



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:04 AM UTC

PDB ID : 6YVT / pdb_00006yvt
Title : HIF prolyl hydroxylase 2 (PHD2/ EGLN1) in complex with MD-253
Authors : Chowdhury, R.; Demetriades, M.; Schofield, C.J.
Deposited on : 2020-04-28
Resolution : 2.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

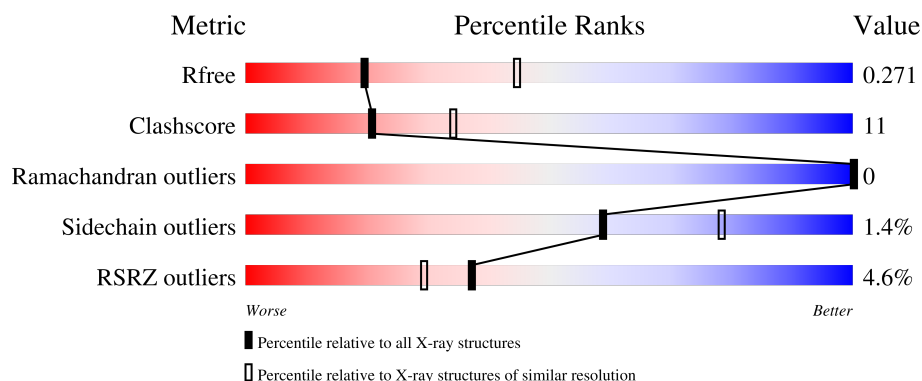
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	252	4% 60%18%22%
1	B	252	4% 62%16%21%
1	C	252	3% 63%14%22%
1	D	252	3% 59%19%21%
1	E	252	4% 59%18%23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	252	3% 60% 18% • 22%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 18029 atoms, of which 8671 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 Egl nine homolog 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	197	Total	C	H	N	O	S	0	0	0
			2877	949	1383	258	276	11			
1	B	199	Total	C	H	N	O	S	0	2	0
			3028	986	1472	272	287	11			
1	C	196	Total	C	H	N	O	S	0	0	0
			2946	960	1432	265	278	11			
1	D	199	Total	C	H	N	O	S	0	0	0
			3007	981	1461	270	284	11			
1	E	194	Total	C	H	N	O	S	0	0	0
			2934	959	1427	260	277	11			
1	F	197	Total	C	H	N	O	S	0	0	0
			2909	954	1398	263	283	11			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	175	GLY	-	expression tag	UNP Q9GZT9
A	176	SER	-	expression tag	UNP Q9GZT9
A	177	HIS	-	expression tag	UNP Q9GZT9
A	178	MET	-	expression tag	UNP Q9GZT9
A	179	ALA	-	expression tag	UNP Q9GZT9
A	180	SER	-	expression tag	UNP Q9GZT9
B	175	GLY	-	expression tag	UNP Q9GZT9
B	176	SER	-	expression tag	UNP Q9GZT9
B	177	HIS	-	expression tag	UNP Q9GZT9
B	178	MET	-	expression tag	UNP Q9GZT9
B	179	ALA	-	expression tag	UNP Q9GZT9
B	180	SER	-	expression tag	UNP Q9GZT9
C	175	GLY	-	expression tag	UNP Q9GZT9
C	176	SER	-	expression tag	UNP Q9GZT9
C	177	HIS	-	expression tag	UNP Q9GZT9
C	178	MET	-	expression tag	UNP Q9GZT9
C	179	ALA	-	expression tag	UNP Q9GZT9

Continued on next page...

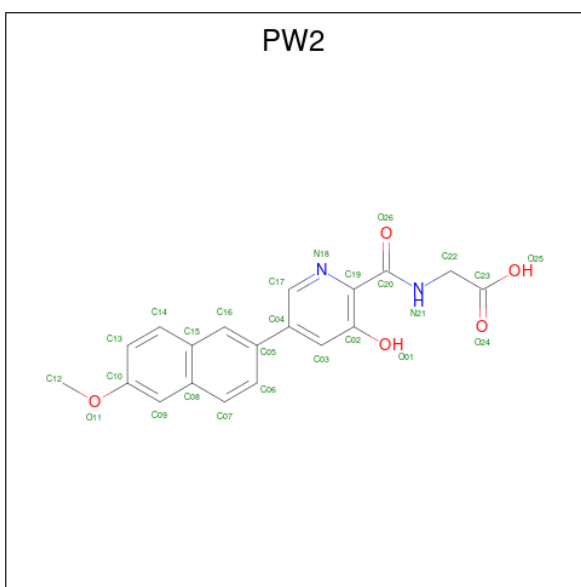
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	180	SER	-	expression tag	UNP Q9GZT9
D	175	GLY	-	expression tag	UNP Q9GZT9
D	176	SER	-	expression tag	UNP Q9GZT9
D	177	HIS	-	expression tag	UNP Q9GZT9
D	178	MET	-	expression tag	UNP Q9GZT9
D	179	ALA	-	expression tag	UNP Q9GZT9
D	180	SER	-	expression tag	UNP Q9GZT9
E	175	GLY	-	expression tag	UNP Q9GZT9
E	176	SER	-	expression tag	UNP Q9GZT9
E	177	HIS	-	expression tag	UNP Q9GZT9
E	178	MET	-	expression tag	UNP Q9GZT9
E	179	ALA	-	expression tag	UNP Q9GZT9
E	180	SER	-	expression tag	UNP Q9GZT9
F	175	GLY	-	expression tag	UNP Q9GZT9
F	176	SER	-	expression tag	UNP Q9GZT9
F	177	HIS	-	expression tag	UNP Q9GZT9
F	178	MET	-	expression tag	UNP Q9GZT9
F	179	ALA	-	expression tag	UNP Q9GZT9
F	180	SER	-	expression tag	UNP Q9GZT9

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0

- Molecule 3 is 2-[[5-(6-methoxynaphthalen-2-yl)-3-oxidanyl-pyridin-2-yl]carbonylamino]ethanoic acid (CCD ID: PW2) (formula: C₁₉H₁₆N₂O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 41	C 19	H 15	N 2	O 5	0	0
3	B	1	Total 41	C 19	H 15	N 2	O 5	0	0
3	C	1	Total 41	C 19	H 15	N 2	O 5	0	0
3	D	1	Total 41	C 19	H 15	N 2	O 5	0	0
3	E	1	Total 41	C 19	H 15	N 2	O 5	0	0
3	F	1	Total 41	C 19	H 15	N 2	O 5	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	O	S	0	0
			5	4	1		

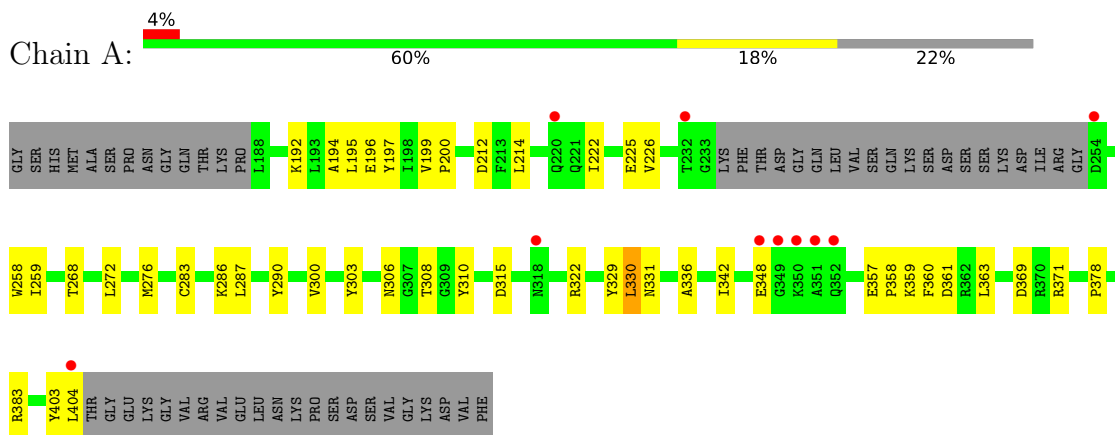
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total 6	O 6	0	0
6	B	7	Total 7	O 7	0	0
6	C	9	Total 9	O 9	0	0
6	D	13	Total 13	O 13	0	0
6	E	14	Total 14	O 14	0	0
6	F	8	Total 8	O 8	0	0

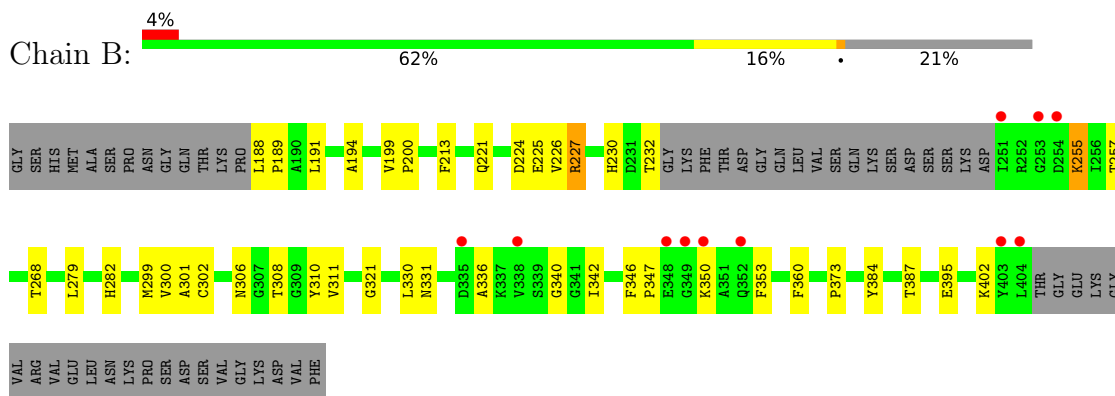
3 Residue-property plots [i](#)

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.

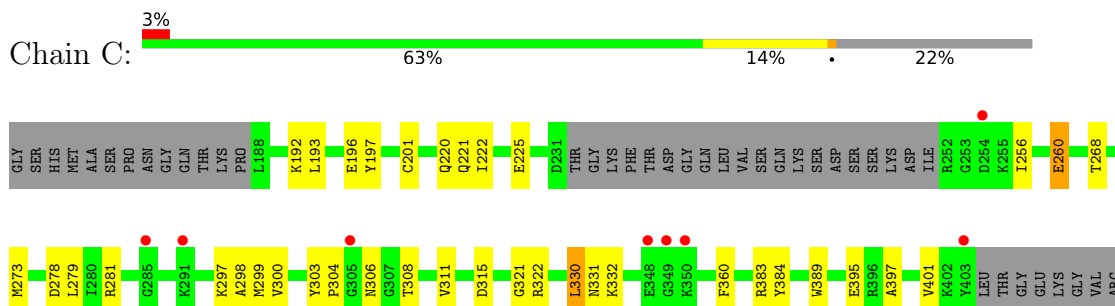
- Molecule 1: Egl nine homolog 1



- Molecule 1: Egl nine homolog 1



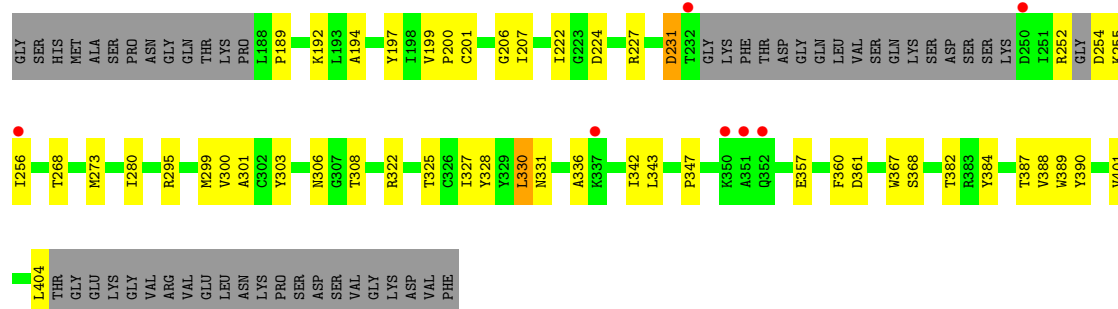
- Molecule 1: Egl nine homolog 1



VAL
GLU
LEU
ASN
MET
LYS
PRO
SER
ASP
GLY
VAL
GLY
LYS
ASP
VAL
PHE

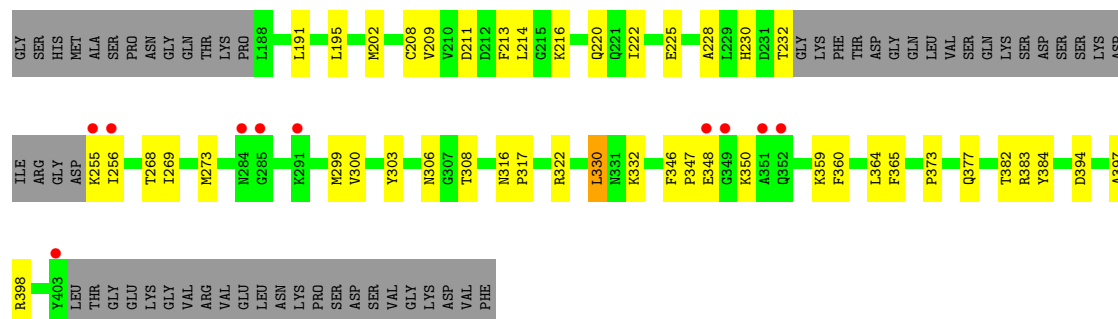
• Molecule 1: Egl nine homolog 1

Chain D: 3% 59% 19% 21%



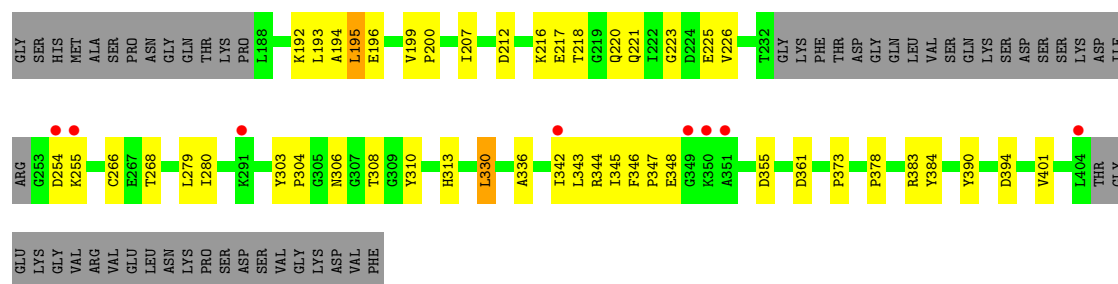
• Molecule 1: Egl nine homolog 1

Chain E: 4% 59% 18% 23%



• Molecule 1: Egl nine homolog 1

Chain F: 3% 60% 18% 22%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.46Å 103.02Å 196.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.75 – 2.85 23.75 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (23.75-2.85) 99.2 (23.75-2.85)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.84Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.237 , 0.266 0.240 , 0.271	Depositor DCC
R_{free} test set	2043 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtrriage
Anisotropy	0.213	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18029	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.45 % 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 8.6664e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, PW2, SO4, GOL

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	0.22	0/1530	0.48	0/2082
1	B	0.22	0/1598	0.47	0/2166
1	C	0.22	0/1550	0.49	0/2103
1	D	0.24	0/1582	0.49	0/2145
1	E	0.21	0/1544	0.48	0/2096
1	F	0.22	0/1547	0.48	0/2104
All	All	0.22	0/9351	0.48	0/12696

There are no bond length outliers.

There are no bond angle outliers.

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	1494	1383	1383	33	0
1	B	1556	1472	1467	31	0
1	C	1514	1432	1433	23	0
1	D	1546	1461	1460	41	0
1	E	1507	1427	1432	39	0
1	F	1511	1398	1399	35	0
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	26	15	0	1	0
3	B	26	15	0	1	0
3	C	26	15	0	4	0
3	D	26	15	0	3	0
3	E	26	15	0	2	0
3	F	26	15	0	1	0
4	E	6	8	8	2	0
5	E	5	0	0	1	0
6	A	6	0	0	0	0
6	B	7	0	0	1	0
6	C	9	0	0	0	0
6	D	13	0	0	1	0
6	E	14	0	0	2	0
6	F	8	0	0	0	0
All	All	9358	8671	8582	199	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 11.

All (199) 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:F:306:ASN:OD1	1:F:308:THR:HG23	1.68	0.94
1:A:336:ALA:HB1	1:A:342:ILE:HD11	1.56	0.85
1:C:306:ASN:OD1	1:C:308:THR:HG23	1.77	0.84
1:D:330:LEU:HD11	1:D:384:TYR:HB2	1.65	0.79
1:D:330:LEU:HD11	1:D:384:TYR:CB	2.14	0.77
1:E:306:ASN:OD1	1:E:308:THR:HG23	1.85	0.77
1:B:299:MET:HE3	1:B:301:ALA:HB2	1.66	0.76
3:C:502:PW2:C06	1:D:401:VAL:HG22	2.16	0.75
1:C:278:ASP:OD1	1:C:281:ARG:NH1	2.21	0.74
1:F:254:ASP:OD1	1:F:255:LYS:N	2.21	0.73
1:C:256:ILE:HA	1:C:300:VAL:O	1.88	0.73
1:E:211:ASP:N	4:E:503:GOL:O1	2.20	0.73
1:C:220:GLN:OE1	1:C:332:LYS:NZ	2.21	0.73
1:D:207:ILE:HD11	1:D:347:PRO:HG3	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:HIS:ND1	1:E:384:TYR:OH	2.22	0.71
1:F:194:ALA:O	1:F:199:VAL:HG23	1.92	0.69
1:B:321:GLY:N	1:B:395:GLU:OE2	2.27	0.67
1:D:325:THR:HG1	1:D:368:SER:HG	1.37	0.67
1:D:255:LYS:NZ	6:D:601:HOH:O	2.27	0.66
1:E:330:LEU:HD11	1:E:384:TYR:HB2	1.78	0.64
1:D:306:ASN:OD1	1:D:308:THR:HG23	1.98	0.64
1:F:336:ALA:HB1	1:F:342:ILE:HD11	1.80	0.63
1:B:336:ALA:HB1	1:B:342:ILE:HD11	1.79	0.62
1:B:224:ASP:OD1	1:B:227[B]:ARG:NH2	2.33	0.62
1:E:228:ALA:O	1:E:232:THR:HG23	2.00	0.62
1:D:194:ALA:O	1:D:199:VAL:HG23	2.01	0.60
1:D:330:LEU:CD1	1:D:384:TYR:HB2	2.30	0.60
1:F:342:ILE:HG21	1:F:355:ASP:HB3	1.83	0.60
1:D:222:ILE:CG1	1:D:268:THR:HG22	2.31	0.60
1:B:330:LEU:HD11	1:B:384:TYR:CB	2.31	0.60
1:E:222:ILE:HG12	1:E:268:THR:HG22	1.82	0.60
1:A:329:TYR:C	1:A:330:LEU:HD23	2.26	0.60
1:F:195:LEU:HD13	1:F:199:VAL:HG21	1.82	0.60
1:E:359:LYS:NZ	5:E:504:SO4:O1	2.24	0.59
1:C:193:LEU:HD23	1:C:279:LEU:HD21	1.83	0.59
1:D:330:LEU:HD11	1:D:384:TYR:HB3	1.85	0.59
1:E:222:ILE:CG1	1:E:268:THR:HG22	2.33	0.58
1:A:222:ILE:CG1	1:A:268:THR:HG22	2.32	0.58
1:D:231:ASP:C	1:D:231:ASP:OD1	2.47	0.58
1:E:330:LEU:HD11	1:E:384:TYR:CB	2.33	0.58
1:B:306:ASN:OD1	1:B:308:THR:HG23	2.03	0.58
1:C:304:PRO:HD2	1:C:308:THR:HG21	1.85	0.57
1:D:343:LEU:HD13	3:D:502:PW2:C22	2.33	0.57
1:E:256:ILE:HA	1:E:300:VAL:O	2.05	0.57
1:F:225:GLU:CD	1:F:268:THR:OG1	2.47	0.57
1:F:216:LYS:O	1:F:220:GLN:HG3	2.05	0.57
1:C:321:GLY:N	1:C:395:GLU:OE2	2.33	0.57
1:D:222:ILE:HG12	1:D:268:THR:HG22	1.87	0.56
1:B:330:LEU:HD11	1:B:384:TYR:HB3	1.87	0.56
1:A:310:TYR:OH	1:C:397:ALA:O	2.20	0.55
1:B:347:PRO:HB2	1:B:350:LYS:HG2	1.89	0.55
1:D:207:ILE:CD1	1:D:347:PRO:HG3	2.36	0.55
1:A:222:ILE:HG13	1:A:268:THR:HG22	1.89	0.54
1:E:303:TYR:HB2	1:E:383:ARG:HB3	1.89	0.54
1:F:303:TYR:HB2	1:F:383:ARG:HB3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:ASP:OD1	1:D:227:ARG:NH2	2.40	0.54
1:D:336:ALA:HB1	1:D:342:ILE:HG13	1.89	0.54
1:D:273:MET:HE2	1:D:295:ARG:NH2	2.23	0.53
1:D:299:MET:HE3	1:D:301:ALA:HB2	1.90	0.53
1:A:192:LYS:HE2	1:A:196:GLU:OE1	2.09	0.53
1:D:327:ILE:HG12	1:D:387:THR:HG23	1.91	0.53
1:B:346:PHE:O	1:B:373:PRO:HD2	2.08	0.53
3:A:502:PW2:N21	3:A:502:PW2:O01	2.42	0.53
1:A:330:LEU:HD23	1:A:330:LEU:N	2.24	0.53
3:B:502:PW2:C06	1:F:401:VAL:HG22	2.39	0.53
1:B:188:LEU:HB3	1:B:189:PRO:CD	2.39	0.52
1:F:348:GLU:O	1:F:348:GLU:CG	2.58	0.52
1:E:211:ASP:HB2	4:E:503:GOL:O1	2.09	0.52
1:E:220:GLN:NE2	1:E:332:LYS:HZ1	2.09	0.51
1:E:330:LEU:CD1	1:E:384:TYR:HB2	2.41	0.51
1:C:299:MET:HE1	3:C:502:PW2:C03	2.41	0.51
1:B:194:ALA:O	1:B:199:VAL:HG23	2.11	0.51
1:A:283:CYS:HB3	1:A:287:LEU:HG	1.93	0.51
1:C:315:ASP:HA	1:D:401:VAL:HG11	1.92	0.51
1:B:311:VAL:HG11	1:F:394:ASP:OD1	2.11	0.51
1:E:225:GLU:CD	1:E:268:THR:HB	2.35	0.51
1:A:357:GLU:HB2	1:A:359:LYS:HG3	1.94	0.50
1:E:397:ALA:O	1:F:310:TYR:OH	2.27	0.50
1:E:191:LEU:HD11	1:E:195:LEU:CD1	2.42	0.50
1:B:331:ASN:O	1:B:360:PHE:HB2	2.12	0.49
1:E:346:PHE:O	1:E:373:PRO:HD2	2.11	0.49
1:E:202:MET:HE1	1:E:365:PHE:HB2	1.93	0.49
1:D:252:ARG:HD3	1:D:254:ASP:O	2.13	0.49
1:D:331:ASN:O	1:D:360:PHE:HB2	2.12	0.49
1:F:225:GLU:CD	1:F:268:THR:HG1	2.20	0.49
1:B:191:LEU:HD12	1:B:282:HIS:HB3	1.94	0.49
1:A:195:LEU:HD21	1:A:286:LYS:HE3	1.94	0.48
1:E:220:GLN:NE2	1:E:332:LYS:NZ	2.61	0.48
1:C:260:GLU:HB2	1:C:297:LYS:HD3	1.95	0.48
1:D:222:ILE:HG13	1:D:268:THR:HG22	1.95	0.48
1:D:252:ARG:CD	1:D:254:ASP:O	2.62	0.48
1:C:222:ILE:HG13	1:C:268:THR:HG22	1.95	0.48
1:D:252:ARG:NH2	1:D:303:TYR:CZ	2.82	0.47
1:A:403:TYR:O	1:A:404:LEU:C	2.57	0.47
1:E:394:ASP:O	1:E:398:ARG:HG3	2.14	0.47
1:B:336:ALA:O	1:B:340:GLY:N	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ILE:HG12	1:A:268:THR:HG22	1.96	0.47
1:F:218:THR:HA	1:F:221:GLN:HG3	1.97	0.47
1:F:308:THR:O	1:F:378:PRO:HA	2.14	0.47
1:D:280:ILE:HG13	1:D:390:TYR:CZ	2.50	0.47
1:A:308:THR:O	1:A:378:PRO:HA	2.15	0.46
1:A:226:VAL:HG21	1:A:330:LEU:CD1	2.45	0.46
1:A:310:TYR:OH	1:C:401:VAL:HG23	2.16	0.46
1:E:348:GLU:O	6:E:601:HOH:O	2.21	0.46
1:E:269:ILE:O	1:E:273:MET:HG3	2.15	0.46
1:F:192:LYS:O	1:F:196:GLU:HB2	2.15	0.46
1:F:345:ILE:O	1:F:347:PRO:HD3	2.15	0.46
1:C:192:LYS:HE3	1:C:196:GLU:OE1	2.15	0.46
1:D:189:PRO:HD2	1:D:192:LYS:HB3	1.98	0.46
1:B:336:ALA:CB	1:B:342:ILE:HD11	2.45	0.46
1:B:310:TYR:OH	1:F:401:VAL:HG23	2.14	0.46
1:A:194:ALA:O	1:A:199:VAL:HG23	2.16	0.46
1:A:303:TYR:HB2	1:A:383:ARG:HB3	1.98	0.46
1:F:348:GLU:O	1:F:348:GLU:HG2	2.16	0.46
1:F:343:LEU:HD21	1:F:345:ILE:HD11	1.97	0.45
1:E:213:PHE:CD2	1:E:214:LEU:HG	2.51	0.45
1:E:216:LYS:O	1:E:220:GLN:HB2	2.16	0.45
1:F:217:GLU:O	1:F:221:GLN:HG3	2.16	0.45
1:E:191:LEU:HD11	1:E:195:LEU:HD12	1.97	0.45
1:F:199:VAL:N	1:F:200:PRO:HD2	2.30	0.45
1:F:225:GLU:OE1	1:F:266:CYS:HA	2.15	0.45
1:C:303:TYR:HB2	1:C:383:ARG:HB3	1.97	0.45
1:E:230:HIS:HA	1:E:255:LYS:CB	2.46	0.45
1:D:303:TYR:O	1:D:382:THR:HA	2.15	0.45
1:D:322:ARG:HD2	1:D:389:TRP:CG	2.52	0.45
1:E:316:ASN:ND2	1:E:322:ARG:O	2.40	0.45
1:F:223:GLY:HA2	1:F:330:LEU:CD1	2.47	0.45
1:A:315:ASP:O	1:A:322:ARG:NH2	2.50	0.45
1:B:387:THR:HG21	6:B:604:HOH:O	2.17	0.45
1:A:369:ASP:OD1	1:A:371:ARG:HB2	2.17	0.45
1:E:202:MET:HE1	1:E:208:CYS:HB3	2.00	0.44
1:C:197:TYR:O	1:C:201:CYS:HB2	2.17	0.44
1:F:344:ARG:NE	1:F:355:ASP:OD1	2.47	0.44
1:D:295:ARG:HD2	1:D:388:VAL:HG11	1.99	0.44
1:A:331:ASN:HD22	1:A:358:PRO:HB2	1.82	0.44
1:B:221:GLN:HB3	1:B:268:THR:HG21	2.00	0.44
1:C:330:LEU:HD11	1:C:384:TYR:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:313:HIS:O	1:F:373:PRO:HA	2.18	0.44
1:A:225:GLU:CD	1:A:268:THR:HB	2.42	0.44
1:D:256:ILE:HA	1:D:300:VAL:O	2.18	0.44
1:B:188:LEU:HB3	1:B:189:PRO:HD2	2.00	0.43
3:D:502:PW2:O01	3:D:502:PW2:N21	2.50	0.43
1:A:199:VAL:HB	1:A:200:PRO:CD	2.49	0.43
1:C:273:MET:HE3	1:C:298:ALA:HB2	2.00	0.43
3:C:502:PW2:C07	1:D:404:LEU:HD13	2.48	0.43
1:F:207:ILE:HD11	1:F:345:ILE:HG21	2.00	0.43
1:C:221:GLN:O	1:C:225:GLU:HG3	2.18	0.43
1:C:330:LEU:HD11	1:C:384:TYR:CB	2.48	0.43
1:A:197:TYR:C	1:A:197:TYR:CD1	2.97	0.43
1:B:336:ALA:HB1	1:B:342:ILE:CD1	2.48	0.43
1:E:377:GLN:OE1	6:E:602:HOH:O	2.21	0.43
1:F:280:ILE:HG13	1:F:390:TYR:CE2	2.54	0.43
1:F:225:GLU:OE1	1:F:268:THR:OG1	2.36	0.43
1:E:299:MET:HE1	3:E:502:PW2:C03	2.48	0.42
1:B:402:LYS:HG3	1:E:317:PRO:CG	2.48	0.42
1:B:199:VAL:N	1:B:200:PRO:HD2	2.34	0.42
1:D:206:GLY:HA2	1:D:367:TRP:NE1	2.34	0.42
1:E:303:TYR:O	1:E:382:THR:HA	2.19	0.42
3:F:502:PW2:O01	3:F:502:PW2:N21	2.52	0.42
1:F:346:PHE:O	1:F:373:PRO:HD2	2.20	0.42
1:D:336:ALA:HB2	1:D:357:GLU:HG2	2.01	0.42
1:A:306:ASN:OD1	1:A:308:THR:HG23	2.19	0.42
1:A:331:ASN:O	1:A:360:PHE:HB2	2.20	0.42
1:D:336:ALA:CB	1:D:342:ILE:HG13	2.50	0.42
1:A:214:LEU:HD11	1:A:272:LEU:HD12	2.01	0.42
1:B:213:PHE:CE1	1:B:279:LEU:HD11	2.55	0.42
1:D:197:TYR:O	1:D:201:CYS:HB2	2.20	0.42
1:D:222:ILE:HG13	1:D:268:THR:CG2	2.50	0.42
1:D:303:TYR:OH	3:D:502:PW2:O01	2.27	0.42
1:B:331:ASN:C	1:B:360:PHE:HB2	2.45	0.41
1:E:347:PRO:HG2	1:E:350:LYS:HE3	2.02	0.41
1:C:331:ASN:O	1:C:360:PHE:HB2	2.20	0.41
3:C:502:PW2:O01	3:C:502:PW2:N21	2.53	0.41
1:A:348:GLU:N	1:A:371:ARG:O	2.50	0.41
1:E:222:ILE:HG13	1:E:268:THR:HG22	2.03	0.41
1:E:209:VAL:HG22	1:E:364:LEU:HD13	2.02	0.41
1:F:193:LEU:HD23	1:F:279:LEU:HD21	2.02	0.41
1:A:258:TRP:O	1:A:259:ILE:HD13	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:VAL:HG13	1:B:300:VAL:CG1	2.51	0.41
1:C:322:ARG:HD2	1:C:389:TRP:CG	2.55	0.41
1:D:328:TYR:OH	1:D:361:ASP:OD1	2.20	0.41
1:F:304:PRO:HD2	1:F:308:THR:HG21	2.03	0.41
1:A:226:VAL:HG13	1:A:300:VAL:HG11	2.02	0.41
1:B:225:GLU:OE2	1:B:268:THR:OG1	2.25	0.41
1:B:255:LYS:HE3	1:B:302:CYS:HB3	2.03	0.41
1:C:256:ILE:HG13	1:C:300:VAL:O	2.21	0.41
1:E:306:ASN:OD1	1:E:306:ASN:C	2.64	0.41
1:A:199:VAL:HB	1:A:200:PRO:HD3	2.03	0.41
1:A:212:ASP:HA	1:A:361:ASP:OD2	2.20	0.41
1:D:199:VAL:N	1:D:200:PRO:HD2	2.36	0.41
1:F:212:ASP:HA	1:F:361:ASP:OD2	2.21	0.41
1:A:290:TYR:OH	1:A:371:ARG:NH2	2.54	0.40
1:A:276:MET:HE2	1:A:363:LEU:HD11	2.02	0.40
1:B:226:VAL:HG13	1:B:300:VAL:HG11	2.04	0.40
1:F:226:VAL:CG1	1:F:384:TYR:CD1	3.05	0.40
1:B:353:PHE:CD1	1:B:353:PHE:C	3.00	0.40
1:E:216:LYS:HA	1:E:360:PHE:HE2	1.86	0.40
1:E:383:ARG:NH2	3:E:502:PW2:O24	2.44	0.40

There are no symmetry-related clashes.

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	193/252 (77%)	184 (95%)	9 (5%)	0	100	100
1	B	197/252 (78%)	193 (98%)	4 (2%)	0	100	100
1	C	192/252 (76%)	189 (98%)	3 (2%)	0	100	100
1	D	193/252 (77%)	189 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	190/252 (75%)	187 (98%)	3 (2%)	0	100	100
1	F	193/252 (77%)	181 (94%)	12 (6%)	0	100	100
All	All	1158/1512 (77%)	1123 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	145/211 (69%)	144 (99%)	1 (1%)	76	88
1	B	156/211 (74%)	151 (97%)	5 (3%)	34	59
1	C	152/211 (72%)	149 (98%)	3 (2%)	48	72
1	D	155/211 (74%)	153 (99%)	2 (1%)	61	79
1	E	153/211 (72%)	152 (99%)	1 (1%)	76	88
1	F	150/211 (71%)	148 (99%)	2 (1%)	61	79
All	All	911/1266 (72%)	897 (98%)	14 (2%)	59	77

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	330	LEU
1	B	227[A]	ARG
1	B	227[B]	ARG
1	B	230	HIS
1	B	255	LYS
1	B	257	THR
1	C	260	GLU
1	C	311	VAL
1	C	330	LEU
1	D	231	ASP
1	D	330	LEU
1	E	330	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	195	LEU
1	F	330	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	372	ASN
1	B	205	HIS
1	B	377	GLN
1	C	318	ASN
1	E	220	GLN
1	E	318	ASN
1	E	377	GLN

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 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	PW2	A	502	2	28,28,28	1.45	1 (3%)	36,39,39	1.67	6 (16%)
5	SO4	E	504	-	4,4,4	0.24	0	6,6,6	0.09	0
3	PW2	E	502	2	28,28,28	1.51	2 (7%)	36,39,39	1.41	5 (13%)
3	PW2	F	502	2	28,28,28	1.47	3 (10%)	36,39,39	1.60	7 (19%)
3	PW2	D	502	2	28,28,28	1.41	2 (7%)	36,39,39	1.84	8 (22%)
3	PW2	B	502	2	28,28,28	1.47	3 (10%)	36,39,39	1.60	6 (16%)
4	GOL	E	503	-	5,5,5	0.09	0	5,5,5	0.23	0
3	PW2	C	502	2	28,28,28	1.44	3 (10%)	36,39,39	1.45	6 (16%)

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	PW2	A	502	2	-	4/15/24/24	0/3/3/3
3	PW2	E	502	2	-	4/15/24/24	0/3/3/3
3	PW2	F	502	2	-	6/15/24/24	0/3/3/3
3	PW2	D	502	2	-	6/15/24/24	0/3/3/3
3	PW2	B	502	2	-	4/15/24/24	0/3/3/3
4	GOL	E	503	-	-	0/4/4/4	-
3	PW2	C	502	2	-	6/15/24/24	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	502	PW2	C20-N21	5.15	1.45	1.33
3	A	502	PW2	C20-N21	5.08	1.45	1.33
3	F	502	PW2	C20-N21	5.06	1.44	1.33
3	B	502	PW2	C20-N21	4.96	1.44	1.33
3	D	502	PW2	C20-N21	4.86	1.44	1.33
3	C	502	PW2	C20-N21	4.85	1.44	1.33
3	B	502	PW2	O26-C20	-2.09	1.18	1.23
3	D	502	PW2	O26-C20	-2.09	1.18	1.23
3	B	502	PW2	O01-C02	2.09	1.40	1.36
3	E	502	PW2	O01-C02	2.06	1.40	1.36
3	F	502	PW2	O26-C20	-2.04	1.18	1.23
3	F	502	PW2	O01-C02	2.02	1.40	1.36
3	C	502	PW2	C08-C15	-2.01	1.37	1.42
3	C	502	PW2	O01-C02	2.00	1.40	1.36

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	PW2	C04-C03-C02	-5.42	116.32	120.72
3	A	502	PW2	C04-C03-C02	-4.71	116.90	120.72
3	B	502	PW2	C04-C03-C02	-4.29	117.24	120.72
3	B	502	PW2	C19-C20-N21	4.17	119.82	115.65
3	C	502	PW2	C04-C03-C02	-4.15	117.35	120.72
3	F	502	PW2	C04-C03-C02	-4.11	117.39	120.72
3	D	502	PW2	C19-C20-N21	4.10	119.74	115.65
3	F	502	PW2	C19-C20-N21	4.01	119.66	115.65
3	E	502	PW2	C19-C20-N21	3.76	119.41	115.65
3	D	502	PW2	C03-C04-C17	3.65	121.01	117.10
3	E	502	PW2	C04-C03-C02	-3.53	117.86	120.72
3	A	502	PW2	C03-C04-C17	3.51	120.87	117.10
3	B	502	PW2	C03-C04-C17	3.13	120.45	117.10
3	A	502	PW2	C06-C05-C04	-3.11	115.89	121.25
3	C	502	PW2	C19-C20-N21	3.07	118.72	115.65
3	A	502	PW2	C20-C19-N18	2.88	120.96	115.81
3	D	502	PW2	C17-C04-C05	-2.82	116.86	121.62
3	E	502	PW2	C17-N18-C19	2.76	122.67	117.92
3	A	502	PW2	C04-C17-N18	-2.65	120.07	124.28
3	A	502	PW2	C03-C04-C05	-2.63	116.43	120.84
3	B	502	PW2	C04-C17-N18	-2.61	120.14	124.28
3	C	502	PW2	C23-C22-N21	-2.57	105.08	113.06
3	F	502	PW2	C03-C04-C17	2.55	119.83	117.10
3	B	502	PW2	O11-C10-C09	-2.45	117.51	124.40
3	D	502	PW2	C04-C17-N18	-2.45	120.38	124.28
3	E	502	PW2	C04-C17-N18	-2.43	120.41	124.28
3	F	502	PW2	C04-C17-N18	-2.41	120.45	124.28
3	C	502	PW2	C03-C04-C17	2.41	119.68	117.10
3	F	502	PW2	C06-C05-C04	-2.39	117.12	121.25
3	F	502	PW2	C17-N18-C19	2.33	121.94	117.92
3	C	502	PW2	C17-N18-C19	2.29	121.86	117.92
3	C	502	PW2	C04-C17-N18	-2.24	120.72	124.28
3	B	502	PW2	C17-N18-C19	2.23	121.76	117.92
3	E	502	PW2	C03-C04-C17	2.20	119.45	117.10
3	D	502	PW2	C06-C05-C16	2.19	121.67	118.03
3	D	502	PW2	C12-O11-C10	-2.12	112.95	117.50
3	D	502	PW2	O11-C10-C09	-2.12	118.45	124.40
3	F	502	PW2	C23-C22-N21	-2.11	106.50	113.06

There are no chirality outliers.

All (30) torsion outliers are listed below:

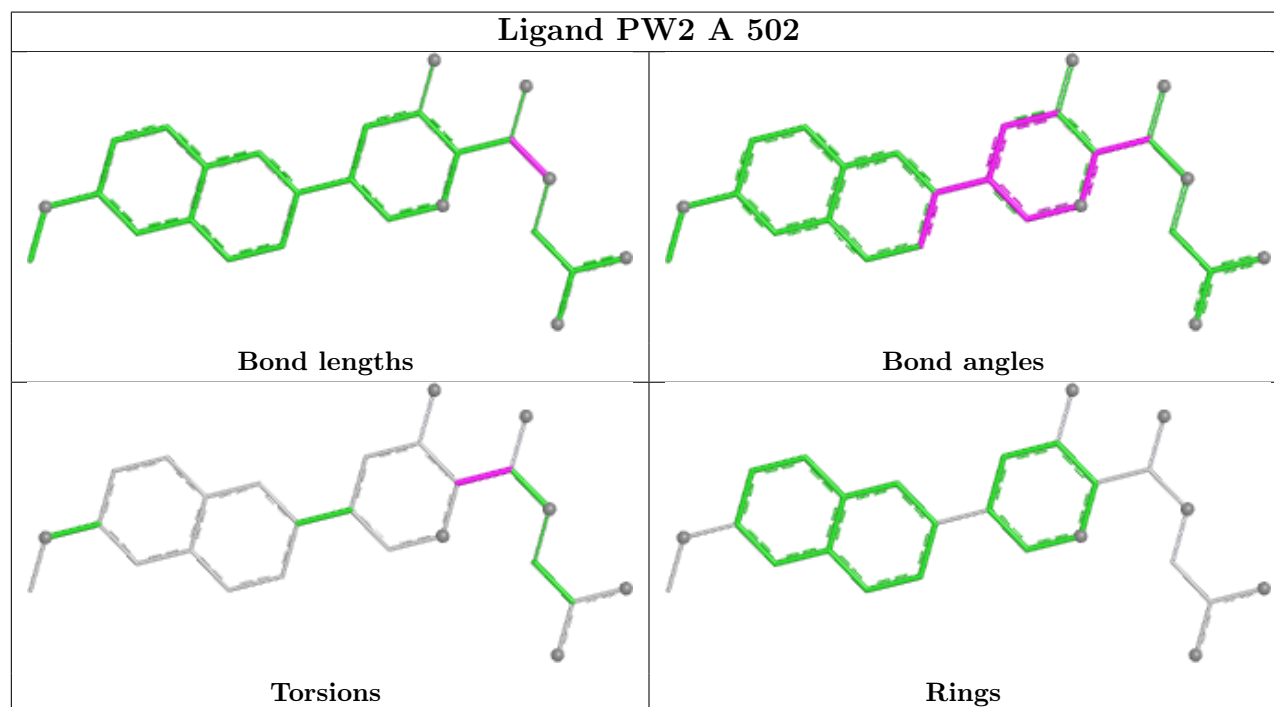
Mol	Chain	Res	Type	Atoms
3	A	502	PW2	C02-C19-C20-N21
3	A	502	PW2	N18-C19-C20-N21
3	A	502	PW2	N18-C19-C20-O26
3	D	502	PW2	C13-C10-O11-C12
3	C	502	PW2	C13-C10-O11-C12
3	D	502	PW2	C09-C10-O11-C12
3	C	502	PW2	C09-C10-O11-C12
3	F	502	PW2	C13-C10-O11-C12
3	F	502	PW2	C09-C10-O11-C12
3	B	502	PW2	N18-C19-C20-O26
3	C	502	PW2	N18-C19-C20-O26
3	D	502	PW2	N18-C19-C20-O26
3	E	502	PW2	N18-C19-C20-O26
3	F	502	PW2	N18-C19-C20-O26
3	B	502	PW2	N18-C19-C20-N21
3	C	502	PW2	N18-C19-C20-N21
3	D	502	PW2	N18-C19-C20-N21
3	E	502	PW2	N18-C19-C20-N21
3	F	502	PW2	N18-C19-C20-N21
3	B	502	PW2	C02-C19-C20-N21
3	C	502	PW2	C02-C19-C20-N21
3	D	502	PW2	C02-C19-C20-N21
3	E	502	PW2	C02-C19-C20-N21
3	F	502	PW2	C02-C19-C20-N21
3	A	502	PW2	C02-C19-C20-O26
3	B	502	PW2	C02-C19-C20-O26
3	C	502	PW2	C02-C19-C20-O26
3	D	502	PW2	C02-C19-C20-O26
3	E	502	PW2	C02-C19-C20-O26
3	F	502	PW2	C02-C19-C20-O26

There are no ring outliers.

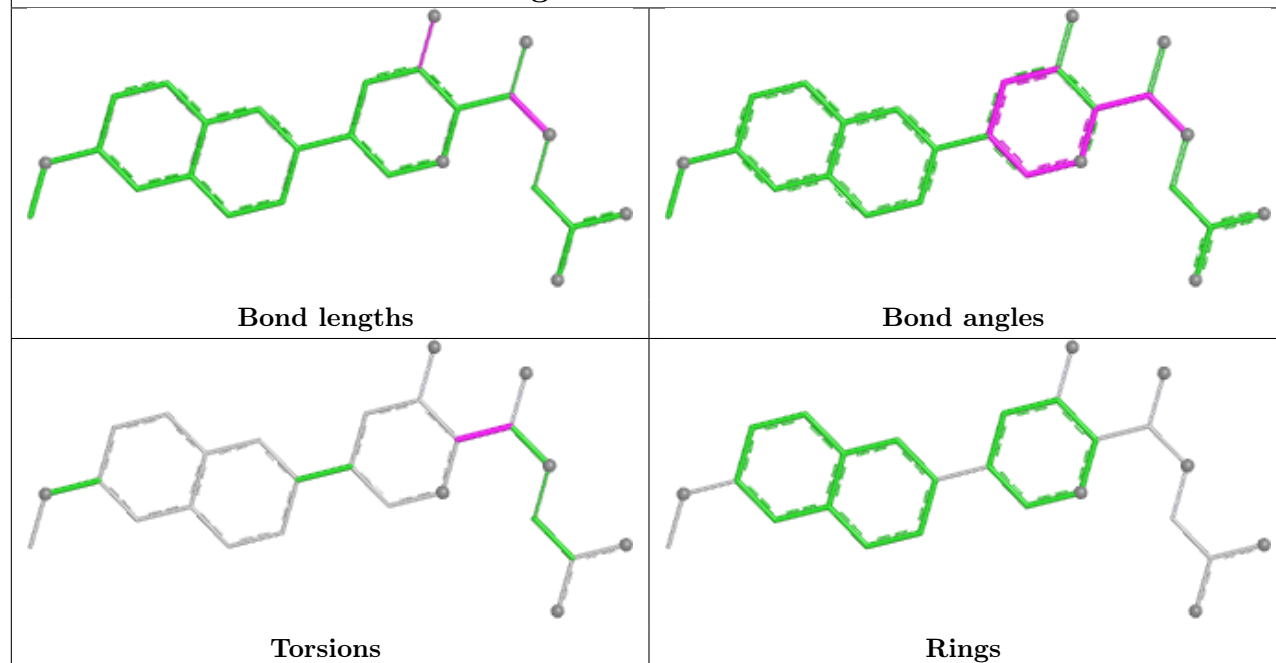
8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	PW2	1	0
5	E	504	SO4	1	0
3	E	502	PW2	2	0
3	F	502	PW2	1	0
3	D	502	PW2	3	0
3	B	502	PW2	1	0
4	E	503	GOL	2	0
3	C	502	PW2	4	0

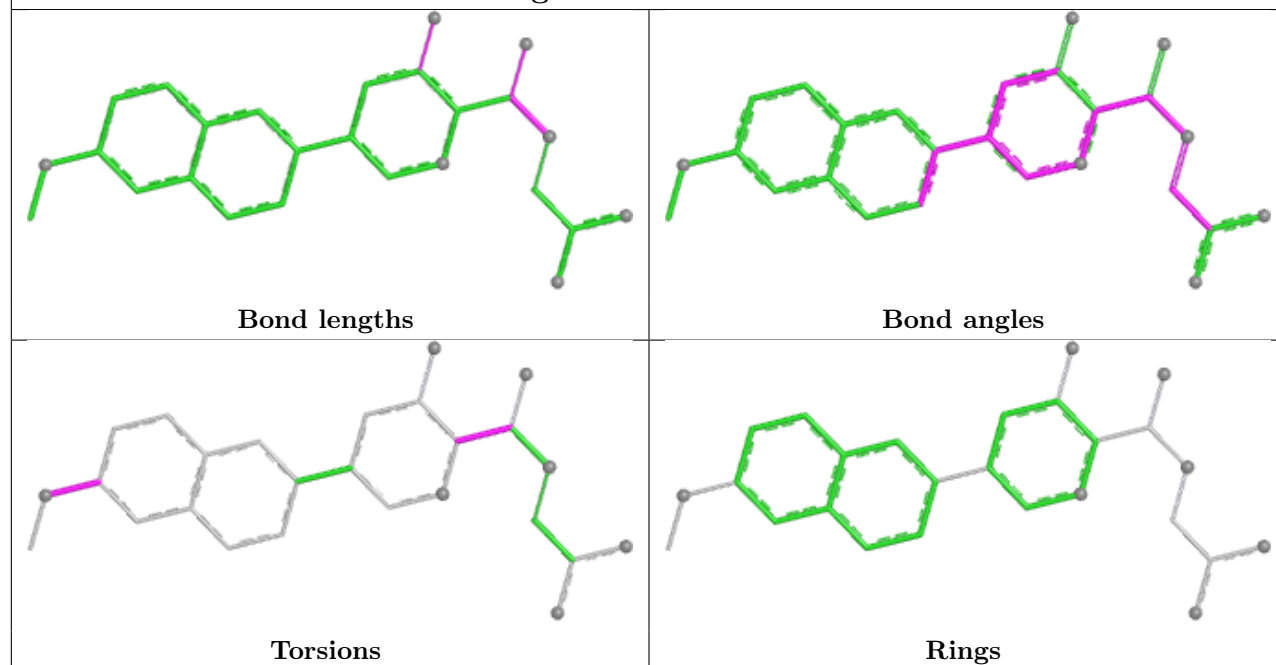
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

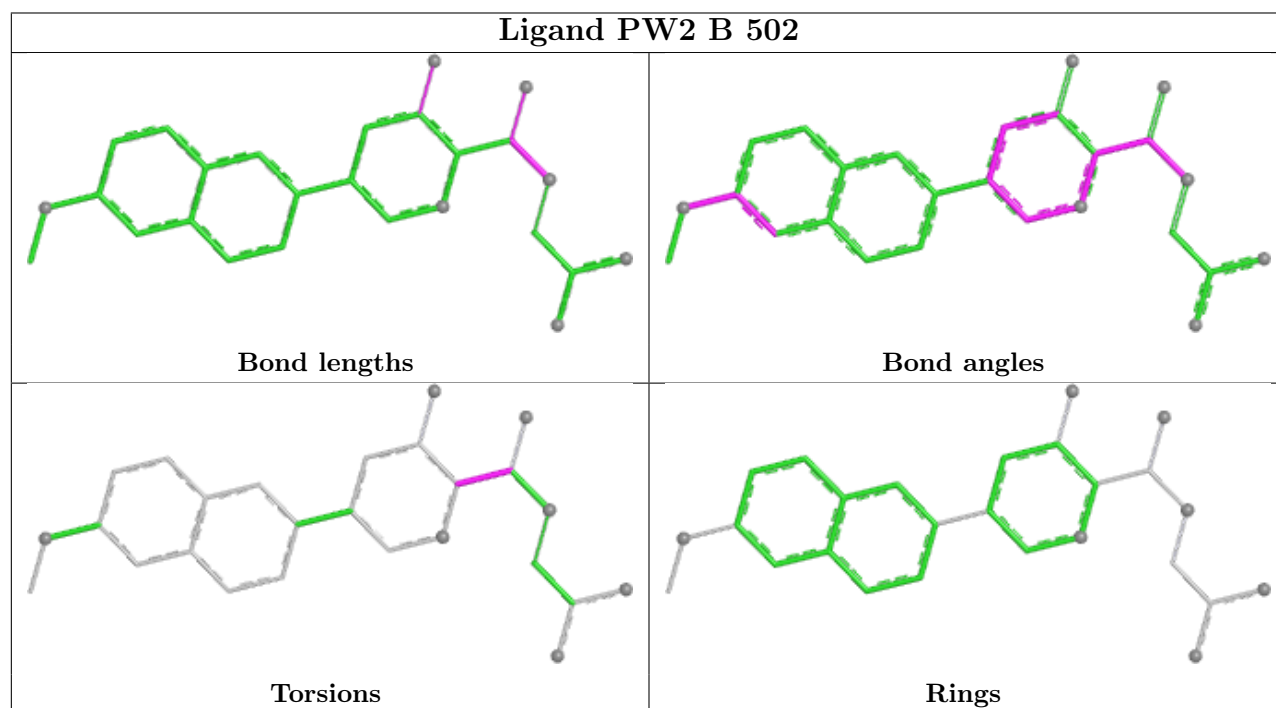
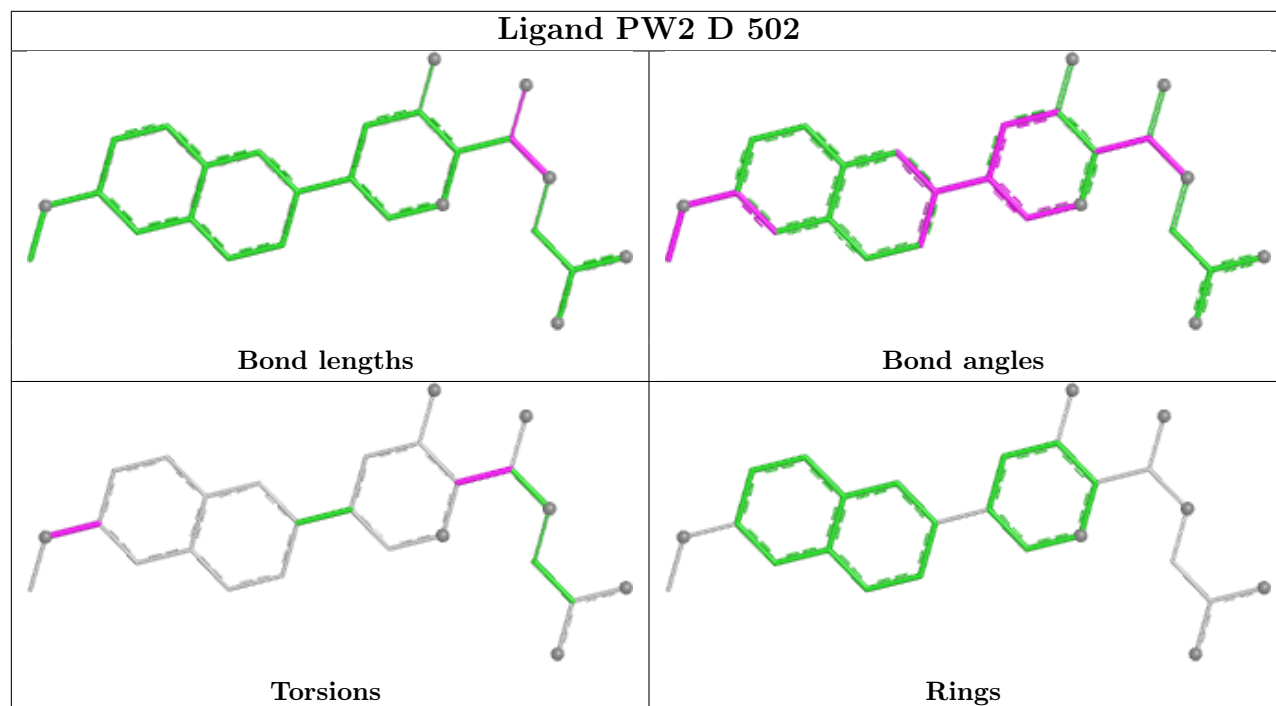


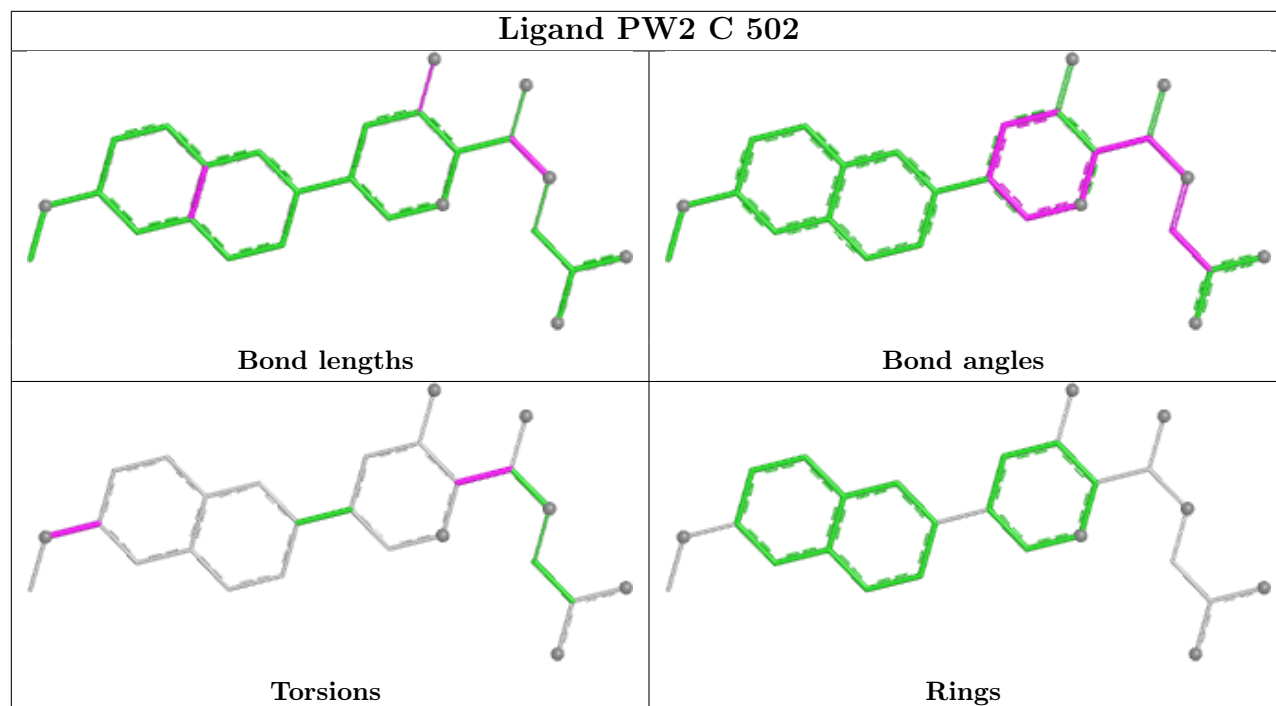
Ligand PW2 E 502



Ligand PW2 F 502







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	197/252 (78%)	0.30	10 (5%) 33 26	30, 54, 80, 98	0
1	B	199/252 (78%)	0.17	11 (5%) 30 23	33, 52, 83, 183	1 (0%)
1	C	196/252 (77%)	0.23	8 (4%) 41 33	34, 50, 83, 132	0
1	D	199/252 (78%)	0.06	7 (3%) 47 37	33, 50, 77, 116	0
1	E	194/252 (76%)	0.22	10 (5%) 33 26	36, 53, 84, 140	0
1	F	197/252 (78%)	0.29	8 (4%) 41 33	35, 57, 85, 149	0
All	All	1182/1512 (78%)	0.21	54 (4%) 37 29	30, 53, 84, 183	1 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	352	GLN	5.7
1	B	352	GLN	5.1
1	C	349	GLY	4.8
1	D	250	ASP	4.7
1	C	350	LYS	4.6
1	B	350	LYS	4.1
1	E	351	ALA	4.1
1	E	284	ASN	4.1
1	F	349	GLY	4.0
1	B	349	GLY	3.6
1	E	349	GLY	3.6
1	A	351	ALA	3.4
1	A	352	GLN	3.4
1	F	350	LYS	3.3
1	A	254	ASP	3.2
1	D	351	ALA	3.2
1	F	351	ALA	3.2
1	C	348	GLU	3.2
1	A	348	GLU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	348	GLU	3.0
1	C	254	ASP	2.9
1	B	254	ASP	2.9
1	F	255	LYS	2.9
1	F	404	LEU	2.8
1	A	404	LEU	2.7
1	D	352	GLN	2.7
1	E	255	LYS	2.6
1	B	338	VAL	2.6
1	A	350	LYS	2.6
1	B	404	LEU	2.6
1	C	291	LYS	2.5
1	C	285	GLY	2.4
1	D	337	LYS	2.4
1	C	403	TYR	2.4
1	D	256	ILE	2.4
1	A	318	ASN	2.3
1	A	349	GLY	2.3
1	A	220	GLN	2.3
1	B	253	GLY	2.3
1	B	348	GLU	2.3
1	E	291	LYS	2.3
1	F	342	ILE	2.3
1	C	305	GLY	2.2
1	F	291	LYS	2.2
1	B	403	TYR	2.2
1	E	403	TYR	2.2
1	E	256	ILE	2.1
1	B	335	ASP	2.1
1	F	254	ASP	2.1
1	B	251	ILE	2.1
1	A	232	THR	2.1
1	D	232	THR	2.0
1	D	350	LYS	2.0
1	E	285	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

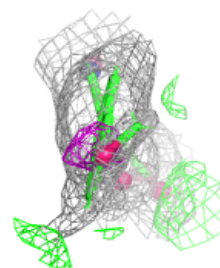
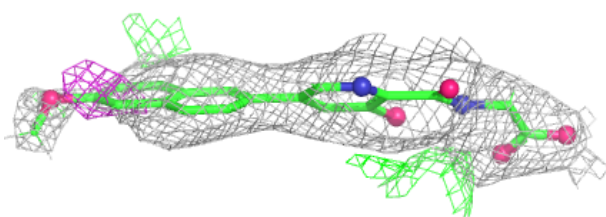
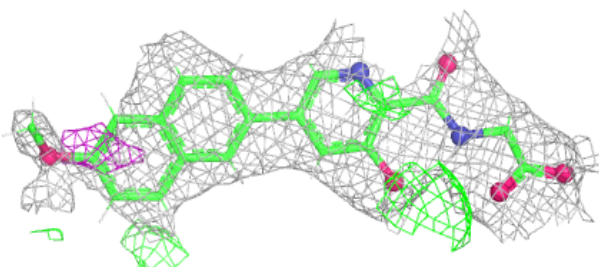
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	E	504	5/5	0.68	0.20	66,71,111,117	0
4	GOL	E	503	6/6	0.73	0.14	41,50,60,63	0
3	PW2	F	502	26/26	0.90	0.12	34,42,65,67	0
3	PW2	A	502	26/26	0.92	0.10	31,47,70,74	0
3	PW2	C	502	26/26	0.93	0.09	31,41,56,57	0
3	PW2	D	502	26/26	0.94	0.09	31,39,65,68	0
3	PW2	E	502	26/26	0.95	0.08	27,37,51,56	0
3	PW2	B	502	26/26	0.95	0.09	32,46,61,67	0
2	MN	A	501	1/1	0.98	0.05	36,36,36,36	0
2	MN	B	501	1/1	0.99	0.03	29,29,29,29	0
2	MN	C	501	1/1	0.99	0.04	32,32,32,32	0
2	MN	D	501	1/1	0.99	0.02	26,26,26,26	0
2	MN	F	501	1/1	0.99	0.02	36,36,36,36	0
2	MN	E	501	1/1	1.00	0.02	31,31,31,31	0

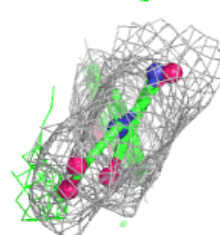
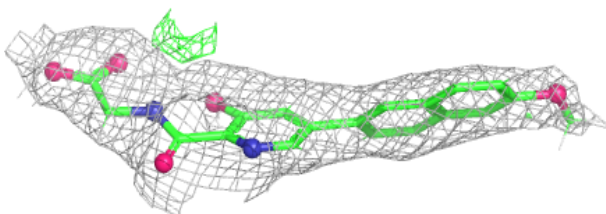
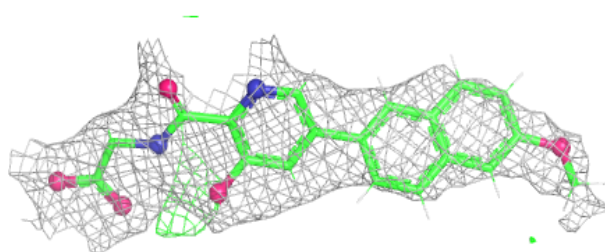
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PW2 F 502:

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

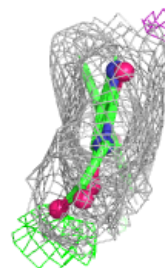
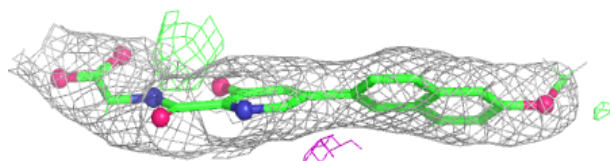
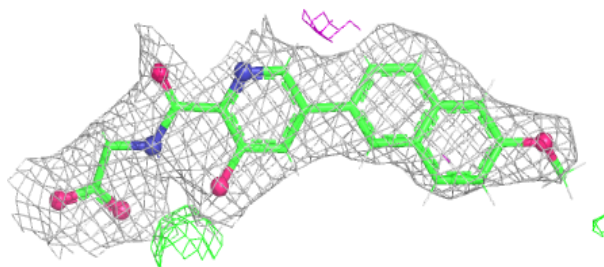
**Electron density around PW2 A 502:**

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

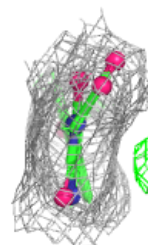
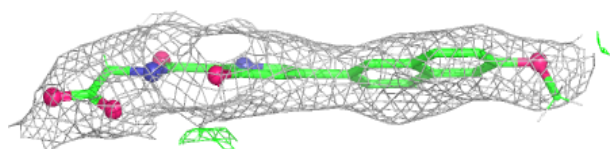
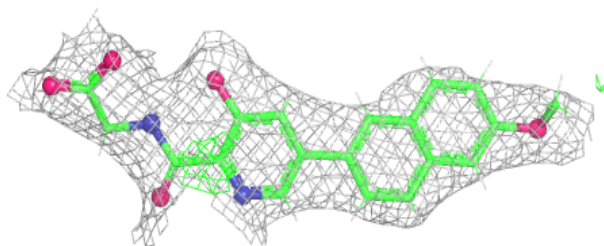


Electron density around PW2 C 502:

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

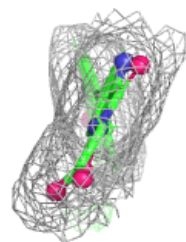
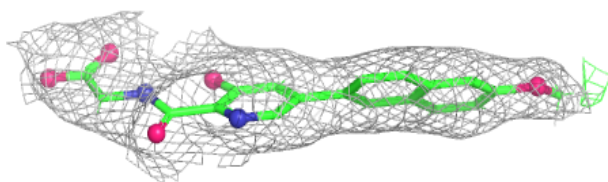
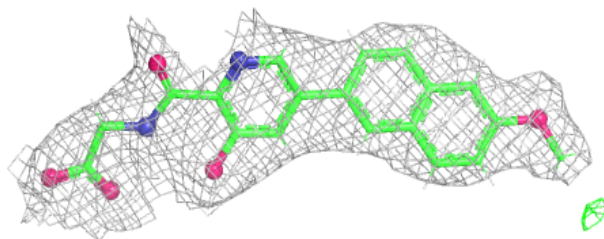
**Electron density around PW2 D 502:**

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

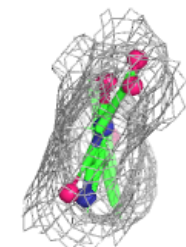
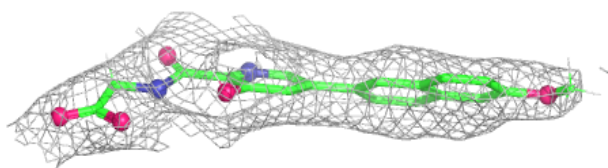
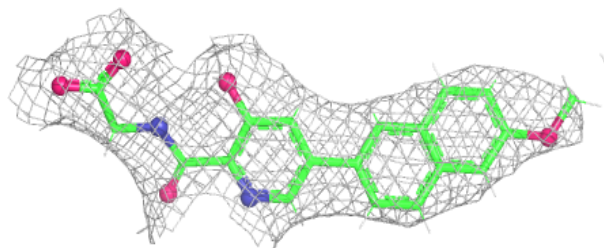


Electron density around PW2 E 502:

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

**Electron density around PW2 B 502:**

$2mF_o-DF_c$ (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.