



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 11:21 AM BST

PDB ID : 1ZYK
Title : Anthranilate Phosphoribosyltransferase in complex with PRPP, anthranilate and magnesium
Authors : Marino, M.; Deuss, M.; Sterner, R.; Mayans, O.
Deposited on : 2005-06-10
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

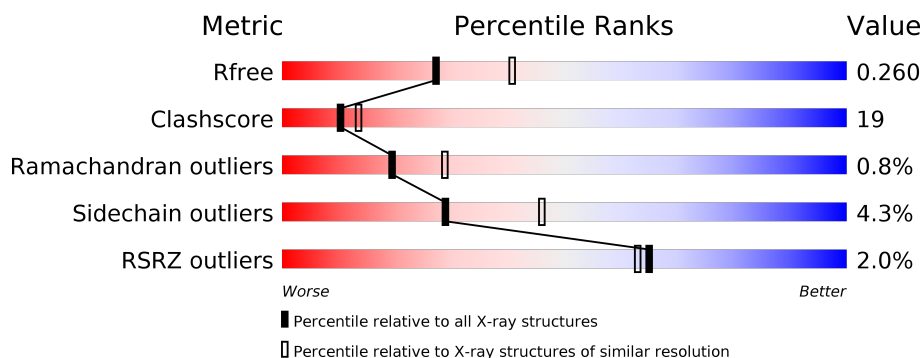
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	345	<div> <div>2%</div> <div>65% 32%</div> <div>.</div> </div>
1	B	345	<div> <div>2%</div> <div>67% 30%</div> <div>.</div> </div>
1	C	345	<div> <div>2%</div> <div>68% 31%</div> <div>..</div> </div>
1	D	345	<div> <div>2%</div> <div>66% 31%</div> <div>.</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PRP	A	601	-	-	X	-
3	PRP	B	602	-	-	X	-
3	PRP	C	603	-	-	X	-
3	PRP	D	604	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11235 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.

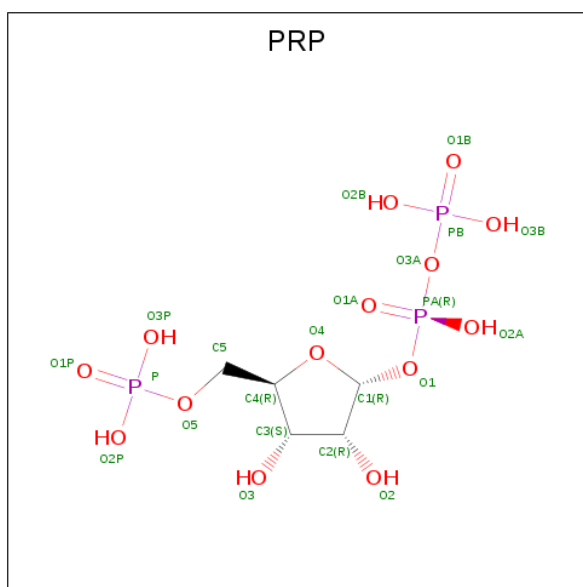
- Molecule 1 is a protein called Anthranilate phosphoribosyltransferase.

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	343	Total	C	N	O	S	0	0	0
			2634	1687	444	496	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).

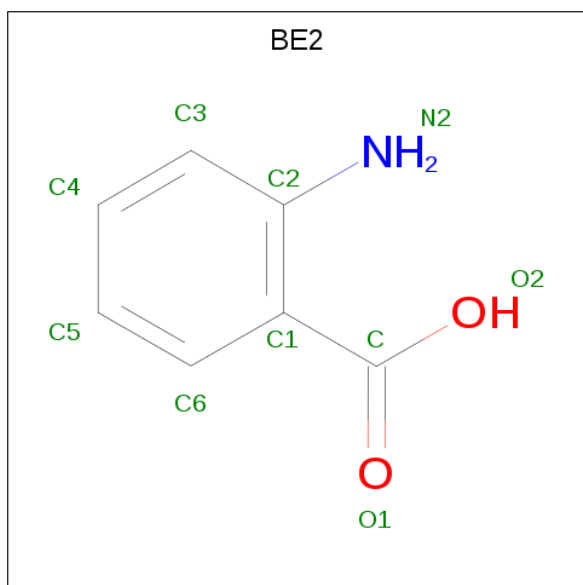
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 1-O-pyrophosphono-5-O-phosphono-alpha-D-ribofuranose (three-letter code: PRP) (formula: C₅H₁₃O₁₄P₃).



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

- Molecule 4 is 2-AMINO BENZOIC ACID (three-letter code: BE2) (formula: $C_7H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	7	1	2		
4	A	1	Total	C	N	O	0	0
			10	7	1	2		
4	B	1	Total	C	N	O	0	0
			10	7	1	2		
4	B	1	Total	C	N	O	0	0
			10	7	1	2		
4	C	1	Total	C	N	O	0	0
			10	7	1	2		
4	C	1	Total	C	N	O	0	0
			10	7	1	2		
4	D	1	Total	C	N	O	0	0
			10	7	1	2		
4	D	1	Total	C	N	O	0	0
			10	7	1	2		

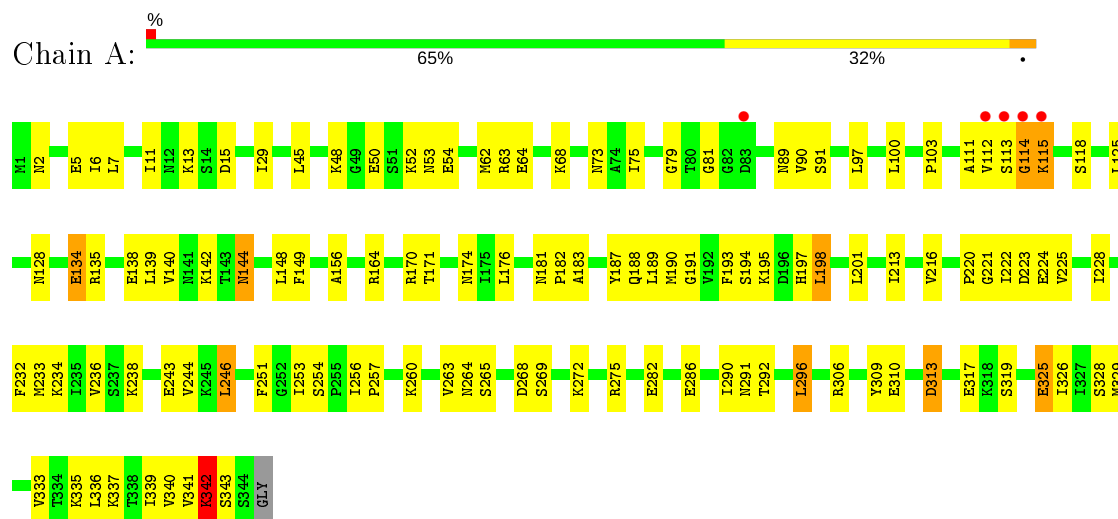
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	160	Total	O	0	0
			160	160		
5	B	105	Total	O	0	0
			105	105		
5	C	111	Total	O	0	0
			111	111		
5	D	129	Total	O	0	0
			129	129		

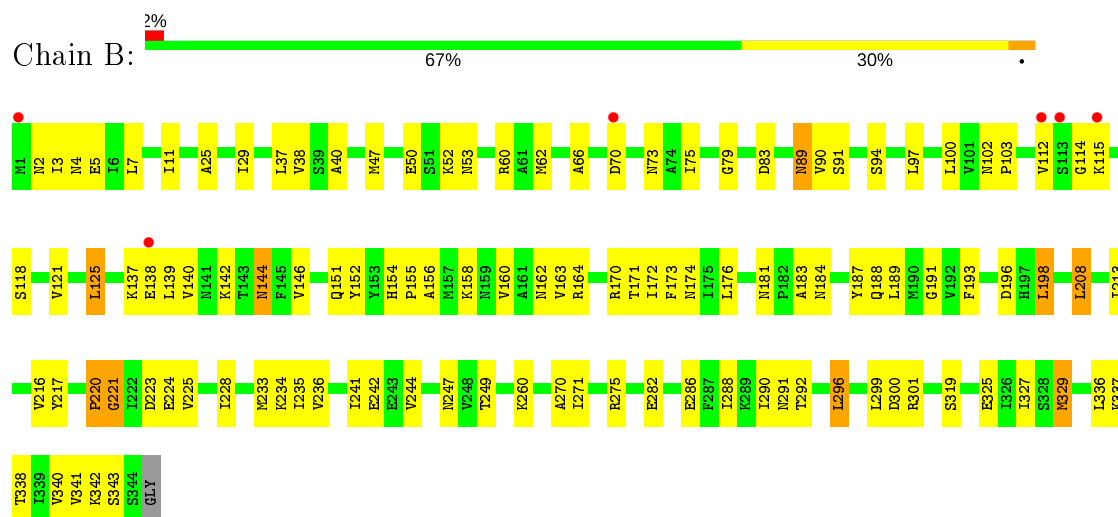
3 Residue-property plots

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

• Molecule 1: Anthranilate phosphoribosyltransferase

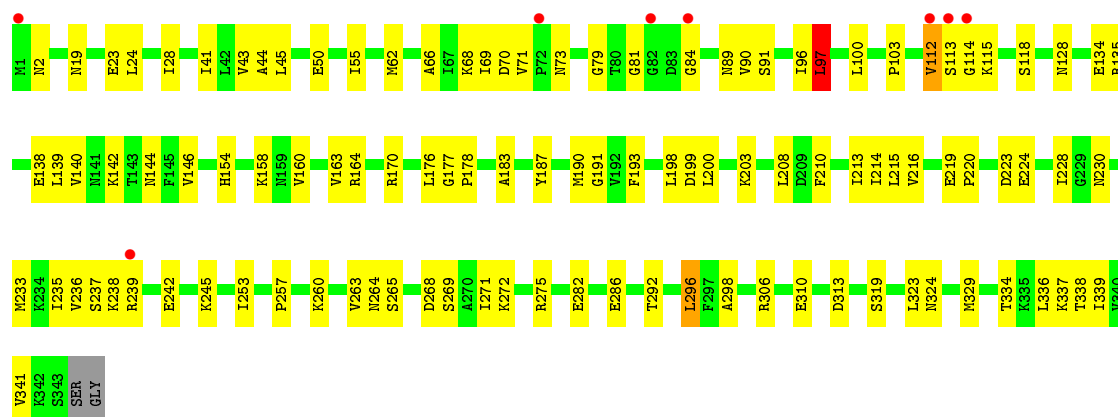


• Molecule 1: Anthranilate phosphoribosyltransferase

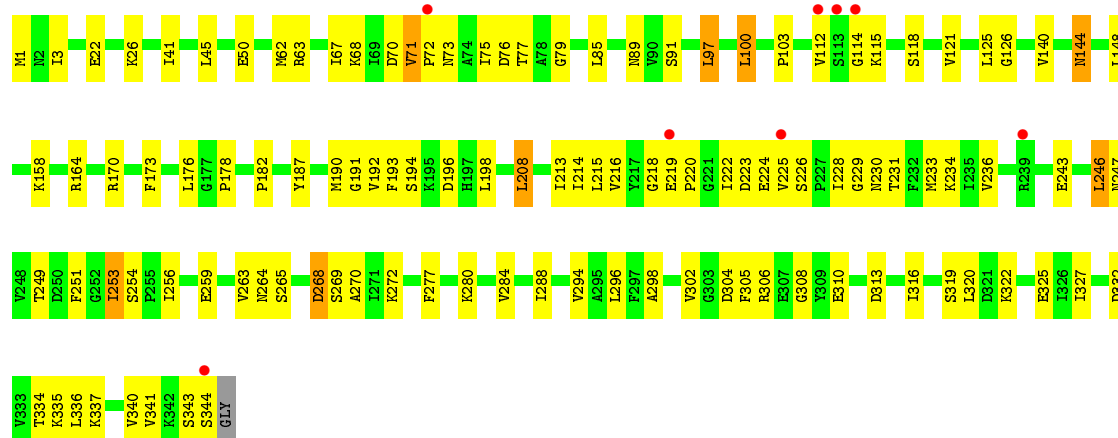


• Molecule 1: Anthranilate phosphoribosyltransferase





• Molecule 1: Anthranilate phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.56 Å 66.10 Å 117.07 Å 90.00° 107.76° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.71 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.40) 98.8 (19.71-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 2.41 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.269 0.200 , 0.260	Depositor DCC
R_{free} test set	624 reflections (1.19%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11235	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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 21.17 % 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 7.4305e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: BE2, MG, PRP

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	0.38	0/2677	0.65	1/3617 (0.0%)
1	B	0.36	0/2677	0.63	0/3617
1	C	0.37	0/2671	0.64	1/3609 (0.0%)
1	D	0.36	0/2677	0.62	0/3617
All	All	0.37	0/10702	0.63	2/14460 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	LYS	CD-CE-NZ	5.24	123.76	111.70
1	C	97	LEU	CA-CB-CG	5.20	127.26	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	104	0
1	B	2640	0	2753	107	0
1	C	2634	0	2748	100	0
1	D	2640	0	2753	98	1
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	7	10	0
3	B	22	0	7	11	0
3	C	22	0	7	10	0
3	D	22	0	7	11	0
4	A	20	0	12	0	0
4	B	20	0	12	0	0
4	C	20	0	12	2	0
4	D	20	0	12	1	0
5	A	160	0	0	15	0
5	B	105	0	0	17	0
5	C	111	0	0	19	0
5	D	129	0	0	6	0
All	All	11235	0	11083	407	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 19.

All (407) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:MET:HE1	1:D:176:LEU:HD13	1.38	1.05
1:A:225:VAL:HB	5:A:963:HOH:O	1.60	1.02
1:A:171:THR:H	1:A:174:ASN:HD22	1.11	0.99
1:A:171:THR:H	1:A:174:ASN:ND2	1.62	0.97
1:B:171:THR:H	1:B:174:ASN:HD22	1.09	0.93
1:B:171:THR:H	1:B:174:ASN:ND2	1.67	0.93
1:B:275:ARG:HG2	1:B:343:SER:HB2	1.52	0.90
1:D:198:LEU:HD21	1:D:234:LYS:HG3	1.54	0.88
1:B:91:SER:HB2	3:B:602:PRP:O1	1.75	0.86
1:A:306:ARG:HH12	1:A:310:GLU:HG3	1.40	0.86
1:B:94:SER:HB2	5:B:909:HOH:O	1.74	0.85
1:B:62:MET:HE1	1:B:176:LEU:HD13	1.58	0.85
1:C:306:ARG:HH12	1:C:310:GLU:HG3	1.42	0.85
1:C:91:SER:HB2	3:C:603:PRP:O1	1.77	0.84
1:A:113:SER:HB2	5:A:809:HOH:O	1.77	0.83
1:B:290:ILE:HG13	5:B:903:HOH:O	1.79	0.80
1:C:97:LEU:HD22	1:C:319:SER:OG	1.81	0.80
1:C:79:GLY:HA3	3:C:603:PRP:O3	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:THR:HB	1:D:246:LEU:HD22	1.64	0.79
1:C:178:PRO:HB3	5:C:909:HOH:O	1.81	0.78
1:C:223:ASP:OD2	3:C:603:PRP:H51	1.84	0.77
1:D:223:ASP:OD2	3:D:604:PRP:H51	1.84	0.77
1:D:280:LYS:NZ	1:D:344:SER:HB3	1.99	0.77
1:B:2:ASN:HB3	1:B:5:GLU:OE2	1.85	0.77
1:D:79:GLY:HA3	3:D:604:PRP:O3	1.86	0.76
1:D:219:GLU:H	1:D:226:SER:HB2	1.49	0.76
1:C:62:MET:HE1	1:C:176:LEU:HD13	1.66	0.76
1:D:332:ASP:OD2	1:D:334:THR:HB	1.85	0.76
1:B:247:ASN:HD22	1:B:249:THR:H	1.32	0.75
1:C:245:LYS:HE2	5:C:907:HOH:O	1.86	0.75
1:C:164:ARG:HD2	5:C:819:HOH:O	1.86	0.75
1:C:118:SER:HB2	3:C:603:PRP:O3B	1.86	0.75
1:D:71:VAL:HA	5:D:911:HOH:O	1.86	0.74
1:D:253:ILE:HG12	1:D:254:SER:N	2.00	0.74
1:A:171:THR:N	1:A:174:ASN:HD22	1.86	0.74
1:D:91:SER:HB2	3:D:604:PRP:O1	1.88	0.74
1:A:253:ILE:HD11	1:A:286:GLU:OE1	1.87	0.73
1:A:164:ARG:HD2	5:A:847:HOH:O	1.88	0.72
1:A:306:ARG:NH1	1:A:310:GLU:HG3	2.04	0.72
1:B:282:GLU:HB2	5:B:908:HOH:O	1.90	0.71
1:B:79:GLY:HA3	3:B:602:PRP:O3	1.91	0.71
1:C:62:MET:CE	1:C:176:LEU:HD13	2.20	0.71
1:D:112:VAL:HA	5:D:931:HOH:O	1.90	0.71
1:B:29:ILE:HG22	1:B:156:ALA:HB1	1.72	0.70
1:B:271:ILE:O	1:B:275:ARG:HG3	1.91	0.70
1:D:97:LEU:HD22	1:D:319:SER:OG	1.91	0.70
1:A:91:SER:HB2	3:A:601:PRP:O1	1.91	0.70
1:B:171:THR:N	1:B:174:ASN:HD22	1.89	0.70
1:C:113:SER:HB2	5:C:913:HOH:O	1.90	0.70
1:B:139:LEU:HA	5:B:904:HOH:O	1.91	0.69
1:C:238:LYS:HG2	5:C:910:HOH:O	1.92	0.69
1:B:118:SER:HB2	3:B:602:PRP:O3B	1.93	0.68
1:A:257:PRO:HG2	5:A:960:HOH:O	1.94	0.68
1:A:13:LYS:HA	1:A:48:LYS:HG3	1.75	0.68
1:A:336:LEU:O	1:A:340:VAL:HG23	1.94	0.68
1:B:191:GLY:C	1:B:223:ASP:HB2	2.14	0.67
1:A:224:GLU:OE2	3:A:601:PRP:H2	1.94	0.67
1:B:225:VAL:HB	5:B:903:HOH:O	1.95	0.67
1:D:198:LEU:CD2	1:D:234:LYS:HG3	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LYS:HB2	5:A:960:HOH:O	1.96	0.66
1:D:336:LEU:O	1:D:340:VAL:HG23	1.96	0.66
1:D:62:MET:HE3	1:D:176:LEU:HB3	1.76	0.66
1:B:62:MET:CE	1:B:176:LEU:HD13	2.26	0.66
1:D:192:VAL:N	1:D:223:ASP:HB2	2.12	0.65
1:D:114:GLY:O	1:D:115:LYS:HB2	1.93	0.65
1:C:191:GLY:C	1:C:223:ASP:HB2	2.16	0.65
1:C:68:LYS:HE3	5:C:914:HOH:O	1.95	0.65
1:A:2:ASN:HB3	1:A:5:GLU:OE1	1.97	0.65
1:C:164:ARG:HH22	4:C:801:BE2:HN21	1.41	0.65
1:B:291:ASN:ND2	5:B:903:HOH:O	2.29	0.65
1:A:238:LYS:HG2	5:A:824:HOH:O	1.96	0.65
1:C:292:THR:HG22	1:C:296:LEU:HD22	1.80	0.64
1:D:268:ASP:O	1:D:272:LYS:HG2	1.98	0.63
1:D:192:VAL:C	1:D:223:ASP:HB3	2.19	0.63
1:B:139:LEU:HD23	5:B:904:HOH:O	1.97	0.63
1:D:97:LEU:O	1:D:100:LEU:HB2	1.98	0.63
1:B:260:LYS:HE2	5:B:882:HOH:O	1.98	0.63
1:C:263:VAL:HG12	1:C:265:SER:H	1.63	0.62
1:C:84:GLY:HA2	5:C:868:HOH:O	1.99	0.62
1:B:162:ASN:HB3	5:B:870:HOH:O	1.99	0.62
1:D:219:GLU:HB2	1:D:230:ASN:O	2.00	0.62
1:B:90:VAL:HG12	1:B:224:GLU:OE2	1.98	0.62
1:C:224:GLU:OE1	3:C:603:PRP:H1	2.00	0.61
1:B:223:ASP:OD2	3:B:602:PRP:H51	2.01	0.61
1:C:62:MET:HE1	1:C:176:LEU:CD1	2.30	0.61
1:C:263:VAL:HG11	1:C:269:SER:HB2	1.82	0.60
1:A:62:MET:HE1	1:A:176:LEU:HD13	1.83	0.60
1:B:90:VAL:CG1	1:B:224:GLU:OE2	2.49	0.60
1:B:247:ASN:ND2	1:B:249:THR:H	1.98	0.60
1:B:62:MET:HE1	1:B:176:LEU:CD1	2.30	0.60
1:B:73:ASN:HD22	1:B:103:PRO:HG3	1.66	0.60
1:C:138:GLU:O	1:C:142:LYS:HG2	2.01	0.60
1:A:216:VAL:HG12	1:A:233:MET:HB3	1.84	0.60
1:A:253:ILE:HG12	1:A:254:SER:N	2.16	0.60
1:A:263:VAL:HG11	1:A:269:SER:HB2	1.83	0.60
1:B:181:ASN:HD21	1:B:183:ALA:HB3	1.65	0.60
1:D:192:VAL:HG12	1:D:194:SER:H	1.67	0.60
1:A:113:SER:HB2	5:A:964:HOH:O	2.01	0.59
1:A:223:ASP:OD2	3:A:601:PRP:H51	2.01	0.59
1:A:191:GLY:C	1:A:223:ASP:HB2	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:MET:CE	1:D:176:LEU:HB3	2.33	0.59
1:A:292:THR:HG22	1:A:296:LEU:HD22	1.85	0.59
1:B:38:VAL:HG12	1:B:163:VAL:HG11	1.85	0.59
1:D:62:MET:HE1	1:D:176:LEU:CD1	2.21	0.59
1:B:154:HIS:N	5:B:905:HOH:O	2.28	0.59
1:B:188:GLN:HG3	1:B:189:LEU:N	2.17	0.59
1:B:338:THR:HG22	1:B:342:LYS:HE3	1.85	0.59
1:C:237:SER:OG	1:C:239:ARG:HG3	2.02	0.59
1:A:118:SER:HB2	3:A:601:PRP:O3B	2.03	0.59
1:A:128:ASN:HB2	5:A:955:HOH:O	2.03	0.58
1:A:97:LEU:HD22	1:A:319:SER:OG	2.02	0.58
1:B:336:LEU:O	1:B:340:VAL:HG23	2.02	0.58
1:D:280:LYS:HZ3	1:D:344:SER:HB3	1.67	0.58
1:A:291:ASN:ND2	5:A:963:HOH:O	2.36	0.58
1:D:115:LYS:HE3	5:D:870:HOH:O	2.03	0.58
1:D:118:SER:HB2	3:D:604:PRP:O3B	2.04	0.58
1:C:245:LYS:HG2	5:C:907:HOH:O	2.03	0.57
1:C:90:VAL:HG12	1:C:224:GLU:OE1	2.04	0.57
1:C:24:LEU:HD11	1:C:41:ILE:HD13	1.86	0.57
1:A:138:GLU:O	1:A:142:LYS:HG2	2.04	0.57
1:A:290:ILE:HG13	5:A:963:HOH:O	2.03	0.57
1:A:282:GLU:HG3	1:A:286:GLU:OE2	2.05	0.57
1:C:73:ASN:HB3	5:C:856:HOH:O	2.05	0.57
1:A:275:ARG:HG3	1:A:343:SER:HB3	1.85	0.57
1:C:89:ASN:HA	3:C:603:PRP:O1A	2.05	0.57
1:A:341:VAL:C	1:A:343:SER:H	2.08	0.56
1:B:138:GLU:O	1:B:142:LYS:HG2	2.05	0.56
1:C:306:ARG:HH12	1:C:310:GLU:CG	2.15	0.56
1:B:70:ASP:H	1:B:137:LYS:CE	2.18	0.56
1:D:263:VAL:HG13	1:D:268:ASP:HB3	1.88	0.56
1:A:341:VAL:O	1:A:343:SER:N	2.38	0.56
1:A:62:MET:CE	1:A:176:LEU:HD13	2.36	0.56
1:D:125:LEU:HD13	1:D:270:ALA:HB1	1.88	0.56
1:A:50:GLU:CD	1:A:50:GLU:H	2.08	0.56
1:D:170:ARG:NH2	1:D:193:PHE:CE2	2.74	0.56
1:A:246:LEU:HD21	1:A:251:PHE:CE2	2.40	0.55
1:B:89:ASN:HA	3:B:602:PRP:O1A	2.06	0.55
1:A:181:ASN:HD21	1:A:183:ALA:HB3	1.72	0.55
1:D:343:SER:O	1:D:344:SER:CB	2.54	0.55
1:B:160:VAL:HG12	1:B:160:VAL:O	2.07	0.55
1:B:213:ILE:HG23	1:B:236:VAL:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:VAL:HA	5:C:854:HOH:O	2.07	0.55
1:D:198:LEU:O	1:D:198:LEU:HD23	2.06	0.55
1:C:19:ASN:O	1:C:23:GLU:HG2	2.07	0.55
1:C:216:VAL:HG12	1:C:233:MET:HB3	1.88	0.55
1:A:90:VAL:HG12	1:A:224:GLU:OE1	2.06	0.54
1:B:224:GLU:OE2	3:B:602:PRP:H1	2.07	0.54
1:C:271:ILE:O	1:C:275:ARG:HG3	2.06	0.54
1:A:148:LEU:HD13	1:A:182:PRO:HB2	1.89	0.54
1:D:228:ILE:HG22	1:D:256:ILE:O	2.08	0.54
1:C:139:LEU:HD23	1:C:329:MET:CE	2.37	0.54
1:D:178:PRO:HA	5:D:820:HOH:O	2.07	0.54
1:A:171:THR:N	1:A:174:ASN:ND2	2.44	0.54
1:A:62:MET:HE1	1:A:176:LEU:CD1	2.38	0.54
1:C:69:ILE:HD11	1:C:183:ALA:HB2	1.89	0.54
1:D:89:ASN:HA	3:D:604:PRP:O1A	2.08	0.54
1:A:181:ASN:ND2	1:A:183:ALA:H	2.05	0.53
1:A:73:ASN:ND2	1:A:103:PRO:HG3	2.23	0.53
1:C:70:ASP:O	1:C:71:VAL:HG22	2.08	0.53
1:D:190:MET:O	1:D:215:LEU:HA	2.09	0.53
1:A:170:ARG:HA	1:A:174:ASN:ND2	2.24	0.53
1:A:335:LYS:O	1:A:339:ILE:HG12	2.08	0.53
1:B:25:ALA:O	1:B:29:ILE:HG13	2.08	0.53
1:D:164:ARG:HD2	5:D:932:HOH:O	2.09	0.53
1:D:302:VAL:HG11	1:D:308:GLY:HA2	1.90	0.53
1:B:70:ASP:H	1:B:137:LYS:HE2	1.74	0.53
1:B:338:THR:O	1:B:342:LYS:HG3	2.09	0.53
1:A:213:ILE:HG23	1:A:236:VAL:HB	1.91	0.52
1:B:125:LEU:HD13	1:B:270:ALA:HB1	1.90	0.52
1:A:256:ILE:HD11	1:A:286:GLU:HB3	1.91	0.52
1:C:164:ARG:NH2	4:C:801:BE2:N2	2.54	0.52
1:D:164:ARG:HH22	4:D:808:BE2:HN21	1.56	0.52
1:B:102:ASN:HD22	1:B:301:ARG:NH2	2.08	0.52
1:D:126:GLY:HA2	1:D:335:LYS:HD2	1.90	0.52
1:B:155:PRO:O	1:B:158:LYS:HG2	2.09	0.52
1:C:263:VAL:HG12	1:C:264:ASN:N	2.25	0.52
1:A:263:VAL:HB	5:A:958:HOH:O	2.09	0.52
1:A:63:ARG:O	1:A:68:LYS:HE3	2.10	0.52
1:B:52:LYS:HE3	1:B:53:ASN:OD1	2.09	0.52
1:C:96:ILE:HD13	1:C:323:LEU:HD13	1.92	0.52
1:D:251:PHE:CE1	1:D:305:PHE:HB3	2.44	0.52
1:A:233:MET:HG3	1:A:244:VAL:HB	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:GLU:OE2	3:D:604:PRP:H2	2.10	0.51
1:B:329:MET:O	1:B:329:MET:HG3	2.11	0.51
1:D:216:VAL:HG12	1:D:233:MET:HB3	1.92	0.51
1:B:170:ARG:NH2	1:B:193:PHE:CE2	2.79	0.51
1:A:2:ASN:CG	1:A:5:GLU:OE1	2.50	0.51
1:D:306:ARG:NH1	1:D:310:GLU:HG3	2.26	0.51
1:D:224:GLU:OE1	3:D:604:PRP:H1	2.11	0.51
1:B:216:VAL:HG12	1:B:233:MET:HB3	1.92	0.51
1:C:199:ASP:OD2	1:C:203:LYS:HE3	2.10	0.51
1:D:219:GLU:N	1:D:220:PRO:HD2	2.26	0.51
1:D:247:ASN:ND2	1:D:249:THR:HG23	2.26	0.51
1:A:263:VAL:HG21	1:A:269:SER:HA	1.92	0.51
1:C:140:VAL:HG23	1:C:146:VAL:HB	1.91	0.51
1:D:263:VAL:HG11	1:D:269:SER:HB2	1.93	0.51
1:C:112:VAL:HA	5:C:904:HOH:O	2.10	0.50
1:C:253:ILE:HD11	1:C:286:GLU:OE1	2.10	0.50
1:A:79:GLY:HA3	3:A:601:PRP:O3	2.11	0.50
1:B:151:GLN:C	5:B:905:HOH:O	2.48	0.50
1:C:213:ILE:HG23	1:C:236:VAL:HB	1.92	0.50
1:C:50:GLU:H	1:C:50:GLU:CD	2.14	0.50
1:C:268:ASP:O	1:C:272:LYS:HG2	2.12	0.50
1:A:198:LEU:HD11	1:A:232:PHE:O	2.12	0.50
1:C:306:ARG:HH11	1:C:306:ARG:HG3	1.76	0.50
1:D:63:ARG:HH22	1:D:208:LEU:HB3	1.75	0.50
1:B:66:ALA:HB2	1:B:154:HIS:CE1	2.46	0.50
1:B:247:ASN:ND2	1:B:249:THR:HG23	2.27	0.50
1:B:7:LEU:O	1:B:11:ILE:HG12	2.11	0.50
1:C:178:PRO:HD3	5:C:909:HOH:O	2.12	0.50
1:B:140:VAL:O	1:B:144:ASN:HA	2.11	0.50
1:C:208:LEU:HB2	1:C:210:PHE:HE1	1.77	0.50
1:C:228:ILE:HB	5:C:832:HOH:O	2.10	0.50
1:A:81:GLY:HA2	3:A:601:PRP:H51	1.94	0.50
1:B:337:LYS:O	1:B:341:VAL:HG23	2.11	0.50
1:D:225:VAL:HG21	1:D:294:VAL:HG21	1.94	0.50
1:C:55:ILE:HD11	1:C:200:LEU:HD21	1.94	0.49
1:C:214:ILE:HD12	1:C:298:ALA:HB2	1.94	0.49
1:C:223:ASP:OD1	3:C:603:PRP:O5	2.30	0.49
1:D:215:LEU:N	1:D:215:LEU:HD12	2.27	0.49
1:C:306:ARG:HG3	1:C:306:ARG:NH1	2.27	0.49
1:B:171:THR:N	1:B:174:ASN:ND2	2.50	0.49
1:B:60:ARG:NH2	5:B:851:HOH:O	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:PRO:HG2	1:C:260:LYS:HG2	1.93	0.49
1:D:70:ASP:O	1:D:71:VAL:HG22	2.12	0.49
1:A:268:ASP:O	1:A:272:LYS:HG2	2.12	0.49
1:A:89:ASN:HA	3:A:601:PRP:O1A	2.12	0.49
1:C:41:ILE:O	1:C:45:LEU:HB2	2.13	0.49
1:D:284:VAL:O	1:D:288:ILE:HG13	2.12	0.49
1:A:190:MET:HE1	1:A:201:LEU:HD13	1.95	0.49
1:B:235:ILE:HB	1:B:242:GLU:HB3	1.95	0.49
1:D:304:ASP:OD2	1:D:306:ARG:HB3	2.13	0.49
1:A:52:LYS:HE3	1:A:53:ASN:OD1	2.12	0.49
1:B:291:ASN:CG	5:B:903:HOH:O	2.50	0.49
1:D:265:SER:OG	1:D:268:ASP:HB2	2.13	0.49
1:A:134:GLU:H	1:A:134:GLU:CD	2.16	0.48
1:D:41:ILE:O	1:D:45:LEU:HB2	2.13	0.48
1:A:170:ARG:NH2	1:A:193:PHE:CE2	2.81	0.48
1:B:236:VAL:HG22	1:B:241:ILE:HG12	1.95	0.48
1:D:191:GLY:C	1:D:223:ASP:HB2	2.34	0.48
1:B:160:VAL:HG12	1:B:164:ARG:HG3	1.94	0.48
1:C:158:LYS:HE2	5:C:899:HOH:O	2.13	0.48
1:D:63:ARG:NH2	1:D:208:LEU:HB3	2.29	0.48
1:D:214:ILE:HD12	1:D:298:ALA:HB2	1.95	0.48
1:A:48:LYS:NZ	1:A:54:GLU:OE2	2.46	0.48
1:C:140:VAL:O	1:C:144:ASN:HA	2.13	0.48
1:C:139:LEU:HD23	1:C:329:MET:HE2	1.96	0.48
1:A:2:ASN:CB	1:A:5:GLU:OE1	2.60	0.48
1:D:247:ASN:HD22	1:D:249:THR:HG23	1.79	0.48
1:B:220:PRO:HD3	1:B:228:ILE:CD1	2.43	0.48
1:D:213:ILE:HG23	1:D:236:VAL:HB	1.96	0.48
1:D:50:GLU:H	1:D:50:GLU:CD	2.13	0.48
1:B:181:ASN:ND2	1:B:183:ALA:H	2.12	0.47
1:C:257:PRO:HG2	1:C:260:LYS:CG	2.44	0.47
1:D:246:LEU:C	1:D:246:LEU:HD23	2.35	0.47
1:A:140:VAL:O	1:A:144:ASN:HA	2.15	0.47
1:A:220:PRO:HD3	1:A:228:ILE:CD1	2.44	0.47
1:A:263:VAL:CG1	1:A:264:ASN:N	2.78	0.47
1:C:213:ILE:CG2	1:C:236:VAL:HB	2.44	0.47
1:C:219:GLU:HG3	1:C:230:ASN:O	2.14	0.47
1:C:142:LYS:HG3	1:C:329:MET:HE3	1.96	0.47
1:A:193:PHE:CE2	1:A:197:HIS:CD2	3.03	0.47
1:D:140:VAL:O	1:D:144:ASN:HA	2.15	0.47
1:D:85:LEU:HD12	1:D:222:ILE:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLU:OE1	3:A:601:PRP:H1	2.14	0.47
1:B:144:ASN:HD22	1:B:144:ASN:HA	1.53	0.47
1:C:160:VAL:HG12	1:C:164:ARG:HG3	1.96	0.47
1:A:75:ILE:HA	1:A:187:TYR:O	2.14	0.47
1:B:213:ILE:CG2	1:B:236:VAL:HB	2.44	0.47
1:B:224:GLU:OE1	3:B:602:PRP:H2	2.15	0.47
1:B:97:LEU:HD22	1:B:319:SER:OG	2.15	0.47
1:B:170:ARG:NH2	1:B:193:PHE:CZ	2.83	0.47
1:B:338:THR:CG2	1:B:342:LYS:HE3	2.45	0.47
1:D:253:ILE:CG1	1:D:254:SER:N	2.74	0.47
1:D:263:VAL:CG1	1:D:264:ASN:N	2.78	0.47
1:A:263:VAL:CG1	1:A:265:SER:H	2.28	0.46
1:B:233:MET:HG3	1:B:244:VAL:HB	1.97	0.46
1:B:75:ILE:HA	1:B:187:TYR:O	2.15	0.46
1:A:90:VAL:CG1	1:A:224:GLU:OE1	2.63	0.46
1:D:91:SER:CB	3:D:604:PRP:O2	2.63	0.46
1:B:29:ILE:HG22	1:B:156:ALA:CB	2.42	0.46
1:B:50:GLU:CD	1:B:50:GLU:H	2.16	0.46
1:C:220:PRO:HD3	1:C:228:ILE:CD1	2.46	0.46
1:D:249:THR:C	1:D:251:PHE:H	2.19	0.46
1:A:2:ASN:O	1:A:6:ILE:HG12	2.16	0.46
1:A:64:GLU:HB2	5:A:878:HOH:O	2.16	0.46
1:D:218:GLY:N	1:D:222:ILE:O	2.44	0.46
1:A:29:ILE:HG22	1:A:156:ALA:HB1	1.98	0.46
1:B:170:ARG:HA	1:B:174:ASN:ND2	2.31	0.46
1:A:251:PHE:HB2	1:A:253:ILE:HG22	1.98	0.45
1:D:216:VAL:HG12	1:D:233:MET:CB	2.46	0.45
1:A:337:LYS:O	1:A:340:VAL:HB	2.16	0.45
1:D:121:VAL:O	1:D:125:LEU:HD22	2.16	0.45
1:D:76:ASP:OD1	1:D:77:THR:N	2.49	0.45
1:A:114:GLY:O	1:A:115:LYS:HD2	2.16	0.45
1:C:177:GLY:N	1:C:178:PRO:HD2	2.32	0.45
1:D:219:GLU:OE1	1:D:229:GLY:HA3	2.16	0.45
1:A:325:GLU:HG3	1:A:326:ILE:N	2.31	0.45
1:B:220:PRO:HD3	1:B:228:ILE:HD13	1.97	0.45
1:B:47:MET:SD	1:C:44:ALA:HA	2.57	0.45
1:C:187:TYR:N	1:C:187:TYR:CD1	2.84	0.45
1:A:328:SER:HA	1:A:333:VAL:HG13	1.98	0.45
1:C:81:GLY:HA2	3:C:603:PRP:H51	1.98	0.45
1:D:173:PHE:HA	1:D:176:LEU:HD12	1.98	0.45
1:D:148:LEU:HD13	1:D:182:PRO:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:O	1:A:11:ILE:HG12	2.16	0.45
1:B:154:HIS:C	5:B:905:HOH:O	2.54	0.45
1:D:316:ILE:HA	1:D:319:SER:OG	2.17	0.45
1:A:263:VAL:HG12	1:A:265:SER:H	1.82	0.45
1:C:334:THR:O	1:C:338:THR:HG23	2.16	0.45
1:D:322:LYS:HD2	1:D:325:GLU:OE1	2.17	0.45
1:C:253:ILE:CD1	1:C:286:GLU:HG2	2.46	0.44
1:A:195:LYS:O	1:A:198:LEU:HB2	2.17	0.44
1:B:3:ILE:HG12	1:B:37:LEU:HD13	2.00	0.44
1:B:52:LYS:HB3	1:B:52:LYS:HE2	1.83	0.44
1:C:91:SER:HG	3:C:603:PRP:C2	2.31	0.44
1:B:172:ILE:HG12	1:B:176:LEU:HD11	1.99	0.44
1:B:125:LEU:CD1	1:B:270:ALA:HB1	2.47	0.44
1:D:337:LYS:O	1:D:341:VAL:HG23	2.18	0.44
1:B:73:ASN:ND2	1:B:103:PRO:HG3	2.33	0.44
1:B:208:LEU:HA	1:B:208:LEU:HD12	1.75	0.44
1:C:115:LYS:HG3	5:C:845:HOH:O	2.17	0.44
1:C:79:GLY:C	5:C:909:HOH:O	2.55	0.44
1:D:280:LYS:HZ1	1:D:344:SER:HB3	1.77	0.44
1:B:223:ASP:CG	3:B:602:PRP:H51	2.38	0.44
1:C:66:ALA:HB2	1:C:154:HIS:CE1	2.52	0.44
1:B:181:ASN:HD22	1:B:184:ASN:N	2.16	0.43
1:C:190:MET:O	1:C:215:LEU:HA	2.18	0.43
1:C:73:ASN:HD22	1:C:103:PRO:HG3	1.82	0.43
1:D:223:ASP:OD1	3:D:604:PRP:O5	2.36	0.43
1:D:1:MET:CE	1:D:3:ILE:HD13	2.48	0.43
1:D:22:GLU:O	1:D:26:LYS:HG3	2.18	0.43
1:B:292:THR:HG22	1:B:296:LEU:HD22	1.99	0.43
1:C:282:GLU:O	1:C:286:GLU:HG3	2.17	0.43
1:A:198:LEU:HD22	1:A:234:LYS:CG	2.48	0.43
1:C:235:ILE:HB	1:C:242:GLU:HB3	2.00	0.43
1:D:72:PRO:HD2	5:D:911:HOH:O	2.18	0.43
1:C:263:VAL:HG13	1:C:268:ASP:HB3	2.01	0.43
1:D:277:PHE:HB3	1:D:320:LEU:HB2	2.00	0.43
1:C:253:ILE:HD13	1:C:286:GLU:HG2	2.01	0.43
1:A:91:SER:OG	3:A:601:PRP:O2	2.30	0.43
1:A:286:GLU:HG2	1:A:309:TYR:OH	2.18	0.43
1:C:191:GLY:HA3	1:C:223:ASP:O	2.19	0.43
1:C:90:VAL:CG1	1:C:224:GLU:OE1	2.66	0.43
1:B:173:PHE:HA	1:B:176:LEU:HD12	1.99	0.42
1:C:142:LYS:HG3	1:C:329:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:LEU:O	1:C:28:ILE:HG13	2.18	0.42
1:D:327:ILE:HD12	1:D:336:LEU:HD22	2.00	0.42
1:B:282:GLU:O	1:B:286:GLU:HG3	2.19	0.42
1:C:170:ARG:NH2	1:C:170:ARG:HB3	2.34	0.42
1:D:73:ASN:ND2	1:D:103:PRO:HG3	2.33	0.42
1:B:73:ASN:HA	5:B:869:HOH:O	2.19	0.42
1:C:62:MET:HE1	1:C:176:LEU:CB	2.50	0.42
1:D:75:ILE:HA	1:D:187:TYR:O	2.18	0.42
1:A:313:ASP:O	1:A:317:GLU:HG3	2.19	0.42
1:C:45:LEU:HA	1:C:45:LEU:HD12	1.90	0.42
1:A:73:ASN:HD22	1:A:103:PRO:HG3	1.83	0.42
1:C:263:VAL:CG1	1:C:264:ASN:N	2.83	0.42
1:A:198:LEU:HD22	1:A:234:LYS:HG3	2.02	0.42
1:D:170:ARG:NH2	1:D:193:PHE:CZ	2.88	0.42
1:A:134:GLU:O	1:A:138:GLU:HG3	2.20	0.42
1:C:208:LEU:HB2	1:C:210:PHE:CE1	2.55	0.42
1:C:223:ASP:CG	3:C:603:PRP:H51	2.39	0.42
1:D:63:ARG:O	1:D:68:LYS:HE3	2.19	0.42
1:B:223:ASP:OD1	3:B:602:PRP:H51	2.19	0.42
1:D:198:LEU:C	1:D:198:LEU:HD23	2.41	0.41
1:D:219:GLU:H	1:D:226:SER:CB	2.24	0.41
1:D:91:SER:OG	3:D:604:PRP:O2	2.35	0.41
1:A:111:ALA:HA	5:A:961:HOH:O	2.19	0.41
1:B:40:ALA:HB1	1:C:43:VAL:HG21	2.02	0.41
1:D:343:SER:O	1:D:344:SER:HB2	2.20	0.41
1:D:223:ASP:CG	3:D:604:PRP:H51	2.40	0.41
1:A:188:GLN:HG3	1:A:189:LEU:N	2.36	0.41
1:B:146:VAL:HG13	1:B:146:VAL:O	2.21	0.41
1:B:223:ASP:OD1	3:B:602:PRP:C5	2.68	0.41
1:D:222:ILE:HD12	1:D:224:GLU:HG3	2.02	0.41
1:B:288:ILE:HA	5:B:909:HOH:O	2.20	0.41
1:B:223:ASP:OD1	3:B:602:PRP:O5	2.37	0.41
1:C:178:PRO:CB	5:C:909:HOH:O	2.54	0.41
1:B:75:ILE:HD12	1:B:299:LEU:HG	2.03	0.41
1:A:264:ASN:O	1:A:265:SER:HB3	2.21	0.41
1:C:134:GLU:HG2	1:C:135:ARG:N	2.35	0.41
1:B:121:VAL:O	1:B:125:LEU:HD22	2.21	0.41
1:C:337:LYS:O	1:C:341:VAL:HG23	2.20	0.41
1:C:163:VAL:HG23	5:C:850:HOH:O	2.20	0.41
1:A:260:LYS:CB	5:A:960:HOH:O	2.61	0.41
1:C:336:LEU:O	1:C:339:ILE:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:ASN:CB	5:C:856:HOH:O	2.65	0.41
1:A:135:ARG:O	1:A:139:LEU:HG	2.21	0.41
1:A:52:LYS:HE2	1:A:52:LYS:HB3	1.90	0.41
1:A:291:ASN:CG	5:A:963:HOH:O	2.60	0.41
1:B:233:MET:CG	1:B:244:VAL:HB	2.50	0.41
1:A:306:ARG:HH12	1:A:310:GLU:CG	2.21	0.40
1:A:335:LYS:HB3	1:A:335:LYS:HE2	1.83	0.40
1:A:224:GLU:CD	3:A:601:PRP:H2	2.40	0.40
1:B:217:TYR:OH	1:B:221:GLY:HA2	2.21	0.40
1:B:198:LEU:HD22	1:B:234:LYS:HG2	2.03	0.40
1:D:192:VAL:O	1:D:223:ASP:HB3	2.21	0.40
1:B:125:LEU:HB3	1:B:327:ILE:HD11	2.02	0.40
1:B:152:TYR:N	5:B:905:HOH:O	2.54	0.40
1:A:222:ILE:HD12	1:A:224:GLU:HG3	2.03	0.40
1:B:118:SER:O	1:B:121:VAL:HG12	2.21	0.40
1:B:3:ILE:HG23	1:B:4:ASN:N	2.36	0.40
1:A:220:PRO:HD3	1:A:228:ILE:HD13	2.02	0.40
1:A:15:ASP:HA	1:A:48:LYS:HZ2	1.86	0.40
1:B:83:ASP:HB2	1:B:221:GLY:O	2.22	0.40
1:C:70:ASP:C	1:C:71:VAL:CG2	2.90	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]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	342/345 (99%)	325 (95%)	13 (4%)	4 (1%)	13 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	342/345 (99%)	327 (96%)	11 (3%)	4 (1%)	13	19
1	C	341/345 (99%)	327 (96%)	11 (3%)	3 (1%)	17	25
1	D	342/345 (99%)	322 (94%)	20 (6%)	0	100	100
All	All	1367/1380 (99%)	1301 (95%)	55 (4%)	11 (1%)	19	29

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	LYS
1	C	2	ASN
1	B	114	GLY
1	A	112	VAL
1	B	89	ASN
1	C	114	GLY
1	C	112	VAL
1	A	221	GLY
1	B	112	VAL
1	A	114	GLY
1	B	221	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/289 (100%)	273 (94%)	16 (6%)	21	35
1	B	289/289 (100%)	277 (96%)	12 (4%)	30	47
1	C	288/289 (100%)	280 (97%)	8 (3%)	43	63
1	D	289/289 (100%)	275 (95%)	14 (5%)	25	41
All	All	1155/1156 (100%)	1105 (96%)	50 (4%)	29	46

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	100	LEU
1	A	115	LYS
1	A	125	LEU
1	A	134	GLU
1	A	144	ASN
1	A	149	PHE
1	A	194	SER
1	A	198	LEU
1	A	243	GLU
1	A	246	LEU
1	A	296	LEU
1	A	313	ASP
1	A	325	GLU
1	A	329	MET
1	A	342	LYS
1	B	100	LEU
1	B	115	LYS
1	B	125	LEU
1	B	144	ASN
1	B	196	ASP
1	B	198	LEU
1	B	208	LEU
1	B	220	PRO
1	B	296	LEU
1	B	300	ASP
1	B	325	GLU
1	B	329	MET
1	C	97	LEU
1	C	100	LEU
1	C	128	ASN
1	C	193	PHE
1	C	198	LEU
1	C	296	LEU
1	C	313	ASP
1	C	324	ASN
1	D	71	VAL
1	D	97	LEU
1	D	100	LEU
1	D	144	ASN
1	D	158	LYS
1	D	196	ASP
1	D	208	LEU

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Mol	Chain	Res	Type
1	D	243	GLU
1	D	246	LEU
1	D	253	ILE
1	D	259	GLU
1	D	268	ASP
1	D	296	LEU
1	D	313	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	151	GLN
1	A	162	ASN
1	A	174	ASN
1	A	181	ASN
1	A	197	HIS
1	A	247	ASN
1	B	89	ASN
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	181	ASN
1	B	211	ASN
1	B	247	ASN
1	C	151	GLN
1	C	197	HIS
1	D	19	ASN
1	D	144	ASN
1	D	151	GLN
1	D	162	ASN
1	D	247	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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
4	BE2	D	808	-	8,10,10	2.25	2 (25%)	9,13,13	1.04	1 (11%)
3	PRP	B	602	2	19,22,22	1.05	0	33,35,35	1.02	2 (6%)
4	BE2	C	801	-	8,10,10	2.44	3 (37%)	9,13,13	1.10	1 (11%)
4	BE2	D	807	-	8,10,10	2.43	3 (37%)	9,13,13	1.01	0
4	BE2	A	806	-	8,10,10	2.55	3 (37%)	9,13,13	1.02	1 (11%)
3	PRP	C	603	2	19,22,22	1.05	0	33,35,35	0.99	2 (6%)
4	BE2	A	802	-	8,10,10	2.54	3 (37%)	9,13,13	0.98	1 (11%)
4	BE2	B	805	-	8,10,10	2.41	2 (25%)	9,13,13	0.91	0
3	PRP	D	604	2	19,22,22	1.01	0	33,35,35	0.99	2 (6%)
4	BE2	B	803	-	8,10,10	2.59	4 (50%)	9,13,13	1.05	1 (11%)
4	BE2	C	804	-	8,10,10	2.36	2 (25%)	9,13,13	0.95	1 (11%)
3	PRP	A	601	2	19,22,22	1.01	0	33,35,35	0.99	2 (6%)

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
4	BE2	D	808	-	-	0/0/4/4	0/1/1/1
3	PRP	B	602	2	-	1/16/33/33	0/1/1/1
4	BE2	C	801	-	-	0/0/4/4	0/1/1/1
4	BE2	D	807	-	-	0/0/4/4	0/1/1/1
4	BE2	A	806	-	-	0/0/4/4	0/1/1/1
3	PRP	C	603	2	-	1/16/33/33	0/1/1/1
4	BE2	A	802	-	-	0/0/4/4	0/1/1/1
4	BE2	B	805	-	-	0/0/4/4	0/1/1/1
3	PRP	D	604	2	-	1/16/33/33	0/1/1/1
4	BE2	B	803	-	-	0/0/4/4	0/1/1/1
4	BE2	C	804	-	-	0/0/4/4	0/1/1/1
3	PRP	A	601	2	-	1/16/33/33	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	802	BE2	C5-C6	5.49	1.50	1.38
4	A	806	BE2	C5-C6	5.45	1.50	1.38
4	D	807	BE2	C5-C6	5.43	1.50	1.38
4	B	803	BE2	C5-C6	5.41	1.50	1.38
4	C	804	BE2	C5-C6	5.36	1.50	1.38
4	C	801	BE2	C5-C6	5.33	1.50	1.38
4	B	805	BE2	C5-C6	5.31	1.50	1.38
4	D	808	BE2	C5-C6	5.30	1.50	1.38
4	B	803	BE2	C1-C	2.96	1.50	1.47
4	A	802	BE2	C1-C	2.79	1.50	1.47
4	A	806	BE2	C6-C1	2.61	1.44	1.40
4	B	803	BE2	C6-C1	2.53	1.43	1.40
4	A	806	BE2	C1-C	2.52	1.49	1.47
4	B	805	BE2	C6-C1	2.51	1.43	1.40
4	C	804	BE2	C6-C1	2.42	1.43	1.40
4	C	801	BE2	C6-C1	2.39	1.43	1.40
4	D	807	BE2	C1-C	2.34	1.49	1.47
4	A	802	BE2	C6-C1	2.30	1.43	1.40
4	C	801	BE2	C1-C	2.22	1.49	1.47
4	D	807	BE2	C6-C1	2.21	1.43	1.40
4	D	808	BE2	C6-C1	2.19	1.43	1.40
4	B	803	BE2	C1-C2	2.01	1.45	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	603	PRP	O1-C1-C2	2.60	111.12	106.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	PRP	O1-C1-C2	2.59	111.11	106.72
3	D	604	PRP	O1-C1-C2	2.51	110.97	106.72
3	A	601	PRP	O1-C1-C2	2.39	110.77	106.72
4	C	801	BE2	C3-C2-N2	-2.32	115.63	120.13
4	B	803	BE2	C3-C2-N2	-2.21	115.85	120.13
4	A	806	BE2	C3-C2-N2	-2.13	116.00	120.13
4	D	808	BE2	C3-C2-N2	-2.11	116.05	120.13
4	A	802	BE2	C3-C2-N2	-2.08	116.09	120.13
3	B	602	PRP	P-O5-C5	2.07	124.01	118.30
3	A	601	PRP	P-O5-C5	2.03	123.88	118.30
4	C	804	BE2	C3-C2-N2	-2.02	116.22	120.13
3	C	603	PRP	P-O5-C5	2.01	123.83	118.30
3	D	604	PRP	P-O5-C5	2.01	123.83	118.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	PRP	C4-C5-O5-P
3	D	604	PRP	C4-C5-O5-P
3	A	601	PRP	C4-C5-O5-P
3	C	603	PRP	C4-C5-O5-P

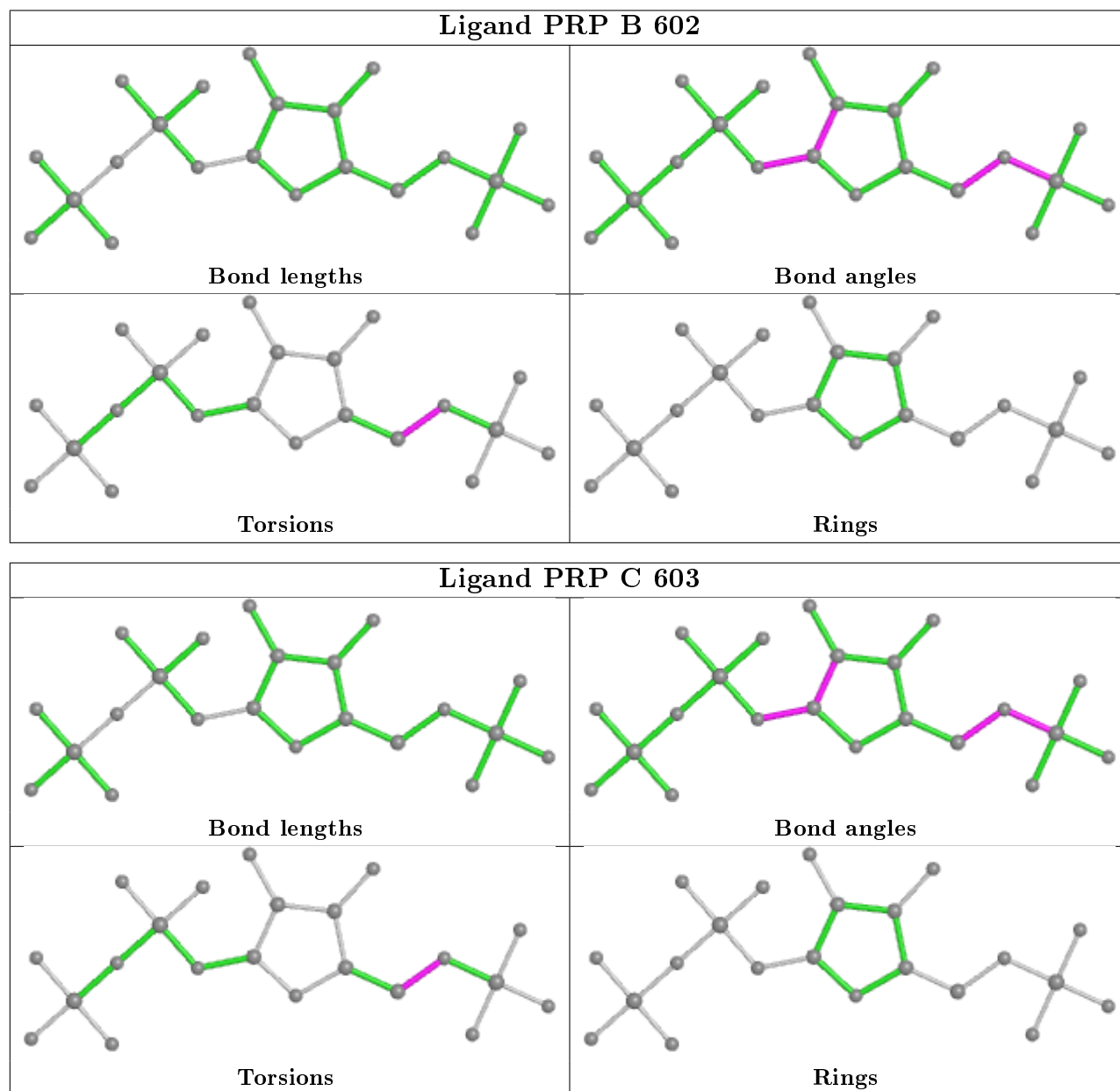
There are no ring outliers.

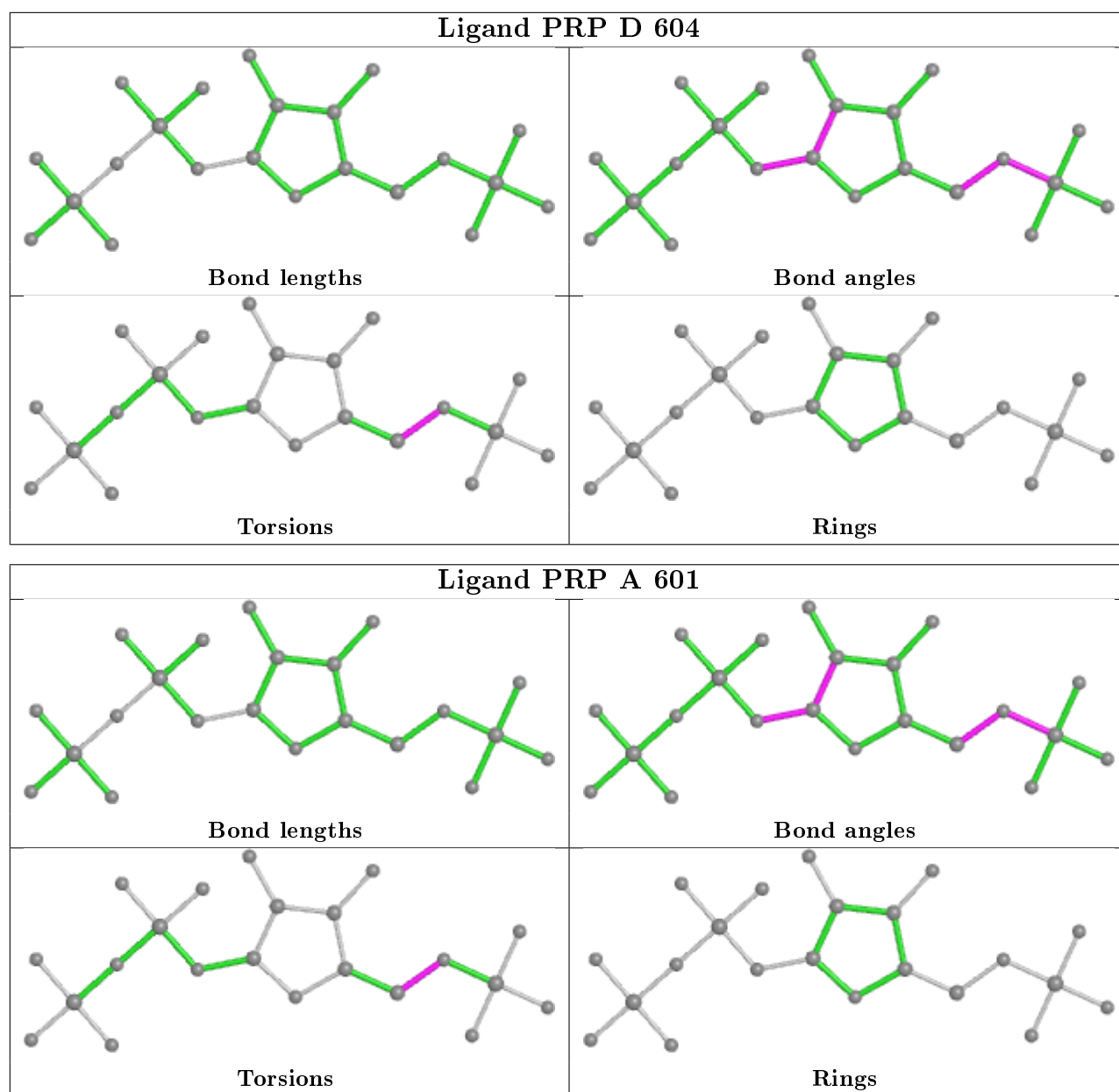
6 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	808	BE2	1	0
3	B	602	PRP	11	0
4	C	801	BE2	2	0
3	C	603	PRP	10	0
3	D	604	PRP	11	0
3	A	601	PRP	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	344/345 (99%)	-0.16	5 (1%) 73 72	19, 35, 52, 73	0
1	B	344/345 (99%)	-0.08	6 (1%) 70 68	21, 38, 63, 82	0
1	C	343/345 (99%)	-0.05	8 (2%) 60 58	21, 37, 53, 81	0
1	D	344/345 (99%)	-0.06	8 (2%) 60 58	20, 37, 59, 73	0
All	All	1375/1380 (99%)	-0.09	27 (1%) 65 63	19, 37, 58, 82	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	113	SER	8.8
1	B	113	SER	7.8
1	C	112	VAL	7.4
1	C	114	GLY	7.2
1	D	113	SER	6.3
1	B	112	VAL	6.1
1	D	112	VAL	5.8
1	A	112	VAL	4.8
1	A	113	SER	4.4
1	D	114	GLY	4.0
1	C	84	GLY	3.7
1	C	1	MET	3.4
1	B	1	MET	3.3
1	C	72	PRO	3.2
1	D	239	ARG	3.0
1	D	219	GLU	2.7
1	D	225	VAL	2.6
1	D	72	PRO	2.6
1	C	82	GLY	2.6
1	B	115	LYS	2.5
1	A	114	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	138	GLU	2.5
1	B	70	ASP	2.5
1	C	239	ARG	2.5
1	D	344	SER	2.4
1	A	115	LYS	2.4
1	A	83	ASP	2.3

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, 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.

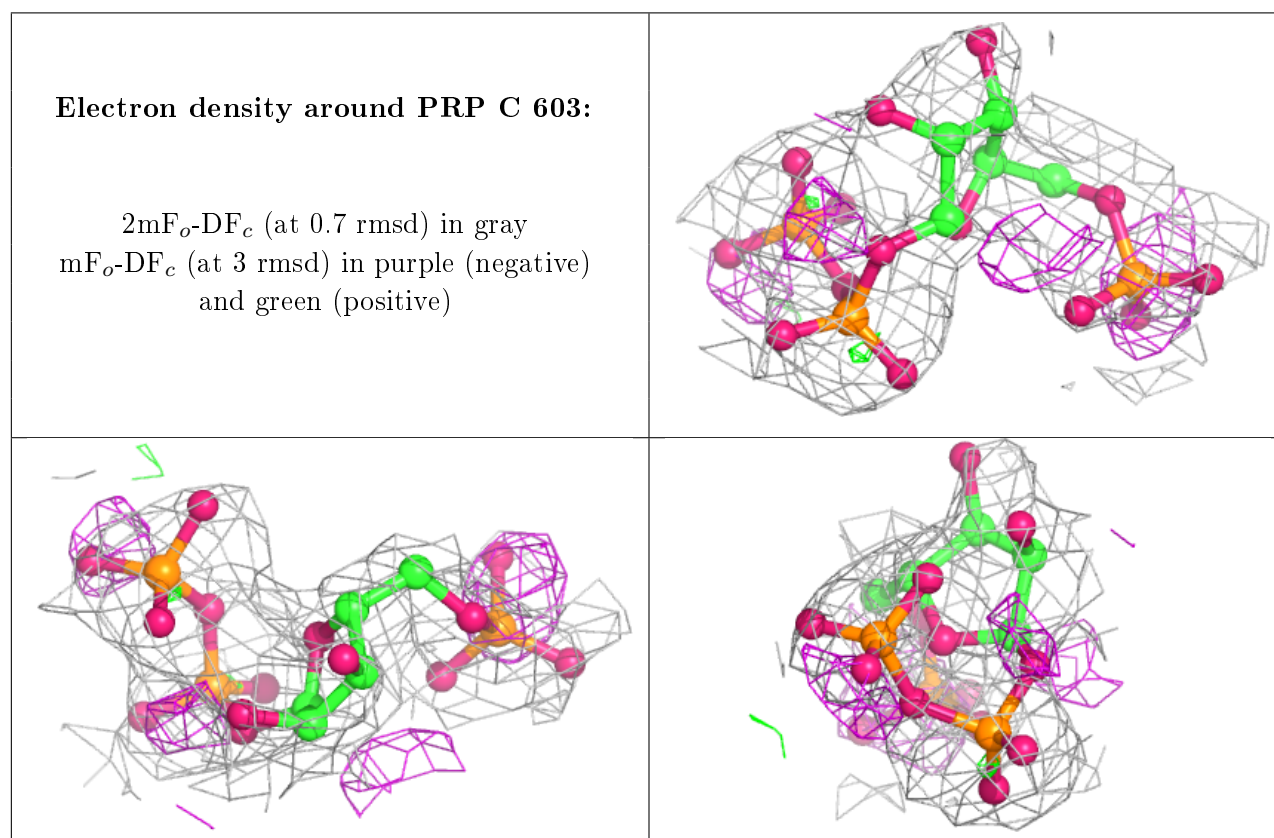
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BE2	B	803	10/10	0.73	0.28	66,68,69,71	0
4	BE2	A	806	10/10	0.77	0.23	65,66,71,71	0
4	BE2	C	804	10/10	0.84	0.24	56,59,61,63	0
2	MG	A	702	1/1	0.86	0.20	81,81,81,81	0
2	MG	B	704	1/1	0.86	0.11	53,53,53,53	0
4	BE2	C	801	10/10	0.88	0.18	77,78,78,78	0
3	PRP	C	603	22/22	0.89	0.25	62,72,87,88	0
2	MG	C	706	1/1	0.90	0.24	78,78,78,78	0
3	PRP	B	602	22/22	0.90	0.22	44,66,80,82	0
2	MG	C	705	1/1	0.91	0.14	70,70,70,70	0
3	PRP	D	604	22/22	0.92	0.19	41,55,71,72	0
3	PRP	A	601	22/22	0.92	0.19	29,54,78,79	0
4	BE2	D	808	10/10	0.92	0.17	47,49,51,52	0
4	BE2	A	802	10/10	0.93	0.16	41,43,45,46	0
4	BE2	B	805	10/10	0.94	0.16	30,36,39,39	0
2	MG	B	703	1/1	0.94	0.15	71,71,71,71	0
4	BE2	D	807	10/10	0.94	0.18	28,31,34,34	0

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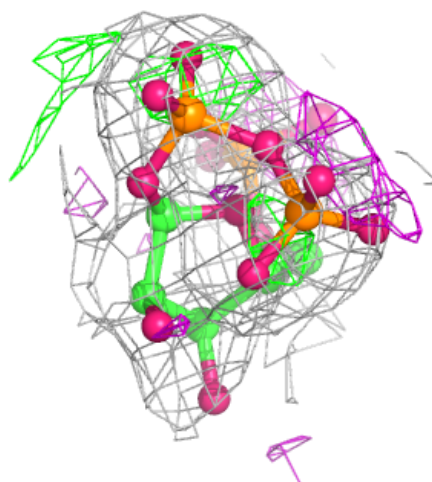
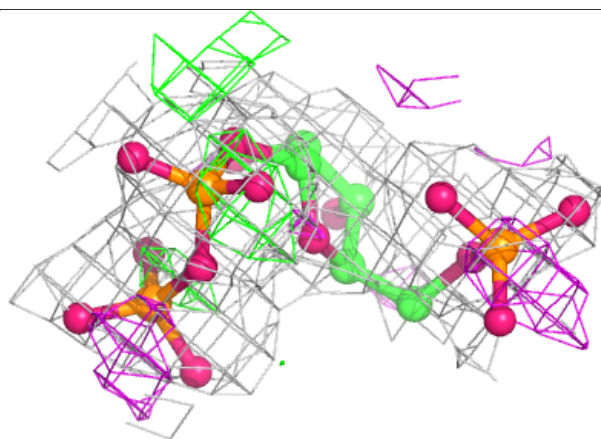
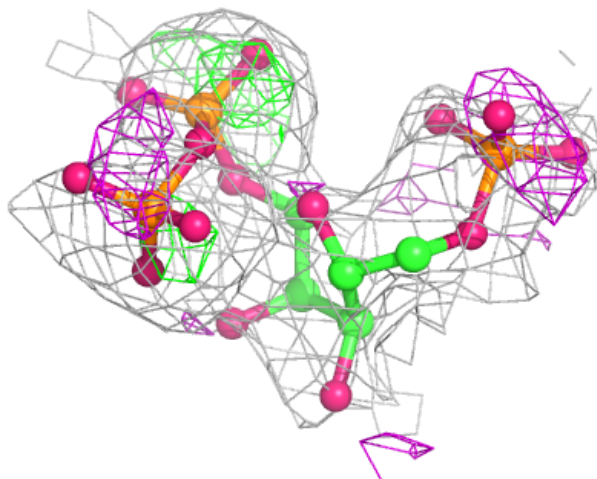
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	D	708	1/1	0.95	0.15	89,89,89,89	0
2	MG	D	707	1/1	0.97	0.16	43,43,43,43	0
2	MG	A	701	1/1	0.97	0.10	70,70,70,70	0

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.



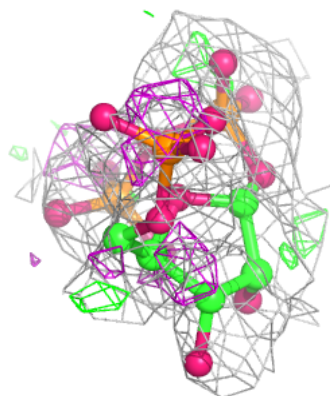
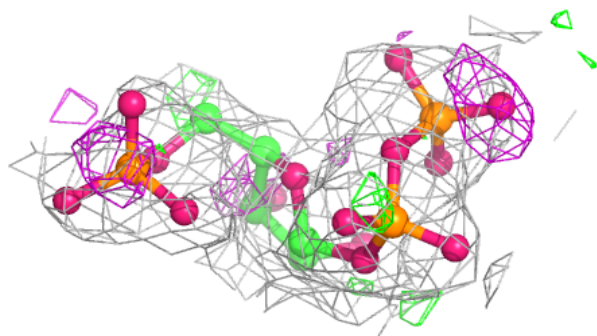
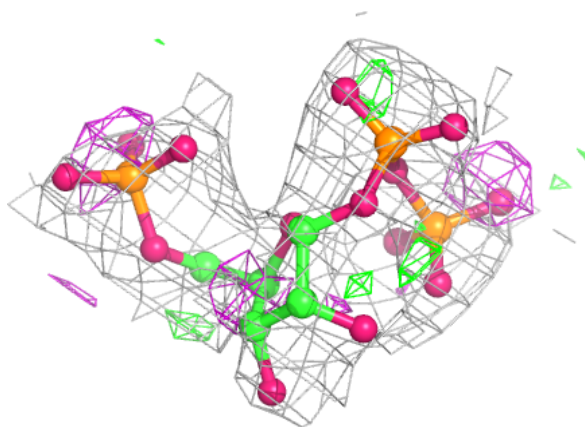
Electron density around PRP B 602:

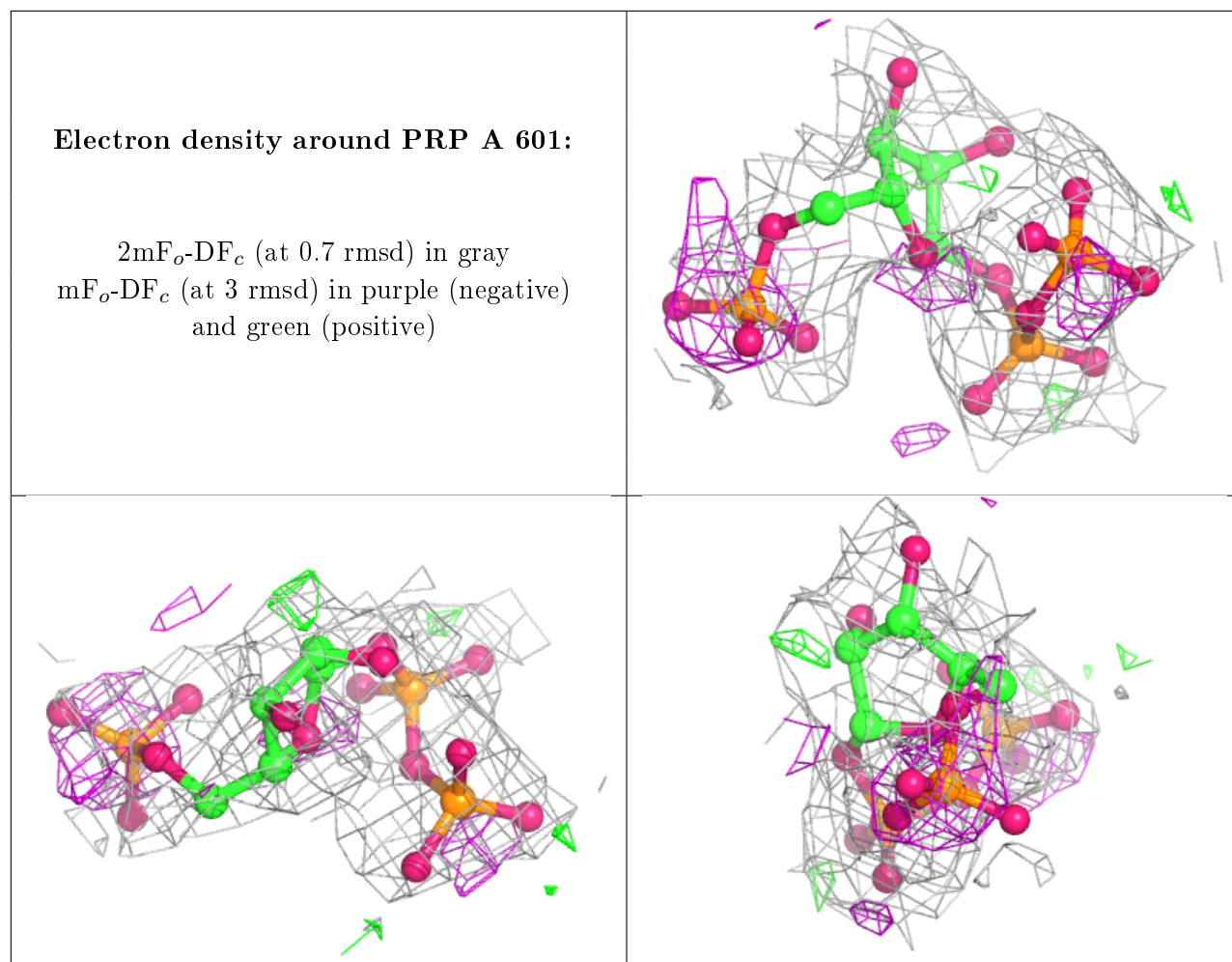
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PRP D 604:

$2mF_o-DF_c$ (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.