Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 12:37 PM EDT

PDB ID	:	1ZXY
Title	:	Anthranilate Phosphoribosyltransferase from Sulfolobus solfataricus in complex with PRPP and Magnesium
Authors	:	Marino, M.; Deuss, M.; Sterner, R.; Mayans, O.
Deposited on	:	2005-06-09
Resolution	:	2.56 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:

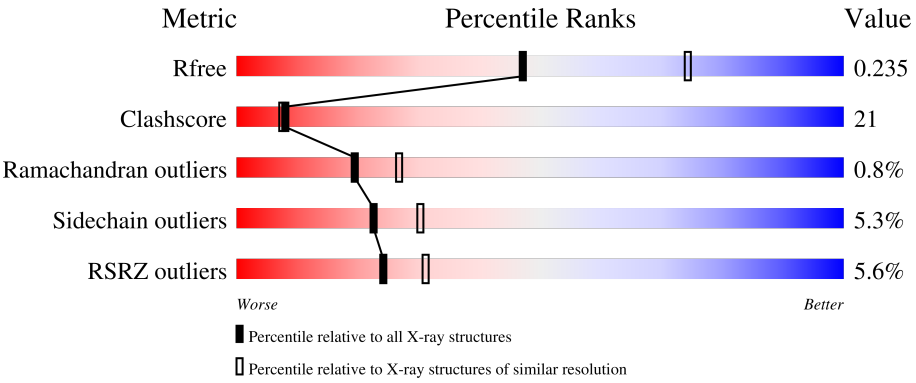
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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 <=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	345	4% 69% 26% .
1	B	345	3% 63% 34% .
1	C	345	7% 65% 32% .
1	D	345	8% 55% 40% .

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	PRP	A	348	-	-	X	-
3	PRP	B	348	-	-	X	-
3	PRP	C	348	-	-	X	-
3	PRP	D	348	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10748 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.

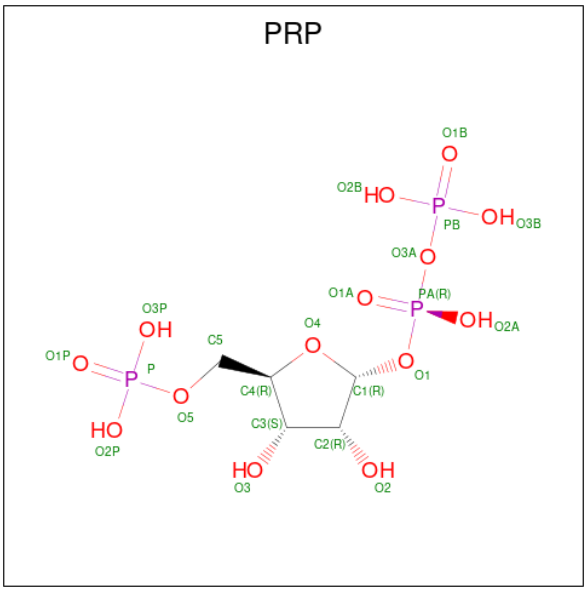
- Molecule 1 is a protein called Anthranilate phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2640	1690	445	498	7			
1	B	344	Total	C	N	O	S	0	0	0
			2640	1690	445	498	7			
1	C	344	Total	C	N	O	S	0	0	0
			2640	1690	445	498	7			
1	D	344	Total	C	N	O	S	0	0	0
			2640	1690	445	498	7			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is 1-O-pyrophosphono-5-O-phosphono-alpha-D-ribofuranose (three-letter code: PRP) (formula: $C_5H_{13}O_{14}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 22 5 14 3	0	0
3	B	1	Total C O P 22 5 14 3	0	0
3	C	1	Total C O P 22 5 14 3	0	0
3	D	1	Total C O P 22 5 14 3	0	0

- Molecule 4 is water.

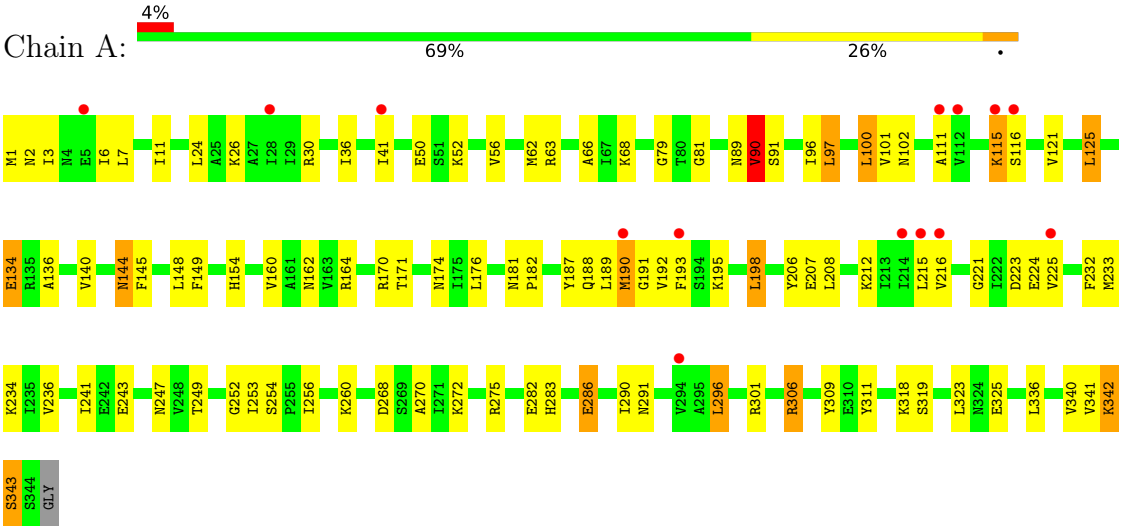
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	22	Total O 22 22	0	0
4	B	21	Total O 21 21	0	0
4	C	28	Total O 28 28	0	0
4	D	21	Total O 21 21	0	0

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.

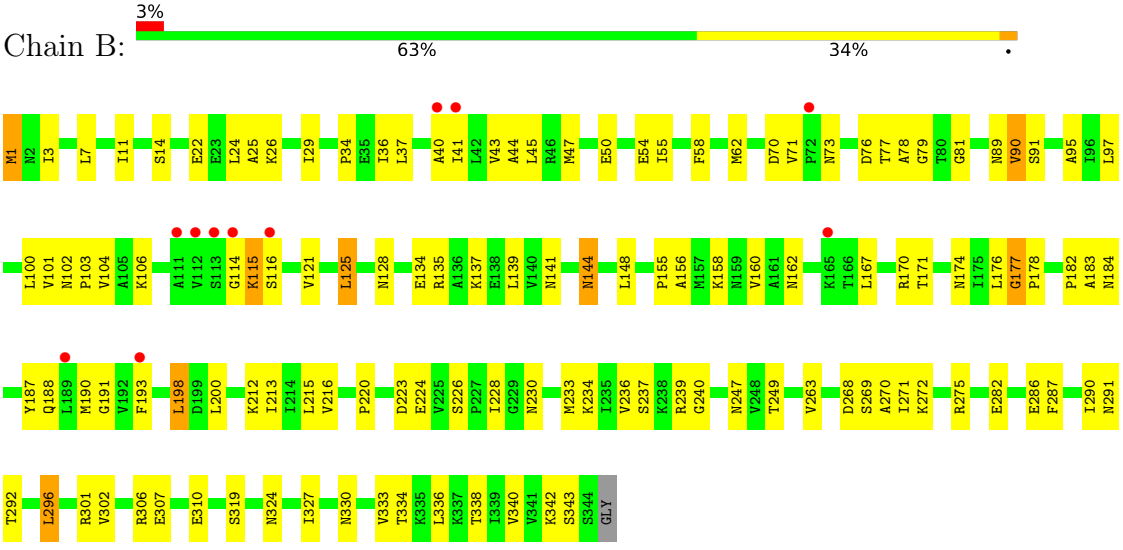
• Molecule 1: Anthranilate phosphoribosyltransferase

Chain A:



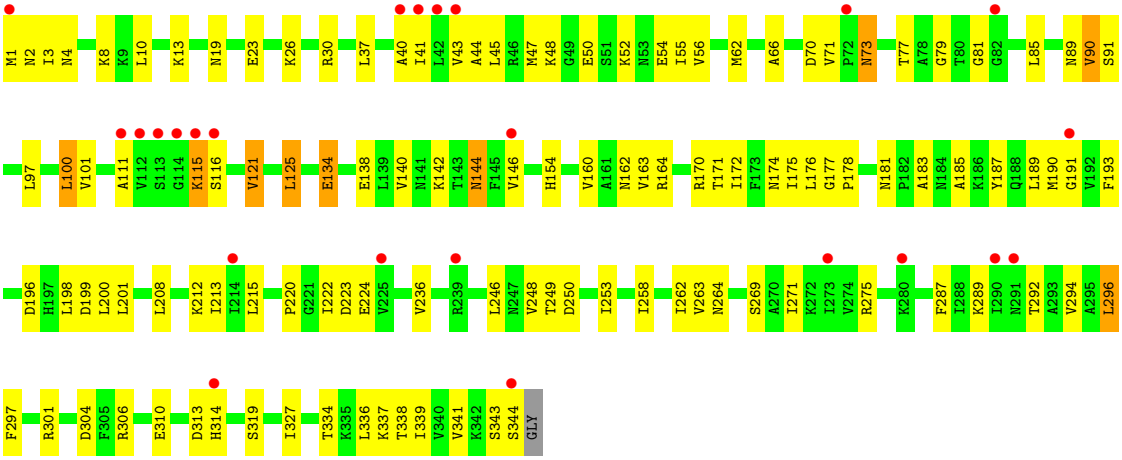
• Molecule 1: Anthranilate phosphoribosyltransferase

Chain B:



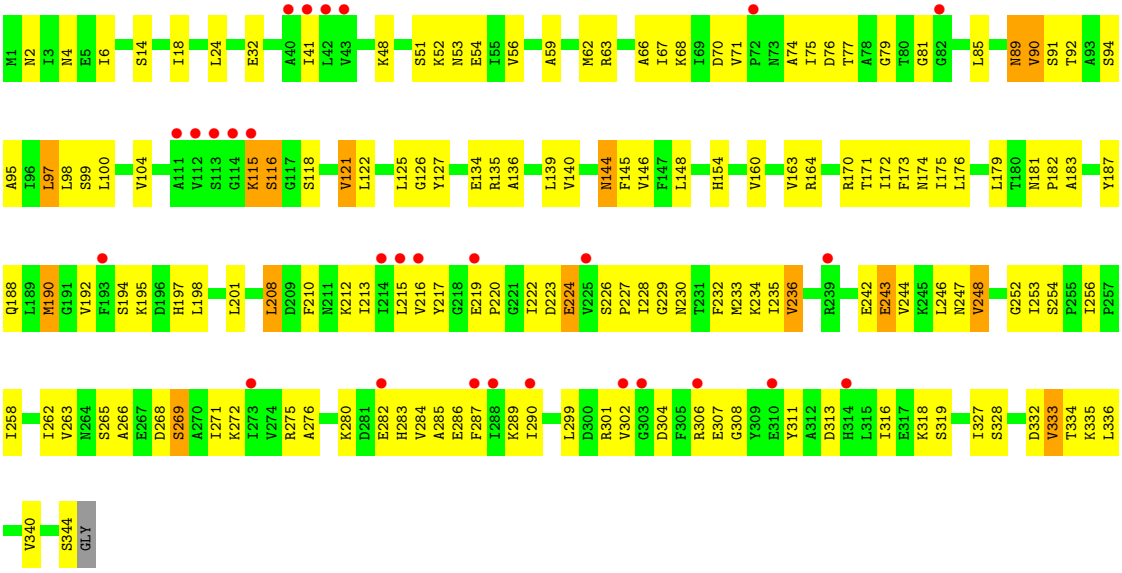
• Molecule 1: Anthranilate phosphoribosyltransferase

Chain C:



• Molecule 1: Anthranilate phosphoribosyltransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	92.69Å 65.81Å 116.72Å 90.00° 107.80° 90.00°	Depositor
Resolution (Å)	20.00 – 2.56 19.84 – 2.56	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.00-2.56) 97.7 (19.84-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	5.87 (at 2.56Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.260 0.191 , 0.235	Depositor DCC
R_{free} test set	503 reflections (1.19%)	wwPDB-VP
Wilson B-factor (Å^2)	69.0	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10748	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6322e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PRP, 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	0.39	0/2677	0.68	2/3617 (0.1%)
1	B	0.38	0/2677	0.67	0/3617
1	C	0.38	0/2677	0.65	0/3617
1	D	0.39	1/2677 (0.0%)	0.65	0/3617
All	All	0.39	1/10708 (0.0%)	0.66	2/14468 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	224	GLU	CG-CD	-5.30	1.44	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	97	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	225	VAL	N-CA-C	-5.01	97.47	111.00

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	2640	0	2753	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2640	0	2753	128	0
1	C	2640	0	2753	98	0
1	D	2640	0	2753	148	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	22	0	6	11	0
3	B	22	0	7	11	0
3	C	22	0	7	9	0
3	D	22	0	7	11	0
4	A	22	0	0	1	0
4	B	21	0	0	6	0
4	C	28	0	0	3	0
4	D	21	0	0	0	0
All	All	10748	0	11039	464	1

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 21.

All (464) 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:62:MET:HE1	1:A:176:LEU:HB3	1.32	1.07
1:A:171:THR:H	1:A:174:ASN:ND2	1.56	1.02
1:B:171:THR:H	1:B:174:ASN:ND2	1.59	1.00
1:B:224:GLU:CD	3:B:348:PRP:H2	1.81	0.99
1:A:282:GLU:O	1:A:286:GLU:HG2	1.66	0.95
1:B:171:THR:H	1:B:174:ASN:HD22	0.98	0.95
1:D:62:MET:HE1	1:D:176:LEU:HD13	1.47	0.95
1:D:171:THR:H	1:D:174:ASN:HD22	1.06	0.94
1:D:253:ILE:HG12	1:D:254:SER:H	1.33	0.94
1:B:237:SER:OG	1:B:239:ARG:HG2	1.67	0.94
1:B:239:ARG:HG3	1:B:240:GLY:H	1.33	0.93
1:A:224:GLU:CD	3:A:348:PRP:H2	1.88	0.93
1:D:198:LEU:HD21	1:D:234:LYS:HG3	1.51	0.91
1:A:171:THR:H	1:A:174:ASN:HD22	0.97	0.91
1:B:239:ARG:HG3	1:B:240:GLY:N	1.86	0.90
1:A:224:GLU:OE1	3:A:348:PRP:H2	1.71	0.90
1:B:275:ARG:HG2	1:B:343:SER:HB2	1.49	0.90
1:C:171:THR:H	1:C:174:ASN:HD22	1.19	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:GLU:CD	3:D:348:PRP:H2	1.93	0.89
1:A:171:THR:N	1:A:174:ASN:HD22	1.70	0.88
1:B:62:MET:HE1	1:B:176:LEU:HD13	1.58	0.86
1:A:91:SER:HB3	3:A:348:PRP:O2	1.78	0.84
1:C:199:ASP:HB2	4:C:362:HOH:O	1.76	0.84
1:D:327:ILE:HD12	1:D:336:LEU:HD22	1.60	0.83
1:D:252:GLY:HA2	1:D:306:ARG:HH21	1.43	0.83
1:D:282:GLU:O	1:D:286:GLU:HG3	1.79	0.82
1:B:282:GLU:O	1:B:286:GLU:HG3	1.79	0.82
1:A:275:ARG:HG3	1:A:343:SER:HB3	1.61	0.82
1:D:224:GLU:OE2	3:D:348:PRP:H2	1.79	0.82
1:A:256:ILE:HD11	1:A:286:GLU:HB2	1.62	0.82
1:B:224:GLU:OE2	3:B:348:PRP:H2	1.78	0.82
1:B:29:ILE:HG22	1:B:156:ALA:HB1	1.60	0.81
1:B:76:ASP:HB3	1:B:188:GLN:HG3	1.59	0.81
1:B:271:ILE:O	1:B:275:ARG:HG3	1.81	0.80
1:D:171:THR:H	1:D:174:ASN:ND2	1.78	0.80
1:D:268:ASP:O	1:D:272:LYS:HG2	1.81	0.79
1:A:253:ILE:HD11	1:A:309:TYR:OH	1.83	0.79
1:C:62:MET:HE1	1:C:176:LEU:HD13	1.62	0.79
1:D:213:ILE:HG23	1:D:236:VAL:HG13	1.65	0.78
1:C:89:ASN:ND2	1:C:116:SER:O	2.15	0.77
1:C:224:GLU:CD	3:C:348:PRP:H2	2.05	0.77
1:D:253:ILE:HG12	1:D:254:SER:N	2.00	0.76
1:B:97:LEU:HD22	1:B:319:SER:OG	1.86	0.76
1:C:81:GLY:HA2	3:C:348:PRP:H51	1.67	0.76
1:A:224:GLU:OE2	3:A:348:PRP:H2	1.85	0.75
1:A:125:LEU:HD13	1:A:270:ALA:HB1	1.68	0.75
1:A:160:VAL:HG12	1:A:164:ARG:HG3	1.66	0.75
1:D:302:VAL:HG13	1:D:307:GLU:HB3	1.69	0.74
1:D:224:GLU:OE1	3:D:348:PRP:H2	1.86	0.74
1:C:97:LEU:HD22	1:C:319:SER:OG	1.87	0.74
1:B:7:LEU:O	1:B:11:ILE:HG12	1.88	0.74
1:B:171:THR:N	1:B:174:ASN:HD22	1.81	0.74
1:A:170:ARG:HA	1:A:174:ASN:ND2	2.02	0.73
1:C:62:MET:CE	1:C:176:LEU:HD13	2.18	0.73
1:D:136:ALA:O	1:D:140:VAL:HG23	1.88	0.73
1:B:271:ILE:HG23	1:B:343:SER:HB3	1.72	0.72
1:D:171:THR:N	1:D:174:ASN:HD22	1.86	0.72
1:D:280:LYS:HE3	1:D:344:SER:O	1.89	0.72
1:D:220:PRO:HG2	1:D:222:ILE:HG13	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:THR:OG1	1:D:118:SER:HB2	1.90	0.72
1:D:208:LEU:HB3	1:D:210:PHE:HE1	1.54	0.71
1:B:224:GLU:OE1	3:B:348:PRP:H2	1.89	0.71
1:D:219:GLU:OE1	1:D:229:GLY:HA3	1.91	0.71
1:D:97:LEU:HD22	1:D:319:SER:OG	1.91	0.71
1:D:285:ALA:O	1:D:289:LYS:HG3	1.91	0.71
1:D:234:LYS:HE2	1:D:243:GLU:OE2	1.91	0.71
1:C:224:GLU:OE2	3:C:348:PRP:H2	1.90	0.71
1:C:91:SER:HB3	3:C:348:PRP:O2	1.92	0.70
1:A:148:LEU:HD13	1:A:182:PRO:HB2	1.74	0.70
1:C:213:ILE:HG23	1:C:236:VAL:HB	1.73	0.70
1:A:268:ASP:O	1:A:272:LYS:HG2	1.92	0.69
1:B:79:GLY:HA3	3:B:348:PRP:O3	1.92	0.69
1:C:134:GLU:CD	1:C:134:GLU:H	1.95	0.69
1:B:62:MET:HE1	1:B:176:LEU:CD1	2.23	0.69
1:B:247:ASN:HD22	1:B:249:THR:H	1.40	0.69
1:D:85:LEU:HD12	1:D:222:ILE:HG12	1.74	0.68
1:B:286:GLU:O	1:B:290:ILE:HG23	1.93	0.68
1:B:292:THR:HG22	1:B:296:LEU:HD22	1.75	0.68
1:D:179:LEU:HD22	1:D:208:LEU:HD23	1.75	0.68
1:B:191:GLY:C	1:B:223:ASP:HB2	2.14	0.68
1:A:286:GLU:O	1:A:290:ILE:HG23	1.94	0.68
1:C:138:GLU:O	1:C:142:LYS:HG2	1.93	0.68
1:D:215:LEU:HD12	1:D:215:LEU:N	2.09	0.68
1:D:302:VAL:CG1	1:D:307:GLU:HB3	2.23	0.67
1:B:188:GLN:OE1	1:B:190:MET:HB2	1.94	0.67
1:A:171:THR:N	1:A:174:ASN:ND2	2.35	0.67
1:B:324:ASN:HD22	1:B:336:LEU:HD23	1.59	0.67
1:D:252:GLY:CA	1:D:306:ARG:HH21	2.08	0.67
1:B:223:ASP:OD2	3:B:348:PRP:H51	1.95	0.67
1:B:336:LEU:O	1:B:340:VAL:HG23	1.95	0.66
1:C:224:GLU:OE1	3:C:348:PRP:H2	1.95	0.66
1:C:327:ILE:HD12	1:C:336:LEU:HD22	1.79	0.65
1:D:89:ASN:HA	3:D:348:PRP:O1A	1.97	0.64
1:C:171:THR:H	1:C:174:ASN:ND2	1.92	0.64
1:A:102:ASN:HD22	1:A:301:ARG:NH2	1.94	0.64
1:D:316:ILE:HA	1:D:319:SER:OG	1.98	0.64
1:D:286:GLU:O	1:D:290:ILE:HG23	1.97	0.63
1:B:77:THR:HB	1:B:91:SER:HB2	1.80	0.63
1:A:336:LEU:O	1:A:340:VAL:HG23	1.99	0.63
1:A:89:ASN:ND2	1:A:116:SER:O	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:N	4:B:368:HOH:O	2.33	0.62
1:B:62:MET:HE3	1:B:176:LEU:HB3	1.80	0.62
1:B:128:ASN:HA	4:B:365:HOH:O	2.00	0.62
1:C:213:ILE:CG2	1:C:236:VAL:HB	2.30	0.62
1:D:223:ASP:OD2	3:D:348:PRP:H51	1.99	0.62
1:B:268:ASP:O	1:B:272:LYS:HG3	1.99	0.62
1:B:170:ARG:NH1	4:B:361:HOH:O	2.32	0.61
1:C:314:HIS:HB3	4:C:370:HOH:O	2.01	0.61
1:D:140:VAL:HG22	1:D:146:VAL:HB	1.81	0.61
1:C:89:ASN:HA	3:C:348:PRP:O1A	2.01	0.61
1:C:301:ARG:HG3	1:C:301:ARG:HH21	1.66	0.60
1:A:191:GLY:C	1:A:223:ASP:HB2	2.21	0.60
1:B:89:ASN:HA	3:B:348:PRP:O1A	2.01	0.60
1:A:253:ILE:HG22	1:A:254:SER:O	2.01	0.60
1:D:271:ILE:O	1:D:275:ARG:HB2	2.01	0.60
1:B:137:LYS:O	1:B:141:ASN:ND2	2.35	0.60
1:D:302:VAL:HG11	1:D:308:GLY:N	2.15	0.59
1:D:91:SER:HB3	3:D:348:PRP:O2	2.02	0.59
1:A:253:ILE:CG2	1:A:254:SER:N	2.65	0.59
1:A:97:LEU:HD22	1:A:319:SER:OG	2.02	0.59
1:A:125:LEU:CD1	1:A:270:ALA:HB1	2.32	0.59
1:A:223:ASP:OD1	3:A:348:PRP:H3	2.02	0.59
1:D:170:ARG:HA	1:D:174:ASN:ND2	2.18	0.59
1:B:102:ASN:HD22	1:B:301:ARG:NH2	2.00	0.59
1:A:2:ASN:O	1:A:6:ILE:HG12	2.02	0.59
1:A:24:LEU:HD11	1:A:41:ILE:HD13	1.84	0.58
1:A:62:MET:HE1	1:A:176:LEU:CB	2.20	0.58
1:B:171:THR:N	1:B:174:ASN:ND2	2.41	0.58
1:B:90:VAL:HG21	1:B:287:PHE:CE2	2.38	0.58
1:B:24:LEU:HD11	1:B:41:ILE:HD13	1.86	0.58
1:A:198:LEU:HD22	1:A:234:LYS:HG3	1.85	0.58
1:C:187:TYR:HA	1:C:212:LYS:O	2.04	0.58
1:D:76:ASP:O	1:D:188:GLN:HB2	2.04	0.58
1:C:343:SER:O	1:C:344:SER:HB2	2.04	0.57
1:B:223:ASP:OD1	3:B:348:PRP:O5	2.23	0.57
1:D:198:LEU:CD2	1:D:234:LYS:HG3	2.30	0.57
1:D:187:TYR:O	1:D:188:GLN:HB3	2.05	0.57
1:A:66:ALA:O	1:A:68:LYS:HE2	2.04	0.57
1:C:190:MET:O	1:C:215:LEU:HA	2.03	0.57
1:D:276:ALA:HB1	1:D:285:ALA:HB2	1.86	0.57
1:C:334:THR:O	1:C:338:THR:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:GLU:HG2	1:D:135:ARG:N	2.19	0.57
1:D:212:LYS:HE3	1:D:235:ILE:CG2	2.35	0.57
1:C:140:VAL:O	1:C:144:ASN:HA	2.03	0.57
1:C:294:VAL:O	1:C:297:PHE:HB3	2.04	0.57
1:C:62:MET:HE1	1:C:176:LEU:CD1	2.34	0.57
1:B:91:SER:HB3	3:B:348:PRP:O2	2.05	0.56
1:C:79:GLY:HA3	3:C:348:PRP:O3	2.04	0.56
1:D:100:LEU:HD21	1:D:318:LYS:HB2	1.87	0.56
1:A:111:ALA:CB	1:A:115:LYS:HA	2.35	0.56
1:A:223:ASP:OD2	3:A:348:PRP:H51	2.06	0.56
1:B:62:MET:CE	1:B:176:LEU:HB3	2.35	0.56
1:D:228:ILE:HG23	1:D:258:ILE:HD11	1.85	0.56
1:A:140:VAL:O	1:A:144:ASN:HA	2.06	0.56
1:B:237:SER:HG	1:B:239:ARG:HG2	1.68	0.56
1:C:90:VAL:HG21	1:C:287:PHE:CE2	2.40	0.56
1:C:191:GLY:C	1:C:223:ASP:HB2	2.26	0.56
1:D:24:LEU:HD11	1:D:41:ILE:HD13	1.88	0.56
1:D:52:LYS:O	1:D:56:VAL:HG23	2.06	0.56
1:B:178:PRO:CG	1:B:190:MET:HE2	2.35	0.56
1:D:148:LEU:HD13	1:D:182:PRO:HB2	1.87	0.55
1:B:263:VAL:HG11	1:B:269:SER:HB2	1.89	0.55
1:A:253:ILE:CD1	1:A:309:TYR:OH	2.54	0.55
1:C:289:LYS:HD3	1:C:313:ASP:HA	1.88	0.55
1:D:97:LEU:O	1:D:100:LEU:HB2	2.05	0.55
1:A:260:LYS:HG2	1:A:283:HIS:CD2	2.42	0.55
1:C:172:ILE:O	1:C:175:ILE:HG12	2.06	0.55
1:A:216:VAL:HG12	1:A:233:MET:HG3	1.89	0.55
1:B:29:ILE:CG2	1:B:156:ALA:HB1	2.36	0.55
1:C:263:VAL:HG11	1:C:269:SER:HA	1.88	0.54
1:D:282:GLU:HG3	1:D:283:HIS:N	2.22	0.54
1:A:50:GLU:CD	1:A:50:GLU:H	2.11	0.54
1:B:50:GLU:H	1:B:50:GLU:CD	2.06	0.54
1:D:208:LEU:HB3	1:D:210:PHE:CE1	2.39	0.54
1:B:263:VAL:HG21	1:B:269:SER:HA	1.90	0.54
1:D:192:VAL:N	1:D:223:ASP:HB2	2.23	0.54
1:D:77:THR:HB	1:D:91:SER:HB2	1.90	0.54
1:D:79:GLY:HA3	3:D:348:PRP:O3	2.07	0.54
1:D:228:ILE:HG21	1:D:258:ILE:HG12	1.90	0.54
1:B:22:GLU:HG2	1:B:26:LYS:HE3	1.89	0.54
1:B:198:LEU:HD13	1:B:234:LYS:HE2	1.90	0.54
1:A:7:LEU:O	1:A:11:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:VAL:HG12	1:D:74:ALA:HB2	1.88	0.54
1:D:302:VAL:HG12	1:D:304:ASP:H	1.72	0.54
1:B:178:PRO:HG2	1:B:190:MET:CE	2.38	0.53
1:D:115:LYS:HD2	1:D:266:ALA:HB2	1.89	0.53
1:D:263:VAL:HG12	1:D:265:SER:H	1.73	0.53
1:C:97:LEU:O	1:C:100:LEU:HB2	2.08	0.53
1:A:252:GLY:HA3	1:A:306:ARG:NH2	2.23	0.53
1:D:63:ARG:O	1:D:68:LYS:HE2	2.08	0.53
1:B:70:ASP:O	1:B:71:VAL:HG22	2.08	0.53
1:A:136:ALA:O	1:A:140:VAL:HG23	2.08	0.53
1:C:3:ILE:HG21	1:C:37:LEU:HD13	1.89	0.53
1:A:253:ILE:HG22	1:A:254:SER:N	2.23	0.53
1:B:306:ARG:O	1:B:310:GLU:HG3	2.09	0.53
1:C:48:LYS:NZ	1:C:54:GLU:OE2	2.42	0.53
1:B:178:PRO:HG2	1:B:190:MET:HE2	1.91	0.53
1:D:90:VAL:HG23	1:D:224:GLU:OE1	2.09	0.53
1:D:140:VAL:O	1:D:144:ASN:HA	2.09	0.53
1:B:55:ILE:HD11	1:B:200:LEU:HD21	1.91	0.53
1:C:62:MET:HE3	1:C:176:LEU:HB3	1.91	0.52
1:D:223:ASP:OD1	3:D:348:PRP:O5	2.28	0.52
1:B:1:MET:HE3	1:B:3:ILE:N	2.25	0.52
1:D:227:PRO:HG3	1:D:287:PHE:CE1	2.44	0.52
1:A:90:VAL:HG11	1:A:291:ASN:ND2	2.25	0.52
1:C:70:ASP:O	1:C:71:VAL:HG22	2.09	0.52
1:C:304:ASP:HB2	4:C:375:HOH:O	2.09	0.52
1:D:216:VAL:HG12	1:D:233:MET:HB3	1.92	0.52
1:D:85:LEU:CD1	1:D:222:ILE:HG12	2.38	0.52
1:D:51:SER:OG	1:D:54:GLU:HG3	2.10	0.52
1:B:73:ASN:HD22	1:B:103:PRO:HG3	1.75	0.52
1:B:77:THR:CB	1:B:91:SER:HB2	2.40	0.51
1:D:224:GLU:OE1	3:D:348:PRP:C2	2.56	0.51
1:A:223:ASP:C	1:A:224:GLU:HG2	2.30	0.51
1:C:55:ILE:HD11	1:C:200:LEU:HD21	1.91	0.51
1:C:13:LYS:HA	1:C:48:LYS:HG3	1.92	0.51
1:D:212:LYS:HE3	1:D:235:ILE:HG23	1.91	0.51
1:C:160:VAL:O	1:C:164:ARG:HG3	2.10	0.51
1:D:190:MET:O	1:D:215:LEU:HA	2.09	0.51
1:A:63:ARG:NH2	1:A:208:LEU:HB3	2.25	0.51
1:B:1:MET:HE1	1:B:3:ILE:HB	1.93	0.51
1:C:41:ILE:O	1:C:45:LEU:HB2	2.11	0.51
1:D:263:VAL:HG13	1:D:268:ASP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ALA:O	1:B:29:ILE:HG13	2.10	0.51
1:D:134:GLU:HG2	1:D:135:ARG:H	1.76	0.51
1:A:247:ASN:HD22	1:A:249:THR:H	1.58	0.51
1:B:34:PRO:HG2	1:B:37:LEU:HD12	1.93	0.50
1:B:90:VAL:CG2	1:B:287:PHE:CE2	2.94	0.50
1:D:213:ILE:CG2	1:D:236:VAL:HG13	2.40	0.50
1:B:213:ILE:HG23	1:B:236:VAL:HB	1.93	0.50
1:D:272:LYS:HB3	1:D:284:VAL:HG21	1.93	0.50
1:A:89:ASN:HA	3:A:348:PRP:O1A	2.11	0.50
1:B:170:ARG:HD3	4:B:361:HOH:O	2.10	0.50
1:D:258:ILE:O	1:D:262:ILE:HG13	2.11	0.50
1:B:224:GLU:OE1	1:B:224:GLU:HA	2.12	0.50
1:B:239:ARG:CG	1:B:240:GLY:N	2.67	0.50
1:D:125:LEU:O	1:D:327:ILE:HD13	2.11	0.50
1:D:282:GLU:HG3	1:D:283:HIS:H	1.77	0.50
1:D:332:ASP:OD2	1:D:334:THR:HB	2.11	0.50
1:D:121:VAL:HG12	1:D:125:LEU:HD21	1.94	0.50
1:A:275:ARG:HG3	1:A:343:SER:CB	2.39	0.49
1:D:122:LEU:HB3	1:D:127:TYR:HB3	1.93	0.49
1:A:96:ILE:HD12	1:A:323:LEU:HD13	1.93	0.49
1:A:62:MET:HE2	1:A:176:LEU:HD13	1.94	0.49
1:A:170:ARG:HA	1:A:174:ASN:HD21	1.76	0.49
1:B:78:ALA:HA	1:B:106:LYS:NZ	2.26	0.49
1:D:59:ALA:O	1:D:63:ARG:HG3	2.12	0.49
1:B:178:PRO:HB2	1:B:190:MET:CE	2.43	0.49
1:B:338:THR:CG2	1:B:342:LYS:HE3	2.43	0.49
1:C:140:VAL:HG23	1:C:146:VAL:HB	1.95	0.49
1:C:70:ASP:O	1:C:71:VAL:CG2	2.61	0.49
1:C:101:VAL:HB	1:C:301:ARG:NH2	2.28	0.49
1:C:171:THR:N	1:C:174:ASN:HD22	1.99	0.49
1:A:91:SER:CB	3:A:348:PRP:O2	2.58	0.49
1:A:134:GLU:CD	1:A:134:GLU:H	2.15	0.49
1:C:85:LEU:O	1:C:262:ILE:HD12	2.13	0.48
1:C:223:ASP:OD2	3:C:348:PRP:H51	2.12	0.48
1:D:222:ILE:HG22	1:D:223:ASP:N	2.28	0.48
1:A:215:LEU:HD12	1:A:215:LEU:N	2.29	0.48
1:B:70:ASP:O	1:B:71:VAL:CG2	2.61	0.48
1:D:76:ASP:OD1	1:D:77:THR:N	2.45	0.48
1:A:170:ARG:NH1	1:A:193:PHE:CZ	2.81	0.48
1:A:198:LEU:HD22	1:A:234:LYS:CG	2.43	0.48
1:B:114:GLY:O	1:B:115:LYS:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ASP:OD1	3:A:348:PRP:O5	2.31	0.48
1:D:66:ALA:HB2	1:D:154:HIS:CE1	2.49	0.48
1:C:301:ARG:HG3	1:C:301:ARG:NH2	2.28	0.48
1:C:337:LYS:O	1:C:341:VAL:HG23	2.14	0.48
1:D:90:VAL:CG2	1:D:224:GLU:OE1	2.62	0.48
1:D:244:VAL:HG12	1:D:246:LEU:CD1	2.43	0.48
1:B:148:LEU:HD13	1:B:182:PRO:HB2	1.96	0.47
1:A:160:VAL:HG12	1:A:160:VAL:O	2.14	0.47
1:A:247:ASN:ND2	1:A:249:THR:H	2.11	0.47
1:B:114:GLY:O	1:B:115:LYS:CD	2.62	0.47
1:B:155:PRO:O	1:B:158:LYS:HG2	2.14	0.47
1:C:52:LYS:O	1:C:56:VAL:HG23	2.15	0.47
1:D:75:ILE:HD12	1:D:299:LEU:HG	1.96	0.47
1:B:47:MET:SD	1:C:44:ALA:HA	2.55	0.47
1:B:62:MET:CE	1:B:176:LEU:HD13	2.39	0.47
1:D:263:VAL:HG11	1:D:269:SER:HB2	1.96	0.47
1:A:341:VAL:O	1:A:343:SER:N	2.47	0.47
1:B:40:ALA:CB	1:C:43:VAL:HG21	2.44	0.47
1:D:99:SER:HB3	1:D:145:PHE:HB2	1.96	0.47
1:C:172:ILE:HG12	1:C:176:LEU:HD11	1.97	0.47
1:C:306:ARG:NH2	1:C:310:GLU:OE1	2.47	0.47
1:B:44:ALA:HA	1:C:47:MET:SD	2.55	0.47
1:D:172:ILE:HG23	1:D:173:PHE:N	2.30	0.47
1:D:230:ASN:HA	1:D:246:LEU:O	2.14	0.47
1:B:160:VAL:HG12	1:B:160:VAL:O	2.14	0.47
1:C:306:ARG:NE	1:C:310:GLU:OE1	2.47	0.47
1:B:193:PHE:O	1:B:193:PHE:CD1	2.68	0.46
1:B:247:ASN:HD22	1:B:249:THR:HB	1.80	0.46
1:D:6:ILE:HG21	1:D:24:LEU:HD22	1.97	0.46
1:C:50:GLU:CD	1:C:50:GLU:H	2.18	0.46
1:D:70:ASP:O	1:D:71:VAL:CG2	2.64	0.46
1:D:121:VAL:HG12	1:D:125:LEU:CD2	2.45	0.46
1:D:135:ARG:CZ	1:D:139:LEU:HD21	2.45	0.46
1:D:228:ILE:CG2	1:D:258:ILE:HG12	2.45	0.46
1:D:70:ASP:O	1:D:71:VAL:HG22	2.15	0.46
1:D:228:ILE:HG22	1:D:256:ILE:O	2.15	0.46
1:A:52:LYS:HD2	1:A:207:GLU:OE2	2.15	0.46
1:D:229:GLY:O	1:D:247:ASN:HA	2.15	0.46
1:A:63:ARG:HH22	1:A:208:LEU:HB3	1.80	0.46
1:C:77:THR:HB	1:C:91:SER:HB2	1.98	0.46
1:D:252:GLY:HA3	1:D:306:ARG:HE	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:PHE:O	1:D:290:ILE:HG12	2.16	0.46
1:A:36:ILE:HD13	1:D:163:VAL:HA	1.97	0.46
1:A:97:LEU:CD2	1:A:319:SER:OG	2.63	0.46
1:B:167:LEU:HD23	1:B:167:LEU:HA	1.82	0.46
1:B:81:GLY:HA2	3:B:348:PRP:H51	1.98	0.46
1:C:170:ARG:HH11	1:C:193:PHE:HE2	1.62	0.46
1:D:328:SER:HA	1:D:333:VAL:HG22	1.97	0.46
1:B:125:LEU:O	1:B:327:ILE:HD13	2.16	0.46
1:C:160:VAL:O	1:C:160:VAL:HG12	2.15	0.46
1:C:170:ARG:NH2	1:C:174:ASN:HB3	2.30	0.46
1:D:215:LEU:N	1:D:215:LEU:CD1	2.78	0.46
1:D:223:ASP:C	1:D:224:GLU:HG2	2.36	0.46
1:A:170:ARG:CA	1:A:174:ASN:ND2	2.77	0.46
1:B:90:VAL:HG11	1:B:291:ASN:ND2	2.30	0.46
1:B:190:MET:O	1:B:215:LEU:HA	2.15	0.46
1:D:302:VAL:HG13	1:D:307:GLU:CB	2.42	0.46
1:A:81:GLY:HA2	3:A:348:PRP:H51	1.99	0.45
1:C:177:GLY:N	1:C:178:PRO:HD2	2.30	0.45
1:C:246:LEU:HD12	1:C:250:ASP:OD2	2.16	0.45
1:B:125:LEU:HD13	1:B:270:ALA:HB1	1.96	0.45
1:C:90:VAL:CG2	1:C:287:PHE:CE2	2.99	0.45
1:C:292:THR:HG22	1:C:296:LEU:HD22	1.97	0.45
1:D:173:PHE:HA	1:D:176:LEU:HD12	1.98	0.45
1:B:170:ARG:HA	1:B:174:ASN:ND2	2.32	0.45
1:D:235:ILE:HB	1:D:242:GLU:HB3	1.98	0.45
1:A:341:VAL:C	1:A:343:SER:H	2.19	0.45
1:C:111:ALA:CB	1:C:115:LYS:HA	2.46	0.45
1:B:247:ASN:ND2	1:B:249:THR:H	2.12	0.45
1:B:213:ILE:CG2	1:B:236:VAL:HB	2.46	0.45
1:B:216:VAL:HG12	1:B:233:MET:HB3	1.99	0.45
1:C:1:MET:HB3	1:C:2:ASN:H	1.46	0.45
1:C:121:VAL:O	1:C:125:LEU:HD22	2.16	0.45
1:B:70:ASP:O	1:B:137:LYS:HE3	2.16	0.45
1:C:181:ASN:ND2	1:C:185:ALA:H	2.15	0.45
1:B:36:ILE:HG13	4:B:349:HOH:O	2.17	0.45
1:B:40:ALA:HB1	1:C:43:VAL:HG21	1.99	0.45
1:B:144:ASN:HD22	1:B:144:ASN:HA	1.61	0.45
1:C:223:ASP:OD1	3:C:348:PRP:O5	2.35	0.45
1:D:160:VAL:HG12	1:D:160:VAL:O	2.17	0.45
1:A:100:LEU:HD21	1:A:318:LYS:HB2	1.99	0.45
1:D:2:ASN:O	1:D:6:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:N	4:A:368:HOH:O	2.50	0.44
1:B:302:VAL:HB	1:B:307:GLU:HB3	2.00	0.44
1:C:271:ILE:O	1:C:275:ARG:HG3	2.17	0.44
1:D:216:VAL:HG12	1:D:233:MET:CB	2.46	0.44
1:A:188:GLN:CG	1:A:189:LEU:N	2.81	0.44
1:C:111:ALA:HB3	1:C:115:LYS:HA	1.98	0.44
1:C:249:THR:HA	1:C:253:ILE:O	2.17	0.44
1:D:301:ARG:O	1:D:302:VAL:HG23	2.18	0.44
1:A:253:ILE:HD11	1:A:309:TYR:HH	1.79	0.44
1:A:26:LYS:O	1:A:30:ARG:HG3	2.17	0.44
1:A:236:VAL:HG22	1:A:241:ILE:HG12	2.00	0.44
1:C:215:LEU:N	1:C:215:LEU:HD12	2.32	0.44
1:D:160:VAL:O	1:D:164:ARG:HG3	2.17	0.44
1:D:248:VAL:O	1:D:253:ILE:HG22	2.18	0.44
1:D:328:SER:HB3	1:D:333:VAL:CG2	2.47	0.44
1:B:198:LEU:CD1	1:B:234:LYS:HE2	2.47	0.44
1:D:316:ILE:HA	1:D:319:SER:HG	1.83	0.44
1:A:160:VAL:O	1:A:160:VAL:CG1	2.66	0.44
1:B:89:ASN:HD21	1:B:116:SER:C	2.22	0.44
1:D:89:ASN:ND2	1:D:116:SER:O	2.43	0.44
1:D:195:LYS:HE2	1:D:232:PHE:CE1	2.52	0.44
1:B:215:LEU:N	1:B:215:LEU:HD12	2.32	0.43
1:D:253:ILE:CD1	1:D:286:GLU:HB3	2.47	0.43
1:D:2:ASN:OD1	1:D:4:ASN:N	2.51	0.43
1:D:91:SER:CB	3:D:348:PRP:O2	2.65	0.43
1:A:1:MET:SD	1:A:3:ILE:HD13	2.59	0.43
1:A:6:ILE:HG21	1:A:24:LEU:HD22	1.99	0.43
1:A:190:MET:O	1:A:215:LEU:HA	2.18	0.43
1:B:22:GLU:O	1:B:26:LYS:HG3	2.18	0.43
1:C:222:ILE:HD11	1:C:224:GLU:HG3	2.01	0.43
1:B:54:GLU:O	1:B:58:PHE:HD1	2.01	0.43
1:A:79:GLY:HA3	3:A:348:PRP:O3	2.19	0.43
1:B:101:VAL:O	1:B:102:ASN:HB2	2.18	0.43
1:B:187:TYR:HA	1:B:212:LYS:O	2.18	0.43
1:D:195:LYS:HG3	1:D:217:TYR:CE2	2.54	0.43
1:B:36:ILE:HD13	1:C:163:VAL:HA	2.00	0.43
1:A:170:ARG:NH1	1:A:193:PHE:CE2	2.87	0.43
1:A:206:TYR:HB2	1:A:241:ILE:HD11	2.01	0.43
1:A:195:LYS:HE2	1:A:232:PHE:CZ	2.54	0.43
1:B:272:LYS:HE2	4:B:366:HOH:O	2.19	0.43
1:B:275:ARG:HG2	1:B:343:SER:CB	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LYS:HB3	1:C:30:ARG:NH1	2.34	0.43
1:C:66:ALA:HB2	1:C:154:HIS:CE1	2.53	0.43
1:D:198:LEU:C	1:D:198:LEU:HD23	2.39	0.43
1:A:111:ALA:HB3	1:A:115:LYS:HA	1.99	0.42
1:B:91:SER:CB	3:B:348:PRP:O2	2.67	0.42
1:B:220:PRO:HD3	1:B:228:ILE:HD13	2.01	0.42
1:D:213:ILE:HG23	1:D:236:VAL:CG1	2.44	0.42
1:B:333:VAL:O	1:B:336:LEU:HB3	2.19	0.42
1:B:338:THR:O	1:B:342:LYS:HG3	2.18	0.42
1:C:181:ASN:HD21	1:C:183:ALA:HB3	1.83	0.42
1:B:90:VAL:CG2	1:B:224:GLU:OE2	2.68	0.42
1:C:4:ASN:O	1:C:8:LYS:HG3	2.19	0.42
1:A:286:GLU:HG2	1:A:286:GLU:H	1.61	0.42
1:B:3:ILE:HD13	1:B:37:LEU:HD13	2.00	0.42
1:D:126:GLY:HA2	1:D:335:LYS:HD2	2.01	0.42
1:D:195:LYS:HG3	1:D:217:TYR:CD2	2.54	0.42
1:A:247:ASN:ND2	1:A:249:THR:HG23	2.35	0.42
1:C:213:ILE:HG23	1:C:213:ILE:O	2.18	0.42
1:D:275:ARG:HG2	1:D:275:ARG:HH11	1.85	0.42
1:B:3:ILE:HG13	1:B:41:ILE:HD11	2.01	0.42
1:D:181:ASN:ND2	1:D:183:ALA:H	2.18	0.42
1:B:55:ILE:HG23	1:B:176:LEU:HD21	2.01	0.42
1:B:191:GLY:HA2	1:B:216:VAL:O	2.20	0.42
3:B:348:PRP:O4	3:B:348:PRP:O3A	2.38	0.42
1:D:75:ILE:HG13	1:D:187:TYR:C	2.40	0.42
1:A:144:ASN:HA	1:A:144:ASN:HD22	1.55	0.41
1:D:18:ILE:HD11	1:D:53:ASN:OD1	2.18	0.41
1:D:198:LEU:HD23	1:D:198:LEU:O	2.20	0.41
1:B:226:SER:HB2	1:B:230:ASN:O	2.20	0.41
1:D:48:LYS:HZ1	1:D:54:GLU:CD	2.22	0.41
1:D:89:ASN:OD1	1:D:121:VAL:HG22	2.19	0.41
1:D:95:ALA:HB1	1:D:104:VAL:HG11	2.02	0.41
1:A:66:ALA:HB2	1:A:154:HIS:ND1	2.35	0.41
1:B:95:ALA:HB1	1:B:104:VAL:HG11	2.03	0.41
1:D:336:LEU:O	1:D:340:VAL:HG23	2.20	0.41
1:D:253:ILE:HD11	1:D:286:GLU:OE1	2.20	0.41
1:B:43:VAL:HG21	1:C:40:ALA:CB	2.51	0.41
1:B:183:ALA:O	1:B:184:ASN:HB3	2.20	0.41
1:B:239:ARG:CG	1:B:240:GLY:H	2.18	0.41
1:C:181:ASN:ND2	1:C:183:ALA:H	2.19	0.41
1:A:187:TYR:HA	1:A:212:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:VAL:HG13	1:C:73:ASN:HD21	1.86	0.41
1:D:81:GLY:HA2	3:D:348:PRP:H51	2.02	0.41
1:D:94:SER:O	1:D:98:LEU:HG	2.20	0.41
1:D:197:HIS:O	1:D:201:LEU:HG	2.20	0.41
1:D:304:ASP:OD1	1:D:306:ARG:N	2.49	0.41
1:B:135:ARG:O	1:B:139:LEU:HG	2.20	0.41
1:C:19:ASN:O	1:C:23:GLU:HG2	2.21	0.41
1:C:101:VAL:HB	1:C:301:ARG:HH22	1.86	0.41
1:C:181:ASN:HD22	1:C:185:ALA:H	1.67	0.41
1:C:336:LEU:O	1:C:339:ILE:HB	2.21	0.41
1:D:219:GLU:HB2	1:D:230:ASN:O	2.19	0.41
1:A:192:VAL:O	1:A:223:ASP:HB3	2.21	0.41
1:B:78:ALA:CA	1:B:106:LYS:HZ2	2.34	0.41
1:B:176:LEU:O	1:B:177:GLY:C	2.60	0.41
1:C:10:LEU:CD1	1:C:41:ILE:HG23	2.50	0.41
1:D:172:ILE:O	1:D:175:ILE:HG12	2.21	0.41
1:D:253:ILE:HD12	1:D:286:GLU:HB3	2.03	0.41
1:A:181:ASN:HA	1:A:182:PRO:HD3	1.82	0.40
1:A:296:LEU:HD21	1:A:311:TYR:HD1	1.86	0.40
1:D:219:GLU:H	1:D:226:SER:HB2	1.85	0.40
1:A:145:PHE:C	1:A:145:PHE:CD2	2.93	0.40
1:A:223:ASP:OD1	1:A:223:ASP:N	2.51	0.40
1:C:89:ASN:CG	1:C:121:VAL:HG21	2.42	0.40
1:C:101:VAL:CG2	1:C:301:ARG:HH22	2.34	0.40
1:A:52:LYS:O	1:A:56:VAL:HG23	2.21	0.40
1:A:190:MET:HG2	1:A:215:LEU:HG	2.02	0.40
1:B:70:ASP:C	1:B:71:VAL:CG2	2.90	0.40
1:C:248:VAL:HG13	1:C:249:THR:N	2.36	0.40
1:D:252:GLY:CA	1:D:306:ARG:HE	2.33	0.40
1:B:43:VAL:HG21	1:C:40:ALA:HB1	2.04	0.40
1:B:333:VAL:HG23	1:B:334:THR:N	2.37	0.40
1:D:222:ILE:HG22	1:D:224:GLU:HG2	2.03	0.40
1:A:101:VAL:O	1:A:102:ASN:HB2	2.21	0.40
1:B:178:PRO:HB2	1:B:190:MET:HE3	2.03	0.40
1:C:90:VAL:HG23	1:C:224:GLU:OE2	2.21	0.40
1:C:201:LEU:HD23	1:C:201:LEU:HA	1.91	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:ILE:CD1	1:D:67:ILE:CD1[2_656]	2.07	0.13

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	342/345 (99%)	324 (95%)	14 (4%)	4 (1%)	13	17
1	B	342/345 (99%)	325 (95%)	14 (4%)	3 (1%)	17	24
1	C	342/345 (99%)	323 (94%)	18 (5%)	1 (0%)	41	50
1	D	342/345 (99%)	310 (91%)	29 (8%)	3 (1%)	17	24
All	All	1368/1380 (99%)	1282 (94%)	75 (6%)	11 (1%)	19	27

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	LYS
1	B	115	LYS
1	C	115	LYS
1	D	115	LYS
1	A	342	LYS
1	D	89	ASN
1	B	330	ASN
1	D	116	SER
1	A	90	VAL
1	B	177	GLY
1	A	221	GLY

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	289/289 (100%)	272 (94%)	17 (6%)	19	25
1	B	289/289 (100%)	277 (96%)	12 (4%)	30	40
1	C	289/289 (100%)	273 (94%)	16 (6%)	21	29
1	D	289/289 (100%)	273 (94%)	16 (6%)	21	29
All	All	1156/1156 (100%)	1095 (95%)	61 (5%)	22	30

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	100	LEU
1	A	121	VAL
1	A	125	LEU
1	A	134	GLU
1	A	144	ASN
1	A	149	PHE
1	A	162	ASN
1	A	190	MET
1	A	198	LEU
1	A	243	GLU
1	A	286	GLU
1	A	296	LEU
1	A	306	ARG
1	A	325	GLU
1	A	342	LYS
1	A	343	SER
1	B	1	MET
1	B	14	SER
1	B	45	LEU
1	B	90	VAL
1	B	100	LEU
1	B	121	VAL
1	B	125	LEU
1	B	134	GLU
1	B	144	ASN
1	B	162	ASN
1	B	198	LEU
1	B	296	LEU
1	C	73	ASN

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Mol	Chain	Res	Type
1	C	90	VAL
1	C	100	LEU
1	C	121	VAL
1	C	125	LEU
1	C	134	GLU
1	C	144	ASN
1	C	162	ASN
1	C	189	LEU
1	C	196	ASP
1	C	198	LEU
1	C	208	LEU
1	C	220	PRO
1	C	258	ILE
1	C	264	ASN
1	C	296	LEU
1	D	14	SER
1	D	32	GLU
1	D	90	VAL
1	D	97	LEU
1	D	121	VAL
1	D	144	ASN
1	D	190	MET
1	D	194	SER
1	D	208	LEU
1	D	236	VAL
1	D	243	GLU
1	D	248	VAL
1	D	269	SER
1	D	311	TYR
1	D	313	ASP
1	D	333	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	144	ASN
1	A	151	GLN
1	A	162	ASN
1	A	174	ASN
1	A	197	HIS
1	A	247	ASN

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Mol	Chain	Res	Type
1	A	283	HIS
1	B	102	ASN
1	B	141	ASN
1	B	144	ASN
1	B	151	GLN
1	B	162	ASN
1	B	174	ASN
1	B	247	ASN
1	B	324	ASN
1	C	144	ASN
1	C	151	GLN
1	C	162	ASN
1	C	174	ASN
1	C	181	ASN
1	C	184	ASN
1	D	107	HIS
1	D	151	GLN
1	D	154	HIS
1	D	162	ASN
1	D	174	ASN
1	D	181	ASN
1	D	247	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 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	PRP	D	348	2	19,22,22	1.03	0	33,35,35	1.16	2 (6%)
3	PRP	C	348	2	19,22,22	0.98	0	33,35,35	1.06	2 (6%)
3	PRP	B	348	2	19,22,22	0.93	0	33,35,35	1.23	3 (9%)
3	PRP	A	348	2	19,22,22	0.92	0	33,35,35	1.33	4 (12%)

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	PRP	D	348	2	-	1/16/33/33	0/1/1/1
3	PRP	C	348	2	-	3/16/33/33	0/1/1/1
3	PRP	B	348	2	-	1/16/33/33	0/1/1/1
3	PRP	A	348	2	-	1/16/33/33	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	348	PRP	O1-C1-C2	3.43	112.52	106.72
3	A	348	PRP	C1-C2-C3	2.98	106.08	102.30
3	D	348	PRP	O1-C1-C2	2.72	111.33	106.72
3	B	348	PRP	C1-C2-C3	2.71	105.73	102.30
3	B	348	PRP	P-O5-C5	2.60	125.46	118.30
3	C	348	PRP	P-O5-C5	2.59	125.43	118.30
3	A	348	PRP	P-O5-C5	2.59	125.42	118.30
3	B	348	PRP	O1-C1-C2	2.55	111.04	106.72
3	D	348	PRP	P-O5-C5	2.35	124.76	118.30
3	C	348	PRP	O1-C1-C2	2.31	110.63	106.72
3	A	348	PRP	C2-C3-C4	2.01	106.55	102.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	348	PRP	C4-C5-O5-P
3	D	348	PRP	C4-C5-O5-P
3	A	348	PRP	C4-C5-O5-P
3	B	348	PRP	C4-C5-O5-P
3	C	348	PRP	O4-C4-C5-O5
3	C	348	PRP	C3-C4-C5-O5

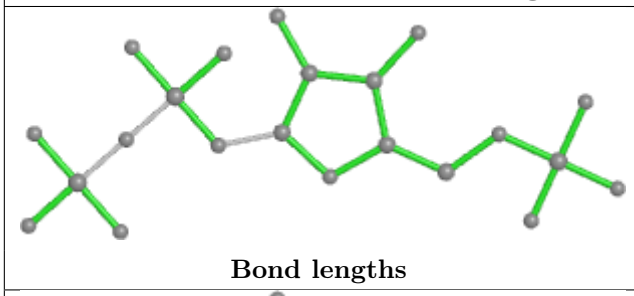
There are no ring outliers.

4 monomers are involved in 42 short contacts:

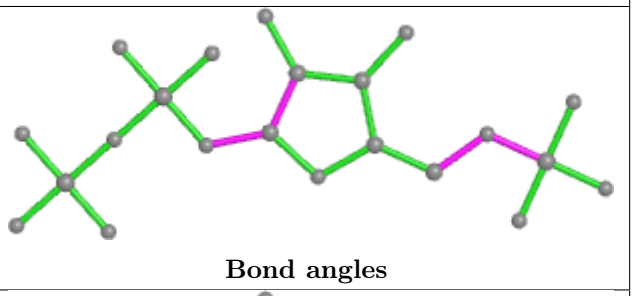
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	348	PRP	11	0
3	C	348	PRP	9	0
3	B	348	PRP	11	0
3	A	348	PRP	11	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

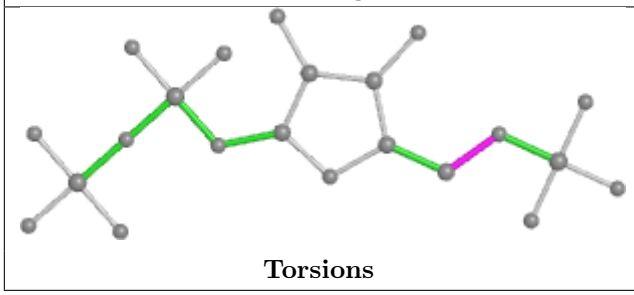
Ligand PRP D 348



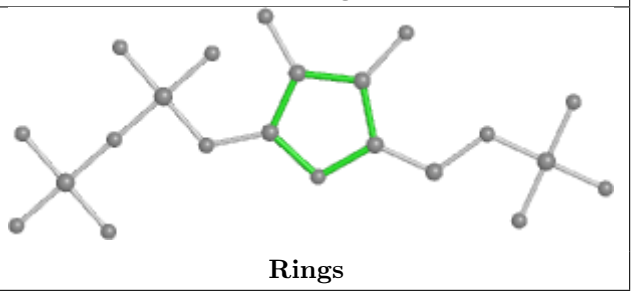
Bond lengths



Bond angles

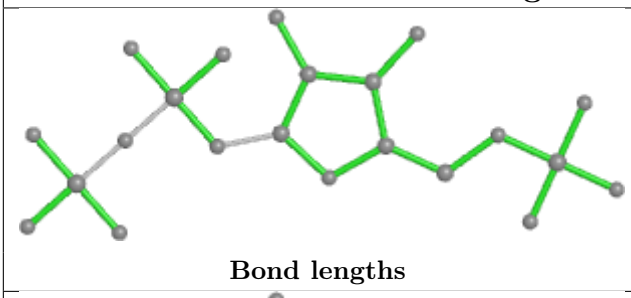


Torsions

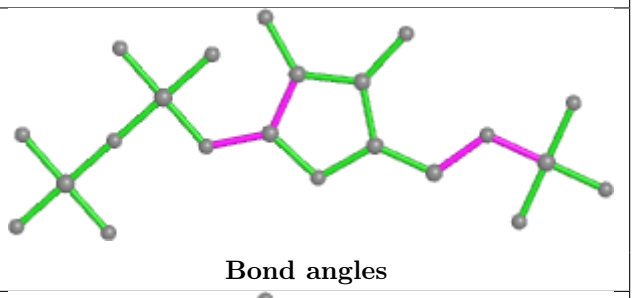


Rings

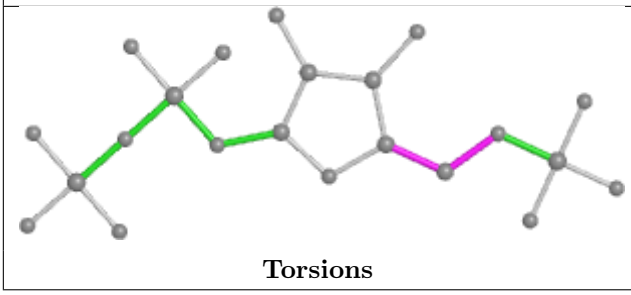
Ligand PRP C 348



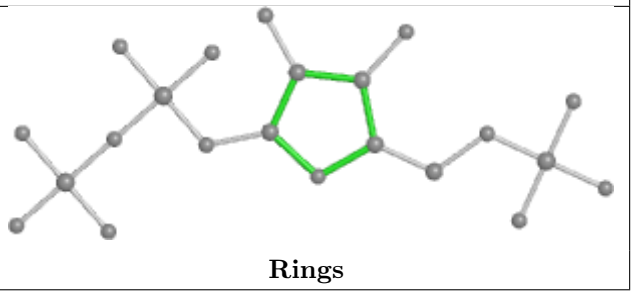
Bond lengths



Bond angles

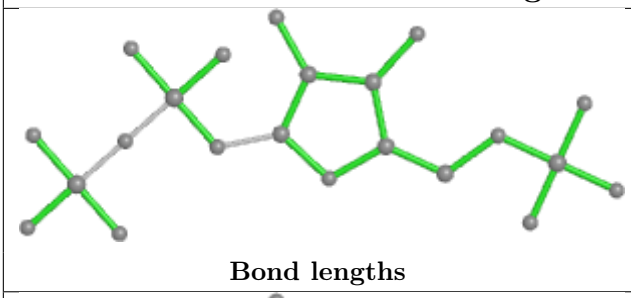


Torsions

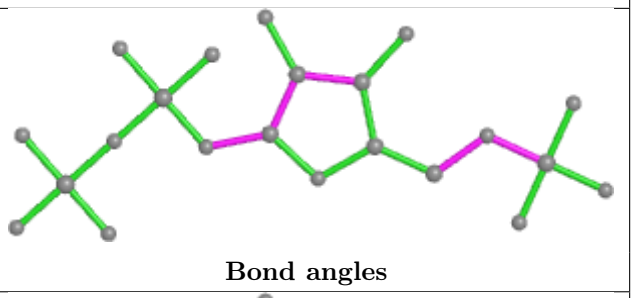


Rings

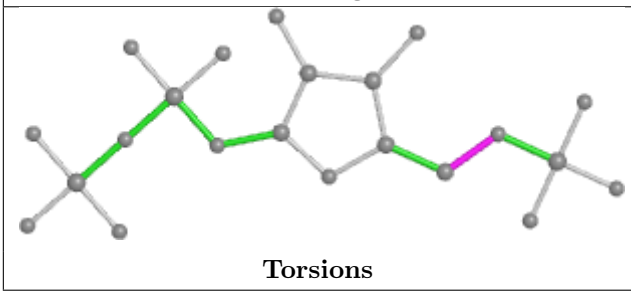
Ligand PRP B 348



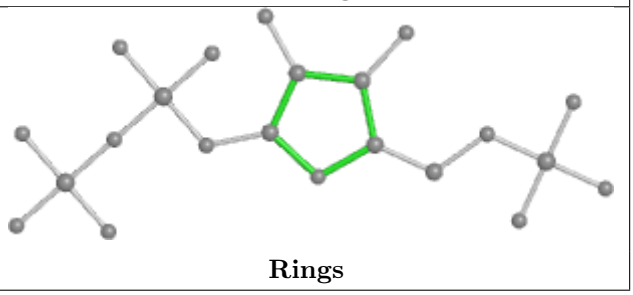
Bond lengths



Bond angles

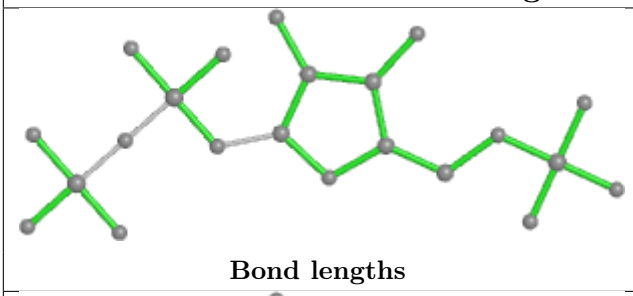


Torsions

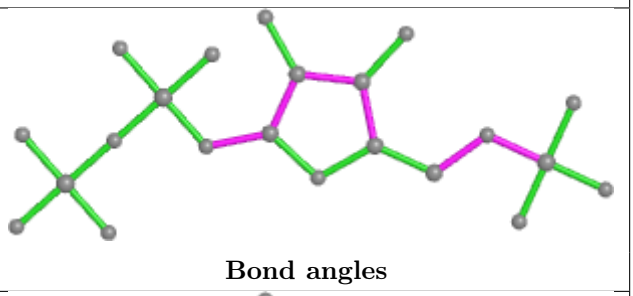


Rings

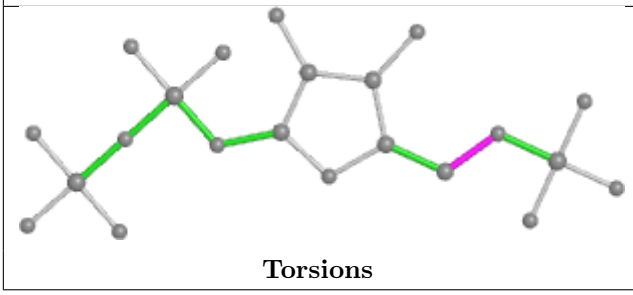
Ligand PRP A 348



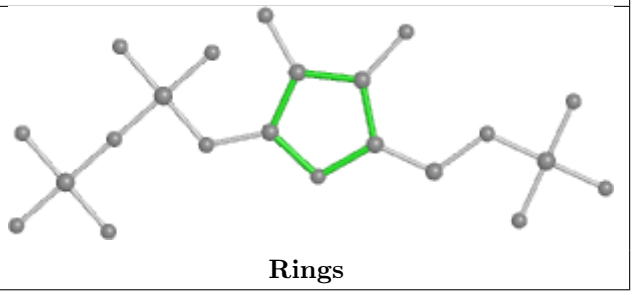
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	344/345 (99%)	0.12	14 (4%)	37	46	47, 60, 74, 96	0
1	B	344/345 (99%)	0.09	11 (3%)	47	57	46, 61, 79, 94	0
1	C	344/345 (99%)	0.19	24 (6%)	16	21	45, 61, 76, 103	0
1	D	344/345 (99%)	0.29	28 (8%)	12	16	50, 67, 87, 99	0
All	All	1376/1380 (99%)	0.17	77 (5%)	24	31	45, 62, 84, 103	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	112	VAL	7.7
1	D	112	VAL	6.6
1	A	112	VAL	5.9
1	D	113	SER	5.8
1	B	111	ALA	4.8
1	C	41	ILE	4.2
1	B	114	GLY	4.0
1	C	112	VAL	4.0
1	C	225	VAL	3.9
1	C	344	SER	3.7
1	D	114	GLY	3.7
1	C	113	SER	3.7
1	D	41	ILE	3.6
1	C	291	ASN	3.6
1	C	116	SER	3.6
1	B	41	ILE	3.4
1	D	111	ALA	3.4
1	D	72	PRO	3.4
1	C	239	ARG	3.4
1	D	306	ARG	3.4
1	D	225	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	116	SER	3.2
1	D	287	PHE	3.2
1	C	273	ILE	3.1
1	D	290	ILE	3.1
1	C	115	LYS	3.0
1	C	82	GLY	3.0
1	C	114	GLY	3.0
1	D	115	LYS	3.0
1	B	40	ALA	2.9
1	D	310	GLU	2.9
1	A	115	LYS	2.9
1	C	42	LEU	2.9
1	B	113	SER	2.9
1	C	72	PRO	2.8
1	D	216	VAL	2.8
1	C	290	ILE	2.7
1	C	43	VAL	2.7
1	A	215	LEU	2.6
1	A	28	ILE	2.6
1	D	314	HIS	2.6
1	A	41	ILE	2.5
1	A	190	MET	2.5
1	C	214	ILE	2.5
1	D	42	LEU	2.5
1	C	191	GLY	2.5
1	D	282	GLU	2.4
1	A	294	VAL	2.4
1	D	288	ILE	2.4
1	D	239	ARG	2.4
1	D	82	GLY	2.4
1	A	111	ALA	2.4
1	B	72	PRO	2.4
1	C	314	HIS	2.4
1	C	40	ALA	2.3
1	A	214	ILE	2.3
1	D	215	LEU	2.3
1	D	40	ALA	2.3
1	A	225	VAL	2.3
1	B	193	PHE	2.3
1	A	216	VAL	2.2
1	C	146	VAL	2.2
1	D	214	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	2.2
1	A	193	PHE	2.2
1	D	302	VAL	2.2
1	D	273	ILE	2.1
1	D	219	GLU	2.1
1	D	43	VAL	2.1
1	C	280	LYS	2.1
1	A	5	GLU	2.1
1	B	116	SER	2.1
1	D	303	GLY	2.1
1	B	165	LYS	2.1
1	B	189	LEU	2.1
1	C	111	ALA	2.0
1	D	193	PHE	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 monosaccharides 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, 95^{th} 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	D	346	1/1	0.87	0.06	50,50,50,50	0
3	PRP	C	348	22/22	0.91	0.18	79,85,97,100	0
3	PRP	D	348	22/22	0.92	0.15	77,86,97,100	0
3	PRP	B	348	22/22	0.93	0.15	62,70,93,95	0
3	PRP	A	348	22/22	0.94	0.14	64,72,94,95	0
2	MG	B	346	1/1	0.94	0.08	52,52,52,52	0
2	MG	C	346	1/1	0.94	0.07	80,80,80,80	0
2	MG	A	346	1/1	0.94	0.12	46,46,46,46	0
2	MG	A	347	1/1	0.97	0.04	54,54,54,54	0

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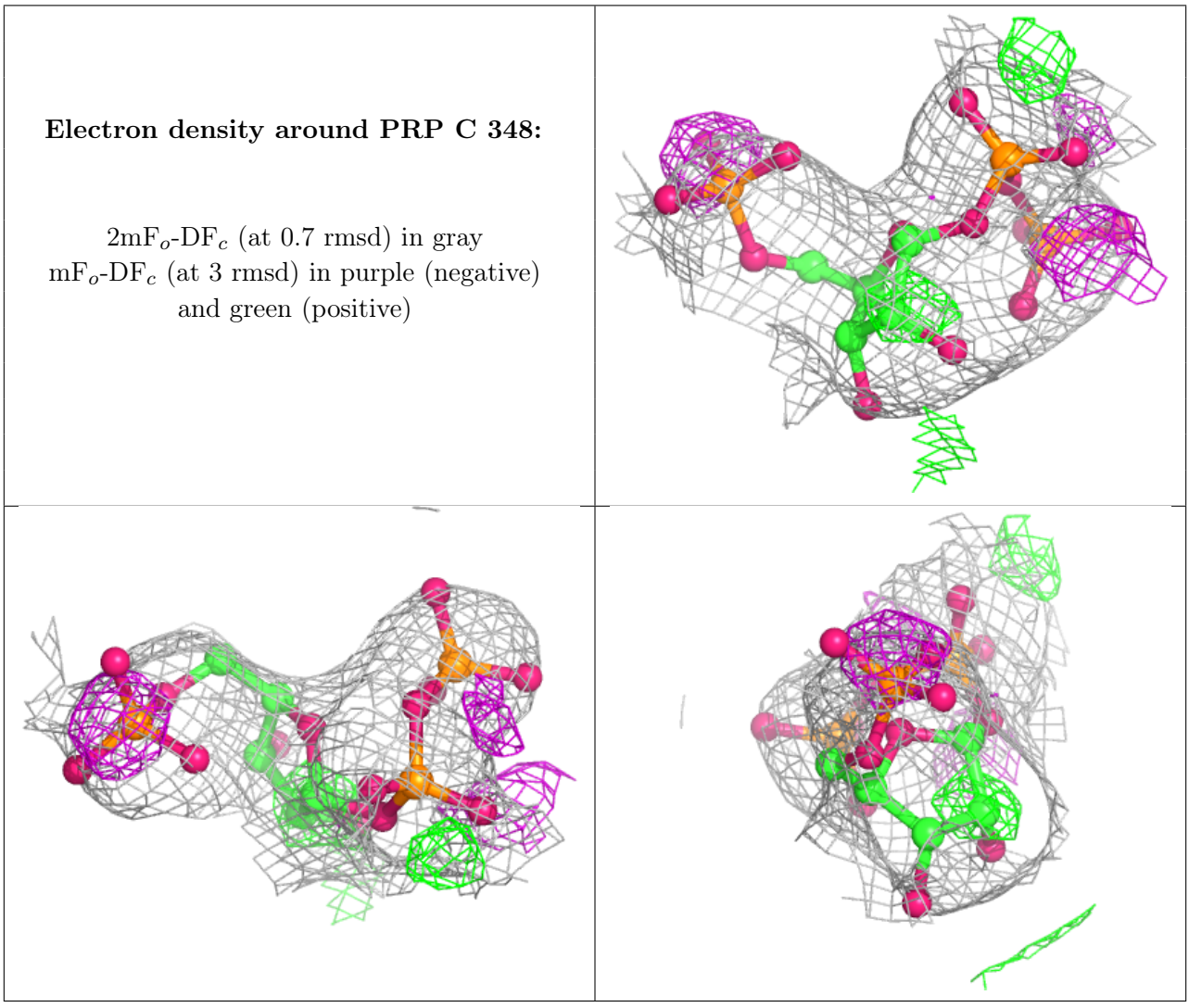
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	D	347	1/1	0.97	0.06	96,96,96,96	0
2	MG	B	347	1/1	0.98	0.09	52,52,52,52	0
2	MG	C	347	1/1	0.99	0.08	78,78,78,78	0

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.

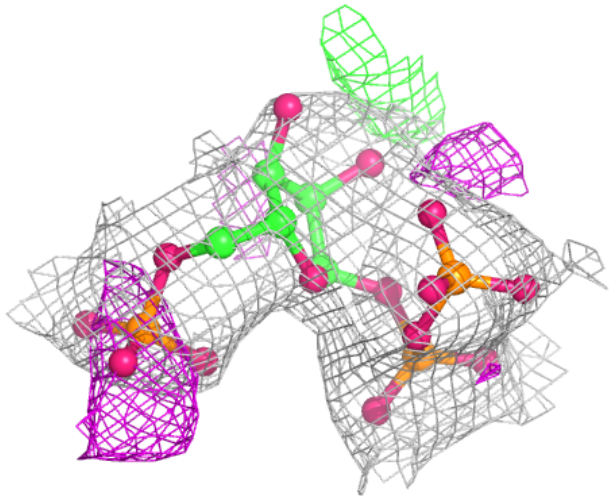
Electron density around PRP C 348:

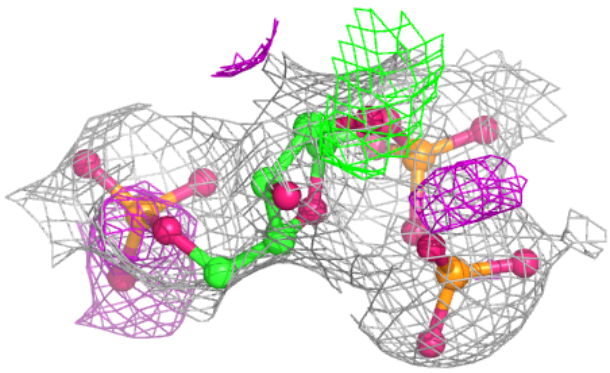
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

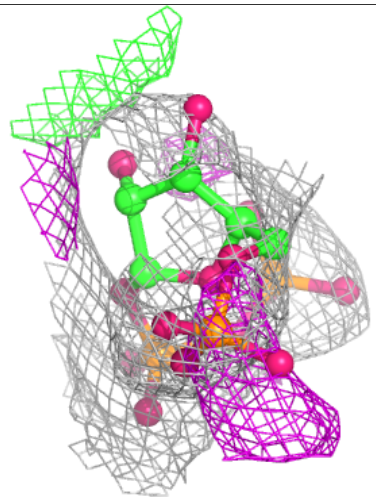


Electron density around PRP D 348:

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

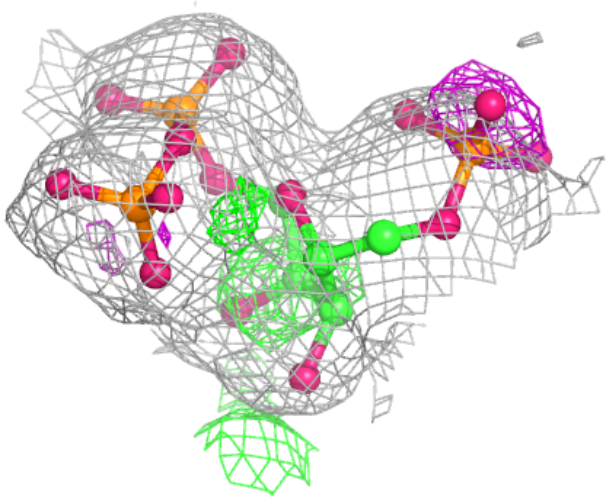


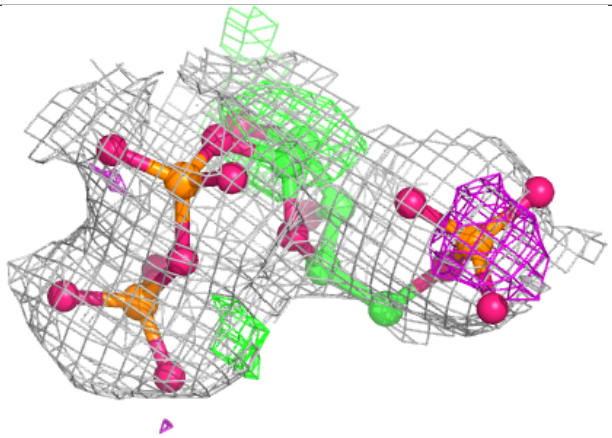


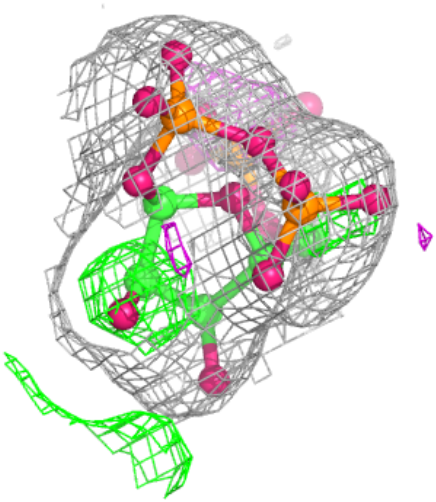


Electron density around PRP B 348:

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

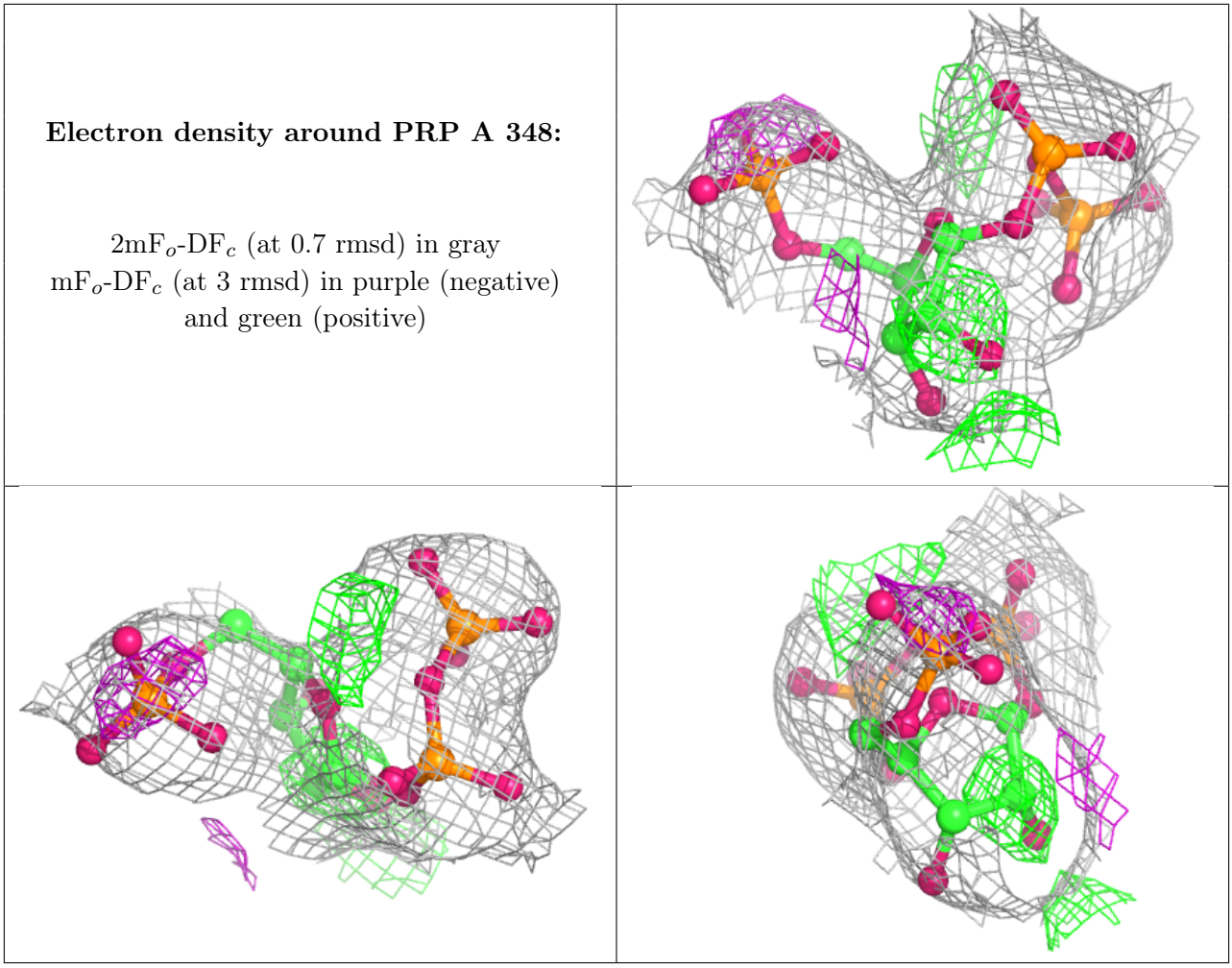






Electron density around PRP A 348:

$2mF_o$-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.