



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2026 – 12:09 PM JST

PDB ID : 9VIJ / pdb\_00009vij  
Title : Crystal structure of fused glycerol dehydratase A177M/M158W variant  
Authors : Park, R.Y.; Seo, M.D.  
Deposited on : 2025-06-18  
Resolution : 3.58 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](mailto: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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
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

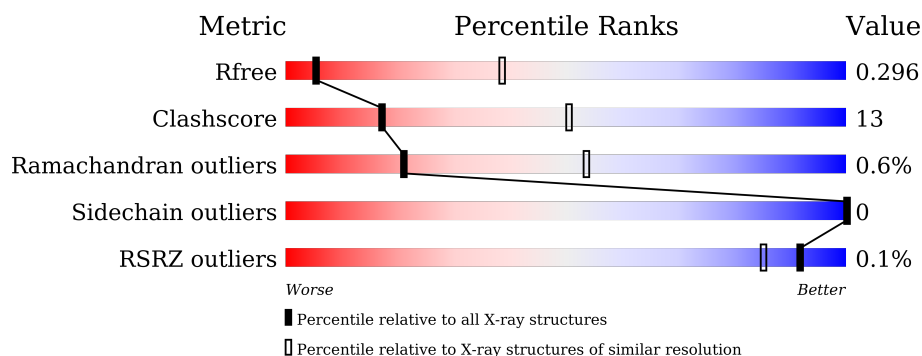
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.58 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	1521 (3.66-3.50)
Clashscore	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)
RSRZ outliers	180081	1520 (3.66-3.50)

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  $\geq 3$ , 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	B	754	<div> <div>74%</div> <div>23%</div> <div>.</div> </div>
1	C	754	<div> <div>71%</div> <div>26%</div> <div>.</div> </div>
2	D	141	<div> <div>72%</div> <div>24%</div> <div>..</div> </div>
2	E	141	<div> <div>82%</div> <div>16%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	B12	C	2601	-	-	X	-
3	B12	C	2602	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13548 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 Glycerol dehydrase alpha subunit,Glycerol dehydrase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	737	Total	C	N	O	S	0	0	0
			5598	3497	980	1088	33			
1	C	735	Total	C	N	O	S	0	0	0
			5624	3515	985	1091	33			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	MET	ALA	engineered mutation	UNP Q59476
B	556	GLN	-	linker	UNP Q59476
B	557	GLY	-	linker	UNP Q59476
B	558	GLY	-	linker	UNP Q59476
B	559	ILE	-	linker	UNP Q59476
B	560	PRO	-	linker	UNP Q59476
B	561	VAL	-	linker	UNP Q59476
B	718	TRP	MET	engineered mutation	UNP O08505
C	177	MET	ALA	engineered mutation	UNP Q59476
C	556	GLN	-	linker	UNP Q59476
C	557	GLY	-	linker	UNP Q59476
C	558	GLY	-	linker	UNP Q59476
C	559	ILE	-	linker	UNP Q59476
C	560	PRO	-	linker	UNP Q59476
C	561	VAL	-	linker	UNP Q59476
C	718	TRP	MET	engineered mutation	UNP O08505

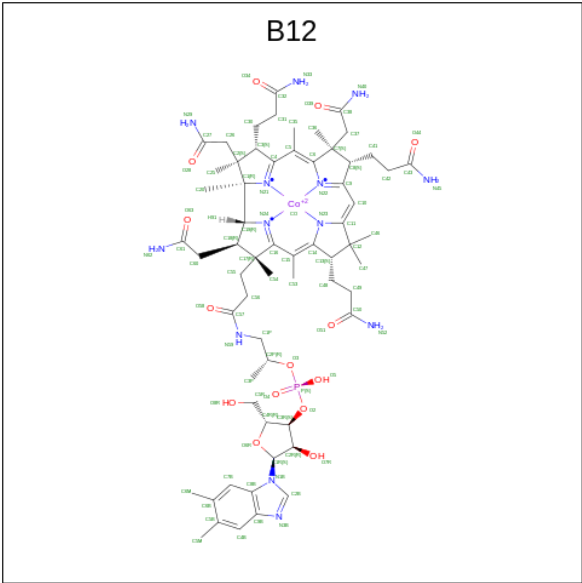
- Molecule 2 is a protein called Glycerol dehydrase gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	136	Total	C	N	O	S	0	0	0
			1061	665	194	198	4			
2	E	138	Total	C	N	O	S	0	0	0
			1083	676	200	203	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	51	CYS	ARG	conflict	UNP Q59475
E	51	CYS	ARG	conflict	UNP Q59475

- Molecule 3 is COBALAMIN (CCD ID: B12) (formula: C<sub>62</sub>H<sub>89</sub>CoN<sub>13</sub>O<sub>14</sub>P) (labeled as "Ligand of Interest" by depositor).

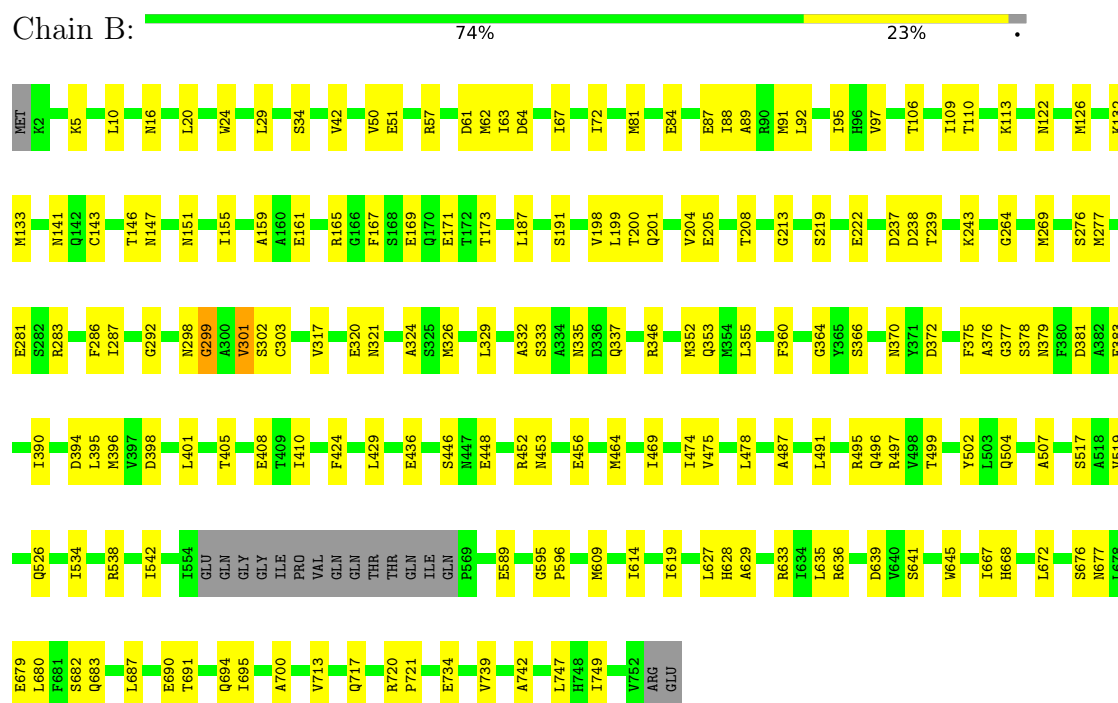


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

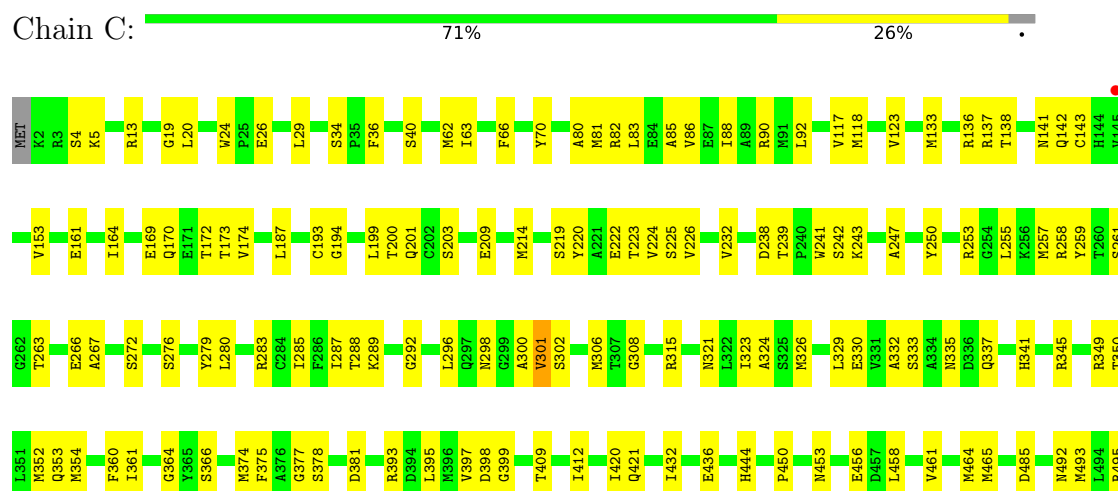
### 3 Residue-property plots

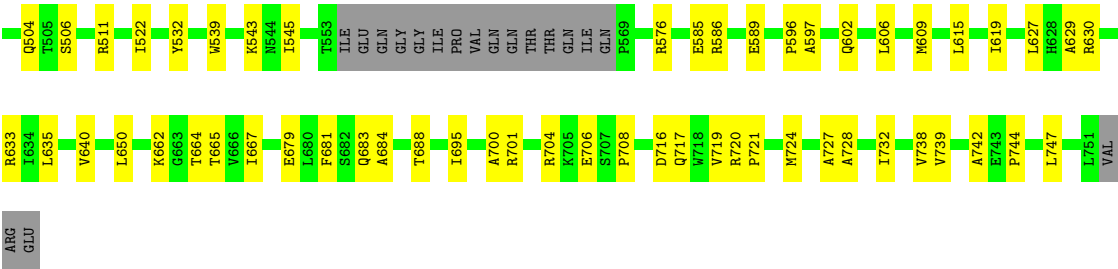
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Glycerol dehydrase alpha subunit, Glycerol dehydrase beta subunit



- Molecule 1: Glycerol dehydrase alpha subunit, Glycerol dehydrase beta subunit

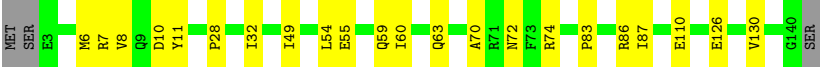
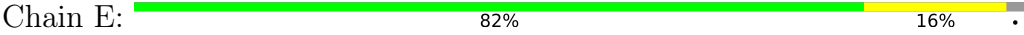




• Molecule 2: Glycerol dehydrase gamma subunit



• Molecule 2: Glycerol dehydrase gamma subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.02Å 157.02Å 383.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.59 – 3.58 29.59 – 3.58	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.59-3.58) 98.8 (29.59-3.58)	Depositor EDS
$R_{merge}$	0.41	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 3.55Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.270 , 0.295 0.270 , 0.296	Depositor DCC
$R_{free}$ test set	1420 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	140.4	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 78.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13548	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: B12

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	B	0.13	0/5691	0.33	1/7716 (0.0%)
1	C	0.12	0/5716	0.31	1/7743 (0.0%)
2	D	0.39	0/1079	0.68	2/1466 (0.1%)
2	E	0.22	0/1102	0.44	0/1496
All	All	0.17	0/13588	0.37	4/18421 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	51	CYS	N-CA-C	-6.54	104.24	111.82
2	D	10	ASP	N-CA-C	-5.93	106.01	113.72
1	B	72	ILE	N-CA-C	5.31	116.23	108.53
1	C	82	ARG	N-CA-C	-5.07	107.09	113.28

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	B	5598	0	5505	144	0
1	C	5624	0	5578	156	0
2	D	1061	0	1041	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1083	0	1066	15	0
3	C	182	0	174	54	0
All	All	13548	0	13364	339	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 13.

All (339) 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)
2:D:23:THR:HG22	2:D:27:LYS:O	1.49	1.12
1:B:720:ARG:HH12	1:C:337:GLN:HB3	1.23	1.01
1:B:237:ASP:O	1:B:238:ASP:OD1	1.78	1.01
1:B:682:SER:HB3	3:C:2602:B12:H201	1.48	0.92
1:C:662:LYS:NZ	3:C:2601:B12:H5R1	1.85	0.91
3:C:2601:B12:H422	3:C:2601:B12:C10	2.02	0.87
3:C:2601:B12:C10	3:C:2601:B12:C42	2.58	0.82
1:B:720:ARG:NH1	1:C:337:GLN:HB3	1.94	0.82
1:B:238:ASP:OD2	1:B:243:LYS:HE3	1.81	0.81
2:D:23:THR:HG23	2:D:27:LYS:H	1.45	0.80
2:D:23:THR:CG2	2:D:27:LYS:H	1.94	0.80
3:C:2602:B12:H2B	3:C:2602:B12:H491	1.62	0.80
1:B:504:GLN:HG3	2:D:11:TYR:CE1	2.17	0.79
1:C:664:THR:OG1	3:C:2601:B12:O5	2.00	0.78
1:C:288:THR:HG21	1:C:296:LEU:HB2	1.65	0.78
1:C:727:ALA:CB	3:C:2601:B12:H3P1	2.13	0.77
1:C:80:ALA:O	1:C:83:LEU:HD13	1.86	0.76
2:D:23:THR:HG21	2:D:27:LYS:HB2	1.67	0.76
1:B:302:SER:HA	1:B:337:GLN:HG3	1.69	0.75
1:B:63:ILE:HG12	1:B:287:ILE:HD11	1.67	0.74
1:B:375:PHE:C	3:C:2601:B12:H621	1.95	0.73
1:C:238:ASP:OD2	1:C:243:LYS:NZ	2.21	0.73
1:B:680:LEU:HD23	3:C:2602:B12:H302	1.71	0.72
3:C:2602:B12:H312	3:C:2602:B12:H353	1.70	0.71
1:C:142:GLN:HB2	1:C:169:GLU:HB2	1.70	0.71
1:C:662:LYS:HZ1	3:C:2601:B12:H5R1	1.53	0.70
1:B:370:ASN:HB3	1:C:717:GLN:HG2	1.73	0.69
1:C:683:GLN:HA	3:C:2601:B12:O4	1.92	0.69
1:B:97:VAL:O	1:B:132:LYS:NZ	2.26	0.69
1:B:239:THR:HG23	2:D:96:PRO:HG3	1.75	0.68
1:C:701:ARG:HE	1:C:708:PRO:HB3	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:ILE:HD13	2:D:54:LEU:HD13	1.76	0.68
1:C:161:GLU:HG3	1:C:409:THR:HG23	1.76	0.67
1:B:424:PHE:HA	1:B:429:LEU:HD12	1.77	0.67
1:B:720:ARG:NH2	1:C:375:PHE:O	2.28	0.67
1:B:396:MET:SD	1:C:315:ARG:NH1	2.68	0.66
1:B:453:ASN:ND2	1:B:456:GLU:OE1	2.24	0.66
1:B:376:ALA:N	3:C:2601:B12:N62	2.44	0.66
1:C:662:LYS:HZ2	3:C:2601:B12:H5R1	1.55	0.66
1:B:366:SER:HB3	1:B:381:ASP:HA	1.78	0.66
1:B:298:ASN:O	1:B:321:ASN:ND2	2.29	0.65
1:B:34:SER:HB2	1:B:276:SER:HB3	1.79	0.65
1:B:410:ILE:HD11	1:C:4:SER:HB2	1.77	0.65
1:C:366:SER:HB3	1:C:381:ASP:HA	1.77	0.65
1:B:680:LEU:HD23	3:C:2602:B12:H253	1.78	0.64
1:B:366:SER:HB2	1:B:378:SER:HB3	1.80	0.64
1:C:335:ASN:OD1	1:C:349:ARG:NH1	2.30	0.64
3:C:2602:B12:N62	3:C:2602:B12:H252	2.12	0.63
1:B:81:MET:HE3	1:B:110:THR:HG23	1.80	0.63
1:B:682:SER:CB	3:C:2602:B12:H201	2.27	0.63
2:E:49:ILE:HD13	2:E:54:LEU:HG	1.81	0.62
2:D:101:GLN:HB2	2:D:137:LEU:HD21	1.81	0.62
1:C:354:MET:HA	1:C:361:ILE:HD13	1.82	0.62
2:D:23:THR:HG22	2:D:27:LYS:C	2.23	0.62
1:B:10:LEU:O	1:B:16:ASN:ND2	2.33	0.61
1:B:335:ASN:HD21	1:B:353:GLN:HB2	1.64	0.61
2:D:23:THR:CG2	2:D:27:LYS:N	2.64	0.61
1:B:609:MET:HG2	1:B:614:ILE:HD11	1.82	0.61
1:B:372:ASP:OD2	1:B:446:SER:N	2.31	0.61
1:B:204:VAL:HG12	1:B:205:GLU:H	1.64	0.61
1:C:136:ARG:HE	1:C:506:SER:HB3	1.65	0.61
1:C:302:SER:HB3	3:C:2602:B12:H13	1.82	0.61
1:B:50:VAL:HA	1:B:57:ARG:HD2	1.83	0.60
1:B:95:ILE:O	1:B:526:GLN:NE2	2.35	0.60
1:B:436:GLU:OE2	1:B:452:ARG:NH1	2.35	0.60
1:C:333:SER:HB2	1:C:353:GLN:HG2	1.82	0.60
3:C:2602:B12:H252	3:C:2602:B12:H621	1.66	0.60
1:B:213:GLY:O	1:B:497:ARG:NH1	2.33	0.60
1:B:375:PHE:C	3:C:2601:B12:N62	2.60	0.59
2:D:59:GLN:O	2:D:63:GLN:HG2	2.02	0.59
1:B:332:ALA:HA	1:B:360:PHE:HB2	1.83	0.59
2:D:11:TYR:O	2:D:13:LEU:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:LEU:HD22	1:C:352:MET:HE3	1.83	0.59
1:B:464:MET:HG3	1:B:469:ILE:HD12	1.85	0.59
1:C:201:GLN:NE2	1:C:222:GLU:OE1	2.34	0.59
1:B:721:PRO:O	1:C:19:GLY:N	2.35	0.59
1:C:395:LEU:HB2	1:C:397:VAL:HG12	1.85	0.59
1:C:173:THR:HG21	3:C:2602:B12:N29	2.19	0.58
1:C:224:VAL:HG21	1:C:257:MET:HE2	1.85	0.58
1:C:266:GLU:HB2	1:C:280:LEU:HD13	1.85	0.58
1:C:633:ARG:HB2	1:C:747:LEU:HD11	1.83	0.58
1:C:332:ALA:HA	1:C:360:PHE:HB2	1.85	0.58
1:C:465:MET:HE2	1:C:465:MET:HA	1.84	0.58
1:C:187:LEU:HD23	1:C:200:THR:HG23	1.86	0.58
1:B:376:ALA:HB2	3:C:2601:B12:N62	2.19	0.58
1:C:201:GLN:HE22	1:C:222:GLU:HB3	1.68	0.58
1:C:492:ASN:HA	1:C:495:ARG:HB2	1.87	0.57
2:E:11:TYR:HD1	2:E:60:ILE:HG21	1.70	0.57
1:B:299:GLY:C	1:B:301:VAL:H	2.13	0.57
1:C:133:MET:HG3	1:C:326:MET:HB3	1.85	0.57
1:C:683:GLN:CA	3:C:2601:B12:O4	2.51	0.57
1:B:42:VAL:HA	1:B:51:GLU:O	2.05	0.57
1:C:86:VAL:O	1:C:90:ARG:HG3	2.04	0.57
1:B:204:VAL:HG12	1:B:205:GLU:N	2.20	0.56
1:B:519:VAL:HA	2:D:64:MET:HE3	1.87	0.56
1:B:62:MET:HG3	2:D:134:ARG:HG3	1.88	0.56
1:B:87:GLU:O	1:B:91:MET:HG3	2.05	0.56
2:D:23:THR:CG2	2:D:27:LYS:HB2	2.34	0.56
1:B:201:GLN:HE22	1:B:222:GLU:HB3	1.71	0.56
1:B:721:PRO:HB2	1:C:341:HIS:CE1	2.41	0.56
1:C:222:GLU:HG3	1:C:258:ARG:HD2	1.88	0.56
1:B:355:LEU:HD22	1:C:123:VAL:HG21	1.88	0.56
1:C:539:TRP:CD1	1:C:543:LYS:HZ2	2.24	0.56
2:D:42:VAL:HG23	2:D:46:ASP:HB2	1.88	0.55
1:C:62:MET:HB3	1:C:241:TRP:HZ3	1.71	0.55
1:B:301:VAL:HG12	1:B:302:SER:N	2.22	0.55
1:C:292:GLY:HA3	2:E:72:ASN:HB2	1.88	0.55
1:C:511:ARG:NH1	1:C:511:ARG:HB3	2.21	0.55
2:E:86:ARG:NH2	2:E:110:GLU:OE1	2.37	0.55
1:C:24:TRP:HB3	1:C:29:LEU:HB2	1.88	0.55
1:B:504:GLN:HG3	2:D:11:TYR:HE1	1.72	0.55
1:C:504:GLN:HG3	2:E:11:TYR:HE1	1.72	0.55
1:B:238:ASP:OD2	1:B:243:LYS:CE	2.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:LYS:HD3	1:C:444:HIS:HB3	1.90	0.54
1:B:146:THR:HG21	1:B:173:THR:HG22	1.89	0.54
1:B:448:GLU:OE2	1:C:5:LYS:HD3	2.07	0.54
1:C:436:GLU:HG2	1:C:450:PRO:HG2	1.88	0.54
1:B:645:TRP:NE1	1:B:672:LEU:O	2.41	0.54
1:C:289:LYS:HD2	1:C:329:LEU:HD21	1.89	0.54
1:B:352:MET:HE3	1:C:395:LEU:HD22	1.89	0.54
2:D:23:THR:HG23	2:D:27:LYS:N	2.17	0.54
1:B:691:THR:O	1:B:695:ILE:HG13	2.07	0.54
2:D:54:LEU:HD23	2:D:77:ALA:HA	1.91	0.54
1:B:668:HIS:NE2	1:B:676:SER:O	2.41	0.53
1:B:680:LEU:CD2	3:C:2602:B12:H253	2.38	0.53
3:C:2602:B12:C19	3:C:2602:B12:C27	2.87	0.53
2:E:126:GLU:O	2:E:130:VAL:HG23	2.09	0.53
1:C:174:VAL:O	3:C:2602:B12:H301	2.08	0.53
1:B:303:CYS:HA	1:C:724:MET:HE1	1.90	0.52
1:C:40:SER:HB2	1:C:81:MET:HE1	1.90	0.52
1:C:172:THR:HB	1:C:187:LEU:HD22	1.90	0.52
1:C:214:MET:HE1	2:E:87:ILE:HG21	1.91	0.52
2:D:41:GLU:HG3	2:D:42:VAL:H	1.74	0.52
1:C:662:LYS:HZ2	3:C:2601:B12:C5R	2.21	0.52
1:B:201:GLN:NE2	1:B:222:GLU:HB3	2.24	0.52
1:B:20:LEU:HD12	1:C:393:ARG:NH1	2.25	0.52
1:C:398:ASP:OD2	1:C:532:TYR:OH	2.22	0.52
1:B:42:VAL:HG12	1:B:81:MET:HG3	1.92	0.52
1:B:298:ASN:ND2	1:B:320:GLU:O	2.43	0.52
1:B:595:GLY:HA3	1:B:734:GLU:OE2	2.10	0.52
1:C:522:ILE:HD12	1:C:522:ILE:H	1.75	0.52
2:E:6:MET:HG3	2:E:10:ASP:HB2	1.90	0.52
1:C:301:VAL:HG12	1:C:302:SER:N	2.24	0.51
1:C:606:LEU:HD11	1:C:727:ALA:HB2	1.92	0.51
1:B:133:MET:HE2	1:B:326:MET:HA	1.93	0.51
1:B:596:PRO:HB3	1:B:635:LEU:HD23	1.92	0.51
2:D:120:ASN:O	2:D:124:VAL:HG23	2.09	0.51
2:E:70:ALA:O	2:E:74:ARG:HG3	2.11	0.51
1:B:264:GLY:H	1:B:277:MET:HG2	1.76	0.51
1:B:475:VAL:HG13	1:B:487:ALA:HB1	1.92	0.51
1:B:680:LEU:HD21	3:C:2602:B12:C20	2.41	0.51
1:B:690:GLU:O	1:B:694:GLN:HG2	2.11	0.51
1:C:203:SER:HB3	1:C:223:THR:HG21	1.93	0.51
1:C:267:ALA:HA	1:C:272:SER:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:54:LEU:HD23	2:D:77:ALA:CA	2.40	0.50
1:B:333:SER:HB2	1:B:353:GLN:HG2	1.93	0.50
1:B:499:THR:HG21	2:D:14:ALA:HB2	1.94	0.50
1:B:720:ARG:HH12	1:C:337:GLN:CB	2.09	0.50
2:D:50:SER:OG	2:D:53:THR:CB	2.60	0.50
1:B:237:ASP:C	1:B:238:ASP:OD1	2.53	0.50
1:B:337:GLN:HE22	1:B:375:PHE:HB3	1.75	0.50
1:C:728:ALA:O	1:C:732:ILE:HG13	2.12	0.50
2:D:23:THR:CG2	2:D:27:LYS:CB	2.90	0.50
1:B:376:ALA:CB	3:C:2601:B12:N62	2.75	0.50
1:B:390:ILE:HD13	1:C:20:LEU:HD11	1.94	0.50
2:D:70:ALA:O	2:D:74:ARG:HG3	2.12	0.50
1:B:639:ASP:OD2	1:B:641:SER:OG	2.30	0.49
1:C:366:SER:HB2	1:C:378:SER:HB3	1.93	0.49
1:B:281:GLU:HG2	1:B:320:GLU:HB2	1.95	0.49
1:C:201:GLN:NE2	1:C:222:GLU:HB3	2.27	0.49
1:C:727:ALA:CB	3:C:2601:B12:C3P	2.87	0.49
1:B:24:TRP:HB3	1:B:29:LEU:HD12	1.95	0.49
1:B:398:ASP:OD1	1:B:538:ARG:NE	2.46	0.49
2:E:59:GLN:O	2:E:63:GLN:HG2	2.13	0.49
1:C:667:ILE:HB	1:C:679:GLU:HB2	1.95	0.48
1:C:684:ALA:N	3:C:2601:B12:O4	2.46	0.48
1:B:713:VAL:HG11	1:C:374:MET:HE1	1.94	0.48
1:C:66:PHE:O	1:C:70:TYR:HB2	2.12	0.48
1:C:136:ARG:NH1	1:C:138:THR:O	2.47	0.48
1:C:586:ARG:HG3	1:C:589:GLU:HB3	1.95	0.48
1:C:80:ALA:O	1:C:83:LEU:CD1	2.57	0.48
1:C:258:ARG:NE	1:C:330:GLU:OE2	2.46	0.48
1:C:609:MET:HE1	1:C:688:THR:HA	1.94	0.48
1:B:474:ILE:O	1:B:478:LEU:HD12	2.13	0.48
1:C:739:VAL:HG23	1:C:742:ALA:HB3	1.95	0.48
1:C:585:GLU:HG3	1:C:630:ARG:CZ	2.43	0.48
1:B:720:ARG:NH2	1:C:337:GLN:OE1	2.37	0.47
2:D:23:THR:HG22	2:D:27:LYS:H	1.75	0.47
1:C:596:PRO:HG2	1:C:738:VAL:HG22	1.95	0.47
1:B:390:ILE:O	1:B:394:ASP:N	2.46	0.47
1:C:83:LEU:N	1:C:83:LEU:HD12	2.30	0.47
1:B:680:LEU:HD21	3:C:2602:B12:H203	1.96	0.47
1:C:225:SER:O	1:C:243:LYS:HE2	2.14	0.47
3:C:2601:B12:H363	3:C:2601:B12:H412	1.57	0.47
1:C:421:GLN:NE2	1:C:432:ILE:O	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:THR:H	1:B:219:SER:HG	1.56	0.47
1:B:633:ARG:HB2	1:B:747:LEU:HD11	1.96	0.47
1:B:264:GLY:N	1:B:277:MET:HG2	2.29	0.47
1:B:346:ARG:HB2	1:B:379:ASN:HD21	1.79	0.47
1:B:635:LEU:HB3	1:B:739:VAL:HG22	1.97	0.46
1:C:63:ILE:HG23	1:C:287:ILE:HD11	1.97	0.46
1:C:222:GLU:HA	1:C:258:ARG:HG2	1.97	0.46
1:C:88:ILE:O	1:C:92:LEU:HG	2.15	0.46
1:C:173:THR:HG21	3:C:2602:B12:H291	1.80	0.46
1:C:306:MET:HE3	1:C:306:MET:HB3	1.78	0.46
1:C:627:LEU:HD13	1:C:700:ALA:HB1	1.97	0.46
1:C:635:LEU:HB3	1:C:739:VAL:HG22	1.98	0.46
1:B:81:MET:HE1	1:B:113:LYS:HB2	1.97	0.46
1:B:171:GLU:HB2	1:B:201:GLN:HE21	1.80	0.46
1:C:259:TYR:HB2	1:C:288:THR:HG23	1.96	0.46
1:B:376:ALA:HB2	3:C:2601:B12:C61	2.46	0.46
1:C:504:GLN:HG3	2:E:11:TYR:CE1	2.50	0.46
1:C:136:ARG:HB2	1:C:506:SER:HB3	1.98	0.46
1:B:191:SER:HB2	1:B:198:VAL:HB	1.98	0.46
1:B:383:GLU:O	1:C:13:ARG:HD2	2.16	0.46
1:C:199:LEU:HD23	1:C:493:MET:HE1	1.96	0.46
1:C:335:ASN:OD1	1:C:350:THR:HA	2.16	0.46
1:C:704:ARG:NH2	1:C:706:GLU:OE2	2.42	0.46
2:D:23:THR:CG2	2:D:27:LYS:CA	2.94	0.46
1:B:292:GLY:HA3	2:D:72:ASN:HB2	1.97	0.45
1:C:200:THR:H	1:C:219:SER:HB2	1.81	0.45
1:C:279:TYR:O	1:C:283:ARG:HG3	2.16	0.45
1:B:63:ILE:HG21	1:B:283:ARG:HE	1.81	0.45
1:C:393:ARG:HD2	1:C:545:ILE:HD12	1.97	0.45
1:B:496:GLN:HB3	1:B:502:TYR:CD1	2.52	0.45
1:C:662:LYS:NZ	3:C:2601:B12:C5R	2.69	0.45
1:B:84:GLU:O	1:B:88:ILE:HD12	2.17	0.45
1:C:650:LEU:HD11	1:C:744:PRO:HG2	1.99	0.45
1:C:727:ALA:HB2	3:C:2601:B12:H3P1	1.96	0.45
2:E:86:ARG:HD2	2:E:86:ARG:HA	1.59	0.45
1:B:324:ALA:O	1:B:329:LEU:HB2	2.17	0.45
2:E:55:GLU:HG3	2:E:59:GLN:NE2	2.32	0.45
3:C:2602:B12:H351	3:C:2602:B12:H372	1.99	0.45
1:C:665:THR:HG21	1:C:695:ILE:HD13	1.98	0.45
1:B:609:MET:HE3	1:B:609:MET:HB2	1.79	0.44
1:C:209:GLU:HG2	1:C:250:TYR:OH	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:ALA:HA	1:C:257:MET:HE3	1.99	0.44
1:C:141:ASN:ND2	1:C:399:GLY:O	2.49	0.44
1:B:495:ARG:HG3	2:D:32:ILE:HG21	1.99	0.44
1:B:680:LEU:CD2	3:C:2602:B12:H302	2.43	0.44
1:C:164:ILE:HD13	1:C:412:ILE:HG21	1.99	0.44
1:B:122:ASN:O	1:B:126:MET:HG3	2.17	0.44
1:B:739:VAL:HG23	1:B:742:ALA:HB3	1.99	0.44
1:C:194:GLY:HA2	1:C:412:ILE:HG12	1.99	0.44
3:C:2602:B12:H351	3:C:2602:B12:C37	2.47	0.44
1:B:161:GLU:O	1:B:165:ARG:HG3	2.18	0.44
1:C:201:GLN:HB3	1:C:220:TYR:CE1	2.53	0.44
2:D:23:THR:CG2	2:D:27:LYS:O	2.42	0.44
2:D:41:GLU:HG3	2:D:42:VAL:N	2.32	0.44
2:D:54:LEU:HD23	2:D:77:ALA:HB2	2.00	0.44
1:B:687:LEU:HD22	1:B:691:THR:HG21	1.99	0.44
3:C:2601:B12:C10	3:C:2601:B12:H421	2.45	0.44
1:B:405:THR:HB	1:B:408:GLU:HG2	1.99	0.44
1:B:677:ASN:HD21	3:C:2602:B12:H311	1.83	0.43
1:B:683:GLN:NE2	3:C:2602:B12:C61	2.80	0.43
1:C:232:VAL:HG21	1:C:266:GLU:HA	1.99	0.43
2:E:7:ARG:HG2	2:E:8:VAL:H	1.83	0.43
1:B:204:VAL:CG1	1:B:205:GLU:H	2.29	0.43
1:C:374:MET:O	3:C:2602:B12:H601	2.17	0.43
1:B:42:VAL:CG1	1:B:81:MET:HG3	2.47	0.43
1:C:34:SER:HB2	1:C:276:SER:HB3	2.01	0.43
1:C:153:VAL:HA	1:C:420:ILE:HG21	2.01	0.43
1:C:485:ASP:OD1	1:C:485:ASP:N	2.49	0.43
3:C:2602:B12:H302	3:C:2602:B12:H253	1.79	0.43
1:B:627:LEU:HD13	1:B:700:ALA:HB1	2.01	0.43
3:C:2601:B12:H602	3:C:2601:B12:H541	1.47	0.43
1:B:317:VAL:O	1:B:320:GLU:HG2	2.18	0.43
1:B:398:ASP:HB2	1:B:534:ILE:HG13	2.00	0.43
1:B:667:ILE:HB	1:B:679:GLU:HB2	2.00	0.43
1:C:321:ASN:HD22	1:C:321:ASN:HA	1.62	0.43
1:C:576:ARG:HG3	1:C:576:ARG:HH11	1.84	0.43
1:B:67:ILE:HG12	1:B:286:PHE:HB3	2.01	0.43
1:C:136:ARG:NE	1:C:506:SER:O	2.51	0.43
3:C:2601:B12:H301	3:C:2601:B12:H253	1.54	0.43
2:D:56:TYR:O	2:D:60:ILE:HG12	2.19	0.43
2:D:126:GLU:O	2:D:130:VAL:HG23	2.19	0.43
2:E:11:TYR:CD1	2:E:60:ILE:HG21	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:LEU:HD12	1:B:491:LEU:HA	1.81	0.42
1:C:137:ARG:HG2	1:C:532:TYR:HB2	2.01	0.42
1:C:453:ASN:HB3	1:C:456:GLU:HB2	2.01	0.42
1:C:615:LEU:O	1:C:619:ILE:HG13	2.19	0.42
1:C:681:PHE:CZ	1:C:695:ILE:HG12	2.55	0.42
3:C:2602:B12:C19	3:C:2602:B12:O28	2.67	0.42
1:B:205:GLU:OE1	1:B:208:THR:N	2.30	0.42
1:C:619:ILE:HG23	1:C:629:ALA:HB3	1.99	0.42
1:B:143:CYS:HB3	1:B:167:PHE:CD1	2.55	0.42
1:C:716:ASP:HB3	1:C:719:VAL:HG23	2.02	0.42
1:B:720:ARG:HB2	1:B:721:PRO:HD3	2.01	0.42
1:C:26:GLU:HG3	1:C:36:PHE:HE2	1.85	0.42
1:C:226:VAL:HG23	1:C:261:SER:HB3	2.01	0.42
1:C:308:GLY:O	1:C:345:ARG:NH2	2.53	0.42
2:D:27:LYS:NZ	2:D:42:VAL:HB	2.35	0.42
1:B:589:GLU:HA	1:B:628:HIS:O	2.19	0.42
1:C:285:ILE:HG12	1:C:296:LEU:HD21	2.02	0.42
3:C:2602:B12:H471	3:C:2602:B12:H482	1.75	0.42
1:C:727:ALA:HB2	3:C:2601:B12:C3P	2.50	0.41
1:B:619:ILE:HG23	1:B:629:ALA:HB3	2.02	0.41
1:C:263:THR:H	1:C:300:ALA:HA	1.85	0.41
1:C:720:ARG:HB3	1:C:721:PRO:HD3	2.01	0.41
1:B:87:GLU:HB3	1:B:91:MET:HE3	2.01	0.41
1:B:239:THR:CG2	2:D:96:PRO:HG3	2.48	0.41
1:C:214:MET:HE2	1:C:253:ARG:HD3	2.03	0.41
2:D:23:THR:HG21	2:D:27:LYS:CB	2.43	0.41
1:C:85:ALA:HB1	1:C:117:VAL:HA	2.03	0.41
1:C:458:LEU:HA	1:C:461:VAL:HG12	2.01	0.41
1:B:89:ALA:HA	1:B:92:LEU:HD12	2.02	0.41
1:B:106:THR:O	1:B:109:ILE:HG12	2.19	0.41
1:C:464:MET:HE2	1:C:464:MET:HB3	1.79	0.41
1:C:717:GLN:H	1:C:717:GLN:HG3	1.68	0.41
2:D:52:GLN:HG2	2:D:56:TYR:CE2	2.55	0.41
1:B:159:ALA:HB2	1:B:187:LEU:HD12	2.03	0.41
1:B:377:GLY:O	1:C:720:ARG:NH2	2.54	0.41
1:C:118:MET:HG3	1:C:323:ILE:HD11	2.02	0.41
1:C:302:SER:OG	1:C:337:GLN:NE2	2.53	0.41
1:B:147:ASN:HD21	1:B:151:ASN:N	2.18	0.41
1:B:636:ARG:HA	1:B:739:VAL:O	2.21	0.41
3:C:2601:B12:C2B	3:C:2601:B12:H492	2.51	0.41
1:B:61:ASP:H	1:B:64:ASP:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:ARG:NH1	1:B:542:ILE:HG13	2.35	0.41
1:C:539:TRP:O	1:C:543:LYS:HG3	2.21	0.41
1:C:576:ARG:HG3	1:C:576:ARG:NH1	2.36	0.41
2:D:11:TYR:C	2:D:13:LEU:N	2.78	0.41
1:B:749:ILE:HD13	1:B:749:ILE:HA	1.93	0.41
1:C:640:VAL:HG13	3:C:2601:B12:HM63	2.03	0.41
1:B:141:ASN:HD22	1:B:401:LEU:HG	1.86	0.40
1:B:169:GLU:OE2	1:B:199:LEU:HD12	2.21	0.40
1:B:269:MET:HE1	3:C:2601:B12:N45	2.36	0.40
1:B:507:ALA:HA	1:B:517:SER:HA	2.03	0.40
1:B:717:GLN:HB2	1:C:377:GLY:HA3	2.02	0.40
1:C:143:CYS:SG	1:C:170:GLN:HG2	2.61	0.40
1:C:255:LEU:HD12	1:C:255:LEU:HA	1.91	0.40
1:B:147:ASN:ND2	1:B:155:ILE:HG12	2.37	0.40
1:C:193:CYS:O	1:C:412:ILE:HD11	2.22	0.40
1:C:239:THR:H	1:C:242:SER:HG	1.63	0.40
1:C:298:ASN:HD21	1:C:324:ALA:HB2	1.86	0.40
1:C:597:ALA:HB1	1:C:602:GLN:HG3	2.03	0.40
3:C:2601:B12:H473	3:C:2601:B12:H482	1.77	0.40
2:D:50:SER:OG	2:D:53:THR:HB	2.21	0.40
1:C:458:LEU:O	1:C:461:VAL:HG12	2.22	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	B	733/754 (97%)	702 (96%)	28 (4%)	3 (0%)	30	60
1	C	731/754 (97%)	696 (95%)	33 (4%)	2 (0%)	36	65
2	D	133/141 (94%)	122 (92%)	8 (6%)	3 (2%)	5	29
2	E	136/141 (96%)	122 (90%)	11 (8%)	3 (2%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1733/1790 (97%)	1642 (95%)	80 (5%)	11 (1%)	21	54

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	83	PRO
1	B	301	VAL
1	B	364	GLY
1	C	364	GLY
1	C	301	VAL
2	D	40	GLY
2	D	45	GLN
1	B	299	GLY
2	E	28	PRO
2	D	42	VAL
2	E	32	ILE

### 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	B	590/620 (95%)	590 (100%)	0	100	100
1	C	599/620 (97%)	599 (100%)	0	100	100
2	D	109/120 (91%)	109 (100%)	0	100	100
2	E	111/120 (92%)	111 (100%)	0	100	100
All	All	1409/1480 (95%)	1409 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	B	73	ASN
1	B	79	GLN

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Mol	Chain	Res	Type
1	B	142	GLN
1	B	297	GLN
1	B	335	ASN
1	B	601	HIS
1	B	602	GLN
1	B	677	ASN
1	B	698	ASN
1	C	142	GLN
1	C	683	GLN
1	C	694	GLN
1	C	737	HIS
2	D	63	GLN
2	D	72	ASN
2	E	65	GLN
2	E	120	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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	B12	C	2602	-	93,101,101	1.46	12 (12%)	146,166,166	3.14	49 (33%)
3	B12	C	2601	-	93,101,101	1.25	12 (12%)	146,166,166	2.30	28 (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
3	B12	C	2602	-	-	29/56/223/223	0/3/11/11
3	B12	C	2601	-	-	28/56/223/223	0/3/11/11

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2602	B12	C14-N23	5.62	1.42	1.35
3	C	2602	B12	C9-N22	4.88	1.43	1.30
3	C	2602	B12	C8B-C9B	4.71	1.48	1.40
3	C	2601	B12	C8B-C9B	4.61	1.48	1.40
3	C	2601	B12	C14-N23	-3.60	1.30	1.35
3	C	2602	B12	C12-C11	-3.54	1.46	1.52
3	C	2601	B12	C9B-N3B	-3.30	1.33	1.39
3	C	2601	B12	C6B-C5B	3.22	1.48	1.40
3	C	2601	B12	C8B-N1B	-2.98	1.33	1.39
3	C	2601	B12	C1-C2	-2.97	1.51	1.58
3	C	2601	B12	C9-N22	2.91	1.38	1.30
3	C	2602	B12	C9B-N3B	-2.87	1.34	1.39
3	C	2602	B12	C6B-C5B	2.80	1.47	1.40
3	C	2601	B12	C19-N24	2.71	1.53	1.48
3	C	2602	B12	C19-N24	2.71	1.53	1.48
3	C	2602	B12	C54-C17	-2.64	1.50	1.54
3	C	2602	B12	C8B-N1B	-2.64	1.34	1.39
3	C	2602	B12	C10-C9	2.57	1.46	1.39
3	C	2601	B12	C14-C15	2.53	1.49	1.38
3	C	2601	B12	C2B-N1B	-2.33	1.33	1.37
3	C	2602	B12	C18-C19	-2.32	1.48	1.53
3	C	2601	B12	C1-C19	-2.27	1.50	1.55
3	C	2601	B12	C11-N23	2.13	1.41	1.37
3	C	2602	B12	C11-N23	2.13	1.41	1.37

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2601	B12	C20-C1-C19	-17.65	92.35	109.36
3	C	2602	B12	C20-C1-N21	-17.39	81.74	110.27
3	C	2602	B12	C20-C1-C2	10.20	130.33	113.28
3	C	2601	B12	C19-C1-N21	9.49	111.88	102.16
3	C	2602	B12	C54-C17-C18	-9.33	99.21	112.98
3	C	2602	B12	C30-C3-C4	8.76	130.02	109.63
3	C	2602	B12	C20-C1-C19	8.75	117.79	109.36
3	C	2602	B12	C18-C17-C16	8.71	111.25	100.67
3	C	2601	B12	C2-C1-C19	7.13	129.86	118.60
3	C	2602	B12	C2-C1-N21	-6.65	92.50	101.77
3	C	2602	B12	C1-C19-C18	6.63	132.77	121.88
3	C	2602	B12	C18-C19-N24	6.58	112.32	102.31
3	C	2602	B12	C1-C2-C3	6.45	109.83	101.60
3	C	2602	B12	C3-C4-C5	-5.75	114.12	123.81
3	C	2602	B12	C48-C13-C14	5.21	121.46	108.49
3	C	2602	B12	C60-C18-C17	-5.03	103.55	115.74
3	C	2601	B12	C1-C19-C18	4.88	129.90	121.88
3	C	2602	B12	C25-C2-C26	-4.87	99.86	109.71
3	C	2601	B12	C54-C17-C18	-4.81	105.88	112.98
3	C	2602	B12	C9-C10-C11	-4.74	119.11	125.97
3	C	2602	B12	C2-C1-C19	-4.50	111.50	118.60
3	C	2602	B12	C35-C5-C6	-4.47	115.32	122.43
3	C	2602	B12	C26-C2-C1	4.29	116.69	110.01
3	C	2602	B12	C48-C13-C12	-3.93	105.60	116.63
3	C	2602	B12	C37-C7-C6	3.90	119.37	107.12
3	C	2601	B12	C8B-C9B-N3B	-3.80	105.78	109.97
3	C	2602	B12	C12-C13-C14	3.77	108.57	102.26
3	C	2602	B12	C12-C11-N23	3.76	117.07	111.83
3	C	2601	B12	C26-C2-C3	3.53	113.65	107.41
3	C	2601	B12	C18-C17-C16	3.45	104.86	100.67
3	C	2602	B12	C60-C18-C19	3.39	123.48	114.62
3	C	2602	B12	O3-C2P-C1P	3.39	113.68	106.92
3	C	2601	B12	C13-C14-C15	-3.34	119.21	124.32
3	C	2601	B12	C48-C13-C14	3.23	116.54	108.49
3	C	2602	B12	C25-C2-C1	3.16	118.54	113.78
3	C	2601	B12	C20-C1-C2	-3.09	108.13	113.28
3	C	2601	B12	C53-C15-C16	3.08	125.68	120.38
3	C	2601	B12	C9B-N3B-C2B	3.08	108.11	104.44
3	C	2601	B12	C55-C17-C16	-3.03	110.67	116.65
3	C	2602	B12	C8B-C9B-N3B	-3.00	106.66	109.97
3	C	2602	B12	C54-C17-C55	2.97	114.15	109.25
3	C	2601	B12	C41-C8-C9	-2.95	105.99	111.19
3	C	2602	B12	C31-C30-C3	2.85	122.96	114.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2602	B12	C7-C6-C5	2.83	132.53	128.07
3	C	2602	B12	C2-C26-C27	2.82	123.15	115.22
3	C	2601	B12	C60-C18-C17	-2.81	108.94	115.74
3	C	2601	B12	C42-C41-C8	-2.77	106.73	114.73
3	C	2602	B12	C54-C17-C16	-2.76	98.05	112.40
3	C	2601	B12	C60-C18-C19	-2.76	107.43	114.62
3	C	2602	B12	O28-C27-N29	-2.71	115.11	122.50
3	C	2602	B12	C7B-C8B-C9B	-2.70	119.31	122.52
3	C	2601	B12	C2P-C1P-N59	-2.66	109.02	112.93
3	C	2602	B12	C55-C56-C57	-2.63	105.49	111.23
3	C	2602	B12	C17-C16-C15	2.60	130.35	126.26
3	C	2602	B12	C5-C4-N21	-2.57	120.01	124.19
3	C	2602	B12	C60-C61-N62	2.53	122.31	116.21
3	C	2602	B12	C3-C4-N21	-2.53	108.80	111.97
3	C	2601	B12	C30-C3-C4	2.51	115.47	109.63
3	C	2601	B12	C48-C13-C12	-2.50	109.61	116.63
3	C	2602	B12	C26-C2-C3	-2.46	103.06	107.41
3	C	2601	B12	C15-C14-N23	2.43	129.23	126.26
3	C	2602	B12	C13-C14-N23	-2.41	105.82	109.10
3	C	2601	B12	C36-C7-C8	-2.35	107.73	112.08
3	C	2602	B12	C10-C11-N23	-2.35	120.41	124.43
3	C	2602	B12	C49-C48-C13	2.29	121.33	114.73
3	C	2601	B12	C15-C16-N24	-2.29	119.13	122.42
3	C	2601	B12	C8B-N1B-C2B	2.28	108.50	106.37
3	C	2602	B12	C15-C16-N24	-2.26	119.17	122.42
3	C	2601	B12	C30-C3-C2	-2.23	114.37	119.09
3	C	2602	B12	C25-C2-C3	-2.21	107.31	112.96
3	C	2602	B12	C30-C31-C32	-2.15	105.30	112.59
3	C	2602	B12	C9B-N3B-C2B	2.09	106.92	104.44
3	C	2602	B12	C47-C12-C46	-2.07	105.85	109.35
3	C	2602	B12	C41-C8-C7	-2.06	108.46	114.14
3	C	2601	B12	C2-C1-N21	2.05	104.62	101.77
3	C	2602	B12	C53-C15-C14	-2.02	114.36	118.43
3	C	2601	B12	C25-C2-C3	-2.00	107.84	112.96

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2601	B12	C2-C3-C30-C31
3	C	2601	B12	C4-C3-C30-C31
3	C	2601	B12	C38-C37-C7-C6

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Mol	Chain	Res	Type	Atoms
3	C	2601	B12	C38-C37-C7-C8
3	C	2601	B12	C42-C41-C8-C7
3	C	2601	B12	C42-C41-C8-C9
3	C	2601	B12	C14-C13-C48-C49
3	C	2601	B12	C16-C17-C55-C56
3	C	2601	B12	C54-C17-C55-C56
3	C	2601	B12	C18-C17-C55-C56
3	C	2601	B12	N59-C1P-C2P-C3P
3	C	2601	B12	N59-C1P-C2P-O3
3	C	2601	B12	C1P-C2P-O3-P
3	C	2601	B12	C3P-C2P-O3-P
3	C	2601	B12	C2P-O3-P-O4
3	C	2601	B12	C2P-O3-P-O2
3	C	2601	B12	C3R-O2-P-O4
3	C	2601	B12	C3R-O2-P-O5
3	C	2602	B12	C1-C2-C26-C27
3	C	2602	B12	C4-C3-C30-C31
3	C	2602	B12	C14-C13-C48-C49
3	C	2602	B12	C18-C17-C55-C56
3	C	2602	B12	C18-C60-C61-O63
3	C	2602	B12	C18-C60-C61-N62
3	C	2602	B12	N59-C1P-C2P-C3P
3	C	2602	B12	N59-C1P-C2P-O3
3	C	2602	B12	C3P-C2P-O3-P
3	C	2602	B12	C3R-O2-P-O5
3	C	2602	B12	O6R-C4R-C5R-O8R
3	C	2602	B12	C3R-C4R-C5R-O8R
3	C	2601	B12	C56-C57-N59-C1P
3	C	2601	B12	O58-C57-N59-C1P
3	C	2601	B12	C3-C30-C31-C32
3	C	2602	B12	C2P-O3-P-O2
3	C	2601	B12	C1-C2-C26-C27
3	C	2601	B12	C17-C55-C56-C57
3	C	2601	B12	C3R-O2-P-O3
3	C	2602	B12	C8-C41-C42-C43
3	C	2602	B12	C13-C48-C49-C50
3	C	2601	B12	C25-C2-C26-C27
3	C	2601	B12	C3-C2-C26-C27
3	C	2602	B12	C3-C2-C26-C27
3	C	2602	B12	C38-C37-C7-C6
3	C	2602	B12	C38-C37-C7-C8
3	C	2602	B12	C3R-O2-P-O4

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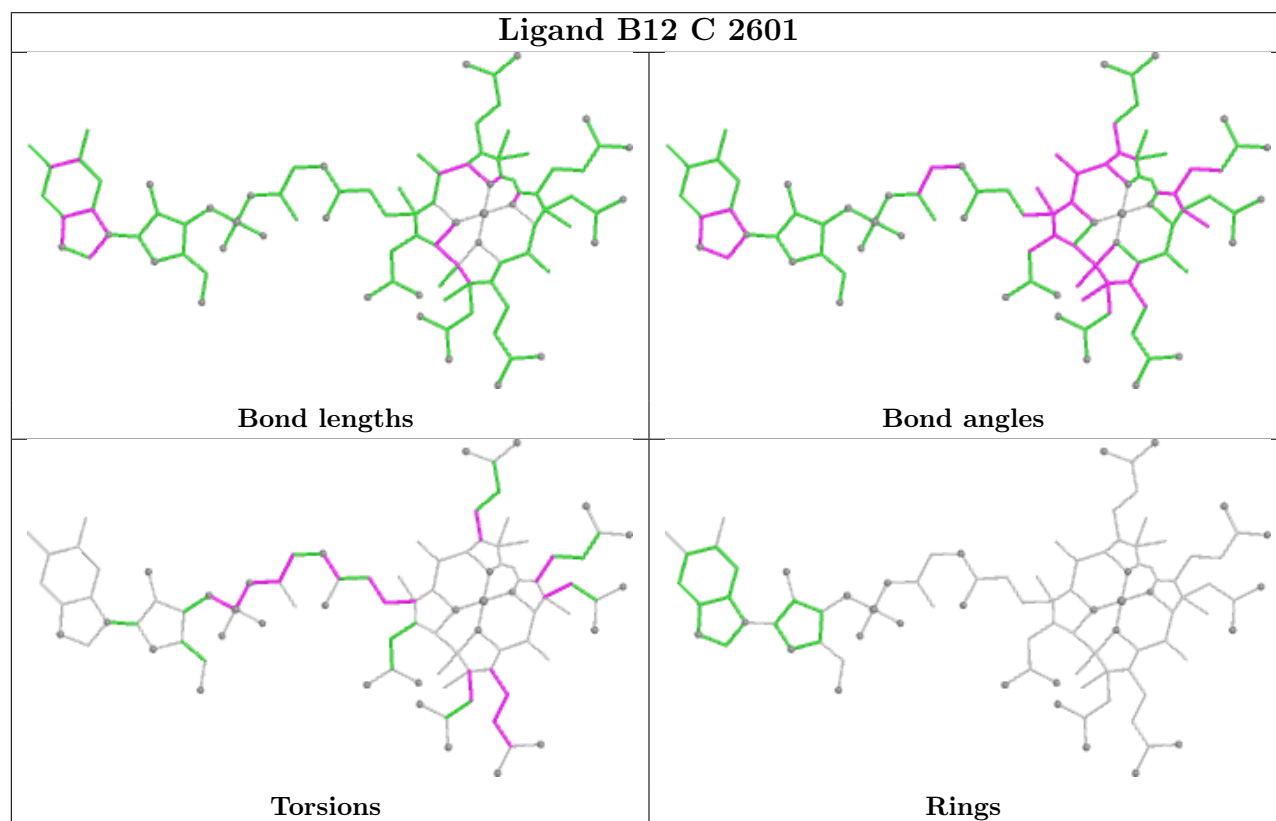
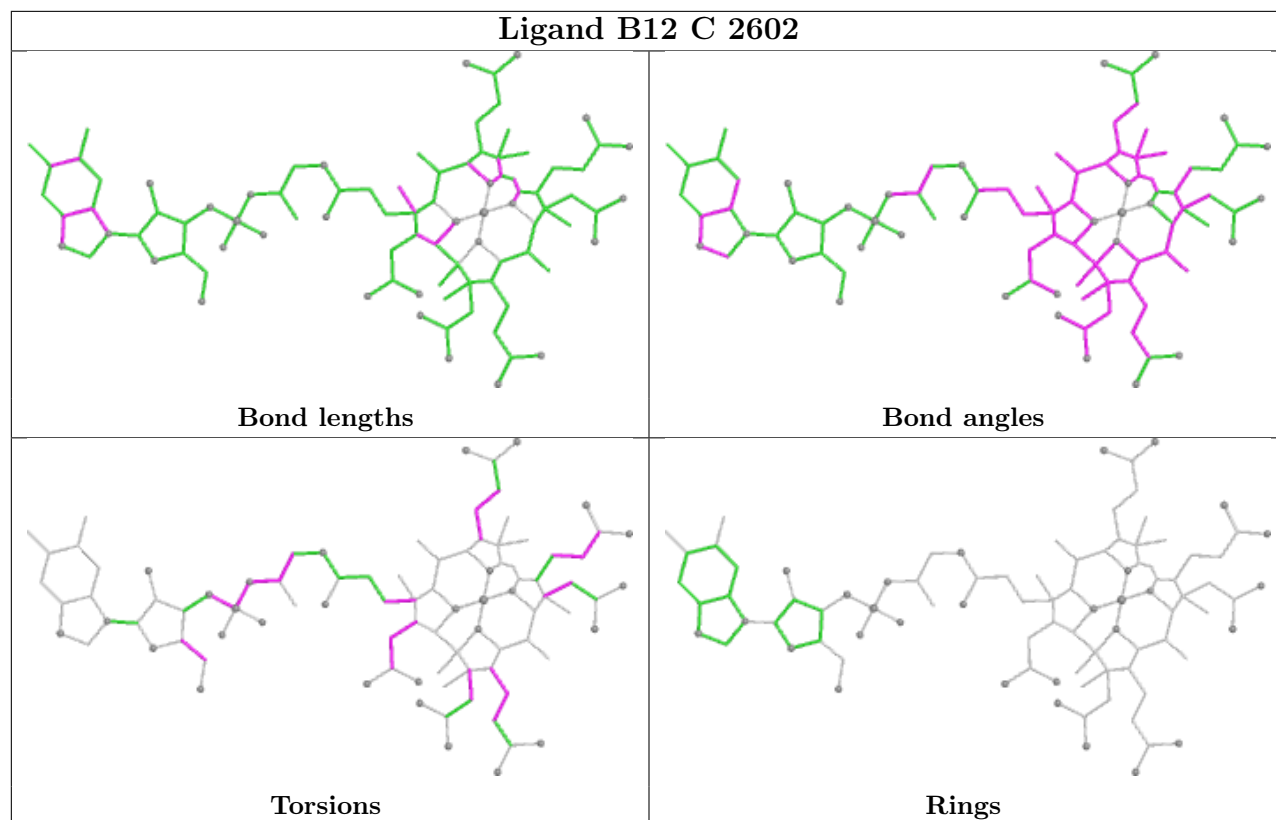
Mol	Chain	Res	Type	Atoms
3	C	2602	B12	C1P-C2P-O3-P
3	C	2602	B12	C25-C2-C26-C27
3	C	2602	B12	C17-C18-C60-C61
3	C	2601	B12	C30-C31-C32-O34
3	C	2602	B12	C3R-O2-P-O3
3	C	2601	B12	C30-C31-C32-N33
3	C	2602	B12	C41-C42-C43-O44
3	C	2602	B12	C19-C18-C60-C61
3	C	2602	B12	C41-C42-C43-N45
3	C	2602	B12	C3-C30-C31-C32
3	C	2602	B12	C2-C3-C30-C31
3	C	2602	B12	C12-C13-C48-C49

There are no ring outliers.

2 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2602	B12	25	0
3	C	2601	B12	29	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	737/754 (97%)	-0.26	0 <a href="#">100</a> <a href="#">100</a>	121, 147, 167, 175	0
1	C	735/754 (97%)	-0.26	1 (0%) <a href="#">92</a> <a href="#">85</a>	122, 145, 170, 182	0
2	D	136/141 (96%)	-0.35	0 <a href="#">100</a> <a href="#">100</a>	155, 168, 179, 183	0
2	E	138/141 (97%)	-0.43	0 <a href="#">100</a> <a href="#">100</a>	145, 159, 173, 175	0
All	All	1746/1790 (97%)	-0.28	1 (0%) <a href="#">92</a> <a href="#">85</a>	121, 149, 172, 183	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	145	VAL	2.1

### 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 oligosaccharides 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	B12	C	2602	91/91	0.81	0.17	102,115,118,123	0

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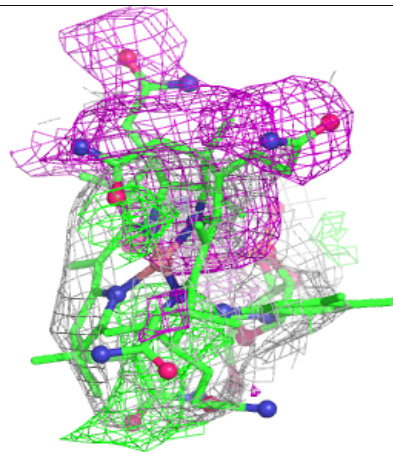
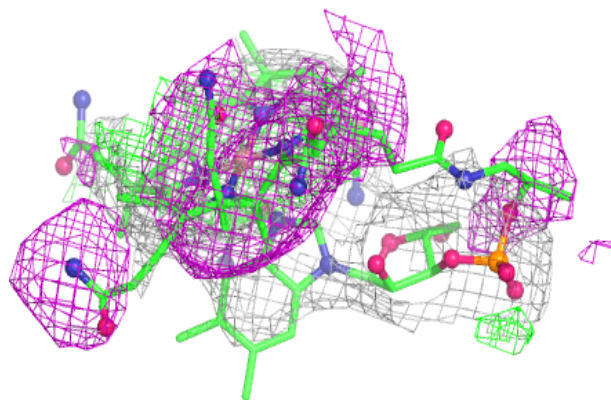
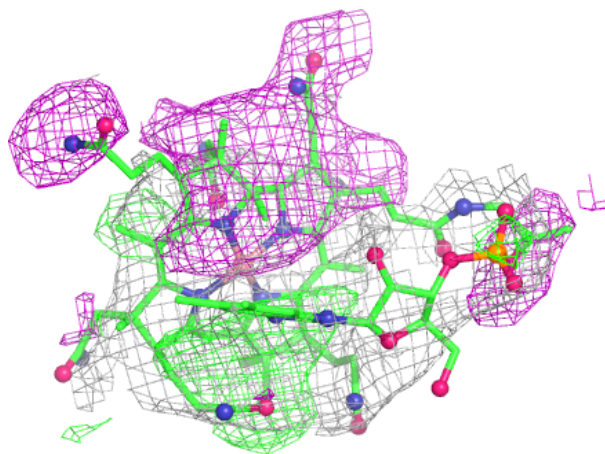
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	B12	C	2601	91/91	0.92	0.12	124,131,138,139	0

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.

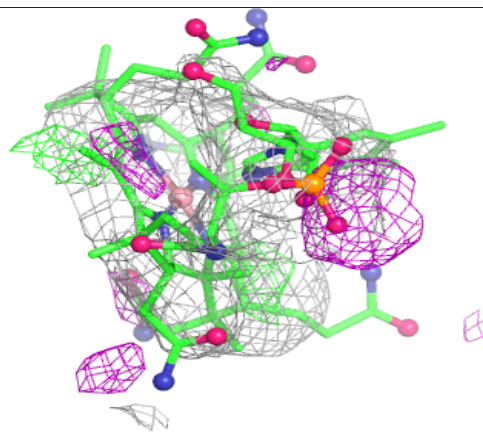
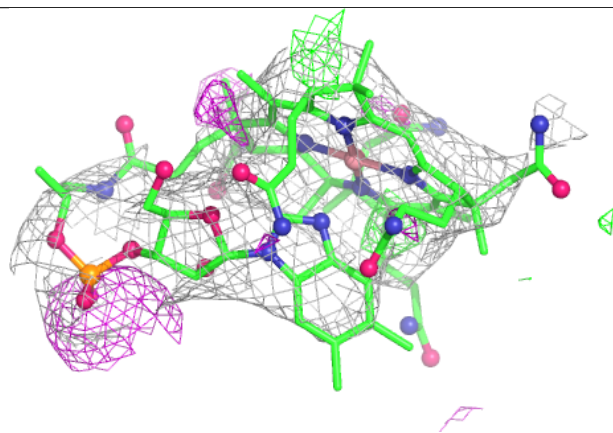
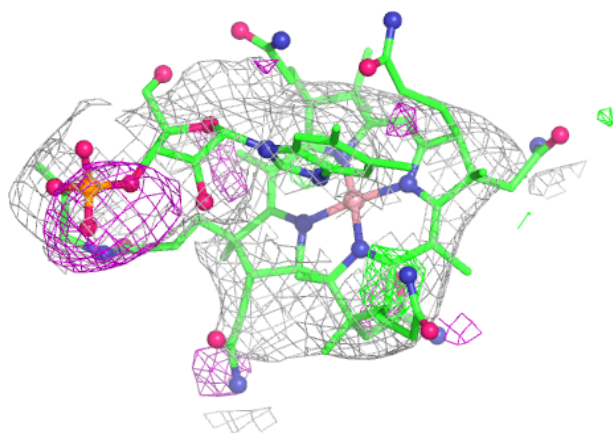
**Electron density around B12 C 2602:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around B12 C 2601:**

$2mF_o-DF_c$  (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.