Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 12:08 PM JST

PDB ID	:	5CUU
Title	:	Crystal structure of Trypanosoma cruzi Vacuolar Soluble Pyrophosphatases in complex with bisphosphonate inhibitor BPH-1260
Authors	:	Liu, W.D.; Yang, Y.Y.; Ko, T.P.; Zheng, Y.Y.; Chen, C.C.; Guo, R.T.
Deposited on	:	2015-07-25
Resolution	:	2.96 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 (i) 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 (i)) were used in the production of this report:

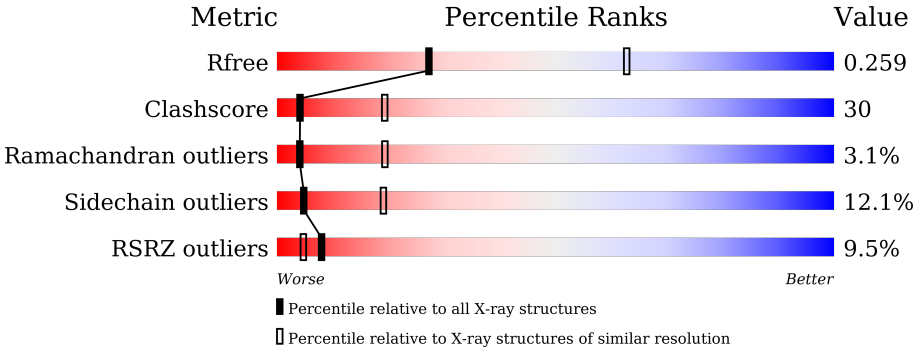
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.96 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	414	5%; 40%, 43%, 8%, 9%
1	B	414	13%; 41%, 44%, 6%, 8%

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	4GA	A	903	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6377 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 Acidocalcisomal pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	378	3091	1994	514	559	24	0	0	0
1	B	379	3096	1997	515	560	24	0	0	0

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q4JH30
A	2	SER	-	expression tag	UNP Q4JH30
A	3	GLU	-	expression tag	UNP Q4JH30
A	4	ASN	-	expression tag	UNP Q4JH30
A	5	LYS	-	expression tag	UNP Q4JH30
A	6	ALA	-	expression tag	UNP Q4JH30
A	7	THR	-	expression tag	UNP Q4JH30
A	8	LEU	-	expression tag	UNP Q4JH30
A	9	MET	-	expression tag	UNP Q4JH30
A	10	GLU	-	expression tag	UNP Q4JH30
A	11	GLY	-	expression tag	UNP Q4JH30
A	12	MET	-	expression tag	UNP Q4JH30
A	13	THR	-	expression tag	UNP Q4JH30
A	14	GLU	-	expression tag	UNP Q4JH30
A	15	LYS	-	expression tag	UNP Q4JH30
A	16	THR	-	expression tag	UNP Q4JH30
A	17	LEU	-	expression tag	UNP Q4JH30
A	18	HIS	-	expression tag	UNP Q4JH30
A	19	SER	-	expression tag	UNP Q4JH30
A	20	PRO	-	expression tag	UNP Q4JH30
A	21	ASN	-	expression tag	UNP Q4JH30
A	22	THR	-	expression tag	UNP Q4JH30
A	23	MET	-	expression tag	UNP Q4JH30
A	24	ALA	-	expression tag	UNP Q4JH30
A	25	GLU	-	expression tag	UNP Q4JH30

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Chain	Residue	Modelled	Actual	Comment	Reference
A	26	VAL	-	expression tag	UNP Q4JH30
A	27	ALA	-	expression tag	UNP Q4JH30
A	28	SER	-	expression tag	UNP Q4JH30
A	29	LEU	-	expression tag	UNP Q4JH30
A	30	HIS	-	expression tag	UNP Q4JH30
A	31	VAL	-	expression tag	UNP Q4JH30
A	411	LYS	-	expression tag	UNP Q4JH30
A	412	GLU	-	expression tag	UNP Q4JH30
A	413	GLU	-	expression tag	UNP Q4JH30
A	414	VAL	-	expression tag	UNP Q4JH30
B	1	MET	-	initiating methionine	UNP Q4JH30
B	2	SER	-	expression tag	UNP Q4JH30
B	3	GLU	-	expression tag	UNP Q4JH30
B	4	ASN	-	expression tag	UNP Q4JH30
B	5	LYS	-	expression tag	UNP Q4JH30
B	6	ALA	-	expression tag	UNP Q4JH30
B	7	THR	-	expression tag	UNP Q4JH30
B	8	LEU	-	expression tag	UNP Q4JH30
B	9	MET	-	expression tag	UNP Q4JH30
B	10	GLU	-	expression tag	UNP Q4JH30
B	11	GLY	-	expression tag	UNP Q4JH30
B	12	MET	-	expression tag	UNP Q4JH30
B	13	THR	-	expression tag	UNP Q4JH30
B	14	GLU	-	expression tag	UNP Q4JH30
B	15	LYS	-	expression tag	UNP Q4JH30
B	16	THR	-	expression tag	UNP Q4JH30
B	17	LEU	-	expression tag	UNP Q4JH30
B	18	HIS	-	expression tag	UNP Q4JH30
B	19	SER	-	expression tag	UNP Q4JH30
B	20	PRO	-	expression tag	UNP Q4JH30
B	21	ASN	-	expression tag	UNP Q4JH30
B	22	THR	-	expression tag	UNP Q4JH30
B	23	MET	-	expression tag	UNP Q4JH30
B	24	ALA	-	expression tag	UNP Q4JH30
B	25	GLU	-	expression tag	UNP Q4JH30
B	26	VAL	-	expression tag	UNP Q4JH30
B	27	ALA	-	expression tag	UNP Q4JH30
B	28	SER	-	expression tag	UNP Q4JH30
B	29	LEU	-	expression tag	UNP Q4JH30
B	30	HIS	-	expression tag	UNP Q4JH30
B	31	VAL	-	expression tag	UNP Q4JH30
B	411	LYS	-	expression tag	UNP Q4JH30

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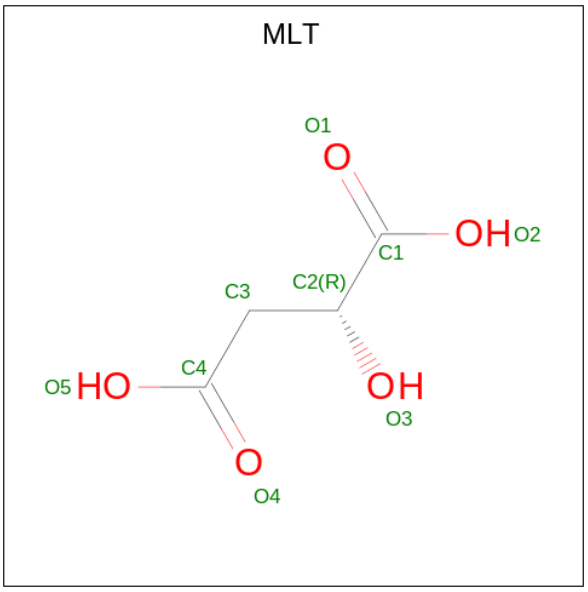
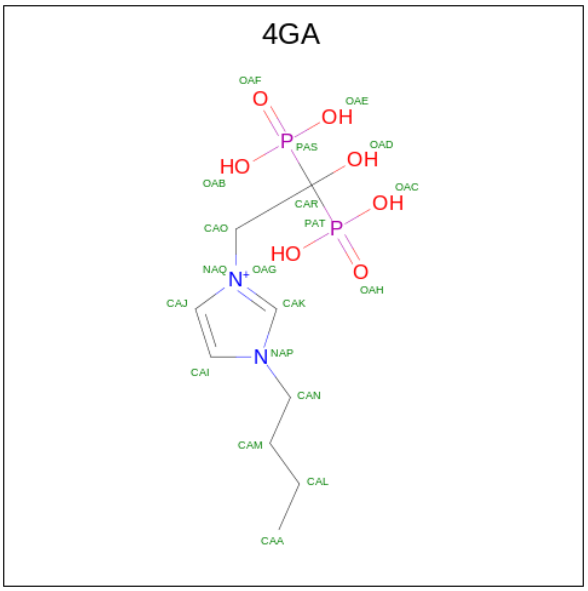
Chain	Residue	Modelled	Actual	Comment	Reference
B	412	GLU	-	expression tag	UNP Q4JH30
B	413	GLU	-	expression tag	UNP Q4JH30
B	414	VAL	-	expression tag	UNP Q4JH30

- Molecule 2 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
2	A	1	9	4	5		0	0
			Total	C	O			
2	A	1	9	4	5		0	0
			Total	C	O			
2	B	1	9	4	5		0	0

- Molecule 3 is 1-butyl-3-(2-hydroxy-2,2-diphosphonoethyl)-1H-imidazol-3-ium (three-letter code: 4GA) (formula: $C_9H_{19}N_2O_7P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	20	9	2	7	2	0	0
			Total	C	N	O	P		
3	B	1	20	9	2	7	2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0
			Total	Mg		
4	B	1	1	1	0	0

- Molecule 5 is water.

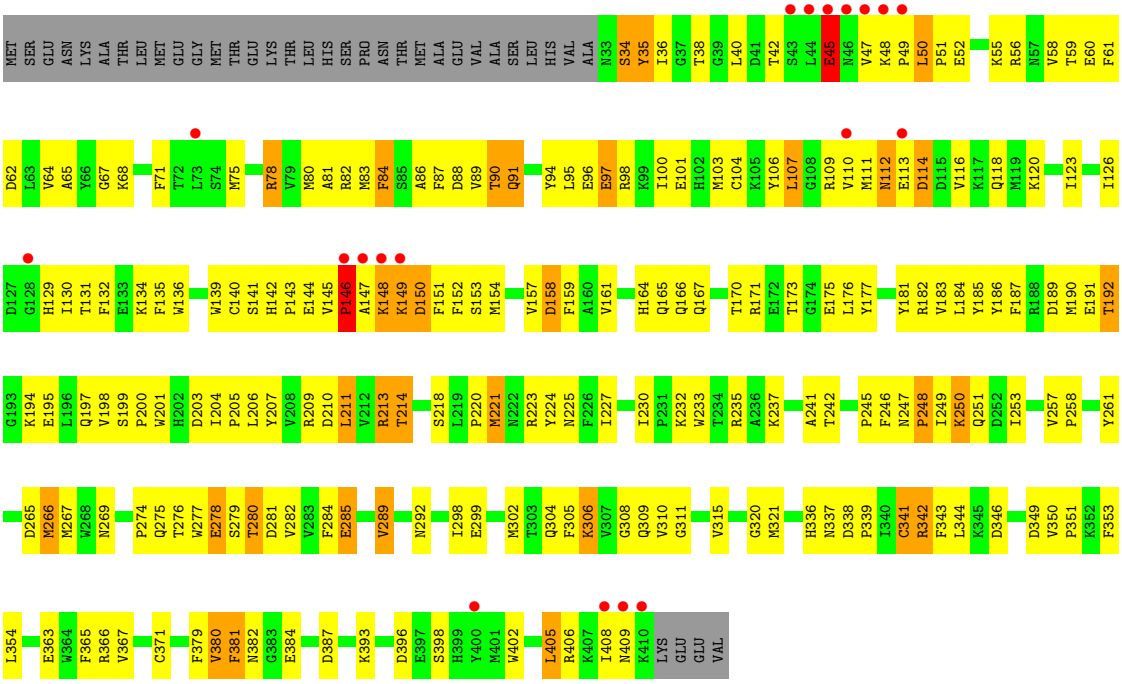
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	70	70	70	0	0
			Total	O		
5	B	51	51	51	0	0

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.

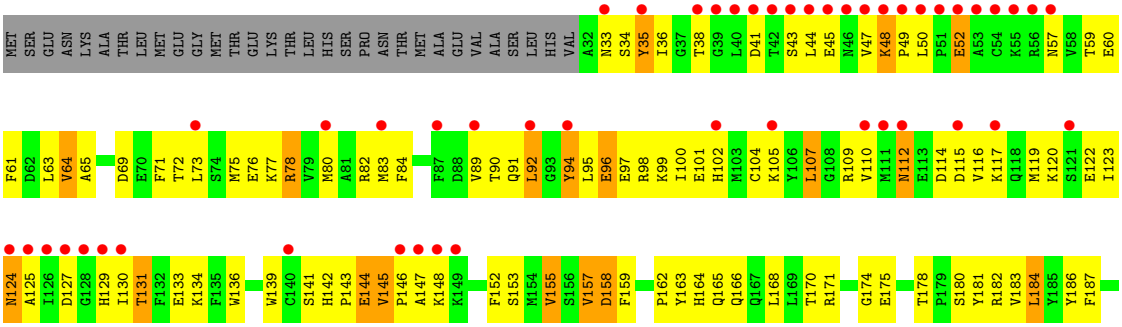
• Molecule 1: Acidocalcisomal pyrophosphatase

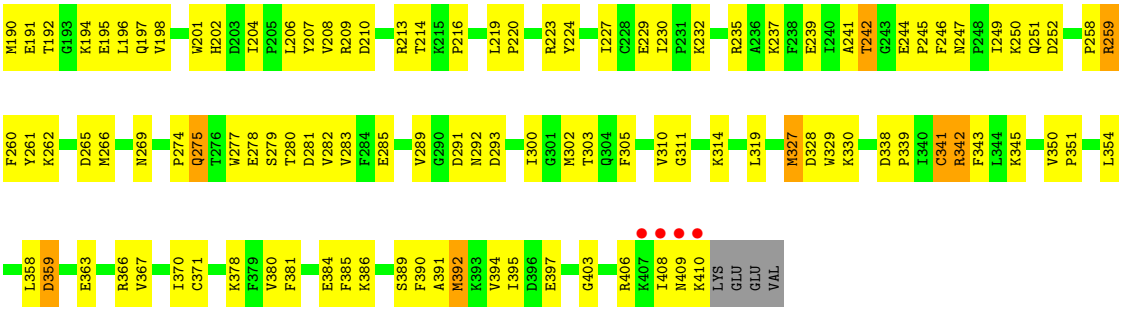
Chain A:



• Molecule 1: Acidocalcisomal pyrophosphatase

Chain B:




M190 E191 T192 G193 K194 E195 L196 Q197 V198 W201 H202 D203 I204 P205 L206 Y207 V208 R209 D210 R213 T214 K215 P216 L219 P220 R223 Y224 I227 C228 E229 I230 P231 K232 R235 A236 K237 F238 E239 I240 A241 T242 G243 E244 P245 F246 N247 P248 I249 K250 Q251 D252 P258 R259
F260 Y261 K262 D265 M266 N269 P274 Q275 T276 W277 E278 S279 T280 D281 V282 V283 F284 E285 V289 G290 D291 N292 D293 I300 G301 M302 T303 Q304 F305 V310 G311 K314 L319 M327 D328 W329 K330 D338 P339 I340 C341 R342 F343 L344 K345 V350 P351 L354
L358 D359 E363 R366 V367 I370 C371 K378 F379 V380 F381 E384 F385 K386 S389 F390 A391 M392 K393 V394 I395 D396 E397 G403 R406 K407 I408 N409 K410 LYS GLU GLU VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	100.78Å 102.63Å 158.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.96 24.84 – 2.96	Depositor EDS
% Data completeness (in resolution range)	94.6 (25.00-2.96) 94.6 (24.84-2.96)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.71 (at 2.94Å)	Xtriage
Refinement program	CNS 1.21	Depositor
R, R_{free}	0.194 , 0.274 0.189 , 0.259	Depositor DCC
R_{free} test set	816 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	69.6	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.034 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6377	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MLT, 4GA, 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	0.71	1/3178 (0.0%)	0.84	0/4297
1	B	0.73	0/3183	0.82	1/4304 (0.0%)
All	All	0.72	1/6361 (0.0%)	0.83	1/8601 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	MET	SD-CE	5.13	2.06	1.77

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	45	GLU	N-CA-C	5.26	125.20	111.00

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	3091	0	3014	208	0
1	B	3096	0	3019	180	0
2	A	18	0	8	5	0
2	B	9	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	20	0	15	5	0
3	B	20	0	15	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	70	0	0	1	0
5	B	51	0	0	4	0
All	All	6377	0	6075	367	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (367) 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:221:MET:SD	1:A:221:MET:CE	2.06	1.43
1:A:78:ARG:HH11	1:A:78:ARG:HB2	0.99	1.11
1:B:144:GLU:O	1:B:146:PRO:HD3	1.54	1.05
1:B:112:ASN:O	1:B:116:VAL:HG23	1.61	1.01
1:B:381:PHE:O	1:B:384:GLU:HG3	1.61	1.00
1:B:227:ILE:HD11	1:B:274:PRO:HB3	1.44	0.99
1:B:100:ILE:HG13	1:B:130:ILE:HD12	1.46	0.97
1:A:192:THR:OG1	1:A:194:LYS:HG2	1.66	0.95
1:A:78:ARG:HB2	1:A:78:ARG:NH1	1.82	0.93
1:B:96:GLU:H	1:B:99:LYS:HE2	1.34	0.90
1:A:184:LEU:HD13	1:A:197:GLN:HE22	1.35	0.90
1:A:266:MET:HA	1:A:266:MET:CE	2.02	0.89
1:A:266:MET:HA	1:A:266:MET:HE3	1.54	0.87
1:A:223:ARG:HH22	2:A:902:MLT:H2	1.40	0.86
1:A:278:GLU:HA	1:A:278:GLU:OE2	1.73	0.85
1:B:143:PRO:O	1:B:144:GLU:HB2	1.74	0.85
1:B:182:ARG:HH11	1:B:182:ARG:HG2	1.42	0.85
1:A:184:LEU:HD13	1:A:197:GLN:NE2	1.92	0.83
1:B:259:ARG:HG3	1:B:259:ARG:HH11	1.40	0.83
1:A:52:GLU:HG3	1:A:75:MET:HE3	1.60	0.83
1:A:298:ILE:HD11	1:A:365:PHE:HE2	1.44	0.82
1:A:112:ASN:O	1:A:116:VAL:HG23	1.80	0.81
1:A:78:ARG:HH11	1:A:78:ARG:CB	1.90	0.81
1:B:146:PRO:HB3	5:B:1032:HOH:O	1.81	0.81
1:A:257:VAL:HG21	1:B:76:GLU:HG2	1.64	0.79
1:B:95:LEU:HD12	1:B:100:ILE:HD13	1.63	0.79
1:B:219:LEU:HD12	1:B:220:PRO:HD2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:PHE:O	1:B:394:VAL:HG23	1.83	0.78
1:A:266:MET:HE2	1:A:267:MET:H	1.49	0.78
1:A:166:GLN:HE21	1:A:187:PHE:HB3	1.48	0.77
1:B:329:TRP:O	1:B:330:LYS:HD3	1.83	0.77
1:B:78:ARG:HH11	1:B:78:ARG:HG2	1.49	0.77
1:A:227:ILE:HD11	1:A:274:PRO:HB3	1.66	0.76
1:A:78:ARG:O	1:A:82:ARG:HG3	1.86	0.76
1:B:219:LEU:HD12	1:B:220:PRO:CD	2.16	0.76
1:B:341:CYS:SG	5:B:1013:HOH:O	2.43	0.75
1:B:342:ARG:HD3	1:B:343:PHE:CZ	2.22	0.74
1:B:117:LYS:HD3	1:B:120:LYS:HD2	1.71	0.73
1:B:78:ARG:HG2	1:B:78:ARG:NH1	2.02	0.73
1:A:55:LYS:HD2	1:A:56:ARG:HG3	1.70	0.73
1:B:90:THR:OG1	1:B:92:LEU:HD22	1.88	0.73
1:B:224:TYR:OH	1:B:392:MET:HG2	1.88	0.73
1:B:72:THR:HG23	1:B:73:LEU:H	1.53	0.72
1:B:182:ARG:HG2	1:B:182:ARG:NH1	2.00	0.72
1:B:166:GLN:HE21	1:B:187:PHE:HB3	1.54	0.72
1:B:35:TYR:HB3	1:B:60:GLU:CG	2.19	0.71
1:A:298:ILE:HD11	1:A:365:PHE:CE2	2.26	0.70
1:B:327:MET:HE2	1:B:327:MET:HA	1.74	0.69
1:A:52:GLU:HG3	1:A:75:MET:CE	2.23	0.69
1:A:152:PHE:HZ	1:B:292:ASN:ND2	1.91	0.69
1:B:359:ASP:OD1	1:B:359:ASP:N	2.26	0.69
1:A:67:GLY:O	1:B:262:LYS:HE3	1.92	0.68
1:A:184:LEU:HD12	1:A:186:TYR:OH	1.93	0.68
1:A:237:LYS:NZ	3:A:903:4GA:HAOA	2.09	0.68
1:B:96:GLU:N	1:B:99:LYS:HE2	2.08	0.68
1:B:131:THR:HG23	1:B:134:LYS:HB2	1.74	0.68
1:A:51:PRO:HG2	1:A:52:GLU:OE2	1.94	0.67
1:B:144:GLU:C	1:B:146:PRO:HD3	2.15	0.67
1:A:152:PHE:CZ	1:B:292:ASN:ND2	2.63	0.67
1:B:35:TYR:HB3	1:B:60:GLU:HG3	1.77	0.66
1:A:157:VAL:CG2	1:B:196:LEU:HD13	2.26	0.66
1:A:88:ASP:O	1:A:91:GLN:NE2	2.29	0.65
1:B:92:LEU:HD23	1:B:92:LEU:H	1.62	0.65
1:A:341:CYS:SG	5:A:1002:HOH:O	2.55	0.64
1:A:165:GLN:HG2	1:A:190:MET:SD	2.37	0.64
1:B:269:ASN:ND2	1:B:305:PHE:H	1.96	0.64
1:A:80:MET:HE3	1:A:80:MET:HA	1.81	0.63
1:A:157:VAL:HG13	1:A:157:VAL:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:GLY:O	1:B:406:ARG:HB2	1.98	0.63
1:A:221:MET:HA	2:A:901:MLT:O2	1.99	0.63
1:B:78:ARG:HH11	1:B:78:ARG:CG	2.11	0.63
1:A:80:MET:HG2	1:A:136:TRP:CZ3	2.35	0.62
1:B:117:LYS:HA	1:B:120:LYS:HG3	1.81	0.62
1:A:292:ASN:ND2	1:B:152:PHE:CE2	2.68	0.62
1:B:269:ASN:HD21	1:B:305:PHE:H	1.47	0.62
1:A:143:PRO:O	1:A:144:GLU:HG2	1.99	0.62
1:A:165:GLN:NE2	1:B:210:ASP:H	1.96	0.62
1:A:104:CYS:O	1:A:109:ARG:HB2	1.99	0.61
1:B:183:VAL:HB	1:B:249:ILE:HB	1.81	0.61
1:A:87:PHE:CE2	1:A:103:MET:HG3	2.36	0.61
1:A:161:VAL:HG23	1:A:161:VAL:O	2.01	0.61
1:A:213:ARG:HG2	1:A:213:ARG:HH11	1.64	0.61
1:B:145:VAL:HG21	1:B:148:LYS:HE3	1.82	0.61
1:A:81:ALA:HA	1:A:132:PHE:CE1	2.36	0.61
1:A:49:PRO:O	1:A:50:LEU:C	2.39	0.61
1:A:110:VAL:HG23	1:A:110:VAL:O	2.01	0.61
1:B:206:LEU:HD23	1:B:207:TYR:CE1	2.35	0.61
1:B:124:ASN:H	1:B:134:LYS:NZ	1.99	0.60
1:B:219:LEU:HD12	1:B:220:PRO:N	2.16	0.60
1:B:280:THR:C	1:B:282:VAL:H	2.05	0.60
1:B:77:LYS:HD2	1:B:136:TRP:HE1	1.67	0.60
1:A:61:PHE:O	1:A:64:VAL:HG12	2.02	0.59
1:B:259:ARG:HH11	1:B:259:ARG:CG	2.14	0.59
1:A:245:PRO:O	1:A:246:PHE:HB2	2.01	0.59
1:B:300:ILE:HD12	1:B:354:LEU:HD12	1.82	0.59
1:B:363:GLU:OE2	1:B:366:ARG:NH2	2.34	0.59
1:A:109:ARG:HB3	1:A:111:MET:HE3	1.84	0.59
1:A:223:ARG:HH22	2:A:902:MLT:C2	2.11	0.59
1:A:106:TYR:OH	1:B:180:SER:HB3	2.03	0.59
1:A:209:ARG:HG2	1:A:221:MET:HE3	1.84	0.59
1:A:278:GLU:OE2	1:A:278:GLU:CA	2.49	0.59
1:B:192:THR:OG1	1:B:194:LYS:HB2	2.03	0.58
1:A:123:ILE:HD12	1:A:134:LYS:HB3	1.85	0.58
1:A:166:GLN:NE2	1:A:187:PHE:HB3	2.17	0.58
1:A:159:PHE:CE1	1:A:161:VAL:HG11	2.38	0.58
1:A:346:ASP:OD1	1:A:387:ASP:HB2	2.04	0.58
1:B:84:PHE:HZ	1:B:94:TYR:HA	1.68	0.58
1:B:327:MET:HA	1:B:327:MET:CE	2.33	0.58
1:B:48:LYS:HB2	1:B:48:LYS:NZ	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:SER:O	1:A:59:THR:HB	2.04	0.57
1:A:109:ARG:HD3	1:A:111:MET:HE3	1.85	0.57
1:A:284:PHE:O	1:A:285:GLU:C	2.42	0.57
1:B:84:PHE:CE1	1:B:95:LEU:HG	2.39	0.57
1:A:298:ILE:CD1	1:A:365:PHE:HE2	2.17	0.57
1:B:116:VAL:O	1:B:120:LYS:HG2	2.05	0.57
1:A:68:LYS:HD2	1:B:371:CYS:SG	2.45	0.56
1:A:276:THR:HB	1:A:398:SER:OG	2.05	0.56
1:A:402:TRP:CZ2	1:A:406:ARG:HD2	2.40	0.56
1:A:306:LYS:O	1:A:309:GLN:HB2	2.04	0.56
1:B:391:ALA:O	1:B:395:ILE:HG13	2.05	0.56
1:A:114:ASP:OD1	1:A:114:ASP:N	2.38	0.56
1:B:48:LYS:O	1:B:48:LYS:HD3	2.05	0.56
1:B:116:VAL:O	1:B:119:MET:HB3	2.06	0.56
1:B:102:HIS:ND1	1:B:105:LYS:HD2	2.20	0.56
1:A:154:MET:HE3	1:B:406:ARG:HH11	1.69	0.56
1:B:72:THR:HG23	1:B:73:LEU:N	2.18	0.56
1:A:171:ARG:NH2	1:A:195:GLU:OE1	2.39	0.55
1:B:358:LEU:HB3	1:B:385:PHE:CE2	2.42	0.55
1:A:167:GLN:HB2	1:A:190:MET:HE3	1.88	0.55
1:A:350:VAL:HB	1:A:351:PRO:HD3	1.88	0.55
1:A:380:VAL:O	1:A:382:ASN:N	2.39	0.55
1:A:292:ASN:HD22	1:B:152:PHE:HZ	1.52	0.55
1:A:40:LEU:HD12	1:A:86:ALA:HB1	1.88	0.55
1:A:214:THR:HG22	1:B:168:LEU:HD22	1.89	0.55
1:B:319:LEU:HD13	1:B:385:PHE:CE1	2.42	0.55
1:A:282:VAL:O	1:A:289:VAL:HA	2.08	0.54
1:A:149:LYS:HB3	1:A:149:LYS:NZ	2.23	0.54
1:A:237:LYS:HZ3	3:A:903:4GA:HAOA	1.73	0.54
1:B:408:ILE:HG23	1:B:409:ASN:N	2.22	0.54
1:A:153:SER:OG	1:B:245:PRO:HA	2.08	0.54
1:B:241:ALA:HB1	1:B:244:GLU:HG3	1.89	0.54
1:B:153:SER:OG	1:B:155:VAL:HG23	2.08	0.54
1:A:242:THR:HA	1:A:247:ASN:ND2	2.23	0.53
1:A:214:THR:HG22	1:B:168:LEU:CD2	2.38	0.53
1:A:218:SER:O	1:A:220:PRO:HD3	2.08	0.53
1:A:235:ARG:HB3	1:A:265:ASP:HA	1.91	0.53
1:B:119:MET:O	1:B:123:ILE:HG13	2.08	0.53
1:B:206:LEU:HB2	1:B:275:GLN:HB3	1.90	0.53
1:A:302:MET:HG2	1:A:338:ASP:OD1	2.09	0.53
1:A:304:GLN:HG2	1:A:305:PHE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:MET:CE	1:A:266:MET:CA	2.83	0.53
1:A:164:HIS:HD2	1:A:189:ASP:OD2	1.91	0.53
1:A:223:ARG:HG3	1:A:336:HIS:CD2	2.44	0.53
1:B:71:PHE:C	1:B:75:MET:HB2	2.29	0.53
1:A:146:PRO:CG	1:A:147:ALA:H	2.22	0.52
1:A:187:PHE:CE1	1:A:198:VAL:HG21	2.44	0.52
1:A:250:LYS:HD3	1:A:251:GLN:O	2.08	0.52
1:A:257:VAL:CG2	1:B:76:GLU:HG2	2.37	0.52
1:A:209:ARG:HG2	1:A:221:MET:CE	2.39	0.52
1:A:247:ASN:O	1:A:248:PRO:O	2.28	0.52
1:A:258:PRO:HD2	1:B:36:ILE:HD13	1.91	0.52
1:A:310:VAL:HG12	1:A:311:GLY:N	2.24	0.52
1:A:321:MET:HG3	1:A:379:PHE:CE2	2.45	0.52
1:A:164:HIS:CD2	1:A:189:ASP:OD2	2.63	0.52
1:B:117:LYS:HA	1:B:120:LYS:CG	2.40	0.52
1:B:157:VAL:HG13	1:B:157:VAL:O	2.09	0.52
1:B:242:THR:HA	1:B:247:ASN:HD22	1.74	0.52
1:A:165:GLN:HE22	1:B:210:ASP:H	1.57	0.52
1:B:328:ASP:OD1	1:B:330:LYS:NZ	2.34	0.52
1:B:116:VAL:HG12	1:B:120:LYS:HE3	1.91	0.52
1:B:206:LEU:HD13	1:B:274:PRO:O	2.09	0.52
1:B:175:GLU:O	1:B:181:TYR:HB2	2.10	0.51
1:A:223:ARG:NH2	2:A:902:MLT:H2	2.18	0.51
1:B:77:LYS:HD2	1:B:136:TRP:NE1	2.25	0.51
1:A:213:ARG:HG2	1:A:213:ARG:NH1	2.25	0.51
1:B:44:LEU:HD22	5:B:1007:HOH:O	2.09	0.51
1:B:381:PHE:CD2	1:B:386:LYS:HG3	2.45	0.51
1:A:116:VAL:HG12	1:A:120:LYS:HE3	1.93	0.51
1:B:64:VAL:CG1	1:B:65:ALA:N	2.73	0.51
1:A:48:LYS:HE2	1:A:48:LYS:HA	1.91	0.51
1:A:80:MET:HE2	1:A:107:LEU:HD11	1.90	0.51
1:A:146:PRO:CD	1:A:147:ALA:H	2.23	0.51
1:B:47:VAL:CG1	1:B:82:ARG:HD2	2.40	0.51
1:B:282:VAL:O	1:B:289:VAL:HA	2.11	0.51
1:B:122:GLU:OE2	1:B:142:HIS:CD2	2.63	0.51
1:A:201:TRP:CZ3	1:A:242:THR:HG22	2.45	0.51
1:B:83:MET:SD	1:B:107:LEU:HD21	2.51	0.51
1:A:157:VAL:O	1:A:158:ASP:C	2.49	0.51
3:A:903:4GA:OAB	3:A:903:4GA:HAK	2.11	0.50
1:B:202:HIS:O	1:B:275:GLN:NE2	2.44	0.50
1:A:146:PRO:HG2	1:A:147:ALA:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:903:4GA:OAC	3:A:903:4GA:OAE	2.28	0.50
1:A:164:HIS:HD2	1:A:189:ASP:CG	2.14	0.50
1:A:173:THR:O	1:A:181:TYR:HA	2.11	0.50
1:B:127:ASP:OD2	1:B:129:HIS:HB2	2.12	0.50
1:B:35:TYR:CB	1:B:60:GLU:HG3	2.40	0.50
1:B:98:ARG:O	1:B:101:GLU:HB3	2.10	0.50
1:B:104:CYS:O	1:B:109:ARG:HB2	2.10	0.50
1:A:230:ILE:CD1	1:A:261:TYR:HE2	2.24	0.50
1:B:92:LEU:HD12	1:B:94:TYR:CE1	2.47	0.50
1:A:205:PRO:HA	1:A:275:GLN:NE2	2.26	0.50
1:A:142:HIS:C	1:A:144:GLU:H	2.15	0.50
1:A:109:ARG:NE	1:A:139:TRP:CZ3	2.78	0.49
1:A:380:VAL:O	1:A:381:PHE:C	2.50	0.49
1:B:43:SER:HB2	5:B:1006:HOH:O	2.11	0.49
1:B:229:GLU:OE2	1:B:239:GLU:HA	2.13	0.49
1:B:291:ASP:OD1	1:B:293:ASP:HB2	2.11	0.49
1:A:164:HIS:CD2	1:A:191:GLU:HB2	2.47	0.49
1:B:201:TRP:CZ3	1:B:242:THR:HG22	2.47	0.49
1:A:176:LEU:O	1:A:177:TYR:HB2	2.13	0.49
1:A:210:ASP:H	1:B:165:GLN:NE2	2.10	0.49
1:A:157:VAL:HG11	1:B:198:VAL:HG12	1.94	0.49
1:B:110:VAL:HG23	1:B:110:VAL:O	2.13	0.49
1:B:165:GLN:HG2	1:B:190:MET:SD	2.53	0.49
1:A:131:THR:HG23	1:A:134:LYS:HB2	1.93	0.49
1:A:183:VAL:HB	1:A:249:ILE:HB	1.95	0.49
1:B:48:LYS:HE3	1:B:78:ARG:HD2	1.93	0.49
1:B:112:ASN:ND2	1:B:115:ASP:OD2	2.44	0.49
1:A:266:MET:HE2	1:A:267:MET:N	2.22	0.49
1:B:72:THR:O	1:B:75:MET:N	2.43	0.49
1:A:103:MET:HE1	1:A:135:PHE:CE2	2.47	0.49
1:A:35:TYR:HA	1:A:60:GLU:HB2	1.95	0.48
1:B:174:GLY:HA3	1:B:181:TYR:HA	1.95	0.48
1:A:141:SER:C	1:A:142:HIS:ND1	2.66	0.48
1:A:408:ILE:HG22	1:A:409:ASN:OD1	2.13	0.48
1:B:381:PHE:CE2	1:B:386:LYS:HG3	2.48	0.48
1:B:47:VAL:HG12	1:B:82:ARG:HD2	1.94	0.48
1:A:366:ARG:HG2	1:A:366:ARG:HH11	1.78	0.48
1:B:95:LEU:HD12	1:B:100:ILE:CD1	2.40	0.48
1:B:157:VAL:O	1:B:158:ASP:C	2.51	0.48
1:A:237:LYS:HZ2	3:A:903:4GA:HAOA	1.79	0.48
1:A:40:LEU:HD12	1:A:86:ALA:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ARG:O	1:A:101:GLU:HB2	2.14	0.48
1:A:280:THR:O	1:A:289:VAL:HG23	2.14	0.48
1:A:141:SER:HB2	1:A:142:HIS:ND1	2.28	0.47
1:B:227:ILE:CD1	1:B:274:PRO:HB3	2.31	0.47
1:B:410:LYS:O	1:B:410:LYS:HG2	2.13	0.47
1:A:170:THR:HG22	1:A:185:TYR:CD2	2.49	0.47
1:B:208:VAL:HB	1:B:223:ARG:HG2	1.96	0.47
1:A:35:TYR:N	1:A:35:TYR:CD1	2.83	0.47
1:A:224:TYR:CD1	1:A:315:VAL:HG23	2.50	0.47
1:B:61:PHE:O	1:B:64:VAL:HG12	2.15	0.47
1:A:232:LYS:HD3	1:A:233:TRP:CZ2	2.50	0.47
1:A:84:PHE:CD1	1:A:84:PHE:C	2.89	0.47
1:A:210:ASP:O	1:B:165:GLN:HG3	2.15	0.47
1:A:230:ILE:HD12	1:A:261:TYR:HE2	1.79	0.47
1:A:366:ARG:HG2	1:A:366:ARG:NH1	2.30	0.47
1:B:408:ILE:CG2	1:B:409:ASN:N	2.78	0.47
1:A:199:SER:HA	1:A:246:PHE:O	2.14	0.47
1:B:145:VAL:HG23	1:B:145:VAL:O	2.15	0.47
1:B:186:TYR:CE1	1:B:197:GLN:HB2	2.50	0.47
1:B:319:LEU:HD13	1:B:385:PHE:CD1	2.50	0.47
1:A:80:MET:HG2	1:A:136:TRP:CE3	2.51	0.46
1:A:96:GLU:O	1:A:98:ARG:N	2.48	0.46
1:A:205:PRO:O	1:A:225:ASN:HB2	2.15	0.46
1:A:146:PRO:CG	1:A:147:ALA:N	2.78	0.46
1:A:353:PHE:O	1:A:354:LEU:HD23	2.15	0.46
1:B:50:LEU:HD13	1:B:78:ARG:HG3	1.96	0.46
1:A:280:THR:C	1:A:282:VAL:H	2.19	0.46
1:A:80:MET:HE2	1:A:107:LEU:CD1	2.45	0.46
1:A:123:ILE:HD11	1:A:134:LYS:O	2.15	0.46
1:A:405:LEU:HG	1:A:405:LEU:O	2.15	0.46
1:B:63:LEU:HD23	1:B:63:LEU:HA	1.66	0.46
1:A:310:VAL:CG1	1:A:311:GLY:N	2.78	0.46
1:A:380:VAL:HG23	1:A:381:PHE:CD2	2.51	0.46
1:A:149:LYS:C	1:A:151:PHE:H	2.18	0.46
1:A:149:LYS:C	1:A:151:PHE:N	2.68	0.46
1:B:310:VAL:HG12	1:B:311:GLY:N	2.31	0.46
1:A:249:ILE:HD12	1:A:308:GLY:HA2	1.98	0.46
1:B:102:HIS:O	1:B:105:LYS:HB3	2.16	0.46
1:B:280:THR:C	1:B:282:VAL:N	2.68	0.46
1:A:159:PHE:CZ	1:A:161:VAL:HG11	2.50	0.45
1:B:34:SER:O	1:B:59:THR:HB	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:HD12	1:A:100:ILE:HD13	1.99	0.45
1:A:343:PHE:O	1:A:344:LEU:HD23	2.16	0.45
1:A:145:VAL:HB	1:A:148:LYS:HB3	1.98	0.45
1:B:164:HIS:O	1:B:165:GLN:C	2.53	0.45
1:B:380:VAL:HG23	1:B:381:PHE:N	2.32	0.45
1:A:136:TRP:CE2	1:A:140:CYS:SG	3.09	0.45
1:A:237:LYS:HE2	1:A:261:TYR:CZ	2.52	0.45
1:B:282:VAL:HG12	1:B:283:VAL:N	2.32	0.45
1:A:94:TYR:CD1	1:A:94:TYR:C	2.90	0.45
1:A:204:ILE:HD13	1:A:310:VAL:HG21	1.99	0.45
1:A:320:GLY:HA3	1:A:380:VAL:HG22	1.97	0.45
1:B:47:VAL:O	1:B:49:PRO:HD3	2.16	0.45
1:A:84:PHE:CD1	1:A:84:PHE:O	2.70	0.45
1:A:90:THR:O	1:A:91:GLN:C	2.54	0.45
1:A:175:GLU:O	1:A:181:TYR:HB2	2.16	0.45
1:B:162:PRO:O	1:B:163:TYR:C	2.55	0.45
1:A:164:HIS:HD2	1:A:189:ASP:OD1	2.00	0.45
1:A:211:LEU:HD13	1:A:211:LEU:HA	1.66	0.45
1:B:170:THR:HA	1:B:184:LEU:O	2.16	0.45
1:A:49:PRO:O	1:A:50:LEU:O	2.35	0.44
1:A:109:ARG:HD3	1:A:111:MET:CE	2.48	0.44
1:A:402:TRP:CH2	1:A:406:ARG:HD2	2.52	0.44
1:A:145:VAL:CB	1:A:148:LYS:HB3	2.48	0.44
1:B:64:VAL:HG13	1:B:65:ALA:N	2.32	0.44
1:A:58:VAL:HG12	1:A:62:ASP:HB2	1.98	0.44
1:B:49:PRO:O	1:B:50:LEU:C	2.55	0.44
1:B:35:TYR:HB3	1:B:60:GLU:CD	2.38	0.44
1:A:146:PRO:HG2	1:A:147:ALA:N	2.32	0.44
1:B:252:ASP:OD2	1:B:259:ARG:HG3	2.17	0.44
1:A:182:ARG:HG2	1:A:182:ARG:HH11	1.82	0.43
1:A:164:HIS:CD2	1:A:189:ASP:OD1	2.71	0.43
1:B:237:LYS:HE2	1:B:261:TYR:CD1	2.53	0.43
1:A:342:ARG:HG3	1:A:343:PHE:CD1	2.54	0.43
1:A:129:HIS:CD2	1:A:129:HIS:N	2.84	0.43
1:A:198:VAL:HB	1:A:203:ASP:OD2	2.19	0.43
1:A:242:THR:HA	1:A:247:ASN:HD22	1.84	0.43
1:B:133:GLU:OE2	1:B:133:GLU:HA	2.18	0.43
1:B:310:VAL:CG1	1:B:311:GLY:N	2.82	0.43
1:A:157:VAL:CG1	1:B:198:VAL:HG12	2.49	0.43
1:A:269:ASN:HB2	1:A:299:GLU:HB3	2.00	0.43
1:B:38:THR:HG22	1:B:83:MET:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:GLU:C	1:B:181:TYR:HB2	2.39	0.43
1:B:237:LYS:HE2	1:B:261:TYR:CE1	2.54	0.43
1:A:38:THR:HG22	1:A:83:MET:HA	2.00	0.43
1:A:292:ASN:ND2	1:B:152:PHE:HE2	2.16	0.43
1:B:237:LYS:O	1:B:251:GLN:HG3	2.19	0.43
1:B:259:ARG:CG	1:B:259:ARG:NH1	2.78	0.43
1:A:45:GLU:H	1:A:45:GLU:HG2	1.60	0.42
1:A:241:ALA:HB2	1:A:250:LYS:HG2	2.00	0.42
1:A:336:HIS:HE1	2:A:901:MLT:O4	2.02	0.42
1:A:349:ASP:O	1:A:353:PHE:HD2	2.02	0.42
1:B:171:ARG:NH2	1:B:195:GLU:OE1	2.52	0.42
1:B:95:LEU:HB3	1:B:99:LYS:HB2	2.02	0.42
1:B:80:MET:HG2	1:B:136:TRP:CE3	2.55	0.42
1:B:145:VAL:CG2	1:B:148:LYS:HE3	2.49	0.42
1:B:280:THR:O	1:B:282:VAL:N	2.53	0.42
1:A:47:VAL:O	1:A:47:VAL:CG2	2.68	0.42
1:A:80:MET:CE	1:A:107:LEU:CD1	2.97	0.42
1:B:92:LEU:HD23	1:B:92:LEU:N	2.31	0.42
1:B:139:TRP:C	1:B:141:SER:H	2.22	0.42
1:A:148:LYS:C	1:A:150:ASP:H	2.23	0.42
1:B:277:TRP:CZ3	1:B:279:SER:HB2	2.55	0.42
1:A:249:ILE:CD1	1:A:308:GLY:HA2	2.49	0.42
1:A:380:VAL:HG23	1:A:381:PHE:HD2	1.85	0.42
1:B:96:GLU:C	1:B:98:ARG:H	2.23	0.42
1:A:36:ILE:H	1:A:36:ILE:HG12	1.50	0.41
1:B:367:VAL:HB	1:B:370:ILE:HD12	2.01	0.41
1:A:64:VAL:HG13	1:A:65:ALA:N	2.35	0.41
1:B:72:THR:CG2	1:B:73:LEU:H	2.19	0.41
1:B:125:ALA:HB1	1:B:129:HIS:O	2.20	0.41
1:B:52:GLU:H	1:B:52:GLU:HG2	1.46	0.41
1:B:204:ILE:HD13	1:B:310:VAL:HG21	2.02	0.41
1:A:201:TRP:CE3	1:A:242:THR:HG22	2.55	0.41
1:A:277:TRP:CZ3	1:A:279:SER:HB2	2.55	0.41
1:B:235:ARG:HB3	1:B:265:ASP:HA	2.02	0.41
1:B:381:PHE:CD2	1:B:386:LYS:CG	3.03	0.41
1:B:96:GLU:O	1:B:98:ARG:N	2.54	0.41
1:A:97:GLU:HG2	1:A:130:ILE:HD11	2.03	0.41
1:A:363:GLU:O	1:A:367:VAL:HG22	2.21	0.41
1:A:393:LYS:HE3	1:A:393:LYS:HB2	1.72	0.41
1:A:251:GLN:HB3	1:A:253:ILE:HD11	2.02	0.41
1:B:232:LYS:H	1:B:269:ASN:ND2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:PRO:HG2	1:B:260:PHE:HE1	1.86	0.41
1:B:278:GLU:OE1	1:B:329:TRP:HD1	2.04	0.41
1:B:245:PRO:O	1:B:246:PHE:HB2	2.21	0.41
1:A:103:MET:HE2	1:A:135:PHE:CZ	2.56	0.40
1:A:200:PRO:HD2	1:A:246:PHE:O	2.21	0.40
1:A:34:SER:HB2	1:A:35:TYR:HD1	1.87	0.40
1:A:80:MET:CE	1:A:107:LEU:HD11	2.52	0.40
1:A:206:LEU:HD23	1:A:207:TYR:CE1	2.56	0.40
1:A:68:LYS:NZ	1:B:262:LYS:O	2.39	0.40
1:B:350:VAL:HB	1:B:351:PRO:HD3	2.03	0.40
1:A:50:LEU:HD12	1:A:60:GLU:CG	2.52	0.40
1:B:99:LYS:C	1:B:101:GLU:N	2.72	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	376/414 (91%)	331 (88%)	33 (9%)	12 (3%)	4 19
1	B	377/414 (91%)	334 (89%)	32 (8%)	11 (3%)	4 21
All	All	753/828 (91%)	665 (88%)	65 (9%)	23 (3%)	4 19

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	146	PRO
1	A	158	ASP
1	A	381	PHE
1	B	91	GLN
1	B	147	ALA

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Mol	Chain	Res	Type
1	A	97	GLU
1	B	144	GLU
1	B	158	ASP
1	A	91	GLN
1	A	107	LEU
1	A	248	PRO
1	B	97	GLU
1	B	145	VAL
1	B	216	PRO
1	B	281	ASP
1	B	107	LEU
1	A	281	ASP
1	A	50	LEU
1	A	285	GLU
1	B	285	GLU
1	A	380	VAL
1	B	155	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	336/367 (92%)	300 (89%)	36 (11%)	6 23
1	B	336/367 (92%)	291 (87%)	45 (13%)	4 15
All	All	672/734 (92%)	591 (88%)	81 (12%)	5 19

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	35	TYR
1	A	42	THR
1	A	45	GLU
1	A	71	PHE
1	A	78	ARG

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Mol	Chain	Res	Type
1	A	84	PHE
1	A	89	VAL
1	A	90	THR
1	A	112	ASN
1	A	113	GLU
1	A	114	ASP
1	A	118	GLN
1	A	126	ILE
1	A	146	PRO
1	A	148	LYS
1	A	149	LYS
1	A	150	ASP
1	A	192	THR
1	A	211	LEU
1	A	213	ARG
1	A	214	THR
1	A	250	LYS
1	A	266	MET
1	A	278	GLU
1	A	280	THR
1	A	289	VAL
1	A	306	LYS
1	A	337	ASN
1	A	339	PRO
1	A	341	CYS
1	A	342	ARG
1	A	371	CYS
1	A	384	GLU
1	A	396	ASP
1	A	405	LEU
1	B	33	ASN
1	B	35	TYR
1	B	41	ASP
1	B	48	LYS
1	B	52	GLU
1	B	57	ASN
1	B	64	VAL
1	B	69	ASP
1	B	78	ARG
1	B	89	VAL
1	B	92	LEU
1	B	94	TYR

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Mol	Chain	Res	Type
1	B	96	GLU
1	B	112	ASN
1	B	114	ASP
1	B	124	ASN
1	B	131	THR
1	B	157	VAL
1	B	159	PHE
1	B	178	THR
1	B	184	LEU
1	B	191	GLU
1	B	209	ARG
1	B	213	ARG
1	B	214	THR
1	B	230	ILE
1	B	242	THR
1	B	250	LYS
1	B	259	ARG
1	B	266	MET
1	B	275	GLN
1	B	302	MET
1	B	303	THR
1	B	314	LYS
1	B	327	MET
1	B	338	ASP
1	B	339	PRO
1	B	341	CYS
1	B	342	ARG
1	B	345	LYS
1	B	359	ASP
1	B	378	LYS
1	B	389	SER
1	B	392	MET
1	B	397	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	164	HIS
1	A	165	GLN
1	A	166	GLN
1	A	197	GLN

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Mol	Chain	Res	Type
1	A	372	GLN
1	A	377	ASN
1	B	33	ASN
1	B	112	ASN
1	B	124	ASN
1	B	142	HIS
1	B	164	HIS
1	B	166	GLN
1	B	197	GLN
1	B	247	ASN
1	B	269	ASN
1	B	292	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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
2	MLT	A	901	-	8,8,8	1.49	2 (25%)	10,10,10	1.76	3 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MLT	B	901	-	8,8,8	1.21	1 (12%)	10,10,10	1.88	3 (30%)
3	4GA	B	902	-	19,20,20	2.13	8 (42%)	26,31,31	1.07	3 (11%)
2	MLT	A	902	-	8,8,8	1.18	1 (12%)	10,10,10	1.41	1 (10%)
3	4GA	A	903	-	19,20,20	2.63	9 (47%)	26,31,31	1.41	5 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLT	A	901	-	-	0/8/8/8	-
2	MLT	B	901	-	-	4/8/8/8	-
3	4GA	B	902	-	-	7/27/27/27	0/1/1/1
2	MLT	A	902	-	-	0/8/8/8	-
3	4GA	A	903	-	-	20/27/27/27	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903	4GA	PAT-OAH	7.07	1.61	1.50
3	B	902	4GA	PAS-OAB	3.71	1.61	1.54
3	B	902	4GA	PAS-OAE	3.70	1.61	1.54
3	A	903	4GA	PAS-OAE	3.69	1.61	1.54
3	A	903	4GA	PAS-OAB	3.68	1.61	1.54
3	B	902	4GA	PAT-OAC	3.67	1.61	1.54
3	A	903	4GA	PAT-OAG	3.65	1.61	1.54
3	B	902	4GA	PAT-OAG	3.62	1.61	1.54
3	A	903	4GA	PAT-OAC	-3.43	1.48	1.54
3	B	902	4GA	PAS-CAR	3.05	1.87	1.85
3	A	903	4GA	PAS-CAR	2.89	1.87	1.85
3	B	902	4GA	PAT-CAR	2.80	1.87	1.85
2	A	901	MLT	O2-C1	-2.75	1.21	1.30
3	A	903	4GA	PAT-CAR	2.71	1.87	1.85
2	A	901	MLT	C2-C1	2.35	1.55	1.52
3	A	903	4GA	CAJ-NAQ	-2.35	1.33	1.37
3	B	902	4GA	CAI-NAP	-2.28	1.33	1.37
3	B	902	4GA	CAJ-NAQ	-2.26	1.33	1.37
3	A	903	4GA	CAI-NAP	-2.17	1.33	1.37
2	B	901	MLT	O2-C1	-2.04	1.23	1.30
2	A	902	MLT	O2-C1	-2.02	1.23	1.30

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	901	MLT	O2-C1-C2	4.15	121.84	112.72
2	A	901	MLT	O2-C1-C2	3.55	120.52	112.72
3	A	903	4GA	OAC-PAT-CAR	3.15	113.22	106.17
2	A	902	MLT	O2-C1-C2	3.04	119.39	112.72
3	A	903	4GA	PAS-CAR-OAD	2.96	114.03	107.30
3	B	902	4GA	PAS-CAR-OAD	2.88	113.84	107.30
2	A	901	MLT	O2-C1-O1	-2.86	117.59	124.09
3	A	903	4GA	OAG-PAT-OAH	-2.86	106.64	113.06
3	A	903	4GA	PAT-CAR-OAD	2.75	113.55	107.30
2	B	901	MLT	O2-C1-O1	-2.67	118.02	124.09
3	B	902	4GA	PAT-CAR-OAD	2.56	113.13	107.30
3	B	902	4GA	PAT-CAR-PAS	-2.35	108.60	112.81
2	B	901	MLT	O5-C4-C3	2.18	121.06	114.07
2	A	901	MLT	O5-C4-C3	2.18	121.05	114.07
3	A	903	4GA	PAT-CAR-PAS	-2.02	109.19	112.81

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	903	4GA	OAD-CAR-PAS-OAB
3	A	903	4GA	OAD-CAR-PAS-OAE
3	A	903	4GA	OAD-CAR-PAS-OAF
3	A	903	4GA	CAO-CAR-PAS-OAB
3	A	903	4GA	CAO-CAR-PAS-OAE
3	A	903	4GA	CAO-CAR-PAS-OAF
3	A	903	4GA	PAT-CAR-PAS-OAE
3	A	903	4GA	PAT-CAR-PAS-OAF
3	A	903	4GA	OAD-CAR-PAT-OAC
3	A	903	4GA	OAD-CAR-PAT-OAG
3	A	903	4GA	OAD-CAR-PAT-OAH
3	A	903	4GA	CAO-CAR-PAT-OAC
3	A	903	4GA	CAO-CAR-PAT-OAG
3	A	903	4GA	CAO-CAR-PAT-OAH
3	A	903	4GA	PAS-CAR-PAT-OAC
3	A	903	4GA	PAS-CAR-PAT-OAG
3	A	903	4GA	PAS-CAR-PAT-OAH
3	B	902	4GA	CAM-CAN-NAP-CAI
3	B	902	4GA	NAQ-CAO-CAR-OAD
3	B	902	4GA	NAQ-CAO-CAR-PAS
3	B	902	4GA	NAQ-CAO-CAR-PAT

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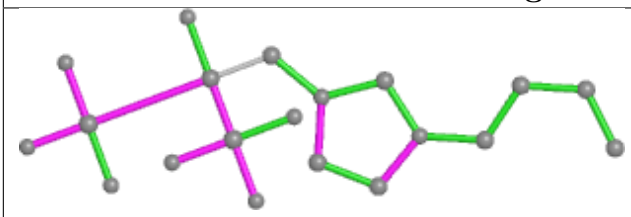
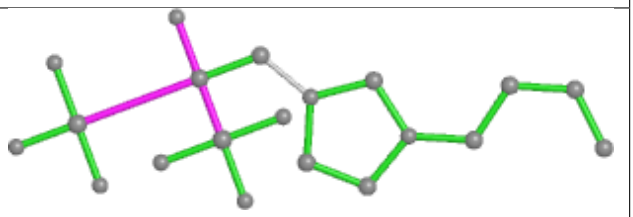
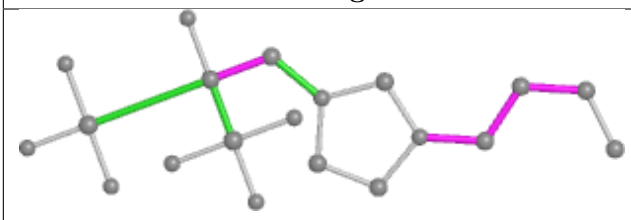
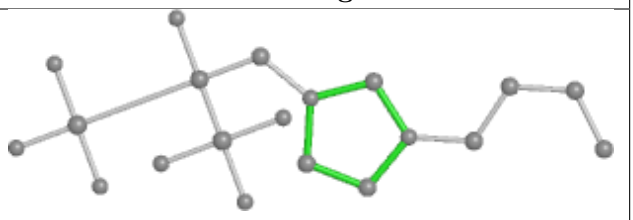
Mol	Chain	Res	Type	Atoms
3	B	902	4GA	CAL-CAM-CAN-NAP
3	B	902	4GA	CAA-CAL-CAM-CAN
3	A	903	4GA	CAA-CAL-CAM-CAN
3	A	903	4GA	PAT-CAR-PAS-OAB
2	B	901	MLT	O1-C1-C2-C3
2	B	901	MLT	O2-C1-C2-C3
3	B	902	4GA	CAM-CAN-NAP-CAK
2	B	901	MLT	O1-C1-C2-O3
3	A	903	4GA	CAM-CAN-NAP-CAK
2	B	901	MLT	O2-C1-C2-O3

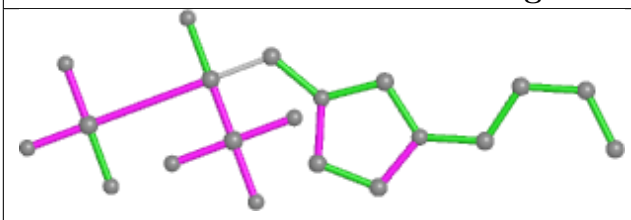
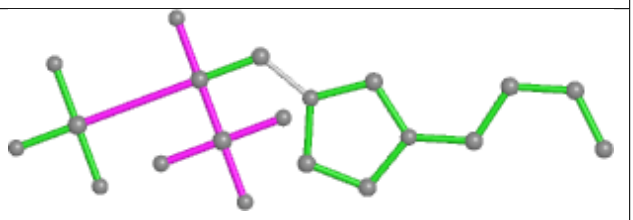
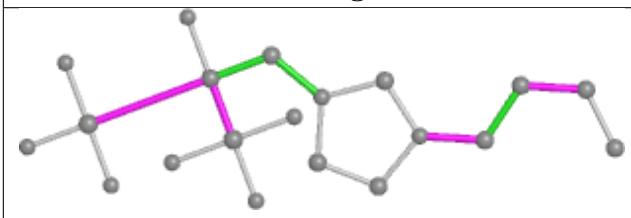
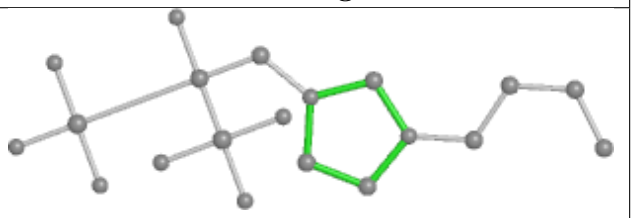
There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	MLT	2	0
2	A	902	MLT	3	0
3	A	903	4GA	5	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 4GA B 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 4GA A 903	
 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	378/414 (91%)	0.17	19 (5%) 28 18	37, 68, 114, 139	0
1	B	379/414 (91%)	0.65	53 (13%) 2 1	37, 67, 158, 184	0
All	All	757/828 (91%)	0.41	72 (9%) 8 5	37, 67, 149, 184	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	PRO	18.7
1	B	49	PRO	11.0
1	B	43	SER	10.9
1	B	45	GLU	9.5
1	A	147	ALA	9.1
1	B	39	GLY	8.4
1	B	44	LEU	8.3
1	B	40	LEU	8.1
1	B	42	THR	8.0
1	B	46	ASN	8.0
1	B	41	ASP	7.6
1	A	46	ASN	7.3
1	B	53	ALA	6.9
1	B	147	ALA	6.4
1	B	54	CYS	6.0
1	B	125	ALA	5.7
1	A	45	GLU	5.4
1	A	44	LEU	5.3
1	B	148	LYS	5.3
1	A	146	PRO	5.2
1	B	126	ILE	5.2
1	B	48	LYS	5.1
1	B	92	LEU	5.1
1	B	52	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	410	LYS	5.0
1	A	148	LYS	4.9
1	B	129	HIS	4.7
1	A	47	VAL	4.7
1	B	50	LEU	4.7
1	B	47	VAL	4.5
1	B	128	GLY	4.3
1	B	111	MET	4.2
1	B	56	ARG	4.2
1	A	149	LYS	4.2
1	B	149	LYS	4.1
1	B	409	ASN	3.7
1	B	55	LYS	3.6
1	B	127	ASP	3.5
1	A	409	ASN	3.4
1	B	38	THR	3.4
1	B	130	ILE	3.3
1	B	87	PHE	3.3
1	A	73	LEU	3.2
1	A	408	ILE	3.2
1	B	146	PRO	3.2
1	B	94	TYR	3.1
1	A	43	SER	2.9
1	B	124	ASN	2.8
1	A	113	GLU	2.8
1	A	48	LYS	2.7
1	A	110	VAL	2.7
1	B	140	CYS	2.6
1	B	102	HIS	2.6
1	B	33	ASN	2.6
1	B	110	VAL	2.6
1	B	115	ASP	2.6
1	B	112	ASN	2.5
1	B	117	LYS	2.4
1	B	35	TYR	2.4
1	B	408	ILE	2.4
1	B	89	VAL	2.4
1	B	105	LYS	2.4
1	A	400	TYR	2.3
1	B	121	SER	2.3
1	A	410	LYS	2.3
1	A	128	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	49	PRO	2.3
1	B	83	MET	2.2
1	B	407	LYS	2.2
1	B	80	MET	2.1
1	B	73	LEU	2.1
1	B	57	ASN	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)

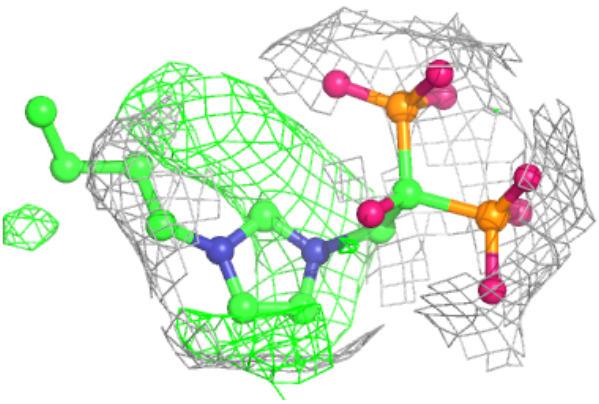
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

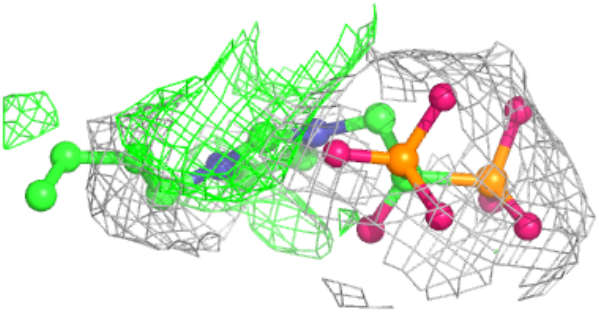
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MLT	A	902	9/9	0.86	0.21	105,106,106,107	0
2	MLT	A	901	9/9	0.89	0.24	82,84,93,93	0
3	4GA	B	902	20/20	0.89	0.12	133,137,138,139	0
3	4GA	A	903	20/20	0.90	0.15	128,135,137,137	0
2	MLT	B	901	9/9	0.90	0.33	77,78,84,85	0
4	MG	A	904	1/1	0.92	0.29	95,95,95,95	0
4	MG	B	903	1/1	0.92	0.09	79,79,79,79	0

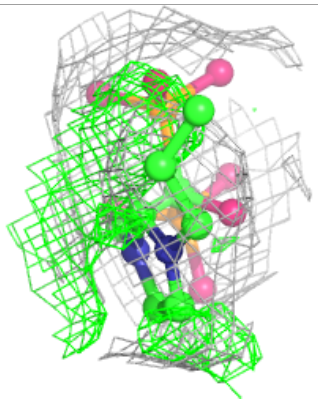
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4GA B 902:

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

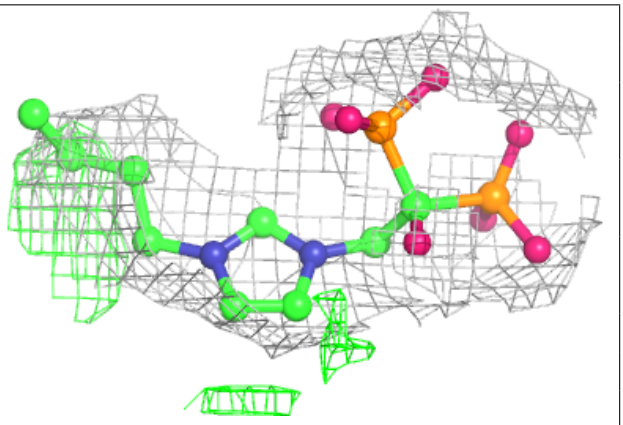


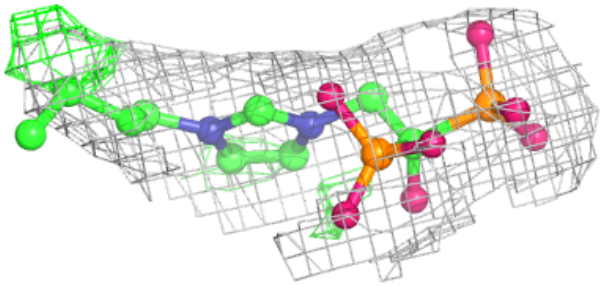


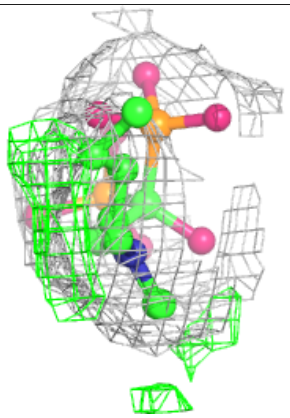


Electron density around 4GA A 903:

$2mF_o$-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.