Full wwPDB X-ray Structure Validation Report (i)

Nov 12, 2024 – 07:01 AM JST

PDB ID	:	8X4R
Title	:	Pyruvate kinase M2 (PKM2) mutant in complex with phenylalanine
Authors	:	Wang, W.C.; Su, T.H.
Deposited on	:	2023-11-15
Resolution	:	2.18 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:

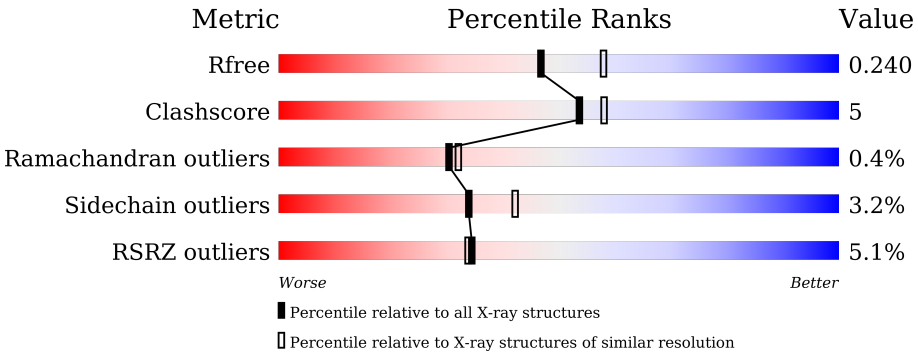
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.18 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}	164625	8336 (2.20-2.16)
Clashscore	180529	9404 (2.20-2.16)
Ramachandran outliers	177936	9297 (2.20-2.16)
Sidechain outliers	177891	9297 (2.20-2.16)
RSRZ outliers	164620	8337 (2.20-2.16)

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	531	3% 87% 9% ·
1	B	531	6% 80% 13% · 6%
1	C	531	5% 79% 15% · 5%
1	D	531	6% 82% 11% · 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15984 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 Pyruvate kinase PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	508	Total	C	N	O	S	0	0	0
			3883	2443	689	726	25			
1	B	499	Total	C	N	O	S	0	0	0
			3818	2402	680	712	24			
1	C	504	Total	C	N	O	S	0	0	0
			3859	2429	685	720	25			
1	D	503	Total	C	N	O	S	0	0	0
			3857	2430	684	719	24			

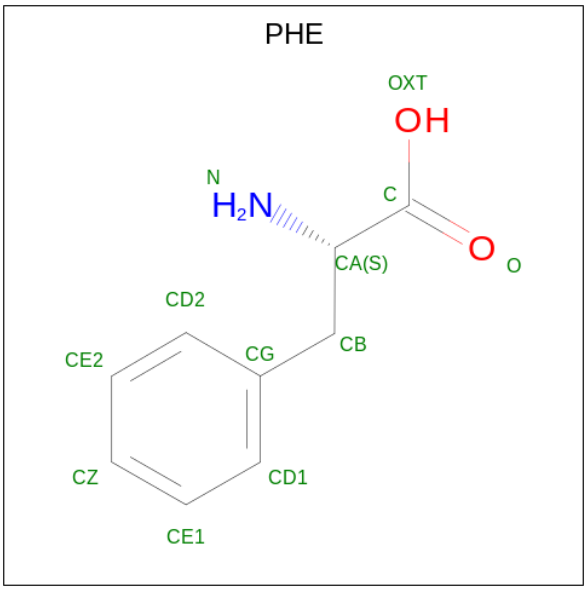
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	405	ALA	THR	engineered mutation	UNP P14618
A	406	ALA	SER	engineered mutation	UNP P14618
A	409	ALA	THR	engineered mutation	UNP P14618
A	454	ALA	THR	engineered mutation	UNP P14618
B	405	ALA	THR	engineered mutation	UNP P14618
B	406	ALA	SER	engineered mutation	UNP P14618
B	409	ALA	THR	engineered mutation	UNP P14618
B	454	ALA	THR	engineered mutation	UNP P14618
C	405	ALA	THR	engineered mutation	UNP P14618
C	406	ALA	SER	engineered mutation	UNP P14618
C	409	ALA	THR	engineered mutation	UNP P14618
C	454	ALA	THR	engineered mutation	UNP P14618
D	405	ALA	THR	engineered mutation	UNP P14618
D	406	ALA	SER	engineered mutation	UNP P14618
D	409	ALA	THR	engineered mutation	UNP P14618
D	454	ALA	THR	engineered mutation	UNP P14618

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0

- Molecule 3 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 12 9 1 2	0	0
3	B	1	Total C N O 12 9 1 2	0	0
3	D	1	Total C N O 12 9 1 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	154	Total O 154 154	0	0
4	B	134	Total O 134 134	0	0

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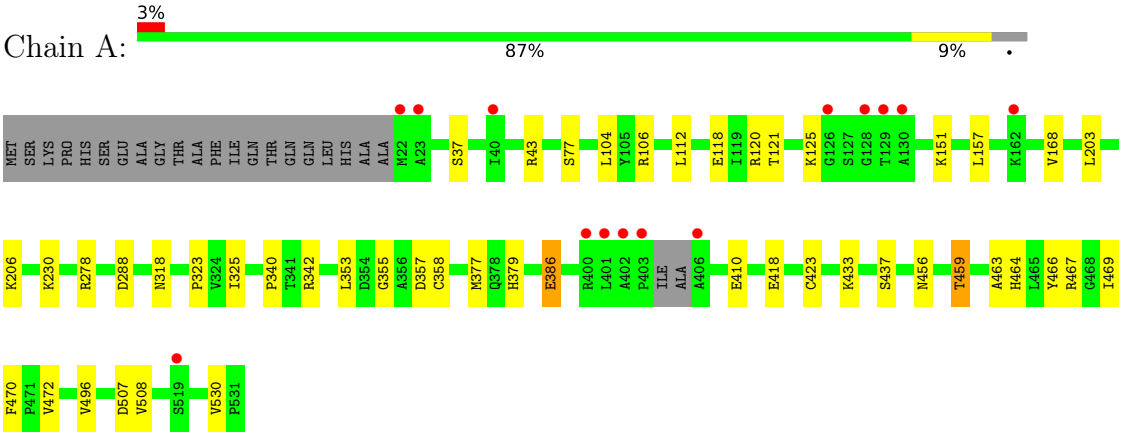
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	122	Total O 122 122	0	0
4	D	117	Total O 117 117	0	0

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.

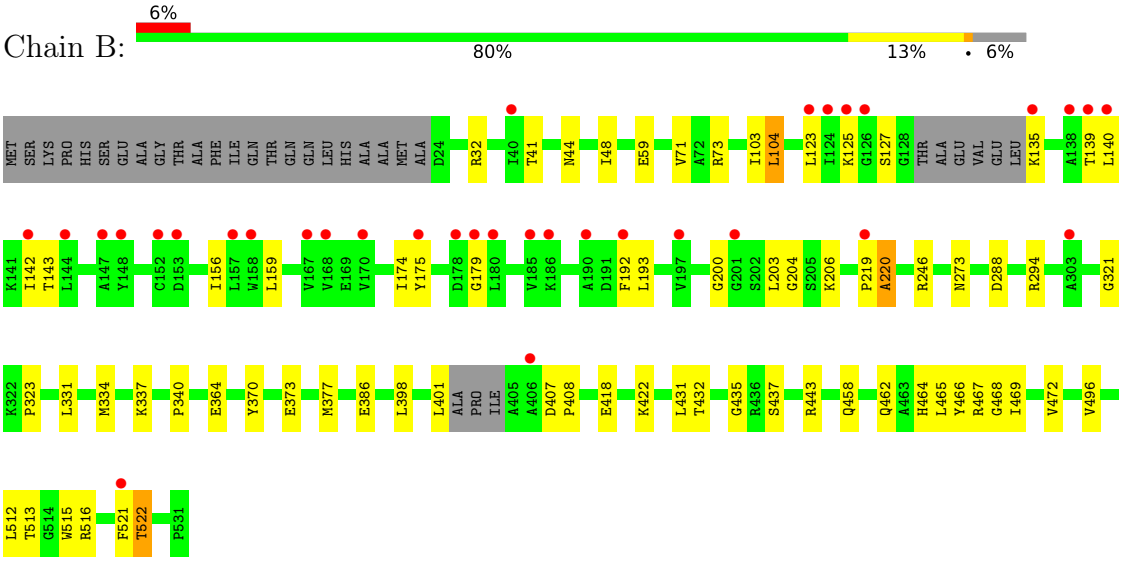
• Molecule 1: Pyruvate kinase PKM

Chain A:



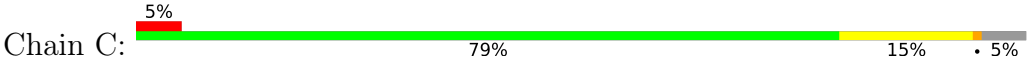
• Molecule 1: Pyruvate kinase PKM

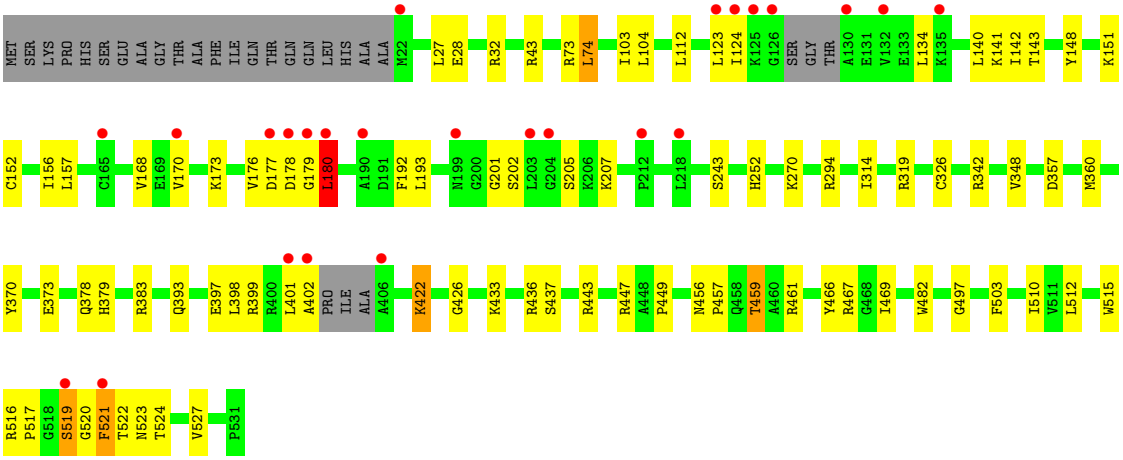
Chain B:



• Molecule 1: Pyruvate kinase PKM

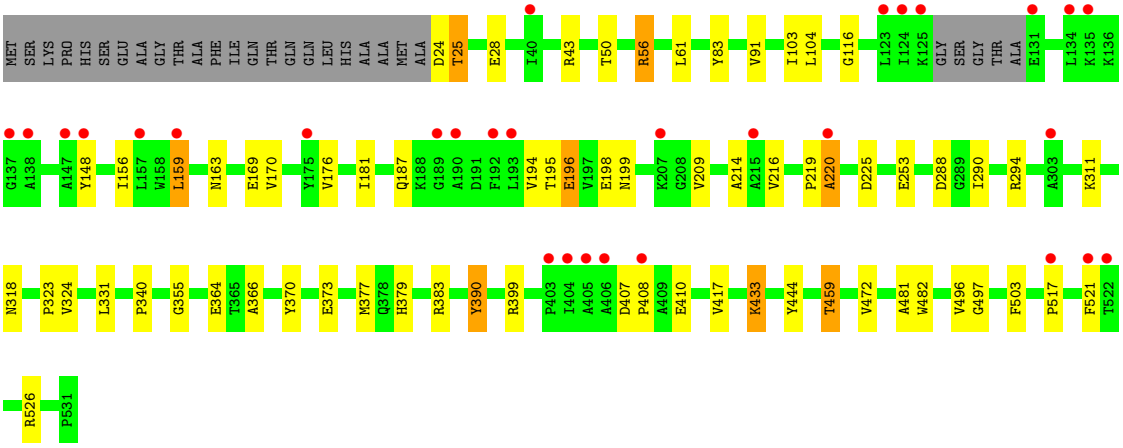
Chain C:





• Molecule 1: Pyruvate kinase PKM

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.14Å 69.40Å 168.82Å 90.00° 106.54° 90.00°	Depositor
Resolution (Å)	27.11 – 2.18 27.11 – 2.18	Depositor EDS
% Data completeness (in resolution range)	95.7 (27.11-2.18) 95.7 (27.11-2.18)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.81 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.198 , 0.240 0.201 , 0.240	Depositor DCC
R_{free} test set	5640 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	37.4	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 28.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15984	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: K

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	0/3945	0.79	0/5324
1	B	0.73	0/3878	0.79	1/5230 (0.0%)
1	C	0.74	0/3919	0.77	0/5286
1	D	0.72	0/3919	0.79	0/5290
All	All	0.72	0/15661	0.78	1/21130 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	73	ARG	NE-CZ-NH2	-5.22	117.69	120.30

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	3883	0	3966	28	0
1	B	3818	0	3900	39	0
1	C	3859	0	3943	50	0
1	D	3857	0	3945	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	0	8	1	0
3	B	12	0	8	1	0
3	D	12	0	8	0	0
4	A	154	0	0	1	0
4	B	134	0	0	1	0
4	C	122	0	0	4	0
4	D	117	0	0	3	0
All	All	15984	0	15778	150	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 5.

All (150) 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:25:THR:HG22	1:D:28:GLU:H	1.46	0.81
1:C:43:ARG:HE	1:C:379:HIS:HD2	1.27	0.80
1:C:179:GLY:O	1:C:180:LEU:HB3	1.83	0.76
1:C:43:ARG:HE	1:C:379:HIS:CD2	2.06	0.73
1:C:516:ARG:HB3	1:C:517:PRO:HD2	1.72	0.71
1:C:482:TRP:CH2	1:C:515:TRP:O	2.44	0.71
1:C:168:VAL:HG21	1:C:193:LEU:HD21	1.72	0.70
1:D:24:ASP:HA	1:D:390:TYR:OH	1.94	0.68
1:B:512:LEU:HB3	1:B:522:THR:HG23	1.78	0.66
1:A:43:ARG:HE	1:A:379:HIS:CD2	2.15	0.65
1:A:423:CYS:HB3	1:A:508:VAL:HG21	1.78	0.65
1:B:437:SER:HA	1:B:521:PHE:CZ	2.32	0.64
1:A:43:ARG:HE	1:A:379:HIS:HD2	1.45	0.63
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.81	0.62
1:C:28:GLU:O	1:C:32:ARG:HG3	2.00	0.62
1:D:103:ILE:HG22	1:D:104:LEU:HD22	1.83	0.61
1:D:195:THR:O	1:D:196:GLU:HB2	2.01	0.61
1:C:177:ASP:HA	1:C:207:LYS:HB3	1.83	0.61
1:B:135:LYS:HA	1:B:200:GLY:HA3	1.83	0.60
1:B:512:LEU:HB3	1:B:522:THR:CG2	2.32	0.60
1:A:125:LYS:HB3	1:A:151:LYS:HA	1.83	0.60
1:C:459:THR:HG22	4:C:753:HOH:O	2.00	0.59
1:B:464:HIS:HD1	3:B:602:PHE:N	2.00	0.59
1:B:246:ARG:HG3	1:B:246:ARG:HH11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:GLY:O	1:C:521:PHE:HB2	2.02	0.58
1:B:422:LYS:HD2	4:B:758:HOH:O	2.02	0.58
1:B:515:TRP:CD1	1:B:516:ARG:HG2	2.38	0.58
1:C:433:LYS:O	1:C:459:THR:HG21	2.03	0.58
1:B:219:PRO:O	1:B:220:ALA:HB3	2.02	0.57
1:C:482:TRP:CZ2	1:C:515:TRP:O	2.57	0.57
1:C:103:ILE:HG22	1:C:104:LEU:HD22	1.86	0.57
1:C:148:TYR:HA	1:C:151:LYS:HB2	1.88	0.56
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.88	0.56
1:C:370:TYR:HB3	1:C:373:GLU:HB2	1.88	0.56
1:A:118:GLU:OE1	1:A:120:ARG:HD3	2.05	0.55
1:A:288:ASP:O	1:A:323:PRO:HD2	2.06	0.55
1:B:472:VAL:HG11	1:B:496:VAL:HG11	1.88	0.55
1:C:73:ARG:HD2	1:C:360:MET:SD	2.47	0.54
1:A:418:GLU:HG2	1:B:418:GLU:OE2	2.07	0.54
1:B:458:GLN:O	1:B:462:GLN:HG3	2.07	0.54
1:D:482:TRP:CD1	1:D:517:PRO:HD3	2.42	0.54
1:C:422:LYS:HE2	4:D:758:HOH:O	2.07	0.54
1:D:481:ALA:HB3	4:D:743:HOH:O	2.06	0.54
1:A:121:THR:O	1:A:206:LYS:HA	2.08	0.54
1:C:134:LEU:HD21	1:C:140:LEU:HD22	1.90	0.54
1:D:43:ARG:HE	1:D:379:HIS:HD2	1.56	0.53
1:A:464:HIS:HD1	3:A:602:PHE:N	2.07	0.53
1:D:219:PRO:O	1:D:220:ALA:CB	2.57	0.53
1:A:456:ASN:HB3	1:A:459:THR:HG23	1.91	0.53
1:D:25:THR:HG22	1:D:28:GLU:N	2.20	0.53
1:B:340:PRO:HG3	1:B:377:MET:HG2	1.90	0.52
1:A:318:ASN:HD21	1:A:355:GLY:HA3	1.75	0.51
1:C:314:ILE:HD11	1:C:326:CYS:SG	2.50	0.51
1:D:417:VAL:HG21	1:D:444:TYR:HB2	1.92	0.51
1:B:44:ASN:HD22	1:B:468:GLY:HA2	1.75	0.51
1:D:43:ARG:HE	1:D:379:HIS:CD2	2.29	0.51
1:C:143:THR:HG21	1:C:156:ILE:HD11	1.93	0.50
1:D:61:LEU:HD13	1:D:91:VAL:HA	1.94	0.50
1:C:141:LYS:HE3	1:C:192:PHE:HB2	1.92	0.50
1:C:523:ASN:O	1:D:526:ARG:HA	2.12	0.49
1:C:319:ARG:HD2	4:C:721:HOH:O	2.13	0.49
1:C:437:SER:OG	1:C:522:THR:HB	2.13	0.49
1:A:353:LEU:CD1	1:D:311:LYS:HE3	2.43	0.49
1:D:370:TYR:HB3	1:D:373:GLU:HB2	1.95	0.49
1:B:401:LEU:HD12	1:C:27:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:GLU:OE2	1:D:444:TYR:OH	2.25	0.48
1:B:522:THR:HG22	1:B:522:THR:O	2.14	0.48
1:A:433:LYS:O	1:A:459:THR:HG21	2.14	0.48
1:B:334:MET:HA	1:B:337:LYS:O	2.14	0.48
1:B:437:SER:OG	1:B:522:THR:HB	2.14	0.47
1:D:148:TYR:CE1	1:D:156:ILE:HD13	2.48	0.47
1:D:288:ASP:O	1:D:323:PRO:HD2	2.14	0.47
1:A:463:ALA:HB1	1:A:469:ILE:HG21	1.96	0.47
1:B:321:GLY:CA	1:B:443:ARG:HG2	2.44	0.47
1:B:143:THR:HB	1:B:156:ILE:HD11	1.97	0.47
1:C:398:LEU:HD13	1:C:443:ARG:O	2.14	0.47
1:A:386:GLU:OE2	1:A:467:ARG:NH1	2.44	0.47
1:B:219:PRO:O	1:B:220:ALA:CB	2.62	0.47
1:D:159:LEU:HD11	1:D:209:VAL:HG11	1.97	0.47
1:D:187:GLN:HB2	1:D:194:VAL:HB	1.96	0.47
1:D:170:VAL:HG12	1:D:170:VAL:O	2.15	0.46
1:D:407:ASP:HB2	1:D:408:PRO:HD2	1.96	0.46
1:B:142:ILE:HB	1:B:193:LEU:HB2	1.97	0.46
1:B:432:THR:O	1:B:432:THR:OG1	2.33	0.46
1:A:157:LEU:HD13	1:A:203:LEU:HD21	1.97	0.46
1:B:331:LEU:O	1:B:364:GLU:HG2	2.15	0.46
1:B:398:LEU:HD13	1:B:443:ARG:O	2.15	0.46
1:C:176:VAL:HG12	1:C:177:ASP:N	2.31	0.46
1:C:43:ARG:HB2	1:C:383:ARG:HG3	1.97	0.45
1:B:407:ASP:HB2	1:B:408:PRO:HD2	1.99	0.45
1:D:482:TRP:CG	1:D:517:PRO:HD3	2.51	0.45
1:D:56:ARG:HD2	1:D:83:TYR:OH	2.17	0.45
1:D:176:VAL:HB	1:D:181:ILE:HB	1.98	0.45
1:C:510:ILE:HD12	1:C:527:VAL:HG22	1.99	0.45
1:A:472:VAL:HG11	1:A:496:VAL:HG11	1.98	0.45
1:C:512:LEU:HA	1:C:524:THR:O	2.17	0.45
1:A:423:CYS:HB3	1:A:508:VAL:CG2	2.43	0.45
1:C:516:ARG:H	1:C:519:SER:CB	2.29	0.45
1:B:321:GLY:HA3	1:B:443:ARG:HG2	1.98	0.44
1:C:456:ASN:CG	1:C:459:THR:HG23	2.38	0.44
1:A:106:ARG:CZ	1:A:470:PHE:CZ	3.01	0.44
1:B:288:ASP:O	1:B:323:PRO:HD2	2.18	0.44
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.52	0.44
1:C:393:GLN:O	1:C:397:GLU:HG3	2.16	0.44
1:B:48:ILE:HG12	1:B:71:VAL:HB	1.99	0.44
1:C:142:ILE:HA	1:C:157:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:SER:HA	1:C:270:LYS:HD3	2.00	0.44
1:D:116:GLY:HA2	1:D:225:ASP:OD2	2.17	0.44
1:D:318:ASN:ND2	4:D:705:HOH:O	2.46	0.44
1:C:516:ARG:H	1:C:519:SER:HB2	1.82	0.43
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.98	0.43
1:D:219:PRO:O	1:D:220:ALA:HB3	2.18	0.43
1:A:357:ASP:HA	1:A:467:ARG:HB2	2.00	0.43
1:D:340:PRO:HG3	1:D:377:MET:HG2	2.01	0.43
1:B:175:TYR:HB3	1:B:179:GLY:HA2	2.00	0.43
1:D:433:LYS:O	1:D:459:THR:HG21	2.17	0.43
1:B:432:THR:HB	1:B:435:GLY:HA2	2.01	0.43
1:C:124:ILE:HA	1:C:152:CYS:O	2.19	0.43
1:C:180:LEU:HD11	1:C:201:GLY:HA3	2.00	0.43
1:C:402:ALA:HA	4:C:809:HOH:O	2.18	0.43
1:C:179:GLY:O	1:C:180:LEU:CB	2.63	0.42
1:D:318:ASN:HD21	1:D:355:GLY:HA3	1.84	0.42
1:C:426:GLY:O	1:C:449:PRO:HD2	2.19	0.42
1:D:331:LEU:O	1:D:364:GLU:HG2	2.20	0.42
1:B:125:LYS:HD3	1:B:125:LYS:HA	1.86	0.42
1:B:386:GLU:OE2	1:B:467:ARG:NH1	2.45	0.42
1:C:457:PRO:O	1:C:461:ARG:HG3	2.20	0.42
1:C:466:TYR:HB2	1:C:469:ILE:HD12	2.01	0.42
1:B:323:PRO:HB3	1:B:465:LEU:O	2.20	0.42
1:C:357:ASP:OD2	1:C:467:ARG:HB2	2.20	0.42
1:A:77:SER:OG	1:A:118:GLU:OE2	2.38	0.41
1:B:370:TYR:HB3	1:B:373:GLU:HB2	2.02	0.41
1:C:177:ASP:O	1:C:178:ASP:HB2	2.21	0.41
1:B:431:LEU:HD22	1:B:513:THR:HG22	2.02	0.41
1:D:50:THR:HG22	1:D:366:ALA:HB2	2.03	0.41
1:D:290:ILE:O	1:D:324:VAL:HA	2.20	0.41
1:C:74:LEU:N	1:C:74:LEU:CD2	2.84	0.41
1:D:497:GLY:HA3	1:D:503:PHE:CZ	2.55	0.41
1:A:278:ARG:NH2	4:A:712:HOH:O	2.53	0.41
1:C:348:VAL:HG11	1:C:378:GLN:HE22	1.85	0.41
1:A:112:LEU:C	1:A:112:LEU:HD23	2.41	0.41
1:C:112:LEU:HD23	1:C:112:LEU:C	2.41	0.41
1:A:340:PRO:HG3	1:A:377:MET:HG2	2.02	0.40
1:A:325:ILE:HG12	1:A:358:CYS:HB2	2.04	0.40
1:A:507:ASP:O	1:A:530:VAL:HG23	2.22	0.40
1:C:252:HIS:HE1	4:C:798:HOH:O	2.03	0.40
1:A:353:LEU:HD12	1:D:311:LYS:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ILE:HG22	1:B:104:LEU:HD13	2.03	0.40
1:B:123:LEU:HD13	1:B:204:GLY:O	2.21	0.40
1:D:198:GLU:O	1:D:199:ASN:C	2.60	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	504/531 (95%)	485 (96%)	19 (4%)	0	100	100
1	B	493/531 (93%)	466 (94%)	25 (5%)	2 (0%)	30	32
1	C	498/531 (94%)	479 (96%)	17 (3%)	2 (0%)	30	32
1	D	499/531 (94%)	473 (95%)	23 (5%)	3 (1%)	22	21
All	All	1994/2124 (94%)	1903 (95%)	84 (4%)	7 (0%)	30	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	220	ALA
1	C	180	LEU
1	B	139	THR
1	B	220	ALA
1	D	196	GLU
1	D	214	ALA
1	C	521	PHE

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	415/432 (96%)	406 (98%)	9 (2%)	47	58
1	B	408/432 (94%)	394 (97%)	14 (3%)	32	39
1	C	412/432 (95%)	396 (96%)	16 (4%)	27	33
1	D	413/432 (96%)	399 (97%)	14 (3%)	32	39
All	All	1648/1728 (95%)	1595 (97%)	53 (3%)	34	42

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	SER
1	A	104	LEU
1	A	168	VAL
1	A	230	LYS
1	A	342	ARG
1	A	386	GLU
1	A	410	GLU
1	A	437	SER
1	A	459	THR
1	B	32	ARG
1	B	41	THR
1	B	59	GLU
1	B	104	LEU
1	B	127	SER
1	B	140	LEU
1	B	159	LEU
1	B	174	ILE
1	B	192	PHE
1	B	203	LEU
1	B	206	LYS
1	B	273	ASN
1	B	294	ARG
1	B	522	THR
1	C	74	LEU
1	C	123	LEU
1	C	170	VAL
1	C	173	LYS
1	C	180	LEU

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Mol	Chain	Res	Type
1	C	202	SER
1	C	205	SER
1	C	294	ARG
1	C	342	ARG
1	C	399	ARG
1	C	401	LEU
1	C	422	LYS
1	C	436	ARG
1	C	447	ARG
1	C	459	THR
1	C	519	SER
1	D	25	THR
1	D	56	ARG
1	D	159	LEU
1	D	163	ASN
1	D	169	GLU
1	D	216	VAL
1	D	253	GLU
1	D	294	ARG
1	D	383	ARG
1	D	390	TYR
1	D	399	ARG
1	D	433	LYS
1	D	459	THR
1	D	521	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	90	ASN
1	A	318	ASN
1	A	379	HIS
1	A	491	ASN
1	B	44	ASN
1	B	90	ASN
1	B	163	ASN
1	B	273	ASN
1	B	378	GLN
1	C	90	ASN
1	C	187	GLN
1	C	274	HIS

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Mol	Chain	Res	Type
1	C	378	GLN
1	C	379	HIS
1	D	90	ASN
1	D	274	HIS
1	D	318	ASN
1	D	378	GLN
1	D	379	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	PHE	B	602	-	11,12,12	0.76	1 (9%)	14,15,15	0.75	0
3	PHE	D	602	-	11,12,12	0.71	1 (9%)	14,15,15	0.75	1 (7%)
3	PHE	A	602	-	11,12,12	0.73	0	14,15,15	0.69	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PHE	B	602	-	-	0/8/8/8	0/1/1/1
3	PHE	D	602	-	-	1/8/8/8	0/1/1/1
3	PHE	A	602	-	-	2/8/8/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	PHE	OXT-C	-2.15	1.23	1.30
3	D	602	PHE	OXT-C	-2.03	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	602	PHE	OXT-C-O	-2.09	119.35	124.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	PHE	C-CA-CB-CG
3	A	602	PHE	N-CA-CB-CG
3	D	602	PHE	O-C-CA-N

There are no ring outliers.

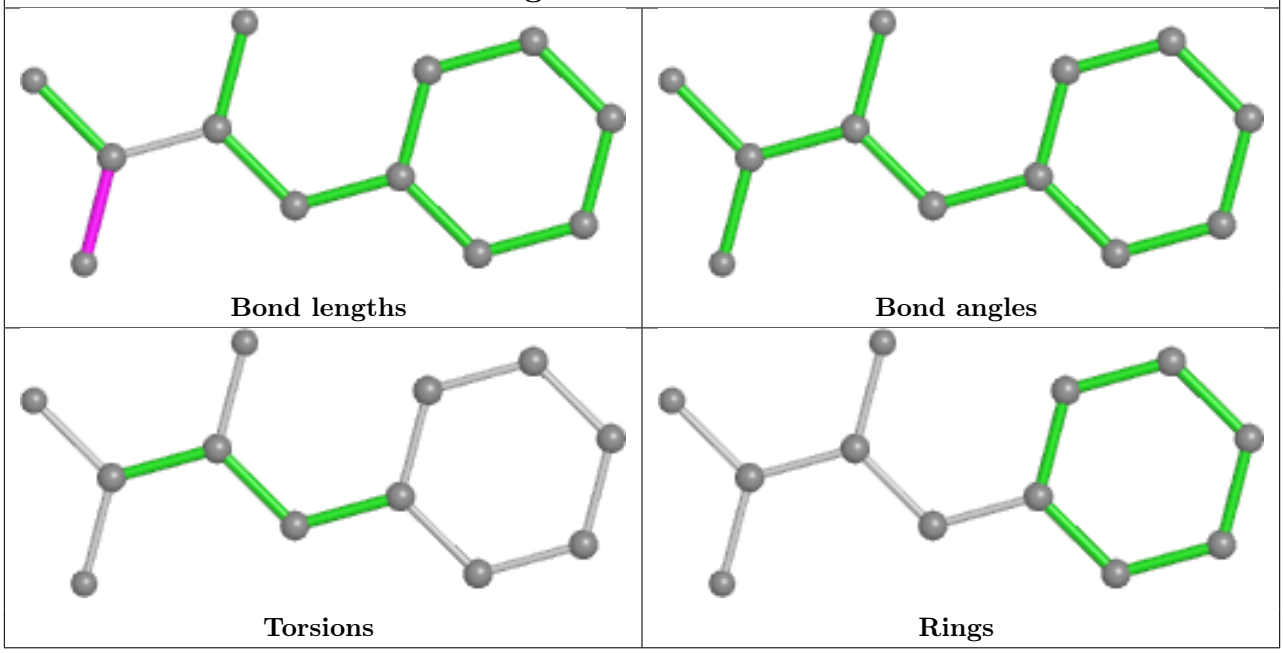
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	PHE	1	0
3	A	602	PHE	1	0

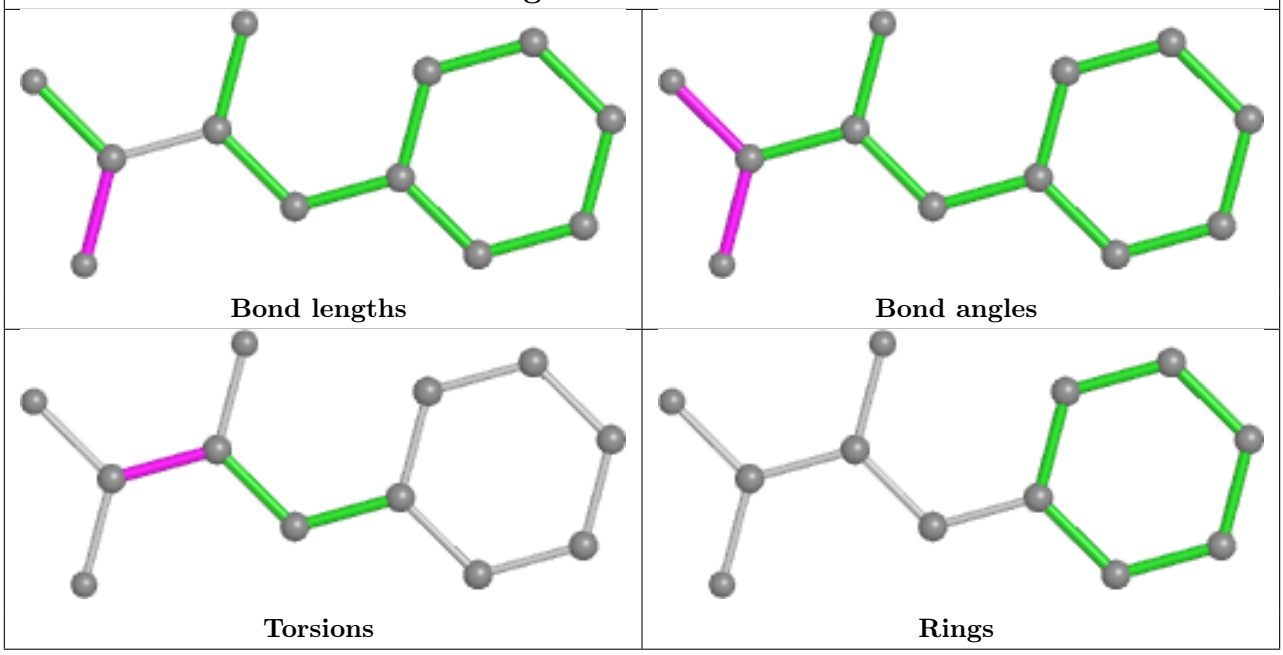
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

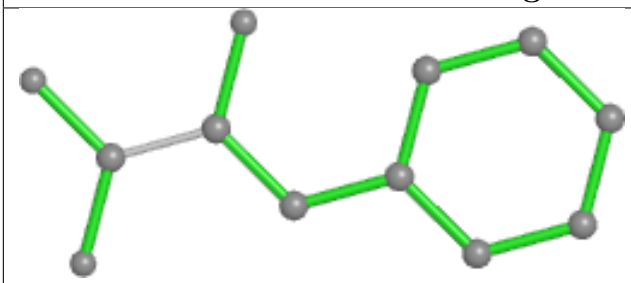
Ligand PHE B 602



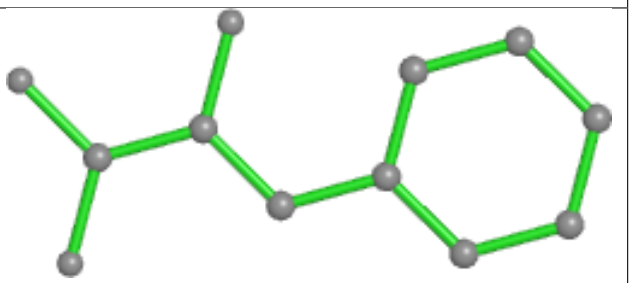
Ligand PHE D 602



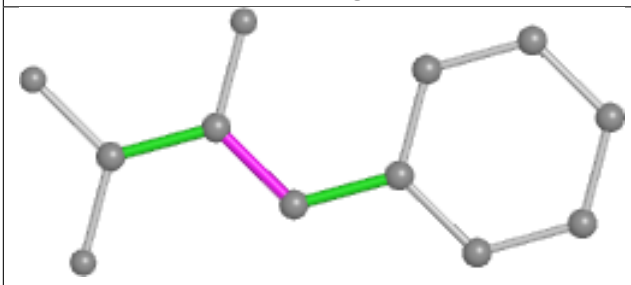
Ligand PHE A 602



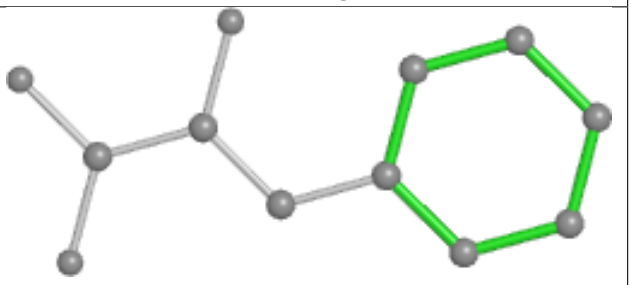
Bond lengths



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	508/531 (95%)	-0.01	14 (2%)	55	54	25, 41, 70, 121	0
1	B	499/531 (93%)	0.14	34 (6%)	25	24	24, 38, 123, 150	0
1	C	504/531 (94%)	0.23	25 (4%)	35	34	27, 45, 93, 133	0
1	D	503/531 (94%)	0.27	30 (5%)	29	28	26, 45, 101, 143	0
All	All	2014/2124 (94%)	0.16	103 (5%)	34	34	24, 42, 102, 150	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	138	ALA	5.5
1	C	130	ALA	4.7
1	B	167	VAL	4.3
1	D	404	ILE	4.3
1	B	147	ALA	4.1
1	B	124	ILE	4.1
1	B	142	ILE	3.9
1	A	129	THR	3.9
1	A	128	GLY	3.8
1	D	137	GLY	3.8
1	C	190	ALA	3.6
1	D	521	PHE	3.6
1	D	124	ILE	3.5
1	B	180	LEU	3.5
1	B	303	ALA	3.5
1	B	521	PHE	3.4
1	D	405	ALA	3.4
1	B	170	VAL	3.4
1	B	144	LEU	3.4
1	B	139	THR	3.3
1	A	406	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	125	LYS	3.3
1	A	403	PRO	3.2
1	C	124	ILE	3.2
1	D	135	LYS	3.1
1	C	402	ALA	3.1
1	C	203	LEU	3.1
1	C	126	GLY	3.1
1	B	138	ALA	3.0
1	D	522	THR	3.0
1	D	403	PRO	3.0
1	C	406	ALA	3.0
1	A	40	ILE	3.0
1	A	130	ALA	3.0
1	D	303	ALA	2.9
1	B	126	GLY	2.9
1	B	186	LYS	2.9
1	D	406	ALA	2.8
1	B	197	VAL	2.8
1	D	40	ILE	2.7
1	B	178	ASP	2.7
1	B	123	LEU	2.7
1	B	157	LEU	2.7
1	A	22	MET	2.7
1	D	220	ALA	2.7
1	C	179	GLY	2.7
1	C	212	PRO	2.7
1	C	22	MET	2.7
1	C	177	ASP	2.7
1	B	140	LEU	2.6
1	C	521	PHE	2.6
1	C	180	LEU	2.6
1	D	123	LEU	2.6
1	B	179	GLY	2.6
1	D	189	GLY	2.6
1	D	192	PHE	2.6
1	D	131	GLU	2.6
1	A	402	ALA	2.5
1	B	153	ASP	2.5
1	B	135	LYS	2.5
1	C	204	GLY	2.5
1	C	519	SER	2.5
1	C	125	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	134	LEU	2.5
1	B	406	ALA	2.5
1	D	148	TYR	2.4
1	C	218	LEU	2.4
1	C	401	LEU	2.4
1	D	408	PRO	2.4
1	B	148	TYR	2.4
1	B	40	ILE	2.4
1	A	23	ALA	2.4
1	D	215	ALA	2.4
1	C	135	LYS	2.4
1	B	168	VAL	2.4
1	A	126	GLY	2.3
1	D	207	LYS	2.3
1	C	165	CYS	2.3
1	B	175	TYR	2.3
1	D	193	LEU	2.3
1	B	190	ALA	2.3
1	D	147	ALA	2.3
1	C	178	ASP	2.2
1	B	158	TRP	2.2
1	B	152	CYS	2.2
1	D	125	LYS	2.2
1	B	201	GLY	2.2
1	A	401	LEU	2.2
1	B	192	PHE	2.1
1	C	123	LEU	2.1
1	C	170	VAL	2.1
1	A	400	ARG	2.1
1	A	519	SER	2.1
1	D	175	TYR	2.1
1	C	199	ASN	2.1
1	D	157	LEU	2.1
1	D	190	ALA	2.1
1	A	162	LYS	2.1
1	D	517	PRO	2.0
1	B	185	VAL	2.0
1	C	132	VAL	2.0
1	D	159	LEU	2.0
1	B	219	PRO	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)

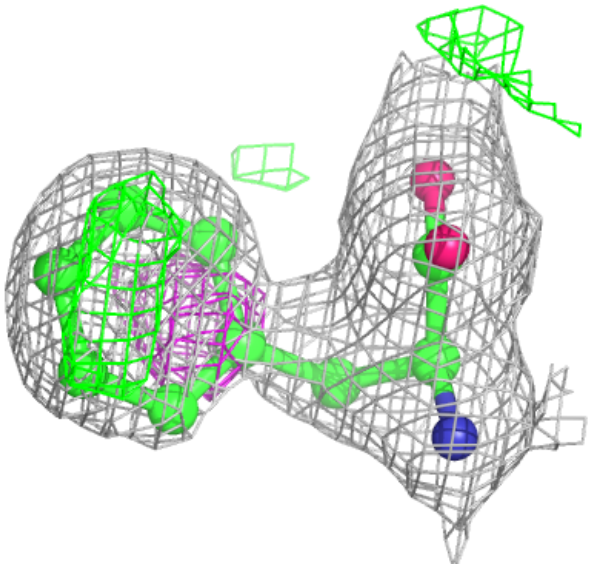
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

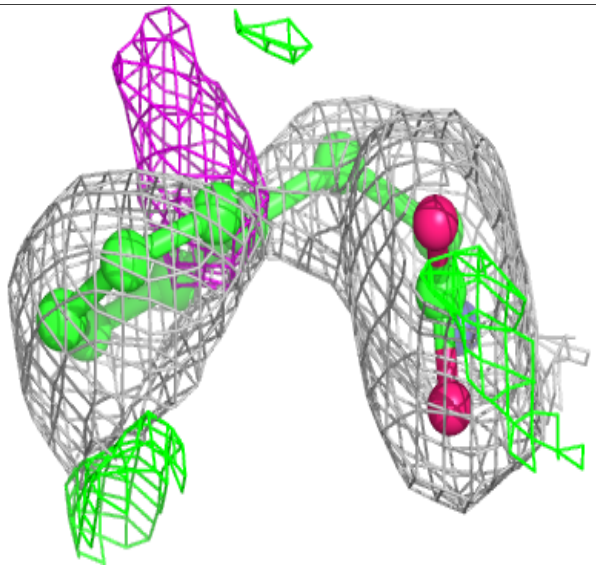
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PHE	A	602	12/12	0.91	0.12	33,39,49,50	0
3	PHE	D	602	12/12	0.92	0.09	32,35,40,42	0
3	PHE	B	602	12/12	0.93	0.09	30,32,36,37	0
2	K	B	601	1/1	0.98	0.14	44,44,44,44	0
2	K	A	601	1/1	0.99	0.04	35,35,35,35	0
2	K	C	601	1/1	0.99	0.13	36,36,36,36	0
2	K	D	601	1/1	0.99	0.09	44,44,44,44	0

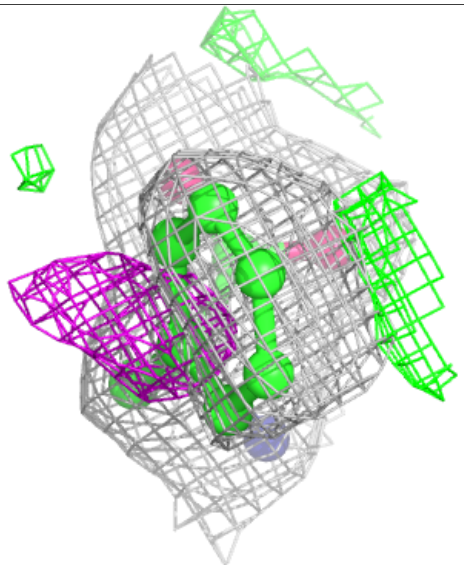
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PHE A 602:

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

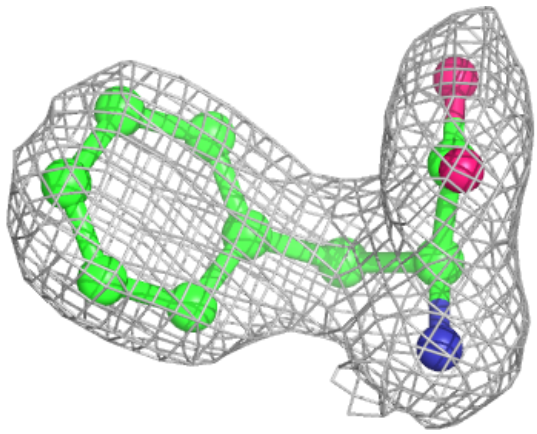


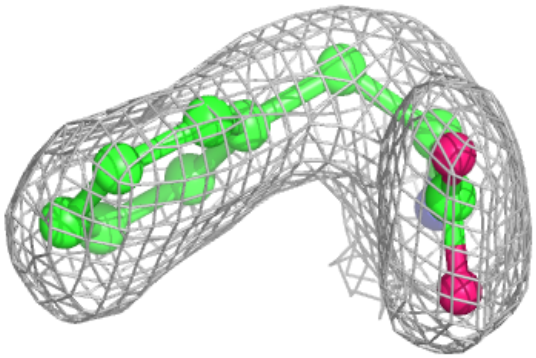


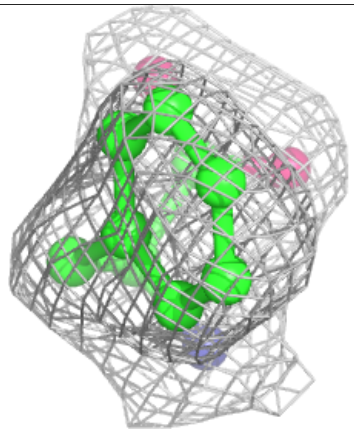


Electron density around PHE D 602:

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

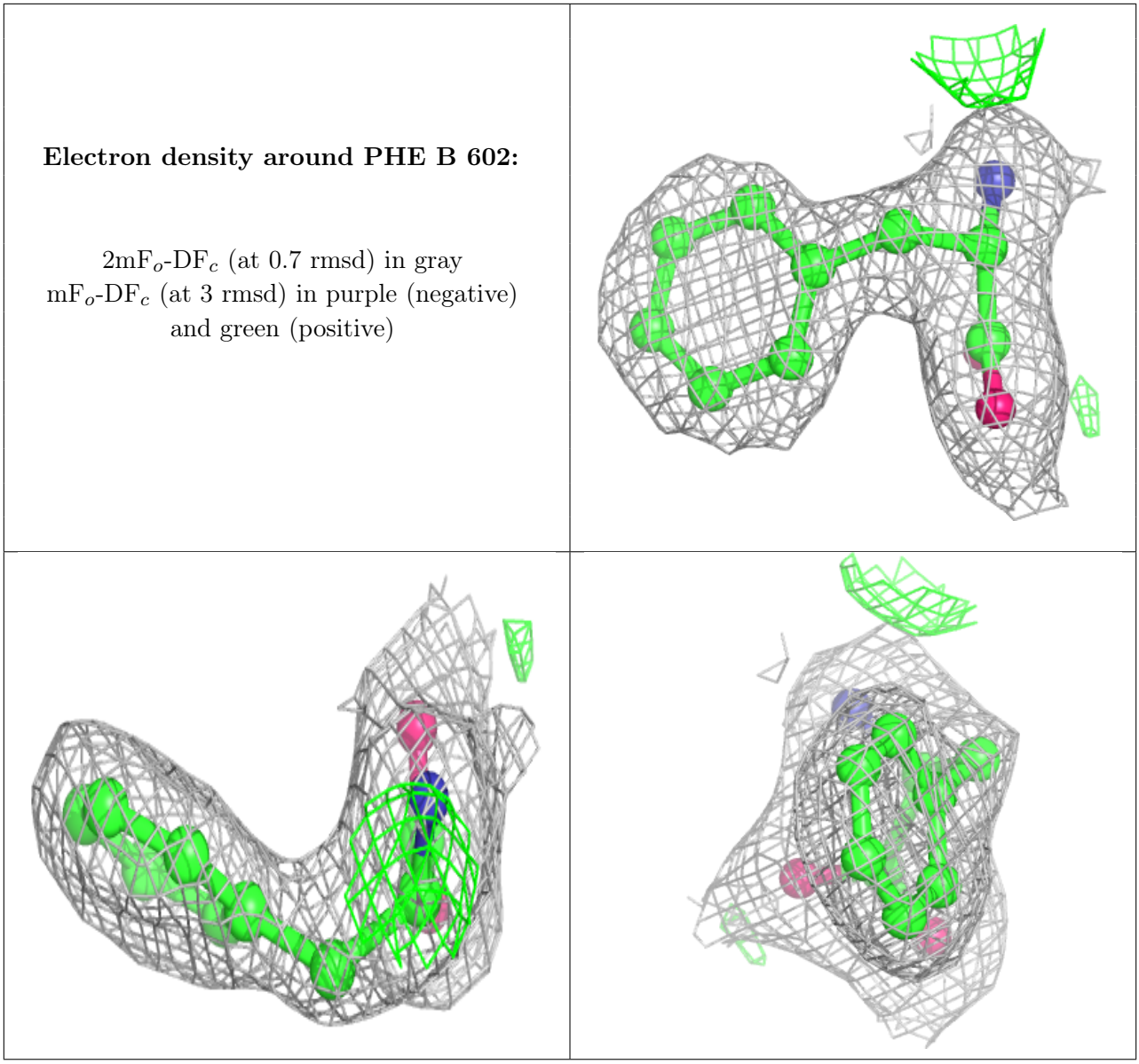






Electron density around PHE B 602:

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



6.5 Other polymers

There are no such residues in this entry.