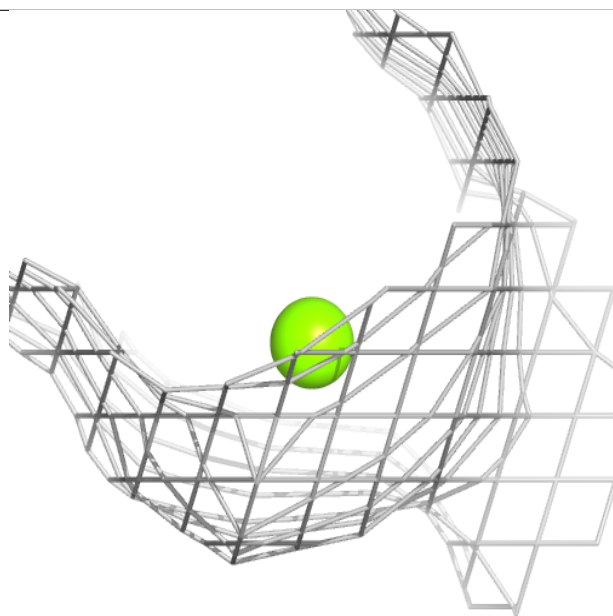
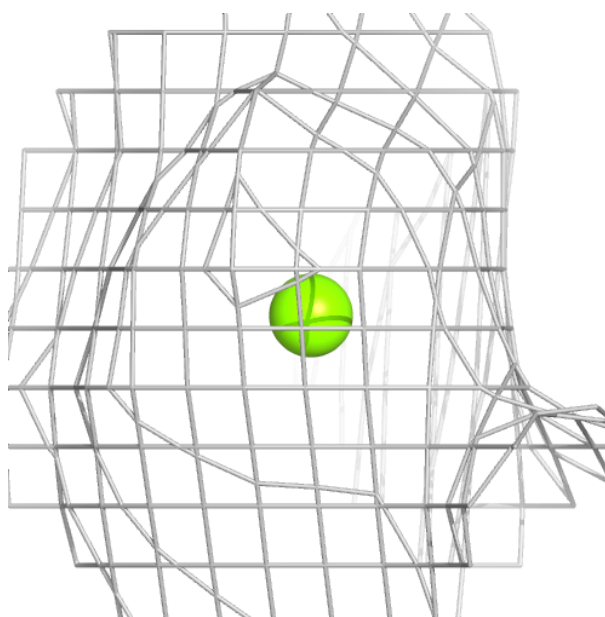
Electron density around MG D 701:

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



Electron density around MG C 703:

$2mF_o-DF_c$ (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.