



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:14 AM UTC

PDB ID : 2PMD / pdb_00002pmd
Title : The structures of aIF2gamma subunit from the archaeon Sulfolobus solfataricus in the GDP-bound form.
Authors : Nikonov, O.S.; Stolboushkina, E.A.; Nikulin, A.D.; Hasenohrl, D.; Blaesl, U.; Manstein, D.J.; Fedorov, R.V.; Garber, M.B.; Nikonov, S.V.
Deposited on : 2007-04-21
Resolution : 2.65 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

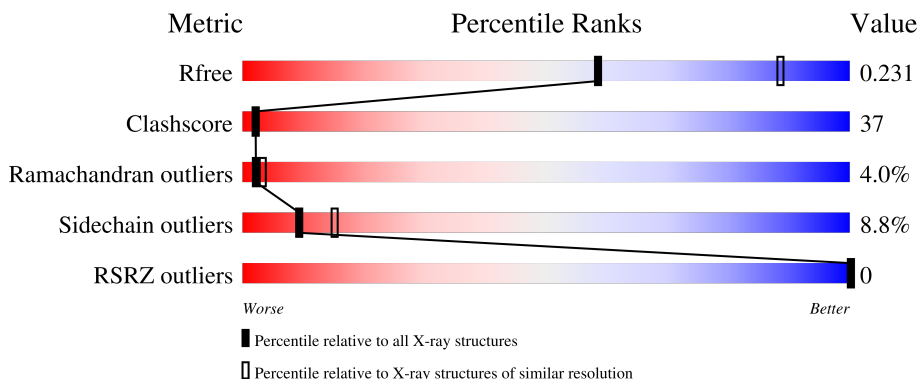
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	415	
1	B	415	

2 Entry composition [i](#)

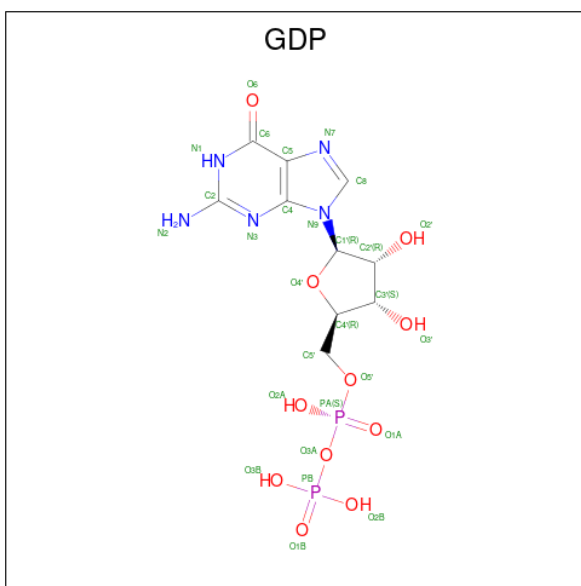
There are 5 unique types of molecules in this entry. The entry contains 6726 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Translation initiation factor 2 gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	414	Total 3212	C 2058	N 548	O 594	S 12	0	0	0
1	B	414	Total 3212	C 2058	N 548	O 594	S 12	0	0	0

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			9	7	2		
4	B	1	Total	O	P	0	0
			9	7	2		
4	B	1	Total	O	P	0	0
			9	7	2		

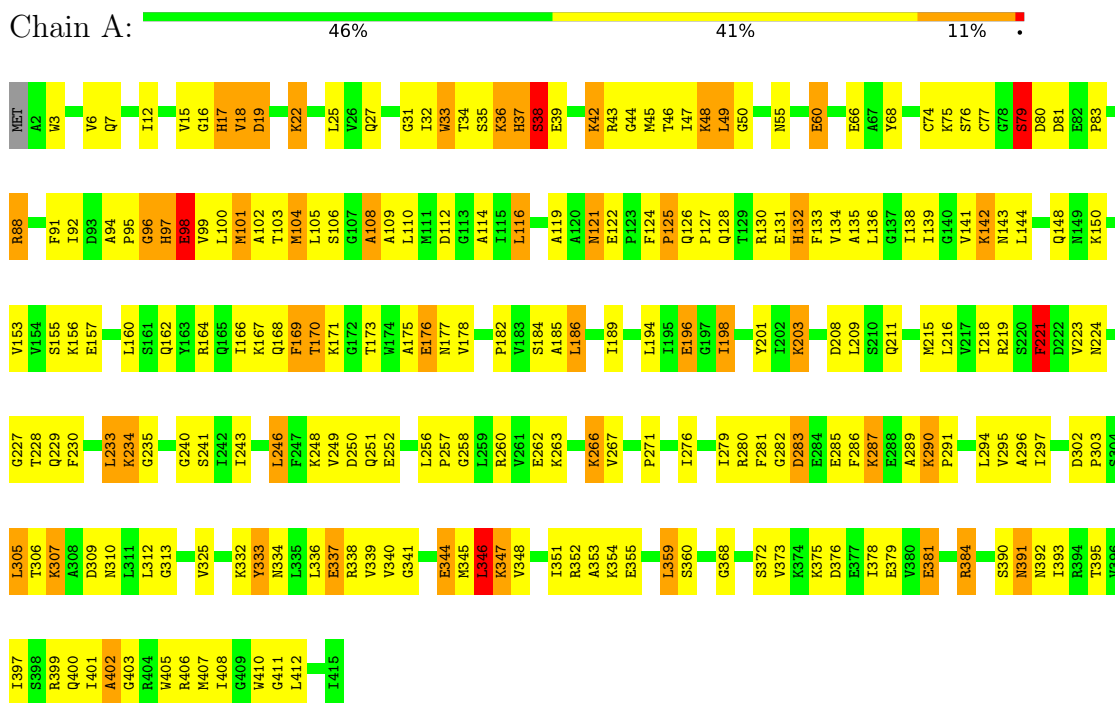
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	71	Total	O	0	0
			71	71		
5	B	89	Total	O	0	0
			89	89		

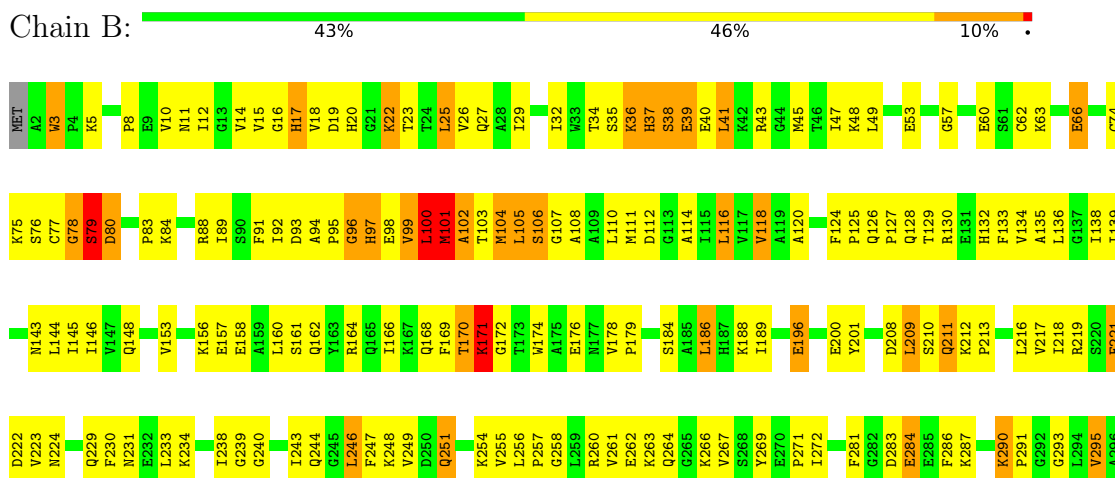
3 Residue-property plots i

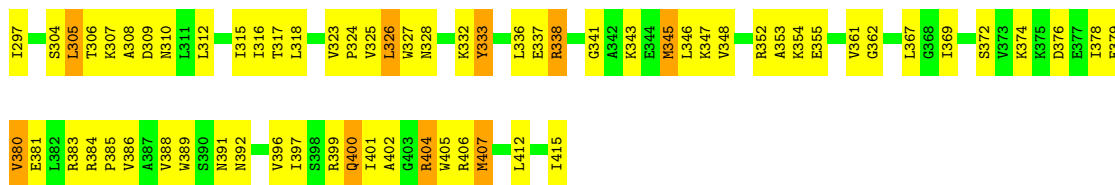
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Translation initiation factor 2 gamma subunit



- Molecule 1: Translation initiation factor 2 gamma subunit





4 Data and refinement statistics i

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	95.06Å 95.06Å 165.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.85 – 2.65 19.85 – 2.65	Depositor EDS
% Data completeness (in resolution range)	89.3 (19.85-2.65) 99.1 (19.85-2.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.64Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.275 0.232 , 0.231	Depositor DCC
R_{free} test set	2426 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l 0.469 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6726	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: GNP, PPV, 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	0.55	0/3271	1.12	30/4430 (0.7%)
1	B	0.56	0/3271	1.16	33/4430 (0.7%)
All	All	0.56	0/6542	1.14	63/8860 (0.7%)

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ASP	N-CA-C	-12.12	97.90	113.17
1	B	102	ALA	N-CA-C	-11.30	99.02	112.92
1	A	169	PHE	N-CA-C	-10.49	102.66	114.62
1	B	400	GLN	OE1-CD-NE2	-9.89	112.71	122.60
1	B	37	HIS	N-CA-C	9.83	124.71	108.49
1	B	80	ASP	CA-CB-CG	9.29	121.89	112.60
1	B	37	HIS	CA-CB-CG	-9.05	104.75	113.80
1	B	37	HIS	CB-CA-C	-8.71	99.04	111.85
1	A	37	HIS	N-CA-C	7.90	127.62	110.80
1	A	109	ALA	N-CA-C	-7.86	103.67	113.18
1	B	80	ASP	CA-C-N	-7.81	108.71	122.07
1	B	80	ASP	C-N-CA	-7.81	108.71	122.07
1	A	37	HIS	N-CA-CB	-7.80	97.30	110.49
1	A	101	MET	CA-C-N	-7.15	111.41	122.49
1	A	101	MET	C-N-CA	-7.15	111.41	122.49
1	B	170	THR	N-CA-C	-7.05	104.25	112.92
1	B	283	ASP	N-CA-C	-7.05	104.83	113.50
1	A	196	GLU	N-CA-C	-6.94	103.64	111.14
1	B	80	ASP	CB-CA-C	-6.93	96.64	110.42
1	A	170	THR	N-CA-C	-6.92	104.03	113.30
1	A	403	GLY	N-CA-C	-6.82	97.01	113.18
1	B	345	MET	N-CA-C	-6.82	103.52	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	GLU	N-CA-C	-6.80	103.94	111.82
1	B	106	SER	N-CA-C	-6.79	105.41	113.21
1	B	400	GLN	CG-CD-NE2	6.68	126.42	116.40
1	A	132	HIS	N-CA-C	-6.68	104.08	111.36
1	A	98	GLU	N-CA-C	6.51	124.66	110.80
1	A	221	PHE	N-CA-C	6.39	116.89	107.88
1	B	221	PHE	N-CA-C	6.26	118.07	108.42
1	B	380	VAL	N-CA-C	6.22	117.44	108.48
1	B	389	TRP	N-CA-C	6.21	120.11	112.54
1	A	381	GLU	N-CA-C	-6.14	101.39	110.48
1	A	333	TYR	N-CA-C	5.97	118.91	110.14
1	A	106	SER	N-CA-C	-5.96	104.47	110.97
1	B	41	LEU	N-CA-C	-5.95	106.56	113.88
1	A	102	ALA	N-CA-C	-5.83	105.49	113.30
1	A	36	LYS	CA-C-N	-5.82	110.43	121.54
1	A	36	LYS	C-N-CA	-5.82	110.43	121.54
1	B	100	LEU	CA-C-N	5.74	132.50	121.54
1	B	100	LEU	C-N-CA	5.74	132.50	121.54
1	B	38	SER	CA-C-N	-5.73	111.60	120.31
1	B	38	SER	C-N-CA	-5.73	111.60	120.31
1	B	101	MET	N-CA-C	5.63	122.80	110.80
1	A	49	LEU	N-CA-C	5.57	118.35	110.50
1	A	384	ARG	CA-C-N	5.56	125.53	120.03
1	A	384	ARG	C-N-CA	5.56	125.53	120.03
1	B	196	GLU	N-CA-C	-5.56	105.22	111.28
1	A	114	ALA	N-CA-C	5.51	117.17	108.96
1	B	333	TYR	N-CA-C	5.50	118.89	110.36
1	B	297	ILE	N-CA-C	5.47	115.73	107.80
1	B	308	ALA	N-CA-C	5.42	117.79	111.02
1	A	88	ARG	N-CA-C	-5.40	100.90	109.59
1	A	112	ASP	N-CA-C	-5.29	107.00	113.50
1	A	38	SER	N-CA-C	5.28	122.03	110.80
1	B	80	ASP	N-CA-C	5.23	121.95	110.80
1	A	79	SER	N-CA-C	5.22	117.61	110.24
1	A	31	GLY	N-CA-C	-5.20	107.87	115.72
1	A	325	VAL	N-CA-C	-5.17	98.59	109.34
1	B	3	TRP	CA-C-N	5.15	124.91	119.76
1	B	3	TRP	C-N-CA	5.15	124.91	119.76
1	A	230	PHE	N-CA-C	5.04	117.42	111.33
1	B	374	LYS	N-CA-C	-5.01	102.04	109.96
1	B	17	HIS	N-CA-C	-5.01	103.34	110.35

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	3212	0	3332	246	0
1	B	3212	0	3332	249	0
2	A	28	0	12	6	0
2	B	28	0	12	2	0
3	A	32	0	13	4	0
4	A	27	0	0	1	0
4	B	27	0	0	0	0
5	A	71	0	0	10	0
5	B	89	0	0	4	0
All	All	6726	0	6701	492	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 37.

All (492) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ALA:HB3	1:A:98:GLU:HA	1.25	1.13
1:B:230:PHE:HA	1:B:233:LEU:HD23	1.38	1.04
1:B:108:ALA:HB1	1:B:139:ILE:HD12	1.46	0.98
1:B:5:LYS:HE2	1:B:284:GLU:HB3	1.48	0.95
1:B:17:HIS:HB2	1:B:129:THR:HG23	1.50	0.93
1:B:36:LYS:HG3	1:B:37:HIS:H	1.35	0.91
1:A:94:ALA:CB	1:A:98:GLU:HA	2.02	0.89
1:B:94:ALA:HB2	1:B:99:VAL:HG13	1.50	0.89
1:A:97:HIS:O	1:A:98:GLU:CB	2.20	0.88
1:A:337:GLU:CD	1:A:337:GLU:H	1.80	0.88
1:B:372:SER:HB3	1:B:379:GLU:HB2	1.58	0.86
1:A:46:THR:HG22	1:A:47:ILE:H	1.39	0.86
1:B:352:ARG:HH21	1:B:355:GLU:HA	1.39	0.85
1:A:46:THR:HA	1:A:219:ARG:HG3	1.59	0.84
1:B:260:ARG:NH2	1:B:267:VAL:HG11	1.93	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ASN:HB3	1:A:412:LEU:HD12	1.57	0.83
1:A:173:THR:HG23	1:A:175:ALA:H	1.43	0.82
1:A:219:ARG:HD3	1:A:309:ASP:OD1	1.80	0.82
1:B:338:ARG:HE	1:B:347:LYS:HE3	1.45	0.82
1:A:99:VAL:HG23	1:A:100:LEU:H	1.45	0.81
1:B:17:HIS:ND1	1:B:128:GLN:HB2	1.95	0.81
1:B:148:GLN:HE21	1:B:162:GLN:HE21	1.28	0.80
1:A:142:LYS:HB3	5:A:428:HOH:O	1.82	0.80
1:B:171:LYS:HA	1:B:171:LYS:HE2	1.61	0.80
1:B:47:ILE:HD13	1:B:219:ARG:HG3	1.65	0.78
1:B:230:PHE:HA	1:B:233:LEU:CD2	2.12	0.77
1:A:97:HIS:O	1:A:98:GLU:HB2	1.82	0.77
1:A:74:CYS:SG	1:A:83:PRO:HB3	2.25	0.76
1:B:367:LEU:HD23	1:B:383:ARG:HH21	1.49	0.76
1:A:312:LEU:HD12	1:A:313:GLY:N	2.02	0.75
1:A:340:VAL:HB	1:A:406:ARG:HH22	1.52	0.75
1:B:247:PHE:HA	1:B:251:GLN:HE22	1.52	0.74
1:A:6:VAL:HG22	1:A:7:GLN:N	2.04	0.73
1:B:168:GLN:O	1:B:171:LYS:HB2	1.88	0.73
1:B:384:ARG:HG2	1:B:385:PRO:HD2	1.71	0.73
1:B:248:LYS:H	1:B:251:GLN:NE2	1.86	0.73
1:B:48:LYS:NZ	1:B:103:THR:HG21	2.04	0.73
1:A:18:VAL:HG12	1:A:128:GLN:HE22	1.54	0.73
1:B:156:LYS:O	1:B:160:LEU:HG	1.88	0.72
1:A:7:GLN:HE22	1:A:290:LYS:H	1.36	0.72
1:B:333:TYR:CE2	1:B:378:ILE:HG23	2.24	0.72
1:B:74:CYS:SG	1:B:83:PRO:HB3	2.29	0.71
1:B:219:ARG:HD3	1:B:309:ASP:OD2	1.90	0.71
1:A:46:THR:HG21	1:A:49:LEU:HD11	1.72	0.71
1:A:6:VAL:HG22	1:A:7:GLN:H	1.55	0.71
1:A:136:LEU:HB3	1:A:141:VAL:HG11	1.74	0.70
1:A:18:VAL:O	1:A:19:ASP:HB2	1.91	0.70
1:B:338:ARG:HA	1:B:347:LYS:HA	1.73	0.70
1:A:144:LEU:HD23	1:A:178:VAL:HG21	1.74	0.70
1:B:209:LEU:HD12	1:B:209:LEU:H	1.56	0.70
1:B:338:ARG:NE	1:B:347:LYS:HE3	2.06	0.70
1:B:218:ILE:HG12	1:B:240:GLY:HA2	1.73	0.69
1:B:230:PHE:CA	1:B:233:LEU:HD23	2.18	0.69
1:B:263:LYS:HD2	1:B:264:GLN:HG2	1.74	0.69
1:A:131:GLU:HA	1:A:134:VAL:HG22	1.76	0.68
1:A:249:VAL:O	1:A:250:ASP:HB2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:THR:C	1:A:219:ARG:HE	2.02	0.68
1:A:344:GLU:CD	1:A:345:MET:H	2.02	0.68
1:A:135:ALA:O	1:A:139:ILE:HG12	1.94	0.67
1:B:36:LYS:HG3	1:B:37:HIS:N	2.07	0.67
1:B:260:ARG:HD2	1:B:269:TYR:OH	1.93	0.67
1:B:77:CYS:O	1:B:78:GLY:C	2.37	0.67
1:A:119:ALA:HB3	1:A:122:GLU:HG3	1.75	0.67
1:B:384:ARG:HD2	1:B:385:PRO:O	1.94	0.67
1:B:23:THR:O	1:B:27:GLN:HG3	1.95	0.67
1:A:37:HIS:O	1:A:38:SER:HB3	1.93	0.67
1:B:209:LEU:HD12	1:B:209:LEU:N	2.10	0.67
1:A:138:ILE:HG21	1:A:407:MET:HE2	1.75	0.67
1:B:260:ARG:HH21	1:B:267:VAL:HG11	1.60	0.67
1:B:126:GLN:HB3	1:B:127:PRO:HD2	1.77	0.67
1:A:150:LYS:O	1:A:153:VAL:HG22	1.95	0.67
1:A:340:VAL:HA	1:A:345:MET:CE	2.25	0.67
1:B:148:GLN:HE21	1:B:162:GLN:NE2	1.93	0.67
1:A:121:ASN:H	1:A:121:ASN:HD22	1.43	0.66
1:A:333:TYR:CE2	1:A:378:ILE:HG23	2.31	0.66
1:B:260:ARG:HB2	1:B:269:TYR:CE2	2.31	0.66
1:A:46:THR:HG22	1:A:47:ILE:N	2.09	0.66
1:A:110:LEU:HD22	1:A:241:SER:HB3	1.77	0.66
1:B:37:HIS:O	1:B:37:HIS:ND1	2.29	0.66
1:B:246:LEU:HD12	1:B:246:LEU:C	2.21	0.65
1:A:359:LEU:HD22	1:A:359:LEU:N	2.12	0.64
1:A:170:THR:HA	1:A:173:THR:HG22	1.80	0.64
1:A:266:LYS:HB2	1:A:266:LYS:NZ	2.12	0.64
1:A:400:GLN:HA	1:A:405:TRP:HA	1.78	0.64
1:A:401:ILE:HG23	1:A:402:ALA:N	2.13	0.63
1:B:392:ASN:HB3	1:B:412:LEU:HD13	1.79	0.63
1:B:99:VAL:HG11	1:B:104:MET:HG2	1.79	0.63
1:B:338:ARG:HG3	1:B:345:MET:HE3	1.80	0.63
1:A:91:PHE:C	1:A:92:ILE:HD12	2.24	0.63
1:B:208:ASP:HB3	1:B:211:GLN:HG3	1.80	0.63
1:A:16:GLY:O	1:A:22:LYS:HD3	1.98	0.63
1:B:248:LYS:O	1:B:251:GLN:HB2	1.98	0.63
1:A:219:ARG:HD2	1:A:221:PHE:CE2	2.34	0.62
1:A:340:VAL:HA	1:A:345:MET:HE1	1.80	0.62
1:B:337:GLU:N	1:B:337:GLU:CD	2.58	0.62
1:B:124:PHE:CE2	1:B:166:ILE:HA	2.35	0.62
1:A:173:THR:HG23	1:A:175:ALA:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:SER:H	1:A:393:ILE:HD11	1.64	0.61
1:A:124:PHE:CE2	1:A:166:ILE:HA	2.35	0.61
1:B:102:ALA:O	1:B:106:SER:HB3	2.00	0.61
1:B:262:GLU:HG2	1:B:267:VAL:HG12	1.82	0.61
1:B:105:LEU:N	1:B:105:LEU:CD2	2.64	0.61
1:B:337:GLU:CD	1:B:337:GLU:H	2.09	0.61
1:B:148:GLN:HG3	1:B:162:GLN:NE2	2.15	0.61
1:B:171:LYS:HE2	1:B:171:LYS:CA	2.31	0.61
1:B:101:MET:CE	1:B:407:MET:SD	2.89	0.60
1:A:156:LYS:O	1:A:160:LEU:HD23	2.01	0.60
1:B:325:VAL:HG12	1:B:385:PRO:HB2	1.82	0.60
1:A:216:LEU:HG	1:A:243:ILE:HG12	1.83	0.60
1:A:395:THR:HG22	1:A:411:GLY:O	2.01	0.60
1:B:16:GLY:H	1:B:22:LYS:HD3	1.64	0.60
1:A:99:VAL:HG12	1:A:104:MET:HG3	1.84	0.60
1:B:105:LEU:HD12	1:B:396:VAL:HG21	1.83	0.60
1:B:105:LEU:C	1:B:107:GLY:H	2.09	0.60
1:B:17:HIS:HB2	1:B:129:THR:CG2	2.29	0.60
1:B:48:LYS:HZ3	1:B:103:THR:HG21	1.65	0.59
1:B:144:LEU:HD23	1:B:178:VAL:HG21	1.84	0.59
1:A:373:VAL:HA	1:A:378:ILE:HG22	1.84	0.59
1:A:353:ALA:O	1:A:354:LYS:HB2	2.01	0.59
1:B:94:ALA:CB	1:B:99:VAL:HG13	2.28	0.59
1:B:254:LYS:HA	1:B:272:ILE:O	2.02	0.59
1:B:401:ILE:CG2	1:B:406:ARG:HD3	2.33	0.59
1:A:224:ASN:HD21	1:A:234:LYS:H	1.51	0.58
1:A:401:ILE:HG23	1:A:402:ALA:H	1.68	0.58
1:B:148:GLN:HG3	1:B:162:GLN:HE21	1.68	0.58
1:A:42:LYS:HG3	5:A:453:HOH:O	2.03	0.58
1:B:78:GLY:O	1:B:79:SER:CB	2.52	0.58
1:B:354:LYS:HA	1:B:369:ILE:HD11	1.86	0.58
1:A:48:LYS:HE2	1:A:103:THR:OG1	2.03	0.58
1:B:27:GLN:HG2	1:B:32:ILE:O	2.04	0.58
1:B:399:ARG:O	1:B:405:TRP:HA	2.03	0.58
1:A:46:THR:HG22	1:A:47:ILE:HG22	1.86	0.57
1:A:280:ARG:CZ	1:A:280:ARG:HB3	2.34	0.57
1:B:37:HIS:O	1:B:37:HIS:CG	2.52	0.57
1:A:121:ASN:HD22	1:A:121:ASN:N	2.02	0.57
1:A:280:ARG:HH12	1:A:283:ASP:C	2.13	0.57
1:A:347:LYS:NZ	1:A:347:LYS:HB2	2.20	0.57
1:A:208:ASP:HB3	1:A:211:GLN:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ILE:HG21	1:B:407:MET:HE3	1.84	0.57
1:A:280:ARG:NH2	1:A:282:GLY:O	2.38	0.57
1:B:37:HIS:HD1	1:B:37:HIS:C	2.13	0.57
1:A:6:VAL:CG2	1:A:7:GLN:H	2.17	0.56
1:A:168:GLN:HA	1:A:171:LYS:HB2	1.87	0.56
1:A:97:HIS:O	1:A:98:GLU:HB3	2.02	0.56
1:A:246:LEU:C	1:A:246:LEU:HD12	2.30	0.56
1:A:391:ASN:C	1:A:391:ASN:HD22	2.14	0.56
1:B:138:ILE:CD1	1:B:407:MET:HB2	2.36	0.56
1:A:215:MET:HE1	1:A:297:ILE:HG13	1.86	0.56
1:B:8:PRO:HG2	1:B:293:GLY:HA3	1.86	0.56
1:B:397:ILE:N	1:B:397:ILE:HD12	2.21	0.56
1:A:68:TYR:CE1	1:A:196:GLU:HG3	2.40	0.56
1:B:133:PHE:O	1:B:174:TRP:HH2	1.89	0.56
1:A:141:VAL:O	1:A:141:VAL:HG13	2.05	0.56
1:B:148:GLN:NE2	1:B:162:GLN:HE21	2.01	0.56
1:B:120:ALA:HA	1:B:162:GLN:HE22	1.70	0.55
1:B:338:ARG:HG3	1:B:338:ARG:HH11	1.71	0.55
1:A:352:ARG:O	1:A:355:GLU:HG2	2.07	0.55
1:A:375:LYS:HG2	1:A:376:ASP:OD2	2.06	0.55
1:B:25:LEU:O	1:B:29:ILE:HG13	2.07	0.55
1:A:127:PRO:HA	1:A:130:ARG:HG3	1.89	0.55
1:A:167:LYS:HE2	5:A:486:HOH:O	2.06	0.55
1:A:312:LEU:HD12	1:A:313:GLY:H	1.68	0.55
1:A:95:PRO:O	1:A:97:HIS:N	2.40	0.54
1:A:260:ARG:HB3	4:A:418:PPV:O11	2.06	0.54
1:B:346:LEU:N	1:B:346:LEU:HD23	2.21	0.54
1:A:42:LYS:HA	5:A:453:HOH:O	2.08	0.54
1:B:153:VAL:HG12	1:B:153:VAL:O	2.07	0.54
1:B:224:ASN:HD21	1:B:234:LYS:H	1.53	0.54
1:B:263:LYS:CD	1:B:264:GLN:HE21	2.20	0.54
1:B:284:GLU:HB2	1:B:286:PHE:CE1	2.43	0.54
1:B:26:VAL:HG11	1:B:34:THR:HG21	1.90	0.54
1:B:37:HIS:ND1	1:B:37:HIS:C	2.65	0.54
1:A:352:ARG:HE	1:A:355:GLU:HB3	1.72	0.54
1:A:279:ILE:HG21	1:A:289:ALA:HB2	1.90	0.54
1:B:184:SER:HB3	1:B:189:ILE:HB	1.89	0.54
1:A:39:GLU:HG2	1:A:43:ARG:HB2	1.88	0.53
1:A:108:ALA:HB1	1:A:139:ILE:HG23	1.89	0.53
1:B:406:ARG:HG2	1:B:406:ARG:HH11	1.73	0.53
1:A:280:ARG:HH21	3:A:417:GNP:H2'	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:VAL:CG2	1:A:7:GLN:N	2.70	0.53
1:B:111:MET:CE	1:B:114:ALA:HB2	2.39	0.53
1:A:12:ILE:O	1:A:91:PHE:HA	2.08	0.53
1:A:249:VAL:HG23	1:A:287:LYS:O	2.08	0.53
1:A:194:LEU:O	1:A:198:ILE:HG23	2.08	0.53
1:A:338:ARG:HB2	1:A:346:LEU:O	2.08	0.53
1:A:209:LEU:HD22	1:A:246:LEU:HD23	1.91	0.53
1:B:345:MET:O	1:B:345:MET:HG3	2.08	0.53
1:A:218:ILE:HA	1:A:312:LEU:HD13	1.91	0.52
1:A:281:PHE:HB2	1:A:286:PHE:CE1	2.44	0.52
1:B:108:ALA:HB1	1:B:139:ILE:CD1	2.27	0.52
1:B:260:ARG:HH12	1:B:262:GLU:CD	2.17	0.52
1:A:256:LEU:HA	1:A:257:PRO:C	2.34	0.52
1:B:48:LYS:HZ2	1:B:103:THR:HG21	1.72	0.52
1:A:39:GLU:CG	1:A:43:ARG:HB2	2.40	0.52
1:B:105:LEU:N	1:B:105:LEU:HD22	2.24	0.52
1:A:130:ARG:HB3	5:A:441:HOH:O	2.08	0.52
1:B:94:ALA:CB	1:B:99:VAL:HG22	2.40	0.52
1:A:42:LYS:HG2	1:A:42:LYS:O	2.10	0.52
1:A:160:LEU:O	1:A:164:ARG:HG2	2.10	0.52
1:B:63:LYS:O	1:B:66:GLU:HG2	2.10	0.52
1:A:136:LEU:HB3	1:A:141:VAL:CG1	2.40	0.52
1:A:79:SER:HB3	1:A:81:ASP:HB2	1.93	0.51
1:A:266:LYS:HB2	1:A:266:LYS:HZ2	1.74	0.51
1:B:125:PRO:HG3	1:B:169:PHE:CE2	2.45	0.51
1:B:135:ALA:HA	1:B:407:MET:HE2	1.90	0.51
1:B:146:ILE:HG13	1:B:178:VAL:HG11	1.91	0.51
1:B:338:ARG:CA	1:B:347:LYS:HA	2.39	0.51
1:B:101:MET:C	1:B:103:THR:H	2.18	0.51
1:A:119:ALA:CB	1:A:122:GLU:HG3	2.39	0.51
1:A:168:GLN:O	1:A:168:GLN:HG2	2.11	0.51
1:A:260:ARG:HH22	1:A:267:VAL:CG1	2.24	0.51
1:A:88:ARG:HG3	1:A:88:ARG:NH1	2.25	0.51
1:A:345:MET:HE2	1:A:345:MET:HA	1.91	0.51
1:A:347:LYS:HB2	1:A:347:LYS:HZ3	1.75	0.51
1:B:317:THR:HG21	1:B:323:VAL:HG21	1.91	0.51
1:B:229:GLN:HG2	5:B:459:HOH:O	2.10	0.51
1:A:258:GLY:HA3	1:A:271:PRO:HA	1.93	0.51
1:B:88:ARG:HG3	1:B:88:ARG:HH11	1.76	0.51
1:B:324:PRO:HD2	1:B:388:VAL:O	2.11	0.51
1:A:3:TRP:CZ2	1:A:83:PRO:HG2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLY:HA2	1:B:230:PHE:CE1	2.46	0.51
1:B:160:LEU:O	1:B:164:ARG:HG2	2.10	0.51
1:B:337:GLU:O	1:B:347:LYS:HB3	2.11	0.51
1:B:116:LEU:HB2	1:B:144:LEU:HD11	1.93	0.51
1:B:130:ARG:O	1:B:134:VAL:HG23	2.11	0.51
1:A:397:ILE:HD12	1:A:410:TRP:HA	1.93	0.50
1:A:17:HIS:C	1:A:17:HIS:CD2	2.89	0.50
1:A:229:GLN:HG2	5:A:474:HOH:O	2.12	0.50
1:A:27:GLN:CD	1:A:33:TRP:HD1	2.20	0.50
1:A:101:MET:O	1:A:105:LEU:CD1	2.59	0.50
1:B:216:LEU:CD1	1:B:243:ILE:HD11	2.42	0.50
1:A:18:VAL:O	1:A:18:VAL:HG13	2.11	0.50
1:A:175:ALA:O	1:A:176:GLU:C	2.54	0.50
1:B:210:SER:O	1:B:211:GLN:C	2.55	0.50
1:A:306:THR:O	1:A:307:LYS:C	2.54	0.50
1:B:16:GLY:N	1:B:22:LYS:HD3	2.25	0.50
1:B:101:MET:HE2	1:B:105:LEU:HD21	1.92	0.50
1:B:388:VAL:HG11	1:B:415:ILE:HG21	1.94	0.50
1:B:263:LYS:HD3	1:B:264:GLN:HE21	1.77	0.49
1:A:98:GLU:HG2	1:A:132:HIS:NE2	2.27	0.49
1:A:228:THR:HG21	1:A:233:LEU:HB3	1.94	0.49
1:B:404:ARG:HH11	1:B:404:ARG:HG2	1.76	0.49
1:A:127:PRO:O	1:A:130:ARG:HG3	2.12	0.49
1:A:406:ARG:HG2	1:A:406:ARG:HH11	1.76	0.49
1:A:99:VAL:HG23	1:A:100:LEU:N	2.21	0.49
1:B:218:ILE:O	1:B:312:LEU:HD13	2.12	0.49
1:B:217:VAL:HG13	1:B:238:ILE:HG23	1.95	0.49
1:B:258:GLY:HA3	1:B:271:PRO:HA	1.94	0.49
1:A:22:LYS:HB2	1:A:22:LYS:NZ	2.28	0.49
1:A:125:PRO:HG3	1:A:169:PHE:CE2	2.48	0.49
1:A:260:ARG:HH22	1:A:267:VAL:HG11	1.77	0.49
1:B:188:LYS:HD2	1:B:188:LYS:N	2.28	0.49
1:B:306:THR:O	1:B:307:LYS:C	2.56	0.49
1:B:111:MET:HE3	1:B:114:ALA:HB2	1.93	0.49
1:A:44:GLY:HA2	3:A:417:GNP:O3'	2.12	0.48
1:A:170:THR:CA	1:A:173:THR:HG22	2.43	0.48
1:B:16:GLY:O	1:B:17:HIS:C	2.55	0.48
1:B:352:ARG:HG2	1:B:353:ALA:N	2.28	0.48
1:B:18:VAL:HG21	1:B:97:HIS:CG	2.47	0.48
1:B:105:LEU:HD11	1:B:396:VAL:HG11	1.95	0.48
1:B:127:PRO:HA	5:B:467:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:SER:HB3	1:A:189:ILE:HB	1.95	0.48
1:A:12:ILE:CD1	1:A:198:ILE:HD12	2.43	0.48
1:B:338:ARG:HB2	1:B:346:LEU:O	2.12	0.48
1:A:16:GLY:O	1:A:17:HIS:C	2.55	0.48
1:A:121:ASN:H	1:A:121:ASN:ND2	2.09	0.48
1:B:10:VAL:HG23	1:B:112:ASP:HB2	1.94	0.48
1:B:157:GLU:HG2	1:B:158:GLU:N	2.29	0.48
1:A:27:GLN:HA	1:A:32:ILE:O	2.14	0.48
1:A:34:THR:HB	1:A:50:GLY:HA3	1.94	0.48
1:B:352:ARG:HE	1:B:355:GLU:HB2	1.78	0.48
1:B:401:ILE:HG23	1:B:401:ILE:O	2.14	0.48
1:A:136:LEU:O	1:A:141:VAL:HG12	2.13	0.47
1:B:96:GLY:O	1:B:97:HIS:CB	2.62	0.47
1:B:262:GLU:HG2	1:B:267:VAL:CG1	2.44	0.47
1:A:148:GLN:NE2	1:A:162:GLN:HB3	2.28	0.47
1:B:132:HIS:O	1:B:136:LEU:HG	2.14	0.47
1:B:18:VAL:HG12	1:B:128:GLN:HE22	1.79	0.47
1:B:407:MET:H	1:B:407:MET:HG2	1.38	0.47
1:A:46:THR:CG2	1:A:47:ILE:H	2.19	0.47
1:A:185:ALA:N	2:A:416:GDP:O6	2.45	0.47
1:B:14:VAL:HB	1:B:93:ASP:HB3	1.97	0.47
1:A:334:ASN:ND2	5:A:478:HOH:O	2.47	0.47
1:A:341:GLY:HA3	1:A:345:MET:O	2.14	0.47
1:B:3:TRP:CZ2	1:B:83:PRO:HG2	2.49	0.47
1:B:88:ARG:HG3	1:B:88:ARG:NH1	2.30	0.47
1:B:209:LEU:H	1:B:209:LEU:CD1	2.14	0.47
1:A:15:VAL:HG23	1:A:116:LEU:HD23	1.96	0.47
1:B:326:LEU:O	1:B:385:PRO:HA	2.15	0.47
1:B:5:LYS:CE	1:B:284:GLU:HB3	2.33	0.47
1:B:12:ILE:HD13	1:B:89:ILE:HD12	1.95	0.47
1:A:224:ASN:HD22	1:A:228:THR:HG21	1.80	0.47
1:A:175:ALA:HA	1:A:178:VAL:HG23	1.97	0.46
1:B:22:LYS:HB2	2:B:416:GDP:O1B	2.15	0.46
1:A:88:ARG:HG3	1:A:88:ARG:HH11	1.79	0.46
1:B:94:ALA:HB1	1:B:99:VAL:HG22	1.98	0.46
1:A:340:VAL:HA	1:A:345:MET:HE2	1.95	0.46
1:A:46:THR:CA	1:A:219:ARG:HG3	2.37	0.46
1:A:224:ASN:ND2	1:A:228:THR:HG21	2.30	0.46
1:A:295:VAL:HG22	1:A:296:ALA:N	2.29	0.46
1:A:305:LEU:O	1:A:310:ASN:HB3	2.16	0.46
1:B:75:LYS:O	1:B:77:CYS:O	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PRO:O	1:B:97:HIS:N	2.48	0.46
1:B:120:ALA:HA	1:B:162:GLN:NE2	2.28	0.46
1:A:203:LYS:HB3	1:A:203:LYS:HZ2	1.80	0.46
1:A:341:GLY:H	1:A:345:MET:HA	1.80	0.46
1:A:194:LEU:O	1:A:198:ILE:CG2	2.63	0.46
1:A:218:ILE:HG12	1:A:240:GLY:HA2	1.97	0.46
1:A:302:ASP:OD1	1:B:222:ASP:OD2	2.34	0.46
1:B:11:ASN:OD1	1:B:293:GLY:N	2.37	0.46
1:B:78:GLY:O	1:B:79:SER:OG	2.34	0.46
1:B:400:GLN:OE1	1:B:400:GLN:HA	2.15	0.46
1:A:280:ARG:HH21	3:A:417:GNP:C2'	2.29	0.46
1:A:290:LYS:HB3	1:A:291:PRO:CD	2.46	0.46
1:A:302:ASP:OD2	1:A:302:ASP:C	2.57	0.46
1:B:328:ASN:HA	1:B:380:VAL:O	2.16	0.46
1:A:32:ILE:CG2	1:A:37:HIS:CE1	2.99	0.46
1:B:105:LEU:CD1	1:B:396:VAL:HG11	2.46	0.46
1:B:105:LEU:HD23	1:B:105:LEU:H	1.81	0.46
1:A:336:LEU:O	1:A:348:VAL:HG21	2.16	0.46
1:B:284:GLU:HB2	1:B:286:PHE:HE1	1.79	0.46
1:B:281:PHE:O	1:B:284:GLU:HG3	2.16	0.45
1:B:101:MET:HE2	1:B:407:MET:SD	2.57	0.45
1:B:179:PRO:HG3	1:B:201:TYR:CD2	2.51	0.45
1:B:196:GLU:O	1:B:200:GLU:HG3	2.17	0.45
1:B:256:LEU:HA	1:B:257:PRO:C	2.41	0.45
1:B:336:LEU:O	1:B:348:VAL:HB	2.15	0.45
1:A:75:LYS:O	1:A:77:CYS:N	2.50	0.45
1:A:248:LYS:O	1:A:251:GLN:HG3	2.16	0.45
1:A:280:ARG:HH12	1:A:283:ASP:CA	2.28	0.45
1:B:255:VAL:HG22	1:B:316:ILE:HD13	1.98	0.45
1:B:338:ARG:CB	1:B:347:LYS:HA	2.47	0.45
1:A:75:LYS:C	1:A:77:CYS:H	2.25	0.45
1:B:105:LEU:CD2	1:B:105:LEU:H	2.30	0.45
1:A:223:VAL:N	5:A:472:HOH:O	2.48	0.45
1:A:399:ARG:HB2	1:A:408:ILE:HD13	1.98	0.45
1:B:37:HIS:O	1:B:41:LEU:HD12	2.16	0.45
1:A:170:THR:HB	1:A:175:ALA:HB3	1.98	0.45
1:A:332:LYS:HA	1:A:376:ASP:O	2.16	0.45
1:B:172:GLY:HA2	1:B:176:GLU:CD	2.42	0.45
1:A:12:ILE:HD13	1:A:198:ILE:HD12	1.98	0.45
1:B:105:LEU:C	1:B:107:GLY:N	2.75	0.45
1:B:105:LEU:CD1	1:B:396:VAL:HG21	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ARG:NE	1:B:43:ARG:HA	2.32	0.44
1:B:260:ARG:HD2	1:B:269:TYR:CZ	2.52	0.44
1:B:369:ILE:HG23	1:B:381:GLU:HB3	1.98	0.44
1:B:224:ASN:HA	5:B:501:HOH:O	2.17	0.44
1:B:144:LEU:HG	1:B:145:ILE:N	2.32	0.44
1:B:186:LEU:HB2	2:B:416:GDP:C5	2.52	0.44
1:B:255:VAL:HG22	1:B:316:ILE:CD1	2.47	0.44
1:B:361:VAL:O	1:B:362:GLY:C	2.60	0.44
1:B:266:LYS:H	1:B:266:LYS:HD2	1.83	0.44
1:A:37:HIS:C	1:A:37:HIS:CD2	2.95	0.44
1:A:198:ILE:O	1:A:198:ILE:HG13	2.12	0.44
1:B:346:LEU:HD23	1:B:346:LEU:H	1.83	0.44
1:A:75:LYS:C	1:A:77:CYS:N	2.75	0.44
1:B:108:ALA:CB	1:B:139:ILE:HD12	2.31	0.44
1:B:261:VAL:O	1:B:261:VAL:HG23	2.18	0.44
1:A:74:CYS:HB2	1:A:79:SER:HB2	2.00	0.44
1:A:99:VAL:O	1:A:103:THR:HB	2.18	0.44
1:A:337:GLU:CD	1:A:337:GLU:N	2.61	0.44
1:A:406:ARG:HG2	1:A:406:ARG:NH1	2.32	0.44
1:A:105:LEU:HD13	1:A:360:SER:OG	2.18	0.44
1:A:203:LYS:HB3	1:A:203:LYS:NZ	2.33	0.44
1:B:266:LYS:HD2	1:B:266:LYS:N	2.32	0.44
1:B:290:LYS:HB3	1:B:291:PRO:CD	2.47	0.44
1:A:101:MET:HE3	1:A:406:ARG:HA	1.98	0.44
1:A:216:LEU:HG	1:A:243:ILE:CG1	2.48	0.44
1:B:138:ILE:CG2	1:B:407:MET:HE3	2.47	0.44
1:A:130:ARG:O	1:A:133:PHE:HB3	2.18	0.43
1:A:218:ILE:HD11	1:A:294:LEU:HD22	2.00	0.43
1:A:18:VAL:O	1:A:19:ASP:CB	2.62	0.43
1:A:55:ASN:HA	1:A:88:ARG:HA	2.00	0.43
1:A:110:LEU:CD2	1:A:241:SER:HB3	2.47	0.43
1:B:60:GLU:OE2	1:B:84:LYS:HE3	2.18	0.43
1:B:95:PRO:O	1:B:96:GLY:C	2.61	0.43
1:B:171:LYS:O	1:B:176:GLU:HG3	2.18	0.43
1:B:11:ASN:HB3	1:B:92:ILE:HD11	1.99	0.43
1:B:94:ALA:HB2	1:B:99:VAL:CG1	2.35	0.43
1:B:401:ILE:CG2	1:B:401:ILE:O	2.66	0.43
1:A:92:ILE:HD12	1:A:92:ILE:N	2.32	0.43
1:B:346:LEU:H	1:B:346:LEU:CD2	2.30	0.43
1:A:39:GLU:CD	1:A:43:ARG:HB2	2.43	0.43
1:A:186:LEU:HB2	2:A:416:GDP:C5	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ARG:NH2	1:A:267:VAL:HG12	2.34	0.43
1:B:224:ASN:HD21	1:B:234:LYS:N	2.16	0.43
1:A:32:ILE:HG23	1:A:37:HIS:NE2	2.34	0.43
1:B:231:ASN:ND2	5:B:444:HOH:O	2.52	0.43
1:B:399:ARG:HG2	1:B:400:GLN:N	2.33	0.43
1:A:333:TYR:HE2	1:A:378:ILE:HG23	1.77	0.43
1:B:146:ILE:HG13	1:B:178:VAL:CG1	2.49	0.43
1:B:327:TRP:CH2	1:B:385:PRO:HD3	2.54	0.43
1:B:353:ALA:C	1:B:355:GLU:H	2.27	0.43
1:A:45:MET:HE2	1:A:219:ARG:CZ	2.49	0.43
1:A:48:LYS:CE	1:A:103:THR:OG1	2.67	0.43
1:B:75:LYS:O	1:B:76:SER:C	2.61	0.43
1:B:286:PHE:N	1:B:286:PHE:CD1	2.87	0.43
1:B:305:LEU:O	1:B:310:ASN:HB3	2.19	0.43
1:B:337:GLU:N	1:B:337:GLU:OE2	2.35	0.43
1:A:124:PHE:CZ	1:A:166:ILE:HA	2.53	0.43
1:A:126:GLN:HB3	1:A:127:PRO:HD2	2.01	0.43
1:A:143:ASN:HB3	1:A:201:TYR:O	2.19	0.43
1:B:94:ALA:O	1:B:95:PRO:C	2.61	0.43
1:A:60:GLU:OE1	1:A:60:GLU:HA	2.18	0.43
1:A:303:PRO:HB2	1:B:304:SER:OG	2.19	0.43
1:A:351:ILE:O	1:A:373:VAL:HG21	2.19	0.43
1:A:359:LEU:HD22	1:A:359:LEU:H	1.80	0.43
1:A:372:SER:HB3	1:A:379:GLU:HG3	2.00	0.43
1:B:98:GLU:HB3	1:B:99:VAL:H	1.76	0.43
1:B:170:THR:O	1:B:171:LYS:C	2.61	0.43
1:B:213:PRO:HG2	1:B:318:LEU:HD11	2.01	0.43
1:B:332:LYS:HA	1:B:376:ASP:O	2.19	0.42
1:A:39:GLU:OE2	1:A:43:ARG:HB2	2.20	0.42
1:A:96:GLY:HA2	2:A:416:GDP:O3B	2.19	0.42
1:B:89:ILE:HD11	1:B:91:PHE:CZ	2.54	0.42
1:A:401:ILE:CG2	1:A:402:ALA:N	2.80	0.42
1:A:42:LYS:HE2	1:A:280:ARG:NH1	2.35	0.42
1:A:142:LYS:HG2	1:A:143:ASN:N	2.34	0.42
1:A:344:GLU:CD	1:A:345:MET:N	2.75	0.42
1:A:392:ASN:HB3	1:A:412:LEU:CD1	2.40	0.42
1:B:40:GLU:OE1	1:B:40:GLU:HA	2.18	0.42
1:B:246:LEU:HD12	1:B:247:PHE:N	2.34	0.42
1:B:341:GLY:HA3	1:B:346:LEU:HD21	2.01	0.42
1:B:343:LYS:O	1:B:343:LYS:HG2	2.19	0.42
1:A:18:VAL:HA	2:A:416:GDP:O2B	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASN:HD21	1:A:233:LEU:HA	1.83	0.42
1:B:367:LEU:HD23	1:B:383:ARG:NH2	2.26	0.42
1:B:405:TRP:CD1	1:B:405:TRP:H	2.36	0.42
1:A:177:ASN:O	1:A:178:VAL:C	2.62	0.42
1:A:280:ARG:HH12	1:A:283:ASP:HA	1.85	0.42
1:A:99:VAL:HA	1:A:104:MET:HG3	2.01	0.42
1:A:142:LYS:HG2	1:A:143:ASN:CG	2.44	0.42
1:A:170:THR:HA	1:A:173:THR:CG2	2.46	0.42
1:A:339:VAL:HG12	1:A:346:LEU:HB3	2.01	0.42
1:B:353:ALA:O	1:B:354:LYS:HB2	2.19	0.42
1:A:46:THR:HG21	1:A:49:LEU:CD1	2.44	0.42
1:A:110:LEU:HD22	1:A:241:SER:CB	2.48	0.42
1:A:280:ARG:HG2	1:A:285:GLU:HG2	2.00	0.42
1:B:212:LYS:HG2	1:B:244:GLN:NE2	2.35	0.42
1:A:49:LEU:HD13	1:A:92:ILE:HG23	2.01	0.42
1:A:186:LEU:HD23	1:A:186:LEU:HA	1.81	0.42
1:A:305:LEU:HD12	1:A:305:LEU:HA	1.80	0.42
1:B:18:VAL:O	1:B:19:ASP:HB2	2.19	0.42
1:B:47:ILE:HG22	1:B:49:LEU:H	1.84	0.42
1:A:160:LEU:HD13	1:A:160:LEU:HA	1.93	0.41
1:A:399:ARG:HB3	1:A:408:ILE:HG21	2.01	0.41
1:B:158:GLU:O	1:B:161:SER:HB3	2.20	0.41
1:A:384:ARG:HD3	5:A:483:HOH:O	2.20	0.41
1:B:3:TRP:CZ2	1:B:57:GLY:HA3	2.56	0.41
1:B:98:GLU:HG3	1:B:100:LEU:CD1	2.49	0.41
1:A:276:ILE:HG23	1:A:297:ILE:HG23	2.02	0.41
1:B:166:ILE:O	1:B:170:THR:HG23	2.20	0.41
1:B:249:VAL:HG23	1:B:287:LYS:O	2.21	0.41
1:A:148:GLN:O	1:A:182:PRO:HA	2.19	0.41
1:B:125:PRO:HG3	1:B:169:PHE:CD2	2.56	0.41
1:B:170:THR:O	1:B:176:GLU:HA	2.21	0.41
1:A:22:LYS:HE3	2:A:416:GDP:O2B	2.20	0.41
1:A:175:ALA:O	1:A:177:ASN:N	2.53	0.41
1:A:227:GLY:O	1:A:228:THR:C	2.61	0.41
1:B:18:VAL:HG23	1:B:97:HIS:HB2	2.03	0.41
1:B:164:ARG:HH11	1:B:164:ARG:HG3	1.86	0.41
1:B:352:ARG:NH2	1:B:355:GLU:HA	2.19	0.41
1:A:186:LEU:HG	2:A:416:GDP:H2'	2.03	0.41
1:A:243:ILE:HD13	1:A:243:ILE:HA	1.86	0.41
1:A:368:GLY:CA	1:A:381:GLU:O	2.69	0.41
1:B:18:VAL:HG12	1:B:128:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASN:ND2	1:A:121:ASN:C	2.77	0.41
1:A:401:ILE:CG2	1:A:402:ALA:H	2.32	0.41
1:B:108:ALA:CB	1:B:139:ILE:CD1	2.97	0.41
1:B:124:PHE:CE1	1:B:125:PRO:HB3	2.56	0.41
1:B:168:GLN:OE1	1:B:168:GLN:HA	2.20	0.41
1:B:346:LEU:N	1:B:346:LEU:CD2	2.83	0.41
1:A:95:PRO:O	1:A:96:GLY:C	2.64	0.41
1:A:169:PHE:CD1	1:A:169:PHE:C	2.99	0.41
1:A:296:ALA:O	3:A:417:GNP:N2	2.51	0.41
1:B:98:GLU:HG3	1:B:100:LEU:HD13	2.02	0.41
1:B:239:GLY:HA2	1:B:295:VAL:O	2.21	0.40
1:A:25:LEU:HA	1:A:185:ALA:HB1	2.03	0.40
1:A:32:ILE:CG2	1:A:37:HIS:NE2	2.84	0.40
1:A:348:VAL:HA	5:A:424:HOH:O	2.21	0.40
1:B:338:ARG:HG3	1:B:338:ARG:NH1	2.36	0.40
1:A:155:SER:OG	1:A:157:GLU:HG2	2.22	0.40
1:A:221:PHE:CD1	1:A:221:PHE:N	2.87	0.40
1:A:336:LEU:O	1:A:348:VAL:CG2	2.70	0.40
1:B:105:LEU:HD11	1:B:407:MET:SD	2.62	0.40
1:B:18:VAL:CG1	1:B:128:GLN:HE22	2.35	0.40
1:B:20:HIS:ND1	1:B:118:VAL:HA	2.36	0.40
1:B:43:ARG:NE	1:B:43:ARG:CA	2.85	0.40
1:A:68:TYR:HE1	1:A:196:GLU:HG3	1.84	0.40
1:B:315:ILE:O	1:B:315:ILE:HG13	2.21	0.40
1:B:323:VAL:HA	1:B:324:PRO:HD3	1.77	0.40
1:B:352:ARG:HH21	1:B:355:GLU:CA	2.22	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	412/415 (99%)	351 (85%)	44 (11%)	17 (4%)	2	3
1	B	412/415 (99%)	356 (86%)	40 (10%)	16 (4%)	2	3
All	All	824/830 (99%)	707 (86%)	84 (10%)	33 (4%)	2	3

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ASP
1	A	38	SER
1	A	48	LYS
1	A	98	GLU
1	B	78	GLY
1	B	80	ASP
1	B	96	GLY
1	B	97	HIS
1	B	101	MET
1	B	402	ALA
1	A	42	LYS
1	A	96	GLY
1	A	142	LYS
1	A	176	GLU
1	A	391	ASN
1	B	22	LYS
1	B	35	SER
1	B	45	MET
1	B	171	LYS
1	A	76	SER
1	A	108	ALA
1	A	307	LYS
1	B	100	LEU
1	B	211	GLN
1	A	97	HIS
1	B	143	ASN
1	B	62	CYS
1	A	35	SER
1	A	346	LEU
1	A	402	ALA
1	B	79	SER
1	B	391	ASN
1	A	18	VAL

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	356/357 (100%)	324 (91%)	32 (9%)	9	14
1	B	356/357 (100%)	325 (91%)	31 (9%)	9	16
All	All	712/714 (100%)	649 (91%)	63 (9%)	9	15

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	22	LYS
1	A	33	TRP
1	A	36	LYS
1	A	60	GLU
1	A	66	GLU
1	A	79	SER
1	A	98	GLU
1	A	104	MET
1	A	116	LEU
1	A	121	ASN
1	A	125	PRO
1	A	186	LEU
1	A	198	ILE
1	A	203	LYS
1	A	221	PHE
1	A	233	LEU
1	A	234	LYS
1	A	246	LEU
1	A	252	GLU
1	A	262	GLU
1	A	263	LYS
1	A	266	LYS
1	A	283	ASP
1	A	287	LYS
1	A	290	LYS
1	A	305	LEU

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Mol	Chain	Res	Type
1	A	337	GLU
1	A	344	GLU
1	A	346	LEU
1	A	347	LYS
1	A	359	LEU
1	B	15	VAL
1	B	25	LEU
1	B	36	LYS
1	B	38	SER
1	B	39	GLU
1	B	53	GLU
1	B	66	GLU
1	B	79	SER
1	B	99	VAL
1	B	101	MET
1	B	104	MET
1	B	105	LEU
1	B	110	LEU
1	B	116	LEU
1	B	118	VAL
1	B	171	LYS
1	B	186	LEU
1	B	209	LEU
1	B	221	PHE
1	B	223	VAL
1	B	246	LEU
1	B	251	GLN
1	B	284	GLU
1	B	290	LYS
1	B	295	VAL
1	B	305	LEU
1	B	326	LEU
1	B	338	ARG
1	B	386	VAL
1	B	404	ARG
1	B	407	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	17	HIS

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Mol	Chain	Res	Type
1	A	27	GLN
1	A	37	HIS
1	A	121	ASN
1	A	128	GLN
1	A	177	ASN
1	A	224	ASN
1	A	391	ASN
1	B	27	GLN
1	B	128	GLN
1	B	162	GLN
1	B	211	GLN
1	B	224	ASN
1	B	251	GLN
1	B	264	GLN
1	B	310	ASN
1	B	334	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](#)

9 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	B	416	-	29,30,30	1.21	1 (3%)	45,47,47	1.81	11 (24%)
4	PPV	A	418	-	6,8,8	2.51	2 (33%)	12,13,13	0.89	0
4	PPV	B	419	-	6,8,8	2.47	2 (33%)	12,13,13	0.91	0
3	GNP	A	417	-	34,34,34	3.65	9 (26%)	47,54,54	1.81	9 (19%)
4	PPV	B	417	-	6,8,8	2.48	2 (33%)	12,13,13	0.91	0
2	GDP	A	416	-	29,30,30	1.31	1 (3%)	45,47,47	1.82	11 (24%)
4	PPV	B	418	-	6,8,8	2.54	2 (33%)	12,13,13	0.89	0
4	PPV	A	419	-	6,8,8	2.50	2 (33%)	12,13,13	0.90	0
4	PPV	A	420	-	6,8,8	2.48	2 (33%)	12,13,13	0.92	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	B	416	-	-	0/16/32/32	0/3/3/3
4	PPV	A	418	-	-	0/6/6/6	-
4	PPV	B	419	-	-	0/6/6/6	-
3	GNP	A	417	-	-	3/18/38/38	0/3/3/3
4	PPV	B	417	-	-	0/6/6/6	-
2	GDP	A	416	-	-	0/16/32/32	0/3/3/3
4	PPV	B	418	-	-	0/6/6/6	-
4	PPV	A	419	-	-	0/6/6/6	-
4	PPV	A	420	-	-	0/6/6/6	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	417	GNP	PB-O3A	10.35	1.71	1.59
3	A	417	GNP	PB-O1B	10.16	1.61	1.46
3	A	417	GNP	PG-O1G	8.21	1.58	1.46
3	A	417	GNP	PG-O2G	5.72	1.72	1.56
3	A	417	GNP	PA-O3A	5.64	1.65	1.59
3	A	417	GNP	PG-O3G	5.63	1.71	1.56
3	A	417	GNP	PB-O2B	5.48	1.71	1.56
2	A	416	GDP	PA-O3A	4.42	1.64	1.59
3	A	417	GNP	PG-N3B	4.15	1.74	1.63
2	B	416	GDP	PA-O3A	4.02	1.63	1.59
3	A	417	GNP	PB-N3B	3.93	1.73	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	418	PPV	P1-O31	3.60	1.61	1.50
4	B	418	PPV	P2-O22	3.60	1.61	1.50
4	A	419	PPV	P2-O22	3.58	1.61	1.50
4	A	418	PPV	P2-O22	3.55	1.61	1.50
4	A	419	PPV	P1-O31	3.54	1.61	1.50
4	B	419	PPV	P2-O22	3.53	1.61	1.50
4	A	420	PPV	P1-O31	3.51	1.61	1.50
4	B	417	PPV	P1-O31	3.51	1.61	1.50
4	B	419	PPV	P1-O31	3.47	1.61	1.50
4	A	418	PPV	P1-O31	3.45	1.61	1.50
4	A	420	PPV	P2-O22	3.41	1.61	1.50
4	B	417	PPV	P2-O22	3.41	1.61	1.50

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	416	GDP	C5-C4-N3	-5.52	119.61	128.39
2	B	416	GDP	C2-N3-C4	5.41	121.62	112.30
2	B	416	GDP	C5-C4-N3	-5.39	119.80	128.39
3	A	417	GNP	C5-C4-N3	-5.39	119.82	128.39
2	A	416	GDP	C2-N3-C4	5.32	121.46	112.30
3	A	417	GNP	C2-N3-C4	5.18	121.23	112.30
3	A	417	GNP	N9-C4-N3	4.47	134.89	125.95
2	A	416	GDP	N9-C4-N3	4.26	134.47	125.95
2	B	416	GDP	N9-C4-N3	4.17	134.30	125.95
2	A	416	GDP	C8-N7-C5	2.92	109.46	104.26
2	B	416	GDP	C8-N7-C5	2.90	109.43	104.26
2	A	416	GDP	C3'-C2'-C1'	2.79	106.75	101.46
3	A	417	GNP	C8-N7-C5	2.69	109.06	104.26
2	B	416	GDP	C6-C5-N7	2.58	134.99	130.29
2	A	416	GDP	C2-N1-C6	-2.50	120.58	125.11
2	B	416	GDP	C3'-C2'-C1'	2.47	106.14	101.46
2	B	416	GDP	C2-N1-C6	-2.46	120.65	125.11
2	A	416	GDP	C6-C5-N7	2.39	134.64	130.29
3	A	417	GNP	O1G-PG-N3B	-2.34	108.33	111.77
2	B	416	GDP	PA-O5'-C5'	-2.32	108.08	121.35
3	A	417	GNP	O6-C6-C5	-2.30	120.47	126.53
2	A	416	GDP	C5-C6-N1	2.27	119.03	113.25
2	B	416	GDP	C5-C6-N1	2.26	119.01	113.25
3	A	417	GNP	C2-N1-C6	-2.24	121.05	125.11
2	A	416	GDP	O6-C6-C5	-2.19	120.76	126.53
2	B	416	GDP	O6-C6-C5	-2.14	120.88	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	417	GNP	C5-C6-N1	2.12	118.64	113.25
2	B	416	GDP	C4-C5-N7	-2.10	107.33	110.67
2	A	416	GDP	C4-C5-N7	-2.10	107.34	110.67
2	A	416	GDP	PA-O5'-C5'	-2.06	109.52	121.35
3	A	417	GNP	C6-C5-N7	2.06	134.04	130.29

There are no chirality outliers.

All (3) torsion outliers are listed below:

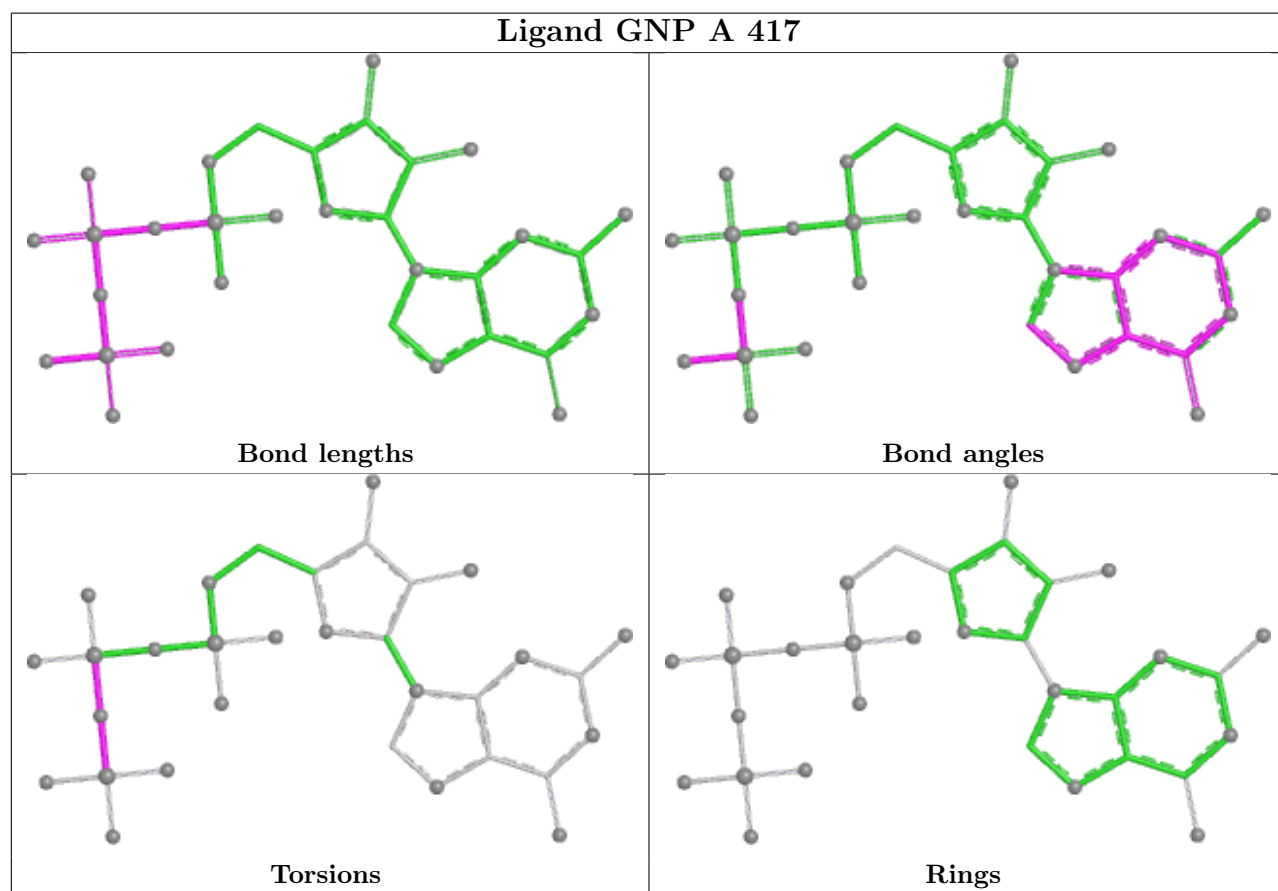
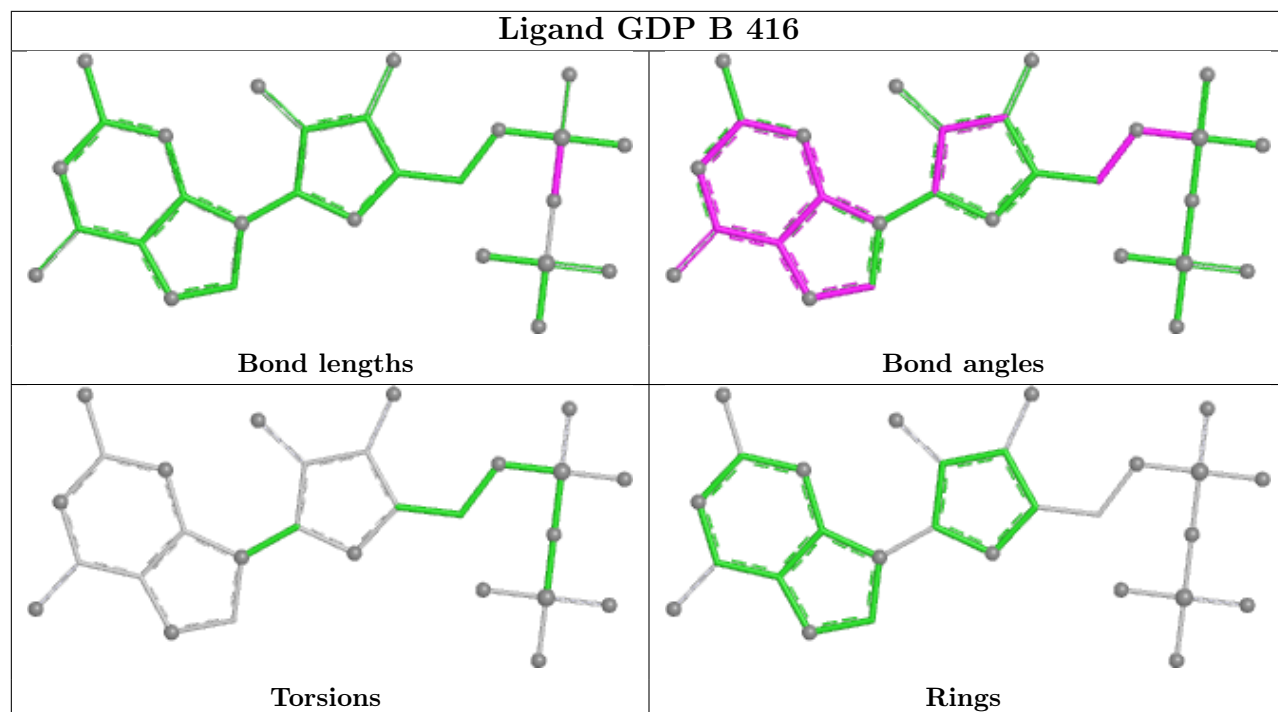
Mol	Chain	Res	Type	Atoms
3	A	417	GNP	PB-N3B-PG-O1G
3	A	417	GNP	PG-N3B-PB-O1B
3	A	417	GNP	PG-N3B-PB-O3A

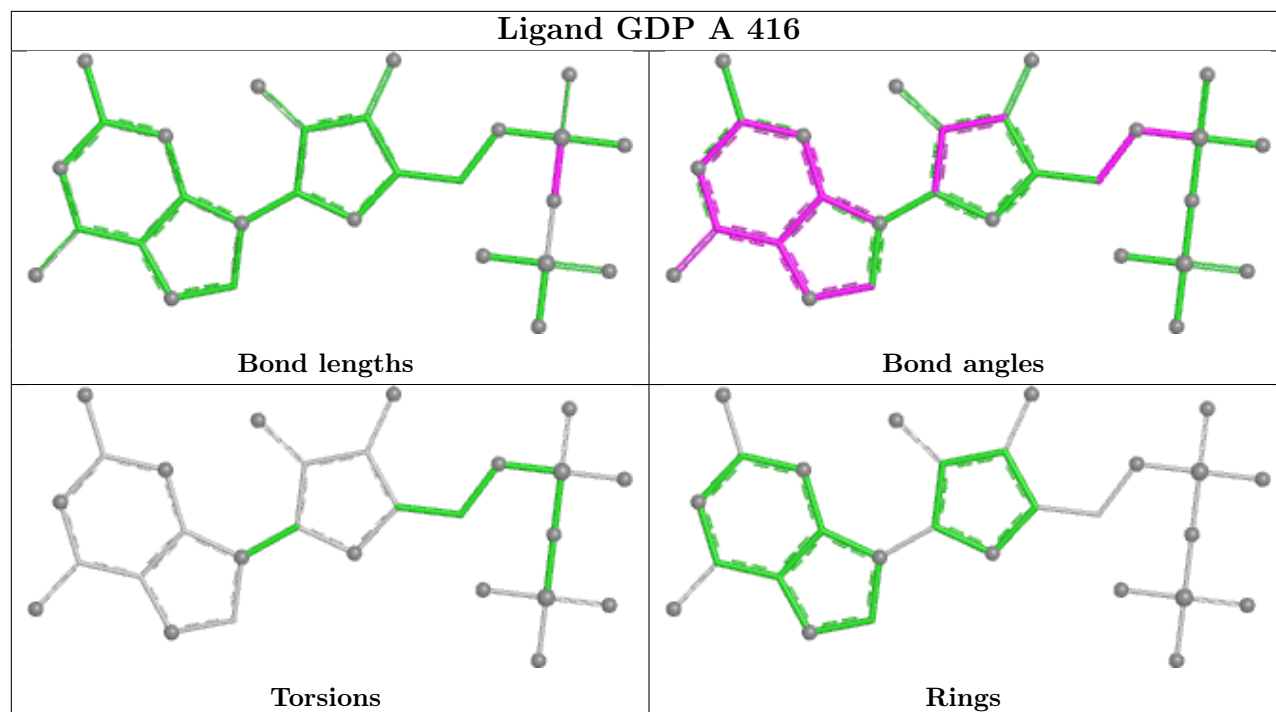
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	416	GDP	2	0
4	A	418	PPV	1	0
3	A	417	GNP	4	0
2	A	416	GDP	6	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	414/415 (99%)	-1.49	0 100 100	31, 53, 122, 162	0
1	B	414/415 (99%)	-1.49	0 100 100	31, 54, 121, 165	0
All	All	828/830 (99%)	-1.49	0 100 100	31, 54, 122, 165	0

There are no RSRZ outliers to report.

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.

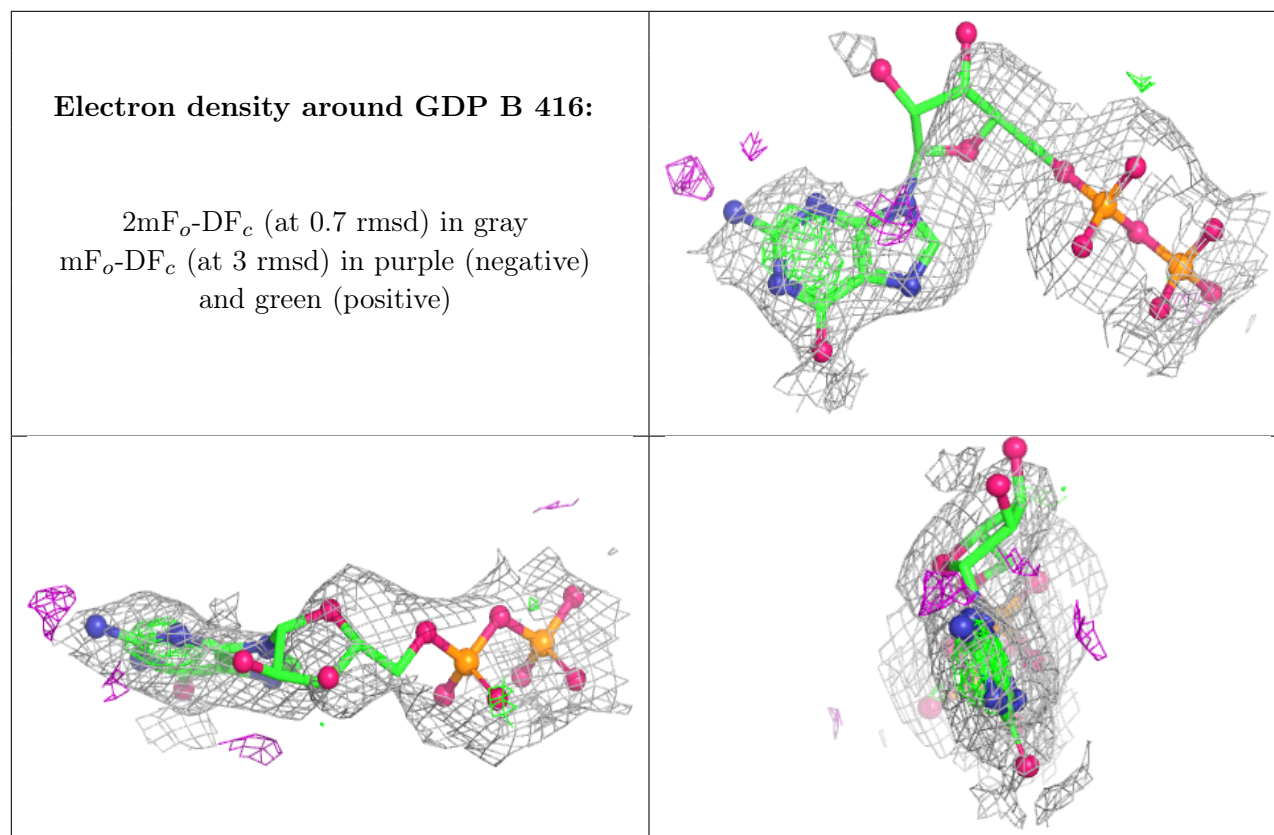
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PPV	A	419	9/9	0.97	0.12	197,197,198,198	0
2	GDP	B	416	28/28	0.98	0.08	127,136,145,146	0
3	GNP	A	417	32/32	0.98	0.09	16,156,168,168	0
4	PPV	A	418	9/9	0.98	0.07	183,184,184,184	0
2	GDP	A	416	28/28	0.98	0.09	118,131,142,143	0
4	PPV	A	420	9/9	0.98	0.07	166,167,168,168	0
4	PPV	B	418	9/9	0.98	0.09	197,198,198,198	0

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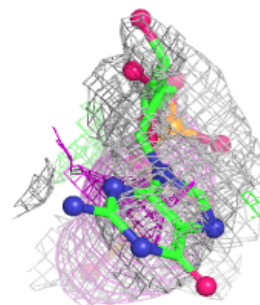
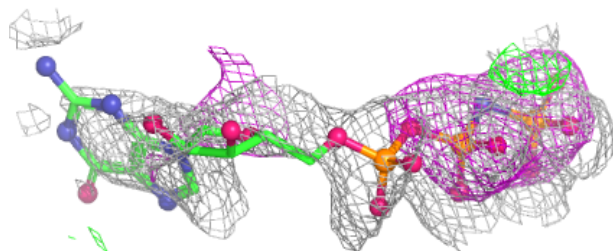
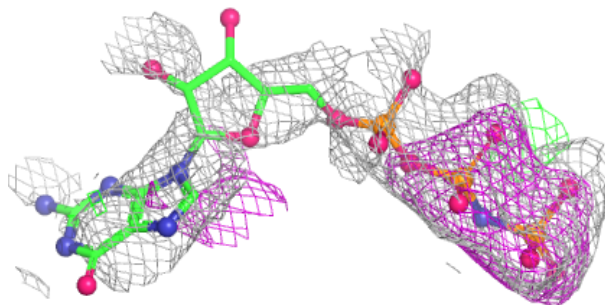
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PPV	B	419	9/9	0.98	0.08	173,174,175,175	0
4	PPV	B	417	9/9	0.99	0.07	182,183,186,186	0

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.

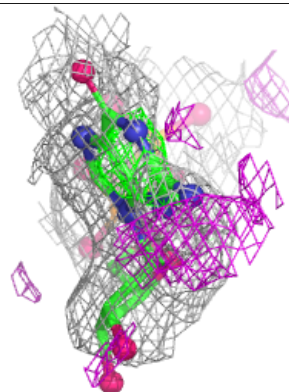
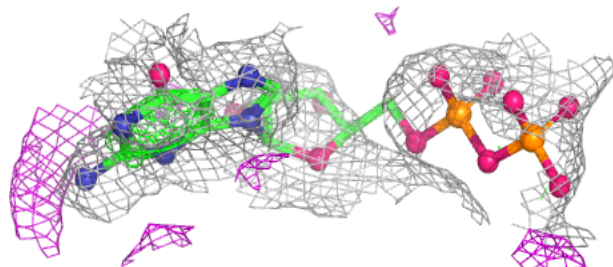
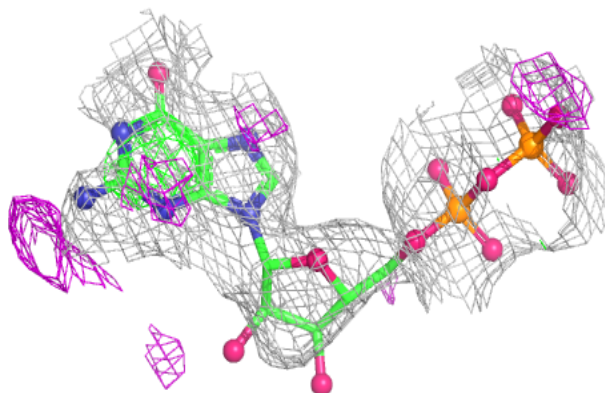


Electron density around GNP A 417:

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

**Electron density around GDP A 416:**

$2mF_o-DF_c$ (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.