



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 09:40 pm BST

PDB ID : 1IWB  
Title : Crystal structure of diol dehydratase  
Authors : Shibata, N.; Masuda, J.; Morimoto, Y.; Yasuoka, N.; Toraya, T.  
Deposited on : 2002-05-01  
Resolution : 1.85 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](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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

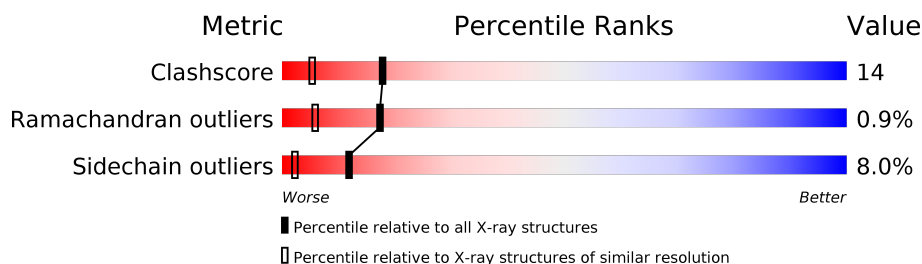
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

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 on 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	554	79% 18% ..
1	L	554	76% 21% ..
2	B	224	53% 23% . 21%
2	E	224	38% 33% 8% 21%
3	G	173	53% 21% . . 21%
3	M	173	55% 20% . . 21%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14446 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 DIOL DEHYDRATASE alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4201	2620	727	825	29			
1	L	551	Total	C	N	O	S	0	0	0
			4200	2620	727	824	29			

- Molecule 2 is a protein called DIOL DEHYDRATASE beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	0	0
			1357	859	244	252	2			
2	E	177	Total	C	N	O	S	0	0	0
			1352	856	243	251	2			

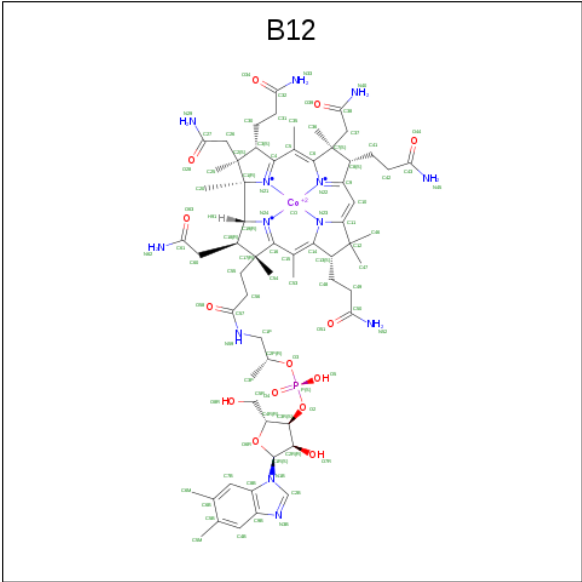
- Molecule 3 is a protein called DIOL DEHYDRATASE gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	137	Total	C	N	O	S	0	0	0
			1093	681	195	214	3			
3	M	137	Total	C	N	O	S	0	0	0
			1093	681	195	214	3			

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	K	0	0
			3	3		
4	L	3	Total	K	0	0
			3	3		

- Molecule 5 is COBALAMIN (three-letter code: B12) (formula: C<sub>62</sub>H<sub>89</sub>CoN<sub>13</sub>O<sub>14</sub>P).

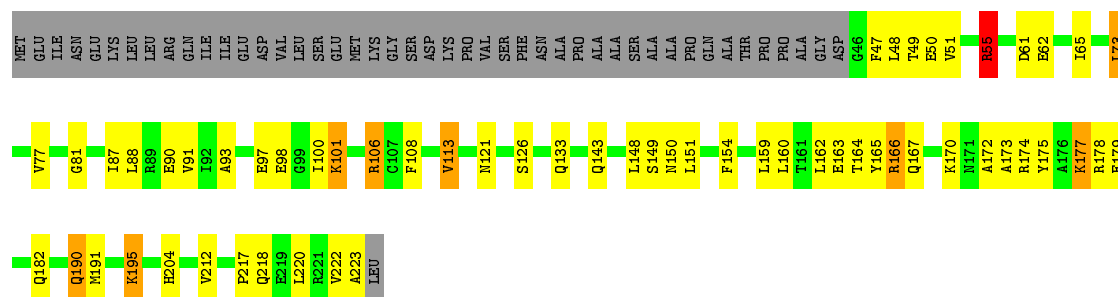


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
5	E	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

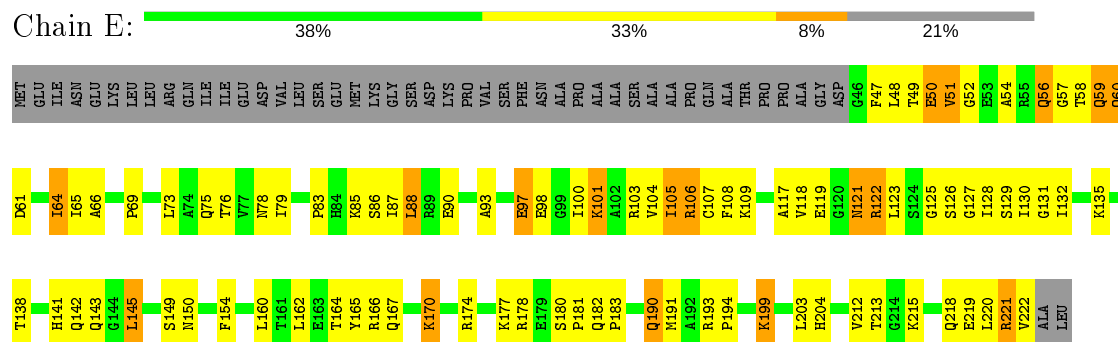
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	335	Total	O	0	0
			335	335		
6	B	89	Total	O	0	0
			89	89		
6	G	70	Total	O	0	0
			70	70		
6	L	330	Total	O	0	0
			330	330		
6	E	54	Total	O	0	0
			54	54		
6	M	84	Total	O	0	0
			84	84		

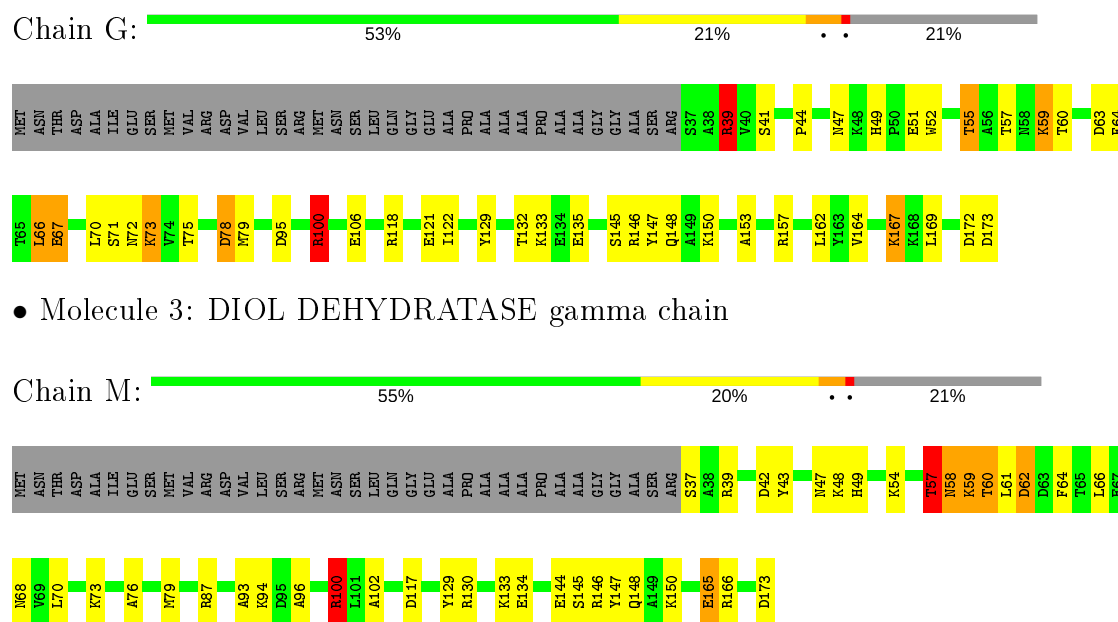




• Molecule 2: DIOL DEHYDRATASE beta chain



• Molecule 3: DIOL DEHYDRATASE gamma chain



• Molecule 3: DIOL DEHYDRATASE gamma chain

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.79 Å   122.40 Å   207.59 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	10.00 – 1.85	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.85)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS, SHELXL-97	Depositor
R, $R_{free}$	0.181 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, 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	A	0.33	0/4273	0.99	9/5787 (0.2%)
1	L	0.34	0/4272	1.01	9/5786 (0.2%)
2	B	0.31	0/1379	0.98	4/1867 (0.2%)
2	E	0.31	0/1374	0.90	1/1860 (0.1%)
3	G	0.31	0/1108	0.96	5/1497 (0.3%)
3	M	0.33	0/1108	1.02	4/1497 (0.3%)
All	All	0.33	0/13514	0.99	32/18294 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	L	0	1
All	All	0	2

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	100	ARG	CD-NE-CZ	10.07	137.69	123.60
2	B	55	ARG	NE-CZ-NH1	9.79	125.19	120.30
2	B	55	ARG	CD-NE-CZ	8.70	135.78	123.60
1	A	345	ARG	NE-CZ-NH1	-8.62	115.99	120.30
3	M	87	ARG	CD-NE-CZ	7.50	134.10	123.60
1	A	364	TYR	CB-CG-CD1	7.32	125.39	121.00
1	A	194	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	370	TYR	CA-CB-CG	6.96	126.63	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	39	ARG	CD-NE-CZ	6.87	133.22	123.60
3	G	146	ARG	CD-NE-CZ	6.78	133.10	123.60
3	G	39	ARG	NE-CZ-NH1	6.61	123.61	120.30
2	B	55	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	L	257	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	5	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	L	345	ARG	NE-CZ-NH1	-6.30	117.15	120.30
2	E	193	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	L	364	TYR	CB-CG-CD1	5.86	124.51	121.00
1	L	252	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	L	2	ARG	NE-CZ-NH1	5.78	123.19	120.30
3	M	87	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	135	ARG	NE-CZ-NH2	5.54	123.07	120.30
3	G	100	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	L	252	ARG	NE-CZ-NH2	5.53	123.07	120.30
3	G	146	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	L	532	ARG	CD-NE-CZ	5.22	130.90	123.60
3	M	130	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	B	106	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	370	TYR	CB-CG-CD1	5.18	124.11	121.00
1	A	68	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	L	449	PRO	C-N-CA	-5.12	108.89	121.70
1	L	2	ARG	CD-NE-CZ	5.11	130.75	123.60
1	A	345	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	GLU	Sidechain
1	L	208	GLU	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4201	0	4138	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	4200	0	4139	99	0
2	B	1357	0	1408	47	0
2	E	1352	0	1403	87	0
3	G	1093	0	1101	38	0
3	M	1093	0	1101	35	0
4	A	3	0	0	0	0
4	L	3	0	0	0	0
5	B	91	0	88	9	0
5	E	91	0	88	5	0
6	A	335	0	0	7	0
6	B	89	0	0	2	0
6	E	54	0	0	3	0
6	G	70	0	0	1	0
6	L	330	0	0	6	0
6	M	84	0	0	2	0
All	All	14446	0	13466	366	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 14.

All (366) 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)
3:M:37:SER:HB3	3:M:39:ARG:HH21	1.32	0.94
2:E:190:GLN:H	2:E:190:GLN:HE21	1.14	0.94
2:B:47:PHE:HA	2:B:223:ALA:HB3	1.52	0.91
1:L:513:GLN:HE22	3:M:47:ASN:HD21	1.13	0.90
2:B:190:GLN:HE21	2:B:190:GLN:H	1.22	0.88
1:L:210:LYS:HE2	1:L:214:LEU:HD11	1.59	0.84
3:M:76:ALA:HA	3:M:79:MET:HE2	1.62	0.80
2:B:55:ARG:HH11	2:B:55:ARG:HG2	1.49	0.78
3:G:60:THR:HG23	3:G:63:ASP:H	1.49	0.77
3:M:100:ARG:HG3	3:M:100:ARG:HH11	1.50	0.77
1:A:494:LYS:HA	1:A:497:LEU:HD12	1.67	0.76
2:E:174:ARG:HE	2:E:181:PRO:HB3	1.50	0.75
2:E:142:GLN:HG3	2:E:145:LEU:HD22	1.69	0.75
2:E:90:GLU:OE1	2:E:166:ARG:HD2	1.87	0.74
1:A:4:LYS:HD2	1:L:441:TYR:O	1.88	0.74
1:A:489:MET:O	1:A:493:GLN:HG2	1.86	0.74
1:L:468:ARG:HB3	1:L:472:GLU:OE2	1.88	0.74
2:B:217:PRO:HD2	6:B:1651:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:79:ILE:HD12	2:E:203:LEU:HD12	1.69	0.73
1:L:404:ARG:HB2	1:L:404:ARG:HH11	1.55	0.72
1:L:453:ILE:HD11	2:E:183:PRO:HD2	1.72	0.71
3:G:57:THR:HG21	3:G:78:ASP:OD1	1.89	0.71
3:G:60:THR:HG23	3:G:63:ASP:N	2.06	0.71
2:E:49:THR:OG1	2:E:221:ARG:HB3	1.90	0.71
1:L:513:GLN:NE2	3:M:47:ASN:HD21	1.87	0.70
3:G:153:ALA:O	3:G:157:ARG:HG3	1.91	0.70
2:B:48:LEU:HD13	2:B:220:LEU:HD13	1.74	0.70
3:G:67:GLU:OE2	3:G:70:LEU:HD12	1.92	0.70
2:B:93:ALA:O	2:B:97:GLU:HB2	1.90	0.69
1:A:42:LYS:HB2	1:A:50:GLU:HB3	1.72	0.69
2:E:60:GLN:OE1	2:E:126:SER:HA	1.93	0.69
2:E:119:GLU:HG2	2:E:122:ARG:HH12	1.58	0.69
2:E:79:ILE:HG13	2:E:199:LYS:NZ	2.08	0.68
2:E:100:ILE:HG22	2:E:101:LYS:O	1.94	0.67
1:L:42:LYS:HB2	1:L:50:GLU:HB3	1.74	0.67
1:A:484:ASP:OD1	1:A:485:VAL:HG23	1.95	0.67
2:E:49:THR:HG23	2:E:221:ARG:O	1.94	0.67
3:G:71:SER:HB2	3:G:73:LYS:HE2	1.76	0.67
1:L:536:GLU:HG3	6:L:3744:HOH:O	1.95	0.66
2:B:113:VAL:HG23	2:B:133:GLN:HG3	1.77	0.66
3:G:60:THR:O	3:G:63:ASP:HB2	1.95	0.66
1:L:57:SER:HB3	6:L:3805:HOH:O	1.95	0.66
1:A:191:GLN:OE1	1:A:492:ILE:HD13	1.96	0.65
2:E:212:VAL:HG22	2:E:215:LYS:HB3	1.79	0.65
3:G:59:LYS:NZ	3:G:59:LYS:HB3	2.11	0.65
2:E:199:LYS:HB3	2:E:199:LYS:NZ	2.11	0.64
2:E:103:ARG:HD2	2:E:219:GLU:OE1	1.98	0.64
1:L:210:LYS:O	1:L:214:LEU:HD13	1.98	0.64
2:B:87:ILE:O	2:B:91:VAL:HG23	1.97	0.64
2:E:48:LEU:HD21	2:E:88:LEU:HD23	1.79	0.63
1:A:471:LEU:O	1:A:475:LYS:HG3	1.99	0.63
3:G:55:THR:HG23	3:G:59:LYS:O	1.98	0.63
2:E:54:ALA:HA	2:E:219:GLU:HB2	1.82	0.62
2:B:90:GLU:OE1	2:B:166:ARG:HG3	2.00	0.62
2:E:79:ILE:HG13	2:E:199:LYS:HZ3	1.65	0.62
1:L:409:ILE:HG23	1:L:440:THR:HG22	1.81	0.61
1:L:513:GLN:HE22	3:M:47:ASN:ND2	1.92	0.61
1:L:404:ARG:HH12	1:L:406:GLU:HG2	1.64	0.61
3:G:133:LYS:HD2	3:G:164:VAL:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:47:PHE:HE2	2:E:88:LEU:HD23	1.66	0.60
1:L:438:ALA:HB1	1:L:448:MET:HE2	1.83	0.60
2:E:58:THR:HG22	2:E:58:THR:O	2.01	0.60
2:B:61:ASP:HB3	2:B:101:LYS:HE2	1.84	0.60
3:G:71:SER:OG	3:G:73:LYS:HD2	2.02	0.59
1:L:462:GLU:HG2	1:L:466:LYS:HG3	1.85	0.59
3:M:59:LYS:HD2	3:M:59:LYS:N	2.18	0.59
1:L:86:LYS:O	1:L:90:MET:HG3	2.02	0.59
1:L:365:SER:HB2	1:L:377:SER:HB3	1.84	0.59
2:E:121:ASN:HB3	2:E:129:SER:OG	2.03	0.59
1:A:528:ALA:HA	6:A:2832:HOH:O	2.01	0.58
2:E:56:GLN:HE21	2:E:57:GLY:H	1.50	0.58
3:G:66:LEU:O	3:G:70:LEU:HG	2.04	0.58
1:L:453:ILE:HD12	1:L:457:ILE:HD12	1.85	0.58
2:E:170:LYS:HD3	2:E:174:ARG:HH11	1.68	0.58
1:L:453:ILE:HD11	2:E:183:PRO:CD	2.33	0.58
1:L:475:LYS:HG2	3:M:70:LEU:HD23	1.86	0.58
2:E:93:ALA:O	2:E:97:GLU:HB2	2.03	0.57
1:A:21:LYS:O	1:L:550:PRO:HG3	2.04	0.57
1:A:175:VAL:O	1:A:178:TYR:HB2	2.05	0.57
1:A:299:SER:OG	1:A:303:ILE:HA	2.04	0.57
2:E:60:GLN:HA	2:E:125:GLY:O	2.04	0.57
1:A:468:ARG:HB3	1:A:472:GLU:OE2	2.04	0.57
2:E:204:HIS:HD2	6:E:1610:HOH:O	1.88	0.57
3:M:54:LYS:HD3	3:M:58:ASN:HA	1.87	0.57
1:A:42:LYS:HB2	1:A:50:GLU:CB	2.35	0.57
1:L:333:SER:HA	1:L:362:SER:OG	2.05	0.57
2:E:132:ILE:HG12	2:E:138:THR:HG23	1.87	0.56
2:E:174:ARG:NE	2:E:181:PRO:HB3	2.19	0.56
1:L:25:GLU:OE2	1:L:25:GLU:HA	2.05	0.56
1:L:494:LYS:O	1:L:498:THR:HG23	2.05	0.56
3:M:76:ALA:HA	3:M:79:MET:CE	2.35	0.56
1:A:434:GLU:HG2	1:A:435:GLU:N	2.19	0.56
2:B:61:ASP:O	2:B:101:LYS:HD2	2.06	0.56
5:B:1601:B12:H362	5:B:1601:B12:H351	1.88	0.56
1:L:442:ALA:HB2	1:L:448:MET:HE1	1.87	0.56
2:E:127:GLY:O	2:E:142:GLN:HA	2.07	0.55
3:M:64:PHE:CE1	3:M:79:MET:HG2	2.41	0.55
2:E:190:GLN:H	2:E:190:GLN:NE2	1.94	0.55
3:M:60:THR:HB	3:M:62:ASP:OD1	2.07	0.55
1:A:23:TRP:HB2	1:L:550:PRO:CG	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:106:ARG:HD2	2:E:108:PHE:CE2	2.42	0.55
1:A:409:ILE:HD13	1:A:441:TYR:HE1	1.71	0.54
2:E:50:GLU:O	2:E:220:LEU:HD23	2.08	0.54
2:E:50:GLU:O	2:E:51:VAL:HB	2.07	0.54
5:E:1602:B12:C2B	5:E:1602:B12:H492	2.37	0.54
1:L:148:LYS:HD2	1:L:450:GLU:HG2	1.88	0.54
2:B:204:HIS:HD2	6:B:1630:HOH:O	1.90	0.54
1:L:258:PHE:O	1:L:295:LEU:HD12	2.08	0.54
1:L:184:ILE:O	1:L:188:VAL:HG23	2.08	0.54
2:B:55:ARG:NH1	2:B:55:ARG:HG2	2.20	0.54
3:M:129:TYR:CD2	3:M:173:ASP:HB3	2.43	0.53
5:B:1601:B12:H492	5:B:1601:B12:C2B	2.39	0.53
2:B:62:GLU:O	2:B:126:SER:HB3	2.09	0.53
1:L:210:LYS:HE2	1:L:214:LEU:CD1	2.34	0.53
2:E:170:LYS:HD3	2:E:174:ARG:NH1	2.24	0.53
1:L:462:GLU:HG3	1:L:466:LYS:HE3	1.89	0.53
1:L:404:ARG:CB	1:L:404:ARG:HH11	2.21	0.52
3:G:44:PRO:HG2	3:G:47:ASN:OD1	2.10	0.52
2:B:98:GLU:O	2:B:177:LYS:HE3	2.10	0.52
2:E:87:ILE:HG12	2:E:165:TYR:CE2	2.45	0.52
1:A:23:TRP:HB2	1:L:550:PRO:HG3	1.90	0.52
1:A:23:TRP:CZ2	1:A:26:GLU:HG3	2.45	0.52
1:L:259:THR:CG2	1:L:296:GLN:HE21	2.22	0.52
1:L:299:SER:OG	1:L:303:ILE:HA	2.10	0.52
1:A:294:GLY:HA3	1:A:329:GLU:HB3	1.91	0.52
3:G:132:THR:OG1	3:G:135:GLU:HG3	2.09	0.52
2:B:100:ILE:HD11	2:B:177:LYS:HD2	1.92	0.51
2:E:119:GLU:HA	2:E:122:ARG:CZ	2.39	0.51
2:E:56:GLN:NE2	2:E:123:LEU:HA	2.25	0.51
1:L:188:VAL:O	1:L:192:VAL:HG23	2.10	0.51
1:L:453:ILE:HD11	2:E:183:PRO:HG2	1.92	0.51
1:A:548:LEU:HD12	1:L:20:VAL:HG12	1.91	0.51
2:E:199:LYS:NZ	2:E:203:LEU:HD11	2.26	0.51
2:E:50:GLU:O	2:E:219:GLU:O	2.29	0.51
1:L:442:ALA:HB2	1:L:448:MET:CE	2.41	0.51
2:E:98:GLU:HG3	2:E:177:LYS:NZ	2.26	0.51
1:L:450:GLU:OE1	1:L:450:GLU:HA	2.10	0.51
1:L:453:ILE:HD12	1:L:457:ILE:CD1	2.41	0.51
2:E:141:HIS:HE1	2:E:145:LEU:HB3	1.75	0.50
3:G:55:THR:HG21	3:G:64:PHE:CZ	2.46	0.50
1:A:548:LEU:HG	1:L:19:PHE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:370:TYR:CZ	1:L:446:LYS:HE3	2.46	0.50
1:L:479:GLN:HG2	6:L:3896:HOH:O	2.10	0.50
3:M:94:LYS:HD3	3:M:102:ALA:CB	2.42	0.50
3:G:71:SER:O	3:G:72:ASN:HB2	2.11	0.50
2:B:148:LEU:HD13	5:B:1601:B12:H411	1.94	0.50
2:E:142:GLN:CG	2:E:145:LEU:HD22	2.41	0.50
2:E:47:PHE:CE2	2:E:88:LEU:HD23	2.44	0.50
1:A:38:LYS:HG2	6:A:2891:HOH:O	2.11	0.50
5:B:1601:B12:H361	5:B:1601:B12:O39	2.12	0.50
2:B:47:PHE:O	2:B:222:VAL:HA	2.11	0.50
2:B:98:GLU:OE1	2:B:174:ARG:HG2	2.12	0.50
2:E:48:LEU:HD21	2:E:88:LEU:CD2	2.42	0.50
2:E:119:GLU:HA	2:E:122:ARG:NH1	2.27	0.49
3:M:146:ARG:HD2	3:M:147:TYR:CZ	2.46	0.49
1:A:458:LYS:HD3	1:A:459:PHE:CE1	2.47	0.49
2:B:61:ASP:HB3	2:B:101:LYS:CE	2.42	0.49
3:M:57:THR:O	3:M:58:ASN:OD1	2.30	0.49
1:L:471:LEU:HD11	3:M:79:MET:HE1	1.94	0.49
3:G:106:GLU:HG3	6:G:224:HOH:O	2.12	0.49
1:A:486:ALA:HB3	3:G:66:LEU:HD11	1.94	0.49
2:E:48:LEU:CD2	2:E:222:VAL:HG13	2.42	0.49
2:E:48:LEU:HD11	2:E:88:LEU:CD2	2.42	0.49
1:A:98:ARG:HG3	1:A:132:MET:CE	2.42	0.49
1:L:334:ASN:ND2	1:L:348:ARG:HD3	2.28	0.49
3:M:165:GLU:HG2	3:M:166:ARG:HG2	1.94	0.49
1:L:56:VAL:HA	1:L:59:PHE:CD1	2.48	0.49
1:A:420:GLN:HG3	1:A:431:ILE:O	2.14	0.48
5:E:1602:B12:H362	5:E:1602:B12:H351	1.95	0.48
3:G:67:GLU:CD	3:G:70:LEU:HD12	2.33	0.48
1:L:302:CYS:O	1:L:306:PRO:HD2	2.13	0.48
2:B:90:GLU:HG3	2:B:162:LEU:HB3	1.94	0.48
1:A:173:VAL:HG21	1:A:176:ALA:HA	1.94	0.48
2:E:142:GLN:O	2:E:145:LEU:HB2	2.13	0.48
2:B:62:GLU:HA	2:B:101:LYS:O	2.13	0.48
2:E:131:GLY:O	2:E:138:THR:HA	2.13	0.48
5:E:1602:B12:H552	5:E:1602:B12:H531	1.94	0.48
1:A:499:GLY:HA2	6:A:2697:HOH:O	2.13	0.48
1:L:148:LYS:HD2	1:L:450:GLU:CD	2.34	0.48
5:B:1601:B12:N29	5:B:1601:B12:H3	2.27	0.48
2:E:121:ASN:HD22	2:E:122:ARG:N	2.12	0.48
1:A:365:SER:HB2	1:A:377:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:370:TYR:OH	1:L:444:GLY:HA3	2.13	0.48
1:L:329:GLU:OE2	1:L:505:SER:HA	2.13	0.48
1:L:408:VAL:O	1:L:411:ILE:HG22	2.14	0.48
1:L:431:ILE:HG22	1:L:431:ILE:O	2.14	0.48
1:L:455:GLU:OE1	1:L:459:PHE:HE1	1.97	0.48
3:G:57:THR:OG1	3:G:59:LYS:HD2	2.14	0.48
1:L:69:TYR:HB2	1:L:289:ALA:HB1	1.95	0.47
1:L:33:SER:HB3	1:L:275:SER:HB3	1.95	0.47
3:M:146:ARG:O	3:M:146:ARG:HG2	2.13	0.47
1:A:331:ALA:HB1	1:A:362:SER:HB3	1.96	0.47
1:L:42:LYS:CB	1:L:50:GLU:HB3	2.43	0.47
2:E:190:GLN:HE21	2:E:190:GLN:N	1.98	0.47
2:E:48:LEU:HD23	2:E:222:VAL:HG13	1.96	0.47
2:B:87:ILE:HG23	2:B:165:TYR:CD1	2.49	0.47
3:G:169:LEU:O	3:G:172:ASP:HB2	2.14	0.47
2:E:56:GLN:HG3	2:E:57:GLY:N	2.29	0.47
1:A:180:PRO:HG3	1:A:464:ILE:HD11	1.95	0.47
1:L:404:ARG:NH1	1:L:406:GLU:HG2	2.29	0.47
2:B:51:VAL:O	2:B:51:VAL:HG23	2.15	0.47
3:G:64:PHE:CE1	3:G:79:MET:HG2	2.50	0.47
1:A:493:GLN:HA	1:A:496:LYS:HE3	1.97	0.47
1:A:69:TYR:HB2	1:A:289:ALA:HB1	1.96	0.47
3:G:39:ARG:HG3	3:G:95:ASP:OD2	2.14	0.47
1:A:205:GLU:OE1	1:A:205:GLU:HA	2.15	0.47
1:L:370:TYR:CE2	1:L:446:LYS:HE3	2.50	0.47
2:E:65:ILE:HD12	2:E:104:VAL:HG22	1.97	0.46
3:G:57:THR:HG23	3:G:78:ASP:HA	1.97	0.46
2:E:119:GLU:HG2	2:E:122:ARG:NH1	2.28	0.46
1:A:259:THR:CG2	1:A:296:GLN:HE21	2.29	0.46
3:G:118:ARG:O	3:G:122:ILE:HG13	2.16	0.46
1:L:479:GLN:HG3	1:L:479:GLN:O	2.15	0.46
2:E:76:THR:HB	6:E:1644:HOH:O	2.16	0.46
1:L:365:SER:HB3	1:L:380:ASP:HA	1.98	0.46
3:G:147:TYR:O	3:G:148:GLN:HB2	2.16	0.46
5:B:1601:B12:H91	5:B:1601:B12:H261	1.66	0.46
2:E:106:ARG:HG2	2:E:108:PHE:CZ	2.50	0.46
1:L:23:TRP:CZ2	1:L:26:GLU:HG3	2.51	0.46
1:L:3:SER:O	1:L:7:GLU:HG3	2.16	0.46
2:B:190:GLN:NE2	2:B:190:GLN:H	2.03	0.46
2:B:160:LEU:HD22	2:B:164:THR:HG21	1.98	0.46
2:E:66:ALA:HB1	2:E:107:CYS:SG	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:72:ASN:ND2	6:L:3775:HOH:O	2.49	0.45
3:M:144:GLU:HG3	3:M:150:LYS:HE3	1.98	0.45
1:A:142:ALA:HB2	1:A:166:PHE:CD1	2.52	0.45
1:A:494:LYS:HA	1:A:497:LEU:CD1	2.43	0.45
3:G:75:THR:O	3:G:79:MET:HG3	2.17	0.45
2:E:60:GLN:OE1	2:E:178:ARG:NH2	2.50	0.45
2:B:113:VAL:CG2	2:B:133:GLN:HG3	2.45	0.45
2:B:177:LYS:O	2:B:178:ARG:HB2	2.17	0.45
2:B:77:VAL:HB	2:B:81:GLY:HA2	1.98	0.45
1:L:259:THR:HG23	1:L:296:GLN:HE21	1.82	0.45
1:L:335:ASP:OD1	1:L:335:ASP:N	2.50	0.45
3:M:54:LYS:CD	3:M:58:ASN:HA	2.46	0.45
1:A:21:LYS:HB2	1:L:550:PRO:HD2	1.99	0.45
1:A:329:GLU:OE2	1:A:505:SER:HA	2.17	0.45
2:B:100:ILE:HG13	2:B:173:ALA:HB1	1.97	0.45
3:G:129:TYR:CD2	3:G:173:ASP:HB3	2.51	0.45
1:L:494:LYS:HE3	3:M:61:LEU:O	2.17	0.45
1:A:38:LYS:HA	6:A:2888:HOH:O	2.17	0.45
5:B:1601:B12:H202	5:B:1601:B12:N3B	2.31	0.45
1:A:483:THR:HG23	3:G:66:LEU:HD13	1.99	0.45
1:A:4:LYS:HE3	6:L:3878:HOH:O	2.17	0.45
1:A:549:ASP:OD1	1:A:551:ASN:ND2	2.50	0.45
1:A:389:VAL:HG11	1:L:344:ARG:HD2	1.99	0.45
3:M:173:ASP:OD1	3:M:173:ASP:N	2.50	0.45
3:G:70:LEU:O	3:G:72:ASN:ND2	2.50	0.44
1:L:499:GLY:HA2	6:L:3741:HOH:O	2.17	0.44
3:M:134:GLU:HB2	6:M:203:HOH:O	2.17	0.44
3:M:43:TYR:O	3:M:48:LYS:HE2	2.17	0.44
1:A:458:LYS:HD3	1:A:459:PHE:CD1	2.52	0.44
1:A:493:GLN:NE2	6:A:2678:HOH:O	2.50	0.44
2:B:172:ALA:O	2:B:175:TYR:HB2	2.16	0.44
2:B:65:ILE:HG21	2:B:88:LEU:HD11	1.99	0.44
2:E:118:VAL:O	2:E:121:ASN:ND2	2.50	0.44
2:E:191:MET:C	2:E:194:PRO:HD2	2.38	0.44
2:E:78:ASN:HB2	2:E:135:LYS:O	2.16	0.44
1:L:231:VAL:HG23	1:L:270:TYR:HB2	2.00	0.44
1:A:549:ASP:O	1:A:551:ASN:N	2.50	0.44
1:L:69:TYR:O	3:M:100:ARG:NE	2.50	0.44
2:E:76:THR:O	2:E:83:PRO:HA	2.17	0.44
2:E:128:ILE:N	2:E:128:ILE:HD12	2.33	0.44
5:E:1602:B12:C55	5:E:1602:B12:H531	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:173:ASP:OD1	3:G:173:ASP:N	2.50	0.44
2:E:75:GLN:NE2	6:E:1617:HOH:O	2.50	0.44
1:L:453:ILE:HD11	2:E:183:PRO:CG	2.48	0.44
1:A:367:VAL:HB	1:A:368:PRO:HD2	1.99	0.44
3:G:39:ARG:HG3	3:G:95:ASP:CG	2.38	0.44
2:E:121:ASN:O	2:E:143:GLN:HG3	2.18	0.44
1:L:334:ASN:ND2	1:L:349:LEU:HA	2.33	0.44
2:B:191:MET:O	2:B:195:LYS:HG3	2.17	0.43
2:E:64:ILE:HG21	2:E:105:ILE:HD12	1.99	0.43
2:B:97:GLU:OE1	2:B:170:LYS:HD2	2.18	0.43
1:L:60:ASP:OD1	1:L:62:ILE:HB	2.18	0.43
2:E:54:ALA:HB2	2:E:219:GLU:N	2.33	0.43
1:L:227:GLY:N	1:L:265:GLU:OE2	2.50	0.43
1:L:386:ASP:O	1:L:390:ILE:HD12	2.18	0.43
3:M:68:ASN:HB3	3:M:73:LYS:HB3	2.00	0.43
2:E:162:LEU:HA	2:E:162:LEU:HD23	1.86	0.43
1:A:199:THR:H	1:A:218:CYS:HB2	1.84	0.43
1:A:35:ASN:HB2	1:A:273:GLY:O	2.19	0.43
1:A:54:LYS:NZ	6:A:2879:HOH:O	2.50	0.43
3:M:42:ASP:HB3	3:M:49:HIS:CD2	2.54	0.43
2:E:117:ALA:HB2	2:E:131:GLY:HA3	2.01	0.43
2:E:180:SER:OG	2:E:180:SER:O	2.29	0.43
1:L:429:PRO:HD3	1:L:459:PHE:CG	2.53	0.43
2:E:199:LYS:HB3	2:E:199:LYS:HZ3	1.80	0.43
1:L:421:ALA:O	1:L:424:ALA:HB3	2.18	0.43
1:A:172:THR:OG1	5:B:1601:B12:N29	2.49	0.43
2:E:160:LEU:HD23	2:E:164:THR:HG21	2.01	0.43
1:A:179:ALA:HB3	1:A:180:PRO:HD3	2.00	0.43
2:E:69:PRO:HA	2:E:106:ARG:HD3	2.01	0.43
3:G:133:LYS:HD2	3:G:164:VAL:CG2	2.48	0.42
1:L:148:LYS:HD2	1:L:450:GLU:CG	2.48	0.42
1:L:421:ALA:HB2	1:L:482:PHE:HE2	1.84	0.42
1:L:533:LEU:HD11	1:L:541:ILE:HD12	2.01	0.42
2:B:50:GLU:HB3	2:B:218:GLN:OE1	2.19	0.42
1:A:370:TYR:OH	1:A:446:LYS:HB2	2.20	0.42
2:B:47:PHE:O	2:B:48:LEU:HD23	2.20	0.42
2:E:98:GLU:HG3	2:E:177:LYS:HZ2	1.85	0.42
1:L:142:ALA:HB2	1:L:166:PHE:CG	2.54	0.42
1:L:152:VAL:HG22	1:L:431:ILE:HG12	2.01	0.42
2:B:98:GLU:OE1	2:B:174:ARG:HD2	2.19	0.42
3:G:49:HIS:HB3	3:G:52:TRP:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:173:VAL:HG21	1:L:176:ALA:HA	2.02	0.42
1:L:490:LEU:HA	1:L:490:LEU:HD12	1.80	0.42
1:A:133:ARG:HD3	1:A:133:ARG:HH11	1.69	0.42
2:B:106:ARG:HD2	2:B:108:PHE:CZ	2.54	0.42
2:B:159:LEU:HD23	2:B:159:LEU:N	2.34	0.42
2:B:177:LYS:HB3	2:B:179:GLU:OE2	2.19	0.42
2:B:73:LEU:HD12	2:B:73:LEU:HA	1.72	0.42
1:A:350:LEU:HA	1:A:353:PHE:HB3	2.01	0.42
3:M:62:ASP:N	3:M:62:ASP:OD2	2.50	0.42
3:M:93:ALA:O	3:M:96:ALA:HB3	2.20	0.42
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.92	0.42
1:A:227:GLY:O	1:A:282:ARG:NH1	2.52	0.42
2:B:160:LEU:CD2	2:B:164:THR:HG21	2.50	0.42
1:A:215:GLY:HA2	6:A:2828:HOH:O	2.19	0.42
1:A:334:ASN:ND2	1:A:349:LEU:HA	2.35	0.42
3:G:167:LYS:HB3	3:G:167:LYS:HE3	1.55	0.42
2:B:154:PHE:HB3	2:B:160:LEU:HD11	2.02	0.42
3:M:133:LYS:HB2	6:M:187:HOH:O	2.20	0.42
3:M:60:THR:HB	3:M:62:ASP:CG	2.40	0.42
1:A:335:ASP:N	1:A:335:ASP:OD1	2.50	0.41
5:B:1601:B12:C55	5:B:1601:B12:H531	2.50	0.41
2:E:154:PHE:HB3	2:E:160:LEU:HD21	2.02	0.41
3:M:39:ARG:HA	3:M:39:ARG:HD3	1.91	0.41
1:A:259:THR:HG23	1:A:296:GLN:HE21	1.86	0.41
1:A:291:GLY:HA2	3:G:100:ARG:HB3	2.01	0.41
1:A:395:LYS:HG2	1:A:395:LYS:O	2.20	0.41
2:E:109:LYS:HG3	2:E:119:GLU:OE2	2.21	0.41
1:A:38:LYS:HA	1:A:39:PRO:HD3	1.92	0.41
1:L:146:ASN:HA	1:L:371:ASP:O	2.20	0.41
1:L:62:ILE:HG12	1:L:286:ILE:HD11	2.01	0.41
3:M:64:PHE:HE1	3:M:79:MET:HG2	1.84	0.41
2:E:109:LYS:HG3	2:E:119:GLU:CD	2.40	0.41
1:A:462:GLU:OE2	1:A:466:LYS:HD2	2.21	0.41
1:A:64:HIS:CD2	3:G:162:LEU:HD22	2.56	0.41
1:L:370:TYR:CE1	1:L:446:LYS:HE3	2.55	0.41
2:E:170:LYS:HB2	2:E:170:LYS:HE2	1.75	0.41
2:B:100:ILE:CG1	2:B:173:ALA:HB1	2.50	0.41
2:B:108:PHE:O	2:B:212:VAL:N	2.49	0.41
1:L:205:GLU:HA	1:L:205:GLU:OE1	2.21	0.41
3:G:57:THR:OG1	3:G:78:ASP:HB3	2.21	0.41
1:L:110:PRO:O	1:L:114:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:47:PHE:CE2	2:E:48:LEU:HG	2.56	0.41
1:A:347:ALA:HA	1:L:350:LEU:HD21	2.02	0.41
1:L:498:THR:HG22	3:M:61:LEU:HD21	2.03	0.41
2:E:174:ARG:HH21	2:E:181:PRO:CB	2.34	0.41
5:E:1602:B12:H363	5:E:1602:B12:H411	1.75	0.40
2:E:64:ILE:O	2:E:130:ILE:N	2.49	0.40
1:L:60:ASP:OD1	1:L:62:ILE:N	2.54	0.40
1:A:455:GLU:O	1:A:458:LYS:HB3	2.22	0.40
2:B:151:LEU:HA	2:B:151:LEU:HD23	1.91	0.40
2:B:47:PHE:HA	2:B:223:ALA:CB	2.38	0.40
2:E:132:ILE:HG23	2:E:138:THR:OG1	2.21	0.40
1:A:102:VAL:HB	1:A:103:PRO:HD3	2.03	0.40
2:E:47:PHE:O	2:E:222:VAL:HA	2.22	0.40
1:L:201:CYS:O	1:L:208:GLU:HG3	2.22	0.40
1:A:262:SER:N	1:A:299:SER:HA	2.37	0.40
1:A:345:ARG:HH11	1:A:345:ARG:HD2	1.62	0.40
1:A:98:ARG:HG3	1:A:132:MET:HE1	2.03	0.40
1:L:163:TRP:O	1:L:401:ARG:NH2	2.50	0.40
1:L:455:GLU:OE1	1:L:458:LYS:HE3	2.20	0.40
1:L:83:ASP:OD2	1:L:86:LYS:N	2.49	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	549/554 (99%)	526 (96%)	17 (3%)	6 (1%)	14 4
1	L	549/554 (99%)	532 (97%)	14 (3%)	3 (0%)	29 15
2	B	176/224 (79%)	169 (96%)	7 (4%)	0	100 100
2	E	175/224 (78%)	161 (92%)	8 (5%)	6 (3%)	3 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	135/173 (78%)	131 (97%)	4 (3%)	0	100	100
3	M	135/173 (78%)	132 (98%)	2 (2%)	1 (1%)	22	9
All	All	1719/1902 (90%)	1651 (96%)	52 (3%)	16 (1%)	17	6

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	50	GLU
2	E	59	GLN
3	M	57	THR
2	E	51	VAL
2	E	52	GLY
1	A	452	ASN
1	A	484	ASP
2	E	61	ASP
1	A	300	VAL
1	L	300	VAL
1	L	484	ASP
2	E	56	GLN
1	A	363	GLY
1	L	363	GLY
1	A	550	PRO
1	A	430	PRO

### 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	450/453 (99%)	425 (94%)	25 (6%)	21	7
1	L	450/453 (99%)	426 (95%)	24 (5%)	22	8
2	B	146/183 (80%)	130 (89%)	16 (11%)	6	1
2	E	146/183 (80%)	122 (84%)	24 (16%)	2	0
3	G	116/141 (82%)	102 (88%)	14 (12%)	5	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	M	116/141 (82%)	105 (90%)	11 (10%)	8 1
All	All	1424/1554 (92%)	1310 (92%)	114 (8%)	12 2

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	PHE
1	A	38	LYS
1	A	77	GLU
1	A	147	VAL
1	A	178	TYR
1	A	211	LEU
1	A	232	PHE
1	A	267	GLN
1	A	348	ARG
1	A	350	LEU
1	A	370	TYR
1	A	404	ARG
1	A	406	GLU
1	A	434	GLU
1	A	458	LYS
1	A	462	GLU
1	A	466	LYS
1	A	475	LYS
1	A	479	GLN
1	A	484	ASP
1	A	490	LEU
1	A	492	ILE
1	A	501	TYR
1	A	534	GLN
1	A	548	LEU
2	B	49	THR
2	B	55	ARG
2	B	73	LEU
2	B	101	LYS
2	B	113	VAL
2	B	121	ASN
2	B	143	GLN
2	B	149	SER
2	B	150	ASN
2	B	163	GLU
2	B	166	ARG

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Mol	Chain	Res	Type
2	B	167	GLN
2	B	177	LYS
2	B	182	GLN
2	B	190	GLN
2	B	195	LYS
3	G	39	ARG
3	G	41	SER
3	G	51	GLU
3	G	55	THR
3	G	59	LYS
3	G	66	LEU
3	G	67	GLU
3	G	73	LYS
3	G	78	ASP
3	G	100	ARG
3	G	121	GLU
3	G	145	SER
3	G	150	LYS
3	G	167	LYS
1	L	1	MET
1	L	28	PHE
1	L	42	LYS
1	L	57	SER
1	L	178	TYR
1	L	191	GLN
1	L	218	CYS
1	L	232	PHE
1	L	348	ARG
1	L	404	ARG
1	L	411	ILE
1	L	437	GLU
1	L	450	GLU
1	L	453	ILE
1	L	455	GLU
1	L	462	GLU
1	L	464	ILE
1	L	479	GLN
1	L	484	ASP
1	L	490	LEU
1	L	501	TYR
1	L	536	GLU
1	L	548	LEU

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Mol	Chain	Res	Type
1	L	551	ASN
2	E	59	GLN
2	E	60	GLN
2	E	64	ILE
2	E	73	LEU
2	E	85	LYS
2	E	86	SER
2	E	88	LEU
2	E	97	GLU
2	E	101	LYS
2	E	105	ILE
2	E	106	ARG
2	E	121	ASN
2	E	122	ARG
2	E	145	LEU
2	E	149	SER
2	E	150	ASN
2	E	167	GLN
2	E	170	LYS
2	E	182	GLN
2	E	190	GLN
2	E	199	LYS
2	E	213	THR
2	E	218	GLN
2	E	221	ARG
3	M	57	THR
3	M	58	ASN
3	M	59	LYS
3	M	60	THR
3	M	62	ASP
3	M	66	LEU
3	M	100	ARG
3	M	117	ASP
3	M	145	SER
3	M	148	GLN
3	M	165	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	ASN
1	A	352	GLN

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Mol	Chain	Res	Type
1	A	465	ASN
1	A	551	ASN
2	B	75	GLN
2	B	121	ASN
2	B	143	GLN
2	B	190	GLN
2	B	204	HIS
3	G	68	ASN
3	G	72	ASN
1	L	45	ASN
1	L	334	ASN
1	L	352	GLN
1	L	513	GLN
1	L	543	ASN
1	L	551	ASN
2	E	56	GLN
2	E	59	GLN
2	E	75	GLN
2	E	121	ASN
2	E	182	GLN
2	E	190	GLN
2	E	204	HIS
2	E	218	GLN
3	M	58	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	$\# Z  > 2$
5	B12	E	1602	-	80,101,101	0.96	2 (2%)	101,166,166	1.37	14 (13%)
5	B12	B	1601	-	80,101,101	0.96	3 (3%)	101,166,166	1.22	12 (11%)

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
5	B12	E	1602	-	-	6/51/223/223	0/3/11/11
5	B12	B	1601	-	-	9/51/223/223	0/3/11/11

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1602	B12	C17-C18	2.67	1.57	1.54
5	E	1602	B12	O58-C57	2.67	1.28	1.23
5	B	1601	B12	O58-C57	2.25	1.27	1.23
5	B	1601	B12	C20-C1	-2.18	1.49	1.53
5	B	1601	B12	C11-C10	-2.06	1.37	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1602	B12	C54-C17-C18	-4.26	106.69	112.98
5	E	1602	B12	C55-C17-C16	4.24	124.06	109.92
5	B	1601	B12	C20-C1-C19	3.72	112.94	109.36
5	E	1602	B12	O58-C57-C56	-3.40	115.80	122.02
5	E	1602	B12	C26-C2-C1	3.18	114.96	110.02
5	E	1602	B12	C1-C19-C18	-3.00	116.96	121.93
5	B	1601	B12	C55-C17-C16	3.00	119.91	109.92
5	B	1601	B12	O58-C57-C56	-2.92	116.68	122.02
5	E	1602	B12	C3-C4-C5	-2.72	121.81	131.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1602	B12	C56-C57-N59	2.64	120.87	116.42
5	E	1602	B12	C25-C2-C3	-2.57	111.66	115.58
5	B	1601	B12	C13-C14-C15	-2.53	122.52	131.68
5	E	1602	B12	C6-C5-C4	-2.52	120.35	124.27
5	B	1601	B12	C16-C15-C14	-2.52	120.35	124.27
5	E	1602	B12	C13-C14-C15	-2.45	122.79	131.68
5	E	1602	B12	C36-C7-C8	-2.41	107.76	112.11
5	B	1601	B12	C3-C4-C5	-2.28	123.41	131.68
5	E	1602	B12	C56-C55-C17	2.26	119.87	115.50
5	B	1601	B12	C1-C2-C3	-2.18	98.85	101.59
5	B	1601	B12	C5-C6-N22	-2.17	120.85	124.81
5	E	1602	B12	C2-C3-C4	2.14	103.92	101.67
5	E	1602	B12	C16-C15-C14	-2.13	120.95	124.27
5	B	1601	B12	C60-C18-C17	2.12	120.86	115.74
5	B	1601	B12	C19-C1-N21	-2.12	100.00	102.16
5	B	1601	B12	C8-C9-N22	2.09	113.73	111.12
5	B	1601	B12	C54-C17-C18	-2.08	109.91	112.98

There are no chirality outliers.

All (15) torsion outliers are listed below:

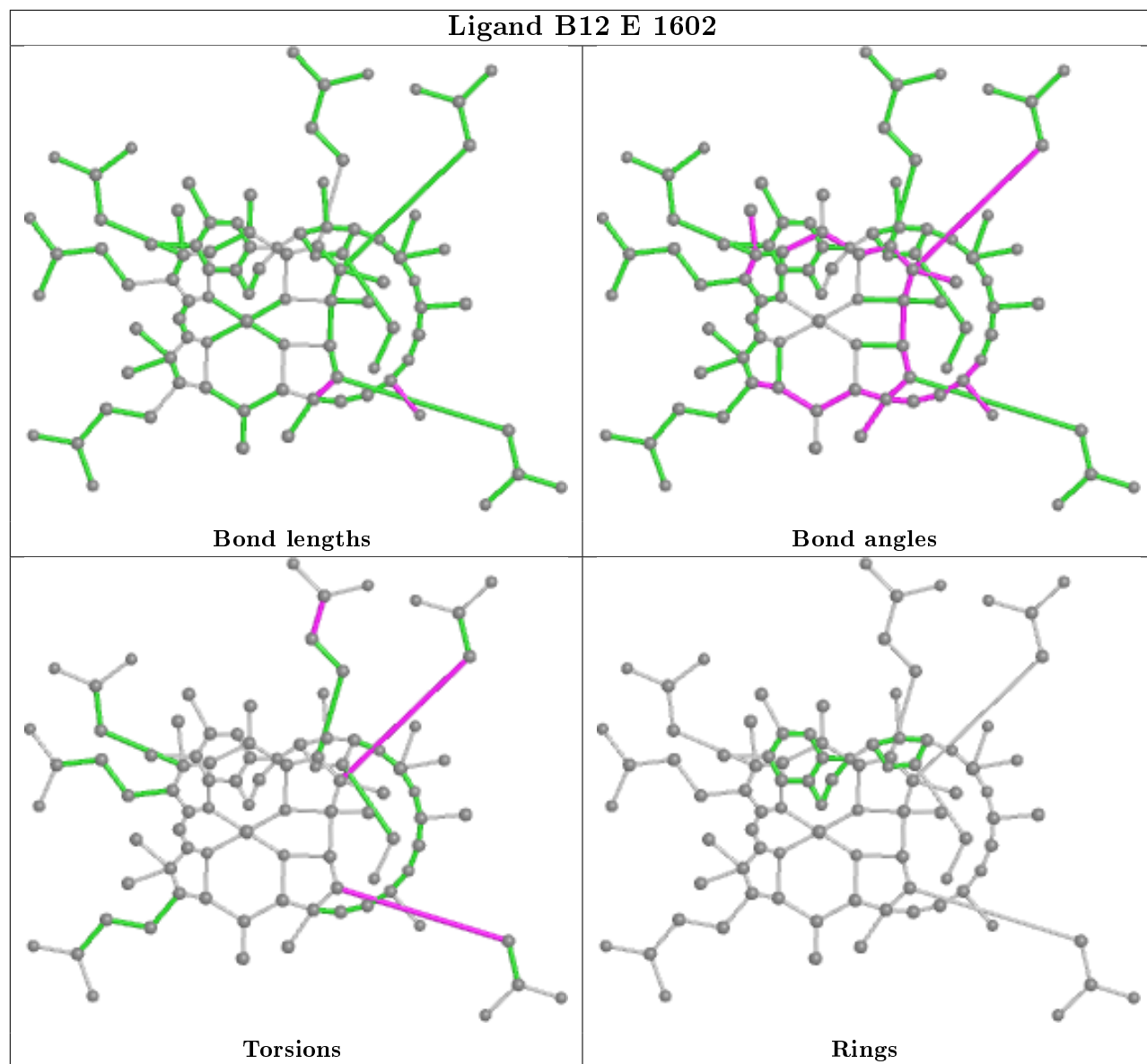
Mol	Chain	Res	Type	Atoms
5	B	1601	B12	C1-C2-C26-C27
5	B	1601	B12	C25-C2-C26-C27
5	B	1601	B12	C3-C2-C26-C27
5	B	1601	B12	C2-C26-C27-N29
5	B	1601	B12	C2-C26-C27-O28
5	B	1601	B12	C2-C3-C30-C31
5	E	1602	B12	C30-C31-C32-O34
5	E	1602	B12	C30-C31-C32-N33
5	E	1602	B12	C1-C2-C26-C27
5	E	1602	B12	C25-C2-C26-C27
5	E	1602	B12	C17-C18-C60-C61
5	E	1602	B12	C19-C18-C60-C61
5	B	1601	B12	C17-C18-C60-C61
5	B	1601	B12	C19-C18-C60-C61
5	B	1601	B12	C4-C3-C30-C31

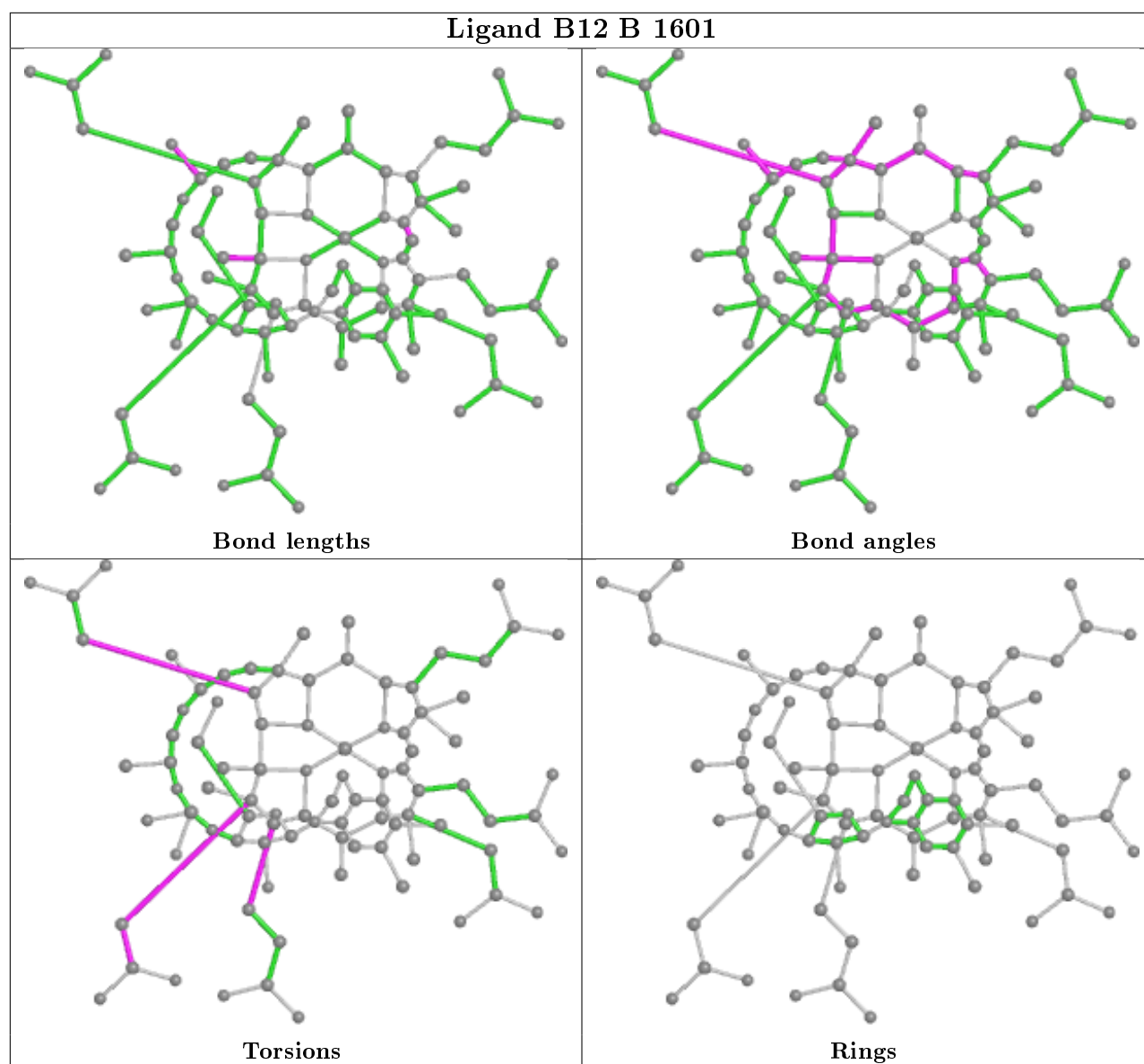
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1602	B12	5	0
5	B	1601	B12	9	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 [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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.