Full wwPDB X-ray Structure Validation Report (i)

Aug 13, 2026 – 09:31 PM JST

PDB ID	:	9VIG / pdb_00009vig
Title	:	Crystal structure of fused glycerol dehydratase L113W variant
Authors	:	Park, R.Y.; Seo, M.D.
Deposited on	:	2025-06-18
Resolution	:	3.02 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:

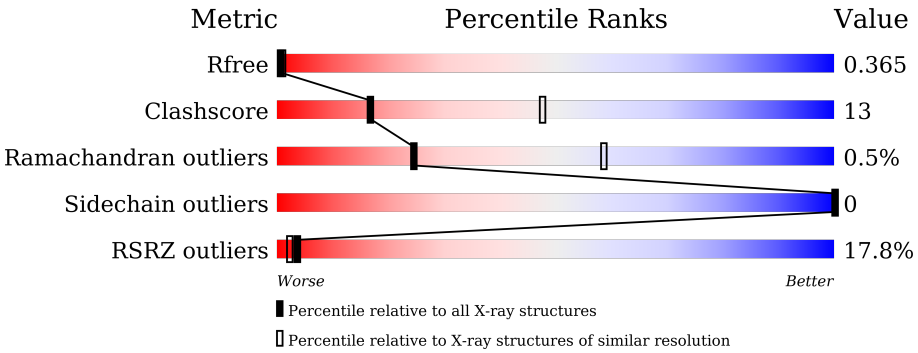
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.02 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	B	754	20% 69% 29%
1	C	754	16% 71% 26%
2	D	141	21% 78% 18%
2	E	141	10% 79% 18%

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	B	2601	-	-	X	-
3	B12	C	2601	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13643 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	738	Total	C	N	O	S	0	0	0
			5641	3522	988	1098	33			
1	C	736	Total	C	N	O	S	0	0	0
			5641	3523	990	1095	33			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	673	TRP	LEU	engineered mutation	UNP O08505
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	673	TRP	LEU	engineered mutation	UNP O08505

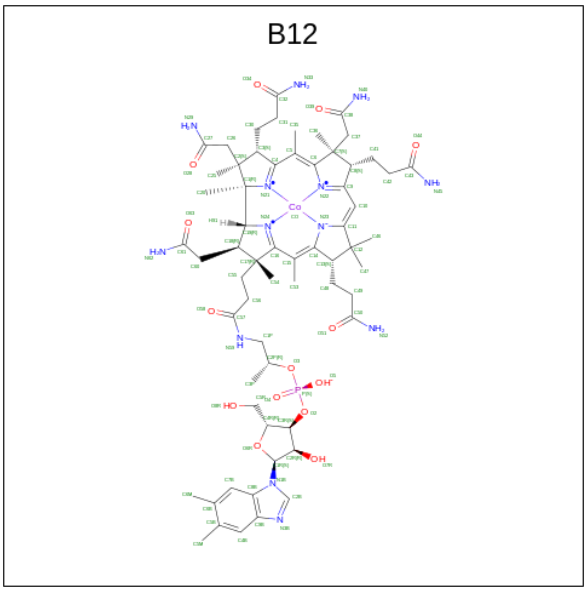
- Molecule 2 is a protein called Glycerol dehydrase gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	136	Total	C	N	O	S	0	0	0
			1073	669	199	201	4			
2	E	138	Total	C	N	O	S	0	0	0
			1106	692	206	204	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: $C_{62}H_{89}CoN_{13}O_{14}P$) (labeled as "Ligand of Interest" by depositor).



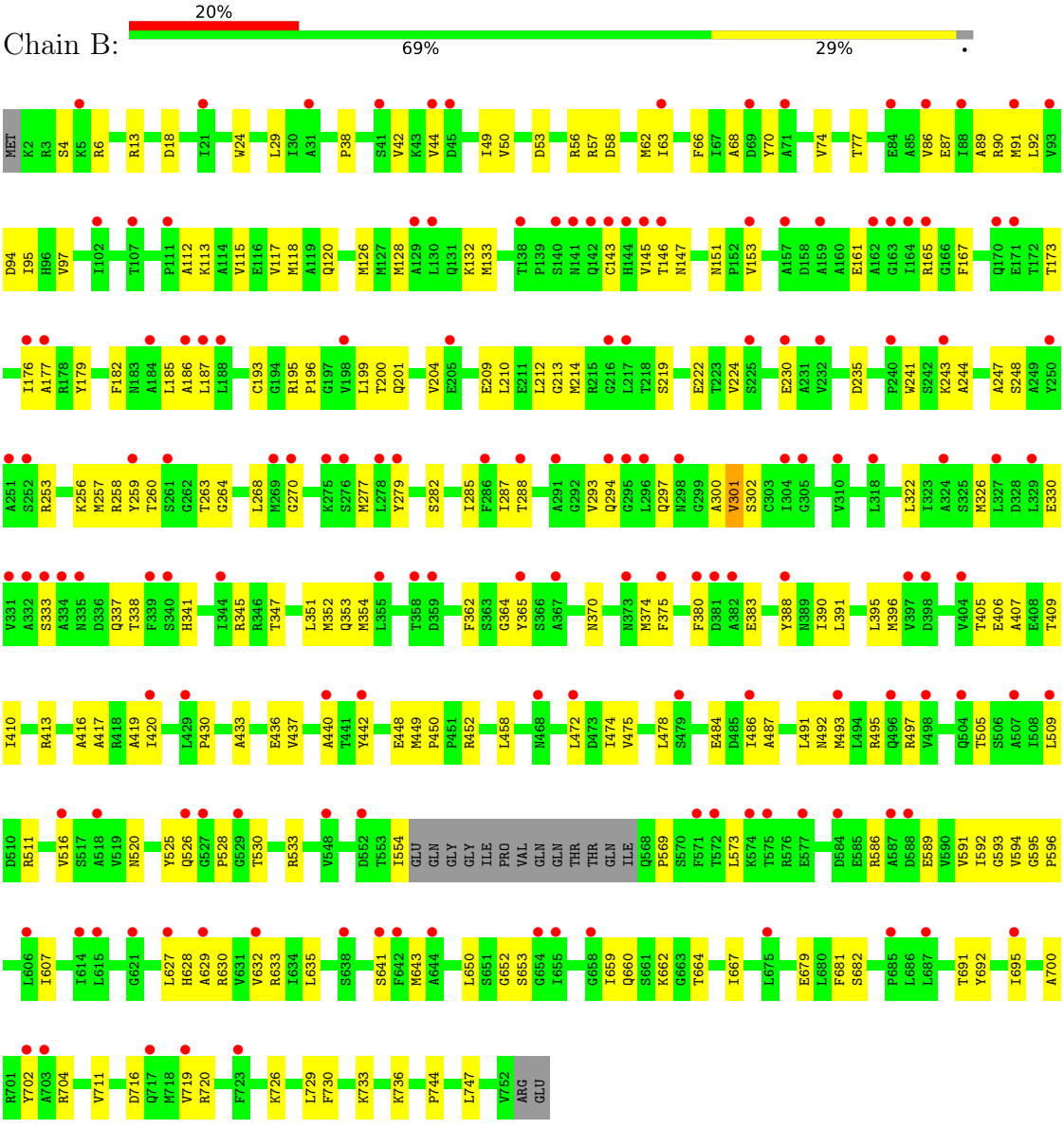
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

3 Residue-property plots (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: Glycerol dehydrase alpha subunit,Glycerol dehydrase beta subunit

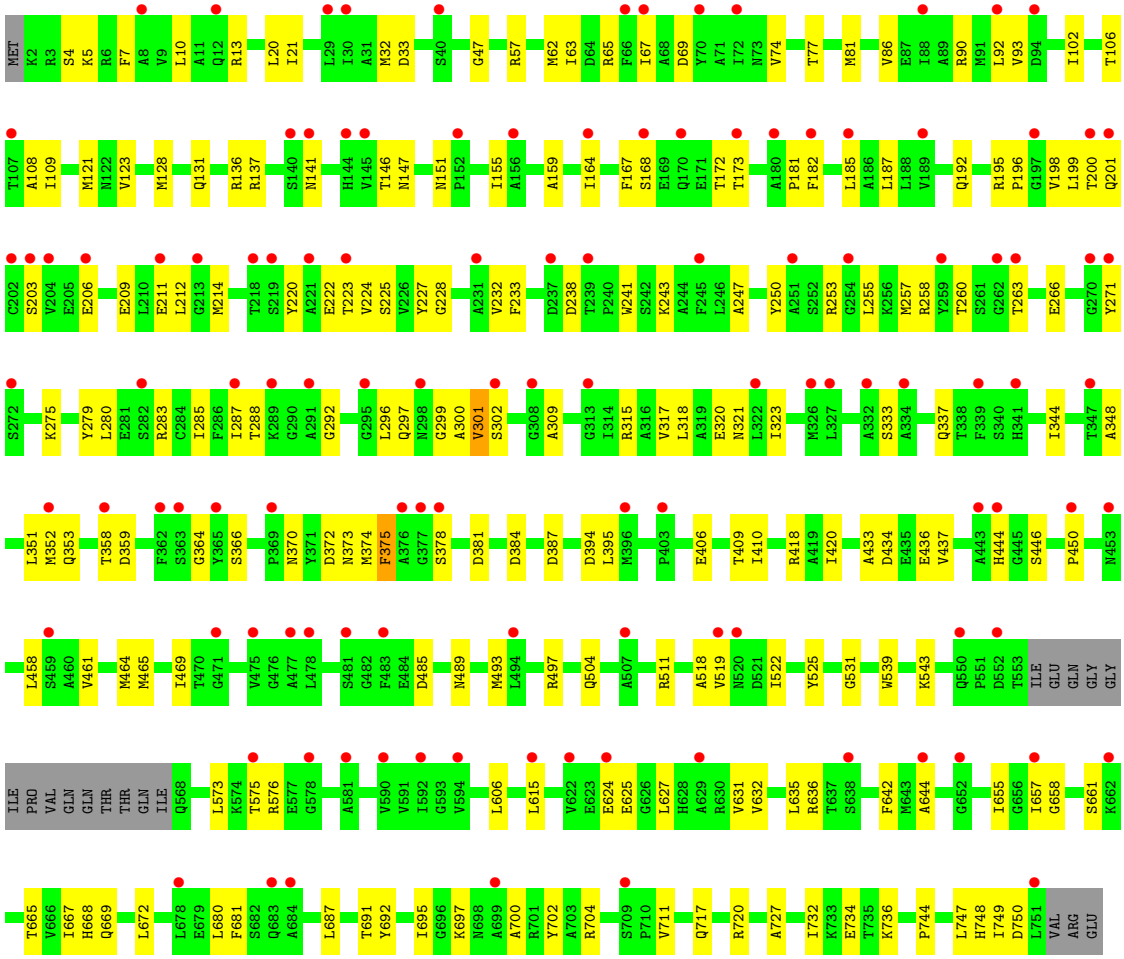
Chain B:



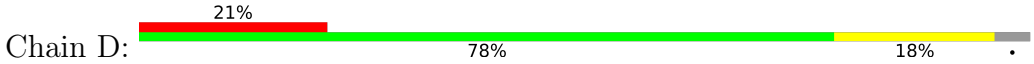
• Molecule 1: Glycerol dehydrase alpha subunit,Glycerol dehydrase beta subunit

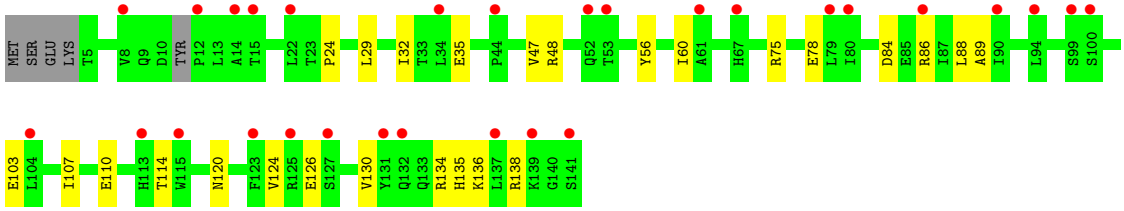
Chain C:



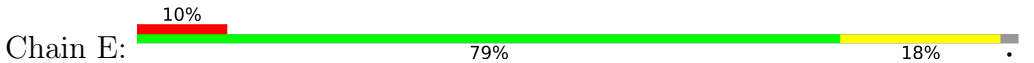


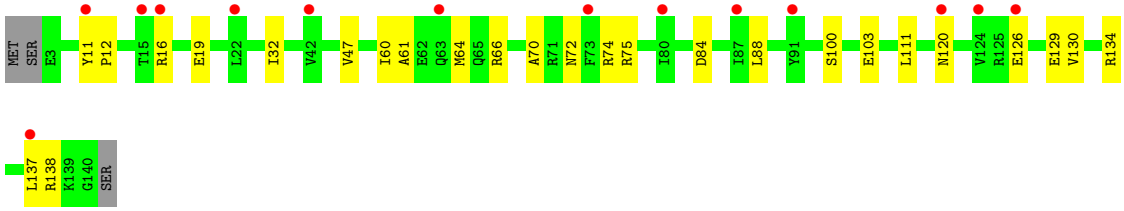
• Molecule 2: Glycerol dehydrase gamma subunit





• Molecule 2: Glycerol dehydrase gamma subunit





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	153.58Å 153.58Å 376.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.02 29.84 – 3.02	Depositor EDS
% Data completeness (in resolution range)	87.2 (29.84-3.02) 87.0 (29.84-3.02)	Depositor EDS
R_{merge}	0.52	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.327 , 0.367 0.326 , 0.365	Depositor DCC
R_{free} test set	1942 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 7.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.75	EDS
Total number of atoms	13643	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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: 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	0/5734	0.39	0/7770
1	C	0.20	0/5734	0.42	1/7767 (0.0%)
2	D	0.72	0/1091	0.84	1/1479 (0.1%)
2	E	0.30	0/1126	0.43	0/1525
All	All	0.27	0/13685	0.46	2/18541 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	375	PHE	N-CA-C	-10.41	97.76	111.71
2	D	89	ALA	N-CA-C	-5.04	106.98	113.23

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	B	5641	0	5578	172	0
1	C	5641	0	5598	156	0
2	D	1073	0	1068	23	0
2	E	1106	0	1113	20	0
3	B	91	0	88	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	91	0	88	21	0
All	All	13643	0	13533	349	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 (349) 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:C:206:GLU:OE2	3:C:2601:B12:N40	1.72	1.21
3:B:2601:B12:H91	3:B:2601:B12:C27	1.70	1.16
3:B:2601:B12:H91	3:B:2601:B12:N29	1.78	0.97
1:B:214:MET:HE1	2:D:88:LEU:HD23	1.44	0.96
1:B:641:SER:HB3	3:C:2601:B12:HM62	1.55	0.88
3:C:2601:B12:H362	3:C:2601:B12:H351	1.55	0.85
1:B:302:SER:HA	1:B:337:GLN:HG3	1.57	0.85
3:B:2601:B12:C27	3:B:2601:B12:C19	2.54	0.84
1:B:214:MET:HE1	2:D:88:LEU:CD2	2.07	0.83
1:C:232:VAL:HG23	1:C:271:TYR:HB2	1.61	0.81
1:B:4:SER:HB2	1:C:410:ILE:HD11	1.67	0.76
1:C:288:THR:HG21	1:C:296:LEU:HB2	1.68	0.75
1:B:516:VAL:HA	1:B:520:ASN:HD21	1.51	0.74
2:E:72:ASN:OD1	2:E:75:ARG:NH2	2.21	0.74
2:E:100:SER:HA	2:E:137:LEU:HD12	1.68	0.74
3:C:2601:B12:H311	3:C:2601:B12:H353	1.72	0.71
1:B:147:ASN:HD21	1:B:151:ASN:H	1.38	0.70
1:C:92:LEU:HD23	1:C:102:ILE:HD13	1.74	0.70
1:C:374:MET:C	3:C:2601:B12:H621	2.00	0.70
1:C:206:GLU:CD	3:C:2601:B12:N40	2.49	0.70
1:C:238:ASP:OD2	1:C:243:LYS:NZ	2.24	0.69
1:C:146:THR:HG21	1:C:173:THR:HG22	1.75	0.69
1:C:172:THR:HB	1:C:187:LEU:HD22	1.75	0.69
1:C:173:THR:OG1	3:C:2601:B12:H262	1.92	0.69
3:B:2601:B12:H302	1:C:680:LEU:HD23	1.74	0.69
1:C:206:GLU:CD	3:C:2601:B12:H402	2.00	0.68
3:B:2601:B12:H362	3:B:2601:B12:H351	1.75	0.67
1:B:650:LEU:HD11	1:B:744:PRO:HG2	1.76	0.67
1:C:657:ILE:HG13	1:C:667:ILE:HD13	1.74	0.67
1:B:282:SER:HA	1:B:285:ILE:HD12	1.76	0.66
1:B:662:LYS:NZ	3:C:2601:B12:H5R1	2.11	0.66
1:B:627:LEU:HD11	1:B:704:ARG:HE	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ASP:HA	1:C:642:PHE:HE2	1.61	0.65
1:B:302:SER:HB3	3:B:2601:B12:C53	2.27	0.65
1:B:627:LEU:HD13	1:B:700:ALA:HB1	1.79	0.64
1:C:372:ASP:OD2	1:C:446:SER:N	2.28	0.64
1:B:433:ALA:HB3	1:B:436:GLU:HG3	1.80	0.64
1:C:418:ARG:NH1	1:C:434:ASP:OD1	2.30	0.64
1:C:655:ILE:HG22	1:C:667:ILE:HD11	1.79	0.63
1:B:733:LYS:O	1:B:736:LYS:HG2	1.98	0.63
1:C:465:MET:HE2	1:C:465:MET:HA	1.80	0.63
1:C:504:GLN:HG3	2:E:11:TYR:HE1	1.64	0.62
1:B:201:GLN:HE22	1:B:222:GLU:HB3	1.64	0.62
1:B:475:VAL:HG21	1:B:491:LEU:HD13	1.82	0.61
1:C:373:ASN:OD1	1:C:375:PHE:HB2	2.01	0.61
1:B:213:GLY:O	1:B:497:ARG:NH1	2.33	0.61
1:B:268:LEU:HD21	3:B:2601:B12:H5R2	1.83	0.61
1:B:630:ARG:NH2	1:B:650:LEU:O	2.34	0.61
1:B:91:MET:HB3	1:B:97:VAL:HG11	1.83	0.60
3:C:2601:B12:H362	3:C:2601:B12:C35	2.28	0.60
2:E:32:ILE:HD12	2:E:32:ILE:H	1.67	0.60
1:B:253:ARG:HD2	2:D:48:ARG:HD3	1.84	0.60
1:B:63:ILE:HG23	1:B:287:ILE:HD11	1.84	0.60
1:B:662:LYS:HZ1	3:C:2601:B12:H5R1	1.67	0.59
1:B:176:ILE:HG21	1:B:458:LEU:HD11	1.84	0.59
2:E:12:PRO:HD2	2:E:16:ARG:HG3	1.83	0.59
1:B:478:LEU:HD22	1:B:486:ILE:HB	1.83	0.59
1:C:128:MET:O	1:C:131:GLN:HG2	2.03	0.59
1:C:222:GLU:O	1:C:260:THR:OG1	2.20	0.59
1:B:199:LEU:HD23	1:B:493:MET:HE1	1.85	0.59
1:B:147:ASN:ND2	1:B:151:ASN:H	2.00	0.59
1:C:625:GLU:OE1	1:C:704:ARG:NH2	2.36	0.59
1:B:86:VAL:HA	1:B:120:GLN:HG3	1.84	0.58
1:C:21:ILE:HG12	1:C:309:ALA:HB1	1.85	0.58
3:C:2601:B12:O39	3:C:2601:B12:H361	2.04	0.58
1:B:147:ASN:HD21	1:B:151:ASN:N	2.02	0.58
1:C:123:VAL:HB	1:C:352:MET:SD	2.44	0.57
1:C:187:LEU:HD23	1:C:200:THR:HG23	1.85	0.57
1:B:395:LEU:HD22	1:C:123:VAL:HG11	1.85	0.57
2:D:56:TYR:O	2:D:60:ILE:HG12	2.04	0.57
1:C:228:GLY:O	1:C:283:ARG:NH1	2.37	0.57
1:B:161:GLU:OE2	1:B:165:ARG:NH1	2.37	0.57
1:C:164:ILE:HD11	1:C:409:THR:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:VAL:O	1:B:132:LYS:NZ	2.37	0.56
1:C:624:GLU:HB3	1:C:697:LYS:HZ3	1.69	0.56
1:B:337:GLN:HE22	1:B:375:PHE:HB3	1.70	0.56
3:B:2601:B12:H302	1:C:680:LEU:CD2	2.35	0.56
1:B:176:ILE:HB	1:B:179:TYR:HD2	1.70	0.56
1:B:338:THR:H	1:C:720:ARG:HH21	1.54	0.56
1:C:63:ILE:HG23	1:C:287:ILE:HD11	1.87	0.56
1:B:365:TYR:CE2	1:B:380:PHE:HB3	2.40	0.56
1:B:526:GLN:N	1:B:530:THR:OG1	2.35	0.56
3:C:2601:B12:C2B	3:C:2601:B12:H492	2.35	0.56
1:C:669:GLN:HB3	1:C:672:LEU:HD12	1.88	0.56
1:B:173:THR:OG1	3:B:2601:B12:H261	2.06	0.56
1:C:318:LEU:HD22	1:C:352:MET:HB3	1.88	0.55
1:B:89:ALA:HA	1:B:92:LEU:HD12	1.86	0.55
1:B:405:THR:HG22	1:B:407:ALA:H	1.72	0.55
1:C:627:LEU:HD13	1:C:700:ALA:HB1	1.88	0.55
2:D:35:GLU:CD	2:D:35:GLU:H	2.14	0.55
1:B:62:MET:HE2	2:D:136:LYS:NZ	2.22	0.55
1:C:199:LEU:HD23	1:C:493:MET:HE1	1.87	0.55
1:B:260:THR:OG1	1:B:297:GLN:NE2	2.39	0.55
1:B:62:MET:HE2	2:D:136:LYS:HZ3	1.71	0.54
1:B:66:PHE:O	1:B:70:TYR:HB2	2.07	0.54
1:C:302:SER:HA	1:C:337:GLN:HG3	1.87	0.54
1:C:106:THR:O	1:C:109:ILE:HG12	2.07	0.54
1:C:224:VAL:HG21	1:C:257:MET:HE2	1.88	0.54
1:C:333:SER:HB2	1:C:353:GLN:HG2	1.89	0.54
3:C:2601:B12:H91	3:C:2601:B12:O28	2.06	0.54
2:E:11:TYR:HA	2:E:60:ILE:HD13	1.90	0.54
1:C:732:ILE:O	1:C:736:LYS:HG2	2.08	0.54
1:B:589:GLU:HA	1:B:628:HIS:O	2.08	0.54
1:C:302:SER:HB3	3:C:2601:B12:H532	1.90	0.54
1:B:374:MET:O	3:B:2601:B12:H601	2.08	0.54
1:C:366:SER:HB3	1:C:381:ASP:HA	1.90	0.53
1:C:147:ASN:HB2	1:C:446:SER:HB3	1.91	0.53
1:B:117:VAL:HG12	1:B:118:MET:HE2	1.89	0.53
1:B:345:ARG:NE	1:C:394:ASP:OD2	2.39	0.53
1:B:128:MET:HE1	1:C:93:VAL:HB	1.89	0.53
1:B:182:PHE:O	1:B:185:LEU:HB3	2.08	0.53
1:C:375:PHE:HA	3:C:2601:B12:H602	1.90	0.53
1:C:681:PHE:CZ	1:C:695:ILE:HG12	2.42	0.53
1:B:133:MET:HE2	1:B:326:MET:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:SER:HB2	3:C:2601:B12:O7R	2.07	0.53
1:C:214:MET:HG2	1:C:253:ARG:HG2	1.89	0.53
1:B:302:SER:HB3	3:B:2601:B12:H532	1.91	0.53
1:C:77:THR:HA	1:C:108:ALA:HB1	1.91	0.52
1:C:573:LEU:HA	1:C:750:ASP:O	2.09	0.52
1:B:259:TYR:HD2	1:B:288:THR:HG23	1.74	0.52
1:C:32:MET:HG2	1:C:33:ASP:H	1.75	0.52
1:C:182:PHE:O	1:C:185:LEU:HG	2.10	0.52
1:B:201:GLN:NE2	1:B:222:GLU:HB3	2.25	0.52
1:B:594:VAL:HA	1:B:659:ILE:HG23	1.91	0.52
1:B:145:VAL:HB	1:B:187:LEU:HD11	1.91	0.51
1:C:86:VAL:O	1:C:90:ARG:HG3	2.10	0.51
1:C:606:LEU:HD21	1:C:727:ALA:HA	1.91	0.51
1:B:478:LEU:HB2	1:B:487:ALA:HB2	1.92	0.51
1:B:177:ALA:HB2	3:B:2601:B12:N33	2.25	0.51
3:B:2601:B12:H531	3:B:2601:B12:H552	1.92	0.51
1:C:539:TRP:O	1:C:543:LYS:HG3	2.11	0.51
2:E:126:GLU:O	2:E:130:VAL:HG23	2.11	0.51
1:C:418:ARG:NE	1:C:437:VAL:HG11	2.27	0.50
1:C:573:LEU:HD12	1:C:615:LEU:HB3	1.92	0.50
1:B:161:GLU:OE1	1:B:413:ARG:HD2	2.11	0.50
1:B:596:PRO:HB3	1:B:635:LEU:HD23	1.93	0.50
1:B:44:VAL:HG21	1:B:74:VAL:HG13	1.94	0.50
1:B:94:ASP:O	1:B:132:LYS:NZ	2.37	0.50
1:B:396:MET:SD	1:C:315:ARG:NH1	2.85	0.50
1:B:200:THR:H	1:B:219:SER:HG	1.57	0.50
1:B:38:PRO:HB2	1:B:53:ASP:HB3	1.94	0.50
1:B:352:MET:HE3	1:C:395:LEU:HD22	1.93	0.50
1:B:395:LEU:HD13	1:C:352:MET:HE3	1.94	0.50
1:C:285:ILE:HG21	1:C:323:ILE:HG22	1.94	0.50
1:C:147:ASN:HA	1:C:372:ASP:HB3	1.93	0.50
1:B:132:LYS:HA	1:B:525:TYR:HB3	1.94	0.49
1:C:228:GLY:HA3	1:C:280:LEU:HB3	1.93	0.49
1:C:644:ALA:HB1	1:C:668:HIS:HB2	1.94	0.49
1:C:65:ARG:NH2	2:E:129:GLU:OE1	2.44	0.49
1:C:185:LEU:HD12	1:C:420:ILE:HD11	1.95	0.49
1:B:716:ASP:HB3	1:B:719:VAL:HG23	1.95	0.49
1:B:244:ALA:HB1	2:D:75:ARG:HH12	1.77	0.49
1:C:232:VAL:HG21	1:C:266:GLU:HA	1.94	0.49
1:C:681:PHE:HE1	1:C:711:VAL:HB	1.78	0.49
1:C:687:LEU:HD23	1:C:692:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:29:LEU:HA	2:D:32:ILE:HD12	1.94	0.49
1:B:256:LYS:HE3	1:B:294:GLN:HE22	1.78	0.49
1:B:475:VAL:HG13	1:B:487:ALA:HB1	1.94	0.49
3:B:2601:B12:C6	3:B:2601:B12:H4B	2.43	0.49
1:C:227:TYR:CD2	1:C:233:PHE:HA	2.48	0.49
1:C:228:GLY:H	1:C:266:GLU:HG2	1.77	0.49
1:C:209:GLU:HG2	1:C:250:TYR:OH	2.12	0.48
1:C:406:GLU:O	1:C:410:ILE:HG12	2.12	0.48
1:B:691:THR:O	1:B:695:ILE:HG23	2.13	0.48
1:B:491:LEU:HA	1:B:491:LEU:HD12	1.70	0.48
2:D:78:GLU:HB2	2:D:120:ASN:ND2	2.28	0.48
2:D:24:PRO:HG3	2:D:48:ARG:HB3	1.95	0.48
1:B:62:MET:HE3	1:B:230:GLU:HG2	1.95	0.48
1:C:32:MET:HG2	1:C:33:ASP:N	2.28	0.48
1:B:679:GLU:HG3	1:B:702:TYR:HE2	1.79	0.48
2:D:103:GLU:CD	2:D:138:ARG:HH22	2.22	0.48
1:B:13:ARG:NH2	1:C:384:ASP:OD1	2.46	0.48
1:B:42:VAL:HG11	1:B:77:THR:HG22	1.95	0.48
1:C:418:ARG:HH12	1:C:434:ASP:CG	2.21	0.48
1:B:302:SER:CB	3:B:2601:B12:H532	2.43	0.48
1:C:373:ASN:C	1:C:375:PHE:H	2.22	0.48
1:C:196:PRO:O	1:C:511:ARG:HA	2.14	0.47
2:E:19:GLU:OE1	2:E:19:GLU:N	2.38	0.47
1:B:475:VAL:HG11	1:B:491:LEU:HD22	1.96	0.47
1:C:263:THR:H	1:C:300:ALA:HA	1.78	0.47
1:B:720:ARG:CZ	1:C:337:GLN:HB3	2.45	0.47
1:C:433:ALA:O	1:C:437:VAL:HG23	2.15	0.47
1:B:50:VAL:HA	1:B:57:ARG:HB2	1.97	0.47
1:B:177:ALA:HB2	3:B:2601:B12:H332	1.80	0.47
1:B:591:VAL:HG22	1:B:630:ARG:HB3	1.96	0.47
1:C:211:GLU:HG3	2:E:88:LEU:HD11	1.97	0.47
1:B:417:ALA:HB1	1:B:437:VAL:HG22	1.96	0.47
1:B:442:TYR:HB3	1:C:4:SER:HA	1.97	0.47
1:B:589:GLU:O	1:B:653:SER:OG	2.24	0.47
1:C:57:ARG:NH2	1:C:69:ASP:OD2	2.47	0.47
1:C:321:ASN:HD22	1:C:353:GLN:HE21	1.63	0.47
1:B:244:ALA:HB1	2:D:75:ARG:NH1	2.30	0.47
2:D:84:ASP:O	2:D:88:LEU:HD23	2.15	0.47
1:B:248:SER:OG	2:D:75:ARG:NE	2.48	0.47
1:B:294:GLN:HB2	1:B:505:THR:HA	1.97	0.47
1:B:440:ALA:HB2	1:B:449:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:ILE:O	1:B:478:LEU:HD12	2.15	0.47
1:C:636:ARG:NH2	1:C:642:PHE:HB3	2.30	0.47
1:B:383:GLU:HB3	1:C:13:ARG:HH11	1.80	0.46
1:C:81:MET:HE3	1:C:81:MET:HB3	1.78	0.46
1:B:681:PHE:HZ	1:B:711:VAL:HB	1.81	0.46
1:B:256:LYS:HE3	1:B:294:GLN:NE2	2.30	0.46
1:B:472:LEU:HD21	2:D:47:VAL:HG21	1.97	0.46
1:B:660:GLN:HG3	1:B:664:THR:HB	1.98	0.46
2:D:86:ARG:HH22	2:D:107:ILE:HG12	1.79	0.46
2:D:110:GLU:O	2:D:114:THR:OG1	2.30	0.46
1:B:247:ALA:HA	1:B:257:MET:HE3	1.98	0.46
3:C:2601:B12:H253	3:C:2601:B12:H301	1.59	0.45
1:B:126:MET:HA	1:B:322:LEU:HD22	1.96	0.45
1:B:362:PHE:CE1	1:B:380:PHE:HB2	2.51	0.45
1:C:47:GLY:HA2	1:C:74:VAL:HG11	1.98	0.45
1:C:358:THR:HG22	1:C:359:ASP:H	1.81	0.45
1:C:655:ILE:HD12	1:C:702:TYR:HB3	1.98	0.45
1:B:24:TRP:H	1:B:29:LEU:HB2	1.81	0.45
1:B:362:PHE:CG	1:B:365:TYR:HB2	2.51	0.45
1:C:375:PHE:HA	3:C:2601:B12:C60	2.45	0.45
1:B:115:VAL:HG11	1:B:279:TYR:HA	1.97	0.45
1:B:146:THR:HB	1:B:374:MET:HG2	1.98	0.45
1:B:18:ASP:OD1	1:B:341:HIS:ND1	2.32	0.45
1:B:430:PRO:HB2	1:B:452:ARG:NH2	2.31	0.45
3:C:2601:B12:H311	3:C:2601:B12:C35	2.45	0.45
1:B:143:CYS:HB3	1:B:167:PHE:CD1	2.52	0.45
1:C:128:MET:HE3	1:C:525:TYR:HE2	1.82	0.45
2:E:103:GLU:CD	2:E:138:ARG:HH22	2.25	0.45
1:C:348:ALA:HA	1:C:351:LEU:HG	1.99	0.45
1:C:658:GLY:O	1:C:665:THR:HA	2.17	0.45
1:C:260:THR:HG23	1:C:297:GLN:NE2	2.32	0.45
1:B:484:GLU:CD	1:B:484:GLU:H	2.25	0.45
1:C:92:LEU:HD12	1:C:121:MET:SD	2.57	0.45
1:B:406:GLU:O	1:B:410:ILE:HG12	2.16	0.45
1:B:592:ILE:HD12	1:B:629:ALA:HB1	1.98	0.45
1:C:436:GLU:HG2	1:C:450:PRO:HG2	1.99	0.45
1:B:354:MET:HE3	1:B:388:TYR:CZ	2.52	0.44
1:C:250:TYR:CD1	1:C:255:LEU:HD23	2.52	0.44
1:C:141:ASN:HB3	1:C:167:PHE:CD1	2.51	0.44
1:C:159:ALA:HB2	1:C:187:LEU:HD12	1.98	0.44
1:C:253:ARG:HH21	2:E:84:ASP:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:LEU:HD13	1:C:497:ARG:CZ	2.48	0.44
1:C:631:VAL:HG12	1:C:747:LEU:HD12	1.98	0.44
3:B:2601:B12:H602	3:B:2601:B12:H541	1.65	0.44
2:D:126:GLU:O	2:D:130:VAL:HG23	2.17	0.44
1:B:153:VAL:HA	1:B:420:ILE:HG21	2.00	0.44
1:B:333:SER:HB2	1:B:353:GLN:HG2	1.99	0.44
1:B:528:PRO:HD3	1:C:93:VAL:HG21	1.98	0.44
1:C:317:VAL:O	1:C:320:GLU:HG2	2.17	0.44
1:B:449:MET:HE3	1:B:449:MET:HB3	1.79	0.44
1:C:137:ARG:NH2	1:C:531:GLY:O	2.50	0.44
1:C:370:ASN:ND2	1:C:378:SER:O	2.42	0.44
2:E:70:ALA:O	2:E:74:ARG:HG3	2.16	0.44
1:B:222:GLU:HB2	1:B:258:ARG:HH11	1.83	0.44
1:C:195:ARG:HB3	1:C:198:VAL:HG23	1.99	0.44
1:C:214:MET:HE2	1:C:253:ARG:NE	2.33	0.44
1:B:259:TYR:CE2	1:B:293:VAL:HG21	2.52	0.44
1:C:518:ALA:O	1:C:522:ILE:HG12	2.18	0.44
1:B:113:LYS:O	1:B:117:VAL:HG23	2.18	0.44
1:B:210:LEU:O	1:B:214:MET:HG3	2.18	0.44
1:C:661:SER:OG	1:C:734:GLU:OE2	2.24	0.44
1:B:241:TRP:CH2	2:D:130:VAL:HG21	2.52	0.44
1:B:258:ARG:HH21	1:B:330:GLU:CD	2.26	0.44
1:B:264:GLY:H	1:B:277:MET:HG2	1.82	0.44
1:B:270:GLY:HA2	1:C:732:ILE:HG12	2.00	0.44
1:B:347:THR:OG1	1:C:344:ILE:HA	2.18	0.44
1:B:733:LYS:HA	1:B:736:LYS:HE3	1.98	0.44
1:C:418:ARG:HG2	1:C:437:VAL:HG11	2.00	0.44
1:C:136:ARG:NH2	1:C:359:ASP:O	2.51	0.43
1:B:726:LYS:HD3	1:B:730:PHE:CE1	2.53	0.43
2:D:120:ASN:O	2:D:124:VAL:HG23	2.18	0.43
1:B:161:GLU:HG3	1:B:409:THR:HG23	2.00	0.43
3:B:2601:B12:H473	3:B:2601:B12:H482	1.37	0.43
1:C:241:TRP:HE1	2:E:126:GLU:CD	2.27	0.43
1:C:632:VAL:CG1	1:C:744:PRO:HB2	2.48	0.43
1:B:436:GLU:HG2	1:B:450:PRO:HG2	2.01	0.43
1:B:692:TYR:HA	1:B:695:ILE:HG12	2.00	0.43
3:B:2601:B12:H253	3:B:2601:B12:H301	1.66	0.43
1:C:250:TYR:HD1	1:C:255:LEU:HD23	1.83	0.43
1:B:300:ALA:O	1:B:301:VAL:C	2.61	0.43
1:C:225:SER:O	1:C:243:LYS:HE2	2.19	0.43
1:B:193:CYS:HA	1:B:486:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:GLN:HG2	1:C:220:TYR:CZ	2.54	0.43
1:B:492:ASN:HA	1:B:495:ARG:HB2	1.99	0.43
1:B:595:GLY:HA2	1:B:643:MET:SD	2.59	0.43
1:C:7:PHE:HA	1:C:10:LEU:HB2	2.00	0.43
1:C:62:MET:HG2	2:E:134:ARG:HG3	2.01	0.43
1:C:181:PRO:HA	1:C:212:LEU:HD21	2.01	0.42
1:B:196:PRO:HG2	1:B:511:ARG:HG3	2.01	0.42
1:B:390:ILE:HD13	1:C:20:LEU:HD11	2.01	0.42
1:B:627:LEU:HD11	1:B:704:ARG:NE	2.31	0.42
1:C:241:TRP:CZ2	2:E:130:VAL:HG21	2.53	0.42
3:B:2601:B12:H4B	3:B:2601:B12:C5	2.50	0.42
1:C:192:GLN:HB3	1:C:489:ASN:HB2	2.02	0.42
1:C:299:GLY:C	1:C:301:VAL:H	2.27	0.42
2:E:111:LEU:HD13	2:E:120:ASN:HB3	2.01	0.42
1:B:264:GLY:N	1:B:277:MET:HG2	2.34	0.42
1:C:203:SER:HB3	1:C:223:THR:HG21	2.01	0.42
1:B:573:LEU:HD12	1:B:573:LEU:HA	1.94	0.42
1:C:275:LYS:HB3	1:C:279:TYR:HD2	1.85	0.42
1:C:458:LEU:HA	1:C:461:VAL:HG12	2.01	0.42
1:B:112:ALA:HA	1:B:115:VAL:HG22	2.00	0.42
1:C:67:ILE:HD11	1:C:287:ILE:HG13	2.01	0.42
2:D:75:ARG:HG2	2:D:120:ASN:OD1	2.20	0.42
1:B:347:THR:O	1:B:351:LEU:HB2	2.19	0.42
1:B:6:ARG:NH2	1:C:444:HIS:O	2.47	0.42
1:C:292:GLY:HA3	2:E:72:ASN:HB2	2.01	0.42
1:C:373:ASN:C	1:C:375:PHE:N	2.78	0.42
2:D:134:ARG:HE	2:D:134:ARG:HB3	1.78	0.42
1:B:90:ARG:O	1:B:94:ASP:HB2	2.19	0.41
1:B:448:GLU:OE2	1:C:5:LYS:HD3	2.20	0.41
1:B:593:GLY:HA2	1:B:632:VAL:O	2.20	0.41
1:C:635:LEU:HD12	1:C:744:PRO:HA	2.02	0.41
1:B:633:ARG:HE	1:B:747:LEU:HD21	1.84	0.41
1:C:691:THR:O	1:C:695:ILE:HG13	2.20	0.41
1:B:56:ARG:HB2	1:B:58:ASP:OD1	2.21	0.41
1:B:153:VAL:HG11	1:B:436:GLU:HB3	2.02	0.41
1:B:186:ALA:O	1:B:187:LEU:C	2.63	0.41
1:B:586:ARG:O	1:B:652:GLY:HA3	2.19	0.41
1:C:384:ASP:O	1:C:387:ASP:HB2	2.20	0.41
1:B:370:ASN:HB3	1:C:717:GLN:HB3	2.02	0.41
1:B:554:ILE:HG13	1:B:729:LEU:HD13	2.02	0.41
1:B:662:LYS:HZ2	3:C:2601:B12:H5R1	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:GLU:HG3	1:C:258:ARG:HD2	2.02	0.41
3:B:2601:B12:H533	3:B:2601:B12:H492	2.01	0.41
1:C:575:THR:HG22	1:C:749:ILE:HD13	2.03	0.41
1:B:526:GLN:H	1:B:530:THR:HG1	1.66	0.41
1:C:247:ALA:HA	1:C:257:MET:HE3	2.03	0.41
1:C:464:MET:HG2	1:C:469:ILE:HG13	2.02	0.41
2:E:61:ALA:O	2:E:66:ARG:HB2	2.21	0.41
1:B:87:GLU:O	1:B:91:MET:HG3	2.21	0.41
1:B:209:GLU:HA	1:B:212:LEU:HD12	2.01	0.41
1:C:418:ARG:HE	1:C:437:VAL:HG11	1.84	0.41
1:B:195:ARG:NH1	1:B:509:LEU:O	2.45	0.41
1:B:263:THR:HB	1:B:277:MET:HG2	2.02	0.41
1:B:388:TYR:HA	1:B:391:LEU:HD12	2.03	0.41
1:B:413:ARG:NH2	1:B:440:ALA:O	2.39	0.41
1:B:667:ILE:HB	1:B:679:GLU:HB2	2.01	0.41
1:B:49:ILE:HD12	1:B:68:ALA:HA	2.03	0.40
1:B:337:GLN:HB3	1:C:720:ARG:CZ	2.51	0.40
1:B:533:ARG:HA	1:B:533:ARG:HD3	1.74	0.40
1:C:151:ASN:O	1:C:155:ILE:HG12	2.22	0.40
1:C:168:SER:HA	1:C:195:ARG:HH21	1.86	0.40
1:B:416:ALA:HA	1:B:419:ALA:HB3	2.04	0.40
1:B:607:ILE:HG22	1:B:607:ILE:O	2.21	0.40
1:B:659:ILE:HA	1:B:664:THR:O	2.21	0.40
1:C:485:ASP:OD1	1:C:485:ASP:N	2.55	0.40
1:B:224:VAL:HG21	1:B:257:MET:HE2	2.03	0.40
1:B:243:LYS:HA	1:B:243:LYS:HD3	1.94	0.40
1:C:255:LEU:HA	1:C:255:LEU:HD12	1.81	0.40
1:C:576:ARG:HG2	1:C:748:HIS:HB2	2.02	0.40
1:B:95:ILE:HG21	1:C:93:VAL:HG23	2.03	0.40
1:C:519:VAL:HG13	2:E:64:MET:HG3	2.04	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	734/754 (97%)	700 (95%)	30 (4%)	4 (0%)	24	59
1	C	732/754 (97%)	682 (93%)	48 (7%)	2 (0%)	36	68
2	D	132/141 (94%)	123 (93%)	8 (6%)	1 (1%)	16	48
2	E	136/141 (96%)	127 (93%)	8 (6%)	1 (1%)	18	51
All	All	1734/1790 (97%)	1632 (94%)	94 (5%)	8 (0%)	24	59

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	301	VAL
1	B	364	GLY
2	D	135	HIS
1	C	364	GLY
1	C	301	VAL
1	B	204	VAL
1	B	569	PRO
2	E	47	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	600/619 (97%)	600 (100%)	0	100	100
1	C	602/619 (97%)	602 (100%)	0	100	100
2	D	113/120 (94%)	113 (100%)	0	100	100
2	E	117/120 (98%)	117 (100%)	0	100	100
All	All	1432/1478 (97%)	1432 (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 (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	73	ASN
1	B	120	GLN
1	B	142	GLN
1	B	183	ASN
1	B	321	ASN
1	B	468	ASN
1	B	604	HIS
1	B	694	GLN
1	C	17	GLN
1	C	142	GLN
1	C	321	ASN
1	C	335	ASN
1	C	341	HIS
1	C	468	ASN
1	C	492	ASN
1	C	526	GLN
1	C	603	HIS
1	C	628	HIS
2	D	63	GLN
2	D	132	GLN
2	E	65	GLN
2	E	116	HIS
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	B	2601	-	93,101,101	1.40	12 (12%)	146,166,166	2.27	34 (23%)
3	B12	C	2601	-	93,101,101	1.26	12 (12%)	146,166,166	1.69	25 (17%)

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	B	2601	-	-	11/56/223/223	0/3/11/11
3	B12	C	2601	-	-	14/56/223/223	0/3/11/11

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2601	B12	C9-N22	5.88	1.46	1.30
3	B	2601	B12	C8B-C9B	4.09	1.47	1.40
3	C	2601	B12	C8B-C9B	4.06	1.47	1.40
3	C	2601	B12	C1-C2	-4.06	1.49	1.58
3	B	2601	B12	C8B-N1B	-3.43	1.32	1.39
3	B	2601	B12	C14-N23	-3.31	1.30	1.35
3	C	2601	B12	C9B-N3B	-3.26	1.33	1.39
3	C	2601	B12	C8B-N1B	-3.21	1.32	1.39
3	B	2601	B12	C1-C2	-3.15	1.51	1.58
3	B	2601	B12	C9B-N3B	-2.97	1.34	1.39
3	C	2601	B12	C6B-C5B	2.96	1.48	1.40
3	C	2601	B12	C9-N22	2.93	1.38	1.30
3	B	2601	B12	C6B-C5B	2.68	1.47	1.40
3	B	2601	B12	C11-N23	2.68	1.42	1.37
3	C	2601	B12	C19-N24	2.68	1.53	1.48
3	B	2601	B12	C8-C9	-2.58	1.45	1.51
3	B	2601	B12	C54-C17	-2.41	1.50	1.54
3	B	2601	B12	C14-C15	2.38	1.48	1.38
3	C	2601	B12	C2B-N1B	-2.33	1.33	1.37
3	C	2601	B12	C14-N23	2.28	1.38	1.35
3	C	2601	B12	C10-C9	2.23	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2601	B12	C11-N23	2.16	1.41	1.37
3	C	2601	B12	C10-C11	-2.06	1.31	1.38
3	B	2601	B12	C2B-N3B	2.04	1.35	1.31

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2601	B12	C1-C19-N24	8.98	116.34	106.24
3	B	2601	B12	C30-C3-C4	7.19	126.35	109.63
3	B	2601	B12	C26-C2-C3	-6.93	95.16	107.41
3	C	2601	B12	C20-C1-C19	-6.71	102.89	109.36
3	B	2601	B12	C18-C19-N24	6.70	112.50	102.31
3	B	2601	B12	C1-C19-C18	-6.41	111.35	121.88
3	B	2601	B12	C2-C1-N21	-5.41	94.22	101.77
3	B	2601	B12	C54-C17-C18	-5.32	105.13	112.98
3	C	2601	B12	C2-C3-C4	5.32	107.67	101.63
3	B	2601	B12	C1-C2-C3	4.83	107.76	101.60
3	C	2601	B12	C54-C17-C18	-4.68	106.07	112.98
3	B	2601	B12	C60-C18-C19	4.33	125.92	114.62
3	C	2601	B12	C25-C2-C1	-4.31	107.29	113.78
3	B	2601	B12	C20-C1-C19	4.19	113.39	109.36
3	B	2601	B12	C9B-C8B-N1B	4.16	107.10	105.35
3	B	2601	B12	C20-C1-C2	4.11	120.16	113.28
3	B	2601	B12	C55-C17-C16	4.08	124.70	116.65
3	B	2601	B12	C48-C13-C12	-4.05	105.27	116.63
3	B	2601	B12	C30-C3-C2	-4.01	110.61	119.09
3	C	2601	B12	C18-C60-C61	-3.91	104.21	113.97
3	B	2601	B12	C36-C7-C8	-3.87	104.93	112.08
3	B	2601	B12	C48-C13-C14	3.78	117.92	108.49
3	B	2601	B12	C18-C17-C16	3.78	105.26	100.67
3	B	2601	B12	C2-C1-C19	-3.69	112.78	118.60
3	B	2601	B12	C7-C8-C9	-3.64	96.24	100.90
3	C	2601	B12	C9-C10-C11	-3.56	120.81	125.97
3	C	2601	B12	C53-C15-C14	-3.48	111.42	118.43
3	B	2601	B12	C25-C2-C26	3.47	116.73	109.71
3	B	2601	B12	C53-C15-C16	-3.46	114.44	120.38
3	C	2601	B12	C3-C4-N21	-3.39	107.72	111.97
3	C	2601	B12	C26-C2-C3	3.37	113.38	107.41
3	C	2601	B12	C53-C15-C16	3.36	126.16	120.38
3	C	2601	B12	C8B-C9B-N3B	-3.35	106.27	109.97
3	C	2601	B12	C41-C8-C7	-3.26	105.16	114.14
3	B	2601	B12	C17-C16-C15	3.22	131.34	126.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2601	B12	C3-C4-N21	-3.18	107.98	111.97
3	B	2601	B12	C53-C15-C14	-3.13	112.12	118.43
3	B	2601	B12	C8B-C9B-N3B	-3.12	106.53	109.97
3	B	2601	B12	C55-C56-C57	-3.10	104.45	111.23
3	C	2601	B12	C12-C11-N23	-3.03	107.60	111.83
3	C	2601	B12	C2-C1-C19	3.03	123.39	118.60
3	C	2601	B12	C30-C3-C2	-3.01	112.73	119.09
3	C	2601	B12	C48-C13-C14	2.98	115.92	108.49
3	C	2601	B12	C30-C31-C32	-2.98	102.49	112.59
3	C	2601	B12	C18-C17-C16	2.97	104.27	100.67
3	C	2601	B12	C10-C9-N22	2.88	129.03	125.73
3	B	2601	B12	C6-C5-C4	-2.69	116.72	121.54
3	B	2601	B12	C15-C16-N24	-2.67	118.58	122.42
3	B	2601	B12	C8-C7-C6	2.52	105.25	100.92
3	C	2601	B12	C9B-C8B-N1B	2.50	106.40	105.35
3	C	2601	B12	C9B-N3B-C2B	2.41	107.30	104.44
3	B	2601	B12	C2-C26-C27	2.39	121.95	115.22
3	C	2601	B12	C56-C55-C17	2.30	119.95	115.52
3	C	2601	B12	C15-C16-N24	-2.24	119.20	122.42
3	B	2601	B12	C3R-C2R-C1R	2.24	104.84	99.89
3	C	2601	B12	C10-C11-N23	2.19	128.17	124.43
3	C	2601	B12	C7B-C8B-C9B	-2.11	120.02	122.52
3	B	2601	B12	C7B-C8B-C9B	-2.01	120.13	122.52
3	B	2601	B12	C4B-C9B-N3B	2.01	133.97	130.51

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2601	B12	C3-C2-C26-C27
3	B	2601	B12	C2-C3-C30-C31
3	B	2601	B12	C4-C3-C30-C31
3	B	2601	B12	C38-C37-C7-C6
3	B	2601	B12	C38-C37-C7-C8
3	B	2601	B12	C14-C13-C48-C49
3	B	2601	B12	N59-C1P-C2P-O3
3	C	2601	B12	C2-C3-C30-C31
3	C	2601	B12	C4-C3-C30-C31
3	C	2601	B12	C18-C17-C55-C56
3	C	2601	B12	C12-C13-C48-C49
3	C	2601	B12	C3R-C4R-C5R-O8R
3	B	2601	B12	C2-C26-C27-N29

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Mol	Chain	Res	Type	Atoms
3	C	2601	B12	O6R-C4R-C5R-O8R
3	B	2601	B12	N59-C1P-C2P-C3P
3	B	2601	B12	C2-C26-C27-O28
3	C	2601	B12	C54-C17-C55-C56
3	C	2601	B12	C8-C41-C42-C43
3	B	2601	B12	C1-C2-C26-C27
3	C	2601	B12	C1-C2-C26-C27
3	C	2601	B12	C25-C2-C26-C27
3	C	2601	B12	C42-C41-C8-C9
3	C	2601	B12	C16-C17-C55-C56
3	C	2601	B12	C19-C18-C60-C61
3	C	2601	B12	C17-C18-C60-C61

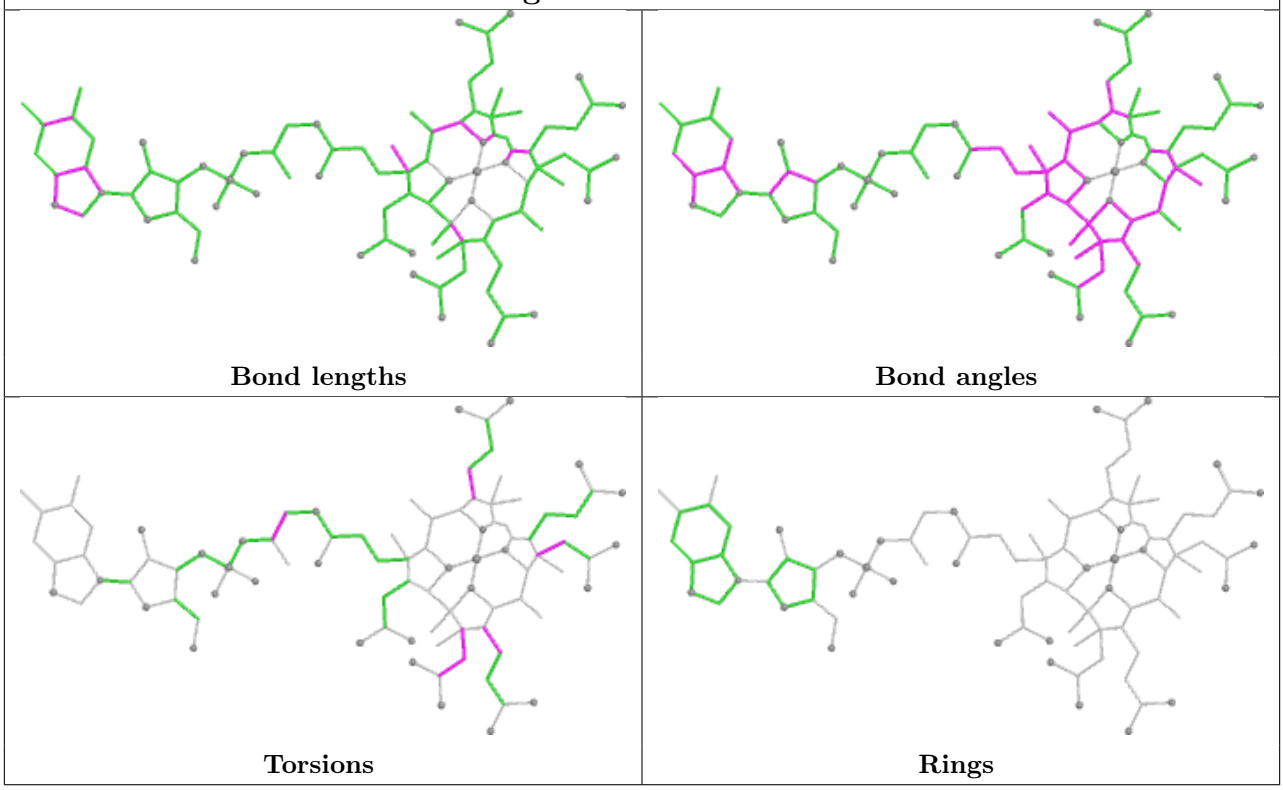
There are no ring outliers.

2 monomers are involved in 42 short contacts:

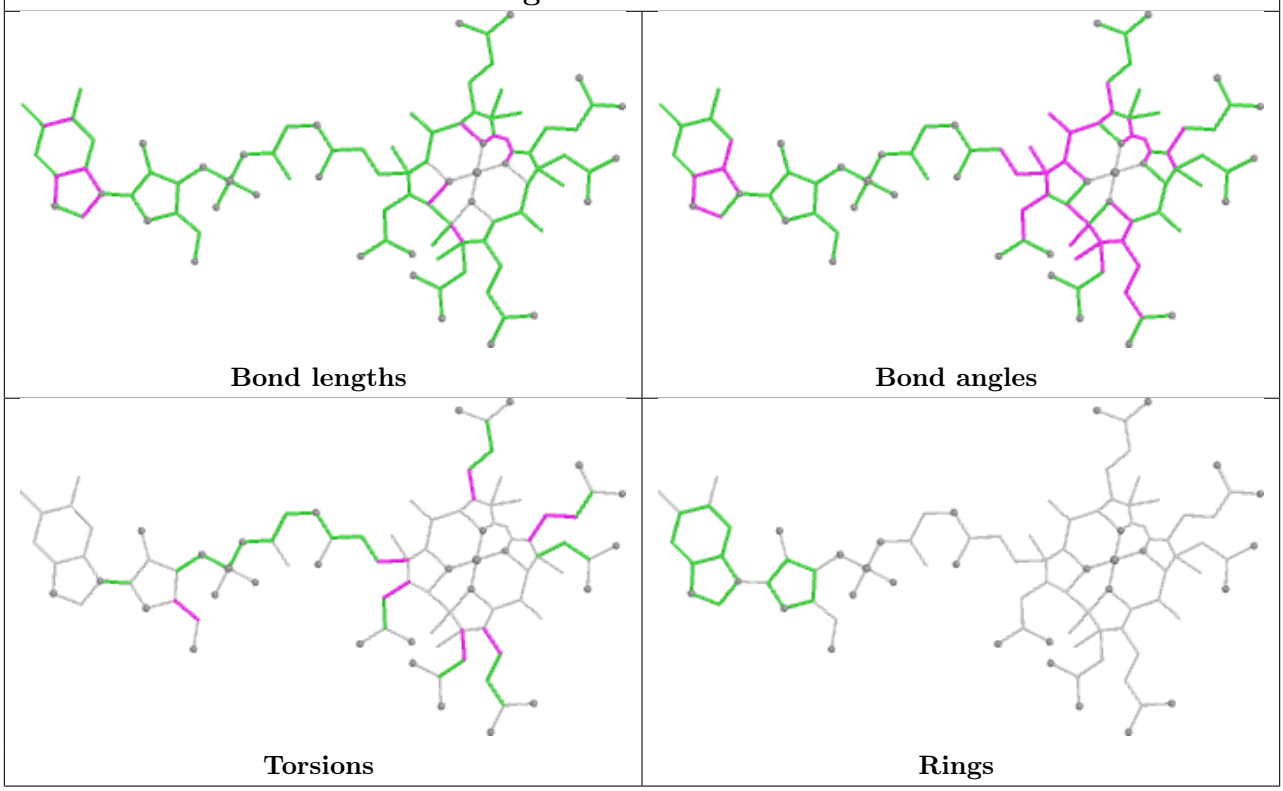
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2601	B12	21	0
3	C	2601	B12	21	0

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 B12 B 2601



Ligand B12 C 2601



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	B	738/754 (97%)	1.38	150 (20%)	3 2	22, 38, 52, 66	0
1	C	736/754 (97%)	1.31	118 (16%)	5 3	22, 32, 43, 61	0
2	D	136/141 (96%)	1.45	29 (21%)	2 1	43, 58, 67, 74	0
2	E	138/141 (97%)	1.17	14 (10%)	12 6	31, 39, 47, 51	0
All	All	1748/1790 (97%)	1.34	311 (17%)	4 2	22, 36, 57, 74	0

All (311) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	615	LEU	5.1
1	C	218	THR	4.7
1	C	245	PHE	4.7
1	C	592	ILE	4.7
2	D	132	GLN	4.6
1	B	107	THR	4.6
1	C	578	GLY	4.4
2	D	125	ARG	4.2
1	B	232	VAL	4.1
1	B	71	ALA	4.1
1	B	225	SER	4.0
1	B	69	ASP	4.0
1	C	295	GLY	3.9
1	C	638	SER	3.9
1	B	340	SER	3.8
1	B	575	THR	3.8
1	C	291	ALA	3.8
1	B	632	VAL	3.8
1	B	129	ALA	3.7
1	B	644	ALA	3.6
1	B	339	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	188	LEU	3.6
1	B	324	ALA	3.5
2	D	100	SER	3.5
2	D	12	PRO	3.5
1	C	590	VAL	3.5
1	B	577	GLU	3.4
2	D	22	LEU	3.4
1	B	584	ASP	3.4
1	B	296	LEU	3.3
1	B	171	GLU	3.3
1	B	334	ALA	3.3
1	C	644	ALA	3.3
1	B	259	TYR	3.3
1	B	278	LEU	3.3
1	C	352	MET	3.3
1	B	332	ALA	3.3
1	B	359	ASP	3.2
1	C	289	LYS	3.2
1	C	145	VAL	3.2
1	B	687	LEU	3.2
1	B	685	PRO	3.2
2	D	141	SER	3.2
2	D	131	TYR	3.2
1	C	363	SER	3.2
1	B	344	ILE	3.2
1	C	156	ALA	3.2
1	C	189	VAL	3.1
1	C	144	HIS	3.1
1	C	141	ASN	3.1
1	C	219	SER	3.1
1	B	527	GLY	3.1
1	B	102	ILE	3.1
1	B	702	TYR	3.1
1	B	548	VAL	3.0
2	D	8	VAL	3.0
1	B	388	TYR	3.0
1	C	254	GLY	3.0
1	C	204	VAL	3.0
1	C	709	SER	3.0
1	B	45	ASP	3.0
1	C	223	THR	3.0
2	D	34	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	63	ILE	3.0
1	B	498	VAL	3.0
1	C	298	ASN	2.9
1	B	31	ALA	2.9
1	C	140	SER	2.9
1	C	231	ALA	2.9
2	E	11	TYR	2.9
1	B	655	ILE	2.9
1	C	376	ALA	2.9
1	B	270	GLY	2.9
1	B	279	TYR	2.9
1	C	66	PHE	2.9
1	C	30	ILE	2.9
1	C	259	TYR	2.8
1	B	177	ALA	2.8
1	B	186	ALA	2.8
1	B	382	ALA	2.8
1	B	275	LYS	2.8
1	B	614	ILE	2.8
1	C	182	PHE	2.8
1	B	365	TYR	2.8
1	B	526	GLN	2.8
1	C	334	ALA	2.8
1	C	624	GLU	2.8
1	B	654	GLY	2.8
1	B	504	GLN	2.8
1	B	93	VAL	2.8
1	B	153	VAL	2.8
1	C	197	GLY	2.8
1	B	518	ALA	2.8
1	B	703	ALA	2.8
1	C	170	GLN	2.8
1	B	240	PRO	2.8
1	C	483	PHE	2.7
1	B	588	ASP	2.7
1	B	243	LYS	2.7
2	E	63	GLN	2.7
1	B	298	ASN	2.7
1	B	145	VAL	2.7
1	B	269	MET	2.7
2	E	73	PHE	2.7
1	B	84	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	252	SER	2.7
1	C	459	SER	2.7
1	B	327	LEU	2.7
1	C	152	PRO	2.7
2	E	126	GLU	2.7
2	E	16	ARG	2.7
1	B	251	ALA	2.7
1	C	477	ALA	2.7
1	B	44	VAL	2.7
1	C	213	GLY	2.7
1	C	377	GLY	2.7
1	B	509	LEU	2.7
1	C	657	ILE	2.6
1	B	367	ALA	2.6
1	C	322	LEU	2.6
1	B	572	THR	2.6
1	C	221	ALA	2.6
1	B	140	SER	2.6
1	B	250	TYR	2.6
1	C	271	TYR	2.6
1	C	237	ASP	2.6
1	B	205	GLU	2.6
1	C	678	LEU	2.6
1	B	331	VAL	2.6
1	B	91	MET	2.6
1	B	329	LEU	2.6
1	B	138	THR	2.6
2	D	15	THR	2.6
1	B	380	PHE	2.6
1	B	305	GLY	2.6
1	B	529	GLY	2.6
1	B	141	ASN	2.6
1	C	494	LEU	2.6
1	B	286	PHE	2.5
1	C	478	LEU	2.5
1	C	684	ALA	2.5
1	B	695	ILE	2.5
1	C	347	THR	2.5
1	C	369	PRO	2.5
1	B	198	VAL	2.5
1	C	622	VAL	2.5
1	B	184	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	581	ALA	2.5
1	B	88	ILE	2.5
1	C	88	ILE	2.5
1	C	475	VAL	2.5
1	B	21	ILE	2.5
1	B	429	LEU	2.5
1	C	341	HIS	2.5
1	B	216	GLY	2.5
1	B	723	PHE	2.5
1	B	165	ARG	2.5
1	C	92	LEU	2.5
2	D	113	HIS	2.5
1	C	550	GLN	2.5
1	C	699	ALA	2.4
1	B	276	SER	2.4
1	B	641	SER	2.4
1	C	202	CYS	2.4
1	B	642	PHE	2.4
1	C	339	PHE	2.4
1	B	288	THR	2.4
1	C	327	LEU	2.4
1	B	111	PRO	2.4
1	B	442	TYR	2.4
1	B	163	GLY	2.4
2	D	127	SER	2.4
2	E	137	LEU	2.4
1	C	507	ALA	2.4
2	E	87	ILE	2.4
1	B	627	LEU	2.4
1	C	302	SER	2.4
1	C	520	ASN	2.4
1	B	587	ALA	2.4
1	B	142	GLN	2.4
1	C	40	SER	2.4
1	C	272	SER	2.4
1	B	472	LEU	2.3
1	B	571	PHE	2.3
2	E	124	VAL	2.3
1	C	107	THR	2.3
1	C	262	GLY	2.3
1	C	263	THR	2.3
1	B	291	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	443	ALA	2.3
1	C	453	ASN	2.3
1	C	94	ASP	2.3
1	B	176	ILE	2.3
1	B	507	ALA	2.3
1	C	251	ALA	2.3
1	C	629	ALA	2.3
2	D	79	LEU	2.3
1	B	717	GLN	2.3
1	B	144	HIS	2.3
1	B	638	SER	2.3
1	C	168	SER	2.3
1	B	355	LEU	2.3
1	C	185	LEU	2.3
1	B	552	ASP	2.3
1	C	552	ASP	2.3
1	B	440	ALA	2.3
2	E	22	LEU	2.3
1	C	378	SER	2.3
1	B	404	VAL	2.3
1	B	146	THR	2.2
1	C	282	SER	2.2
2	D	99	SER	2.2
1	B	230	GLU	2.2
1	B	304	ILE	2.2
2	D	80	ILE	2.2
1	C	362	PHE	2.2
1	C	662	LYS	2.2
1	B	479	SER	2.2
1	B	373	ASN	2.2
1	C	206	GLU	2.2
1	C	308	GLY	2.2
2	D	14	ALA	2.2
2	D	104	LEU	2.2
2	D	115	TRP	2.2
1	B	310	VAL	2.2
2	E	42	VAL	2.2
1	B	496	GLN	2.2
1	B	468	ASN	2.2
1	C	29	LEU	2.2
2	D	94	LEU	2.2
1	B	159	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	403	PRO	2.2
2	D	123	PHE	2.2
1	C	575	THR	2.2
1	B	486	ILE	2.2
1	B	130	LEU	2.2
1	B	187	LEU	2.2
1	B	217	LEU	2.2
1	B	629	ALA	2.2
1	C	8	ALA	2.2
1	B	658	GLY	2.2
1	C	450	PRO	2.2
1	C	471	GLY	2.2
1	C	652	GLY	2.2
1	B	381	ASP	2.2
1	B	398	ASP	2.2
1	C	200	THR	2.1
1	C	70	TYR	2.1
1	C	365	TYR	2.1
1	C	67	ILE	2.1
1	C	72	ILE	2.1
1	C	164	ILE	2.1
1	B	606	LEU	2.1
1	B	615	LEU	2.1
1	C	201	GLN	2.1
1	B	157	ALA	2.1
1	B	295	GLY	2.1
2	D	86	ARG	2.1
2	E	120	ASN	2.1
1	C	444	HIS	2.1
1	C	594	VAL	2.1
1	C	358	THR	2.1
2	E	91	TYR	2.1
1	B	318	LEU	2.1
1	C	180	ALA	2.1
2	D	61	ALA	2.1
1	B	333	SER	2.1
1	C	519	VAL	2.1
1	B	675	LEU	2.1
1	C	287	ILE	2.1
2	E	15	THR	2.1
1	B	493	MET	2.1
1	B	294	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	12	GLN	2.1
1	C	683	GLN	2.1
2	D	52	GLN	2.1
1	B	621	GLY	2.1
1	C	270	GLY	2.1
1	B	375	PHE	2.1
1	B	420	ILE	2.1
2	D	67	HIS	2.1
2	D	137	LEU	2.1
1	B	41	SER	2.1
1	B	516	VAL	2.1
1	B	719	VAL	2.1
1	B	335	ASN	2.1
1	B	574	LYS	2.1
2	D	139	LYS	2.1
2	D	53	THR	2.1
1	B	86	VAL	2.0
1	C	481	SER	2.0
1	B	164	ILE	2.0
2	D	90	ILE	2.0
2	E	80	ILE	2.0
1	C	173	THR	2.0
1	C	239	THR	2.0
1	C	332	ALA	2.0
1	C	313	GLY	2.0
2	D	44	PRO	2.0
1	B	397	VAL	2.0
1	B	261	SER	2.0
1	C	203	SER	2.0
1	C	326	MET	2.0
1	C	396	MET	2.0
1	B	162	ALA	2.0
1	B	358	THR	2.0
1	B	5	LYS	2.0
1	B	143	CYS	2.0
1	B	170	GLN	2.0
1	C	211	GLU	2.0
1	C	751	LEU	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 oligosaccharides in this entry.

6.4 Ligands (i)

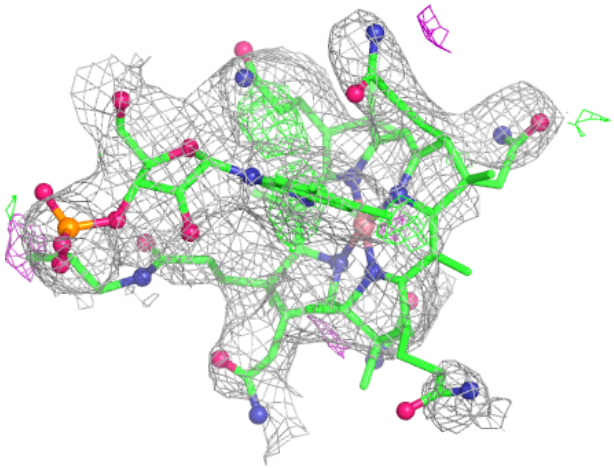
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

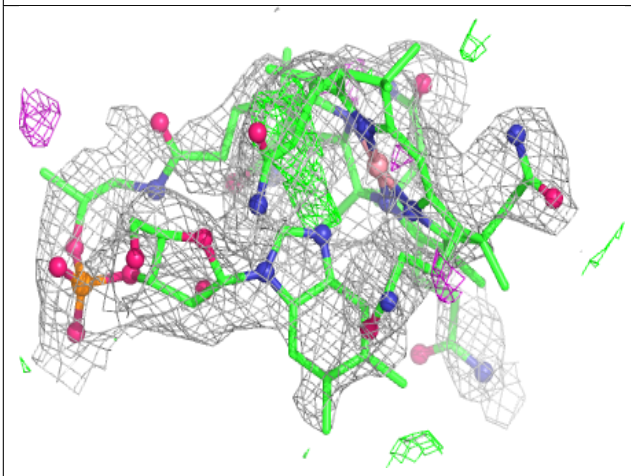
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	B12	B	2601	91/91	0.79	0.20	26,33,55,70	0
3	B12	C	2601	91/91	0.85	0.19	24,28,45,53	0

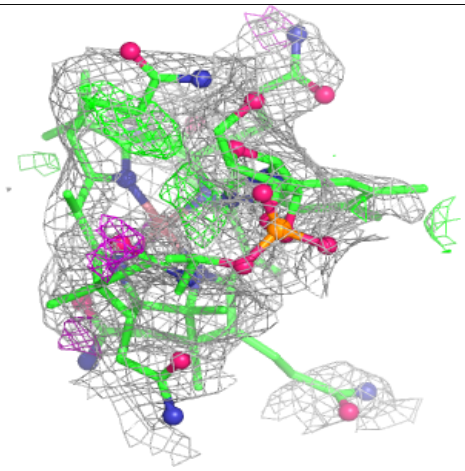
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B12 B 2601:

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

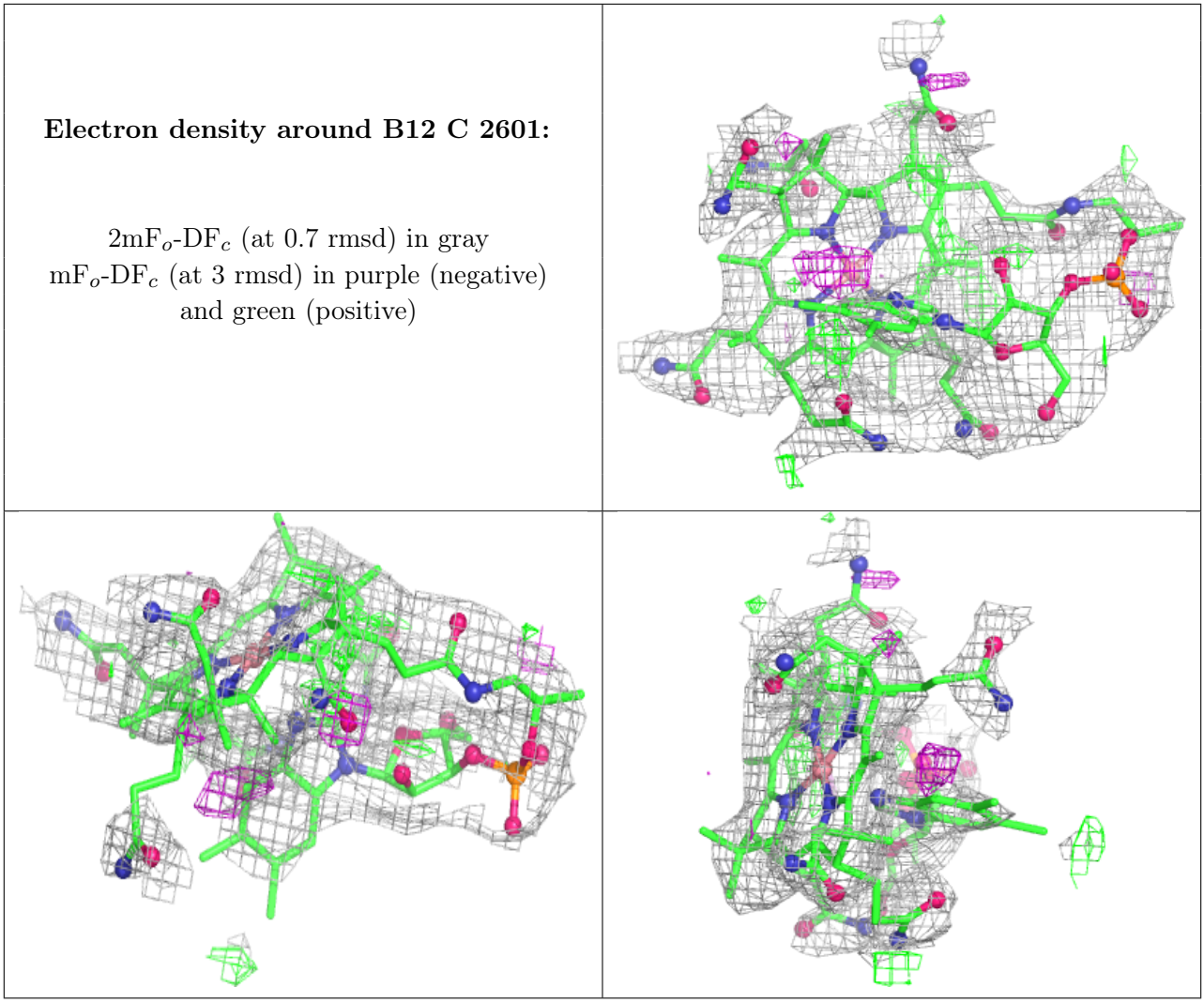






Electron density around B12 C 2601:

$2mF_o$-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.