



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2022 – 06:40 PM EDT

PDB ID : 7U3A
Title : Structure of the Streptomyces venezuelae GlgX-c-di-GMP complex
Authors : Schumacher, M.A.
Deposited on : 2022-02-26
Resolution : 3.34 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

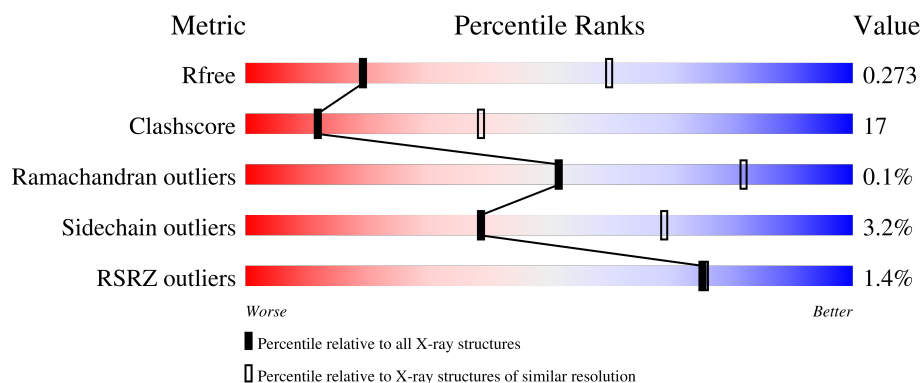
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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}	130704	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	709	<div> <div>%</div> <div>59% 37% ..</div> </div>
1	B	709	<div> <div>2%</div> <div>65% 32% ..</div> </div>
1	C	709	<div> <div>%</div> <div>63% 33% ..</div> </div>
1	D	709	<div> <div>2%</div> <div>64% 32% ..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22242 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 Glycogen debranching enzyme GlgX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	693	Total	C	N	O	S	0	0	0
			5523	3473	997	1029	24			
1	B	693	Total	C	N	O	S	0	0	0
			5517	3468	998	1027	24			
1	C	691	Total	C	N	O	S	0	0	0
			5507	3462	995	1027	23			
1	D	693	Total	C	N	O	S	0	0	0
			5511	3467	996	1025	23			

There are 36 discrepancies between the modelled and reference sequences:

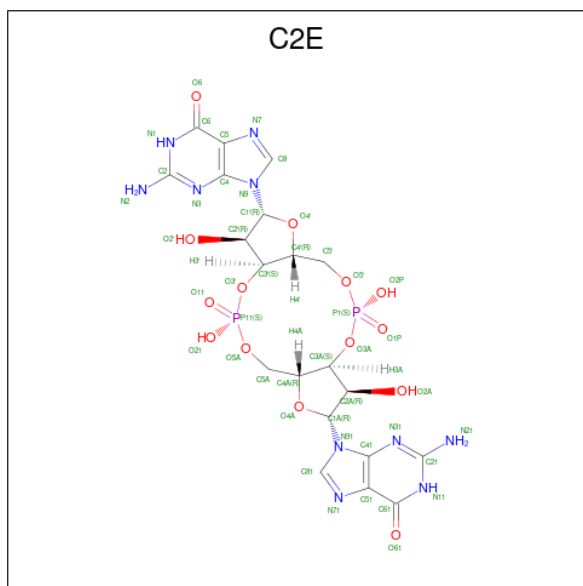
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A5P2ALW6
A	-1	SER	-	expression tag	UNP A0A5P2ALW6
A	0	HIS	-	expression tag	UNP A0A5P2ALW6
A	103	VAL	ILE	conflict	UNP A0A5P2ALW6
A	192	ARG	LYS	conflict	UNP A0A5P2ALW6
A	296	ALA	SER	conflict	UNP A0A5P2ALW6
A	297	ASP	ASN	conflict	UNP A0A5P2ALW6
A	303	MET	THR	conflict	UNP A0A5P2ALW6
A	682	GLN	GLU	conflict	UNP A0A5P2ALW6
B	-2	GLY	-	expression tag	UNP A0A5P2ALW6
B	-1	SER	-	expression tag	UNP A0A5P2ALW6
B	0	HIS	-	expression tag	UNP A0A5P2ALW6
B	103	VAL	ILE	conflict	UNP A0A5P2ALW6
B	192	ARG	LYS	conflict	UNP A0A5P2ALW6
B	296	ALA	SER	conflict	UNP A0A5P2ALW6
B	297	ASP	ASN	conflict	UNP A0A5P2ALW6
B	303	MET	THR	conflict	UNP A0A5P2ALW6
B	682	GLN	GLU	conflict	UNP A0A5P2ALW6
C	-2	GLY	-	expression tag	UNP A0A5P2ALW6
C	-1	SER	-	expression tag	UNP A0A5P2ALW6
C	0	HIS	-	expression tag	UNP A0A5P2ALW6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	103	VAL	ILE	conflict	UNP A0A5P2ALW6
C	192	ARG	LYS	conflict	UNP A0A5P2ALW6
C	296	ALA	SER	conflict	UNP A0A5P2ALW6
C	297	ASP	ASN	conflict	UNP A0A5P2ALW6
C	303	MET	THR	conflict	UNP A0A5P2ALW6
C	682	GLN	GLU	conflict	UNP A0A5P2ALW6
D	-2	GLY	-	expression tag	UNP A0A5P2ALW6
D	-1	SER	-	expression tag	UNP A0A5P2ALW6
D	0	HIS	-	expression tag	UNP A0A5P2ALW6
D	103	VAL	ILE	conflict	UNP A0A5P2ALW6
D	192	ARG	LYS	conflict	UNP A0A5P2ALW6
D	296	ALA	SER	conflict	UNP A0A5P2ALW6
D	297	ASP	ASN	conflict	UNP A0A5P2ALW6
D	303	MET	THR	conflict	UNP A0A5P2ALW6
D	682	GLN	GLU	conflict	UNP A0A5P2ALW6

- Molecule 2 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula: C₂₀H₂₄N₁₀O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	B	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

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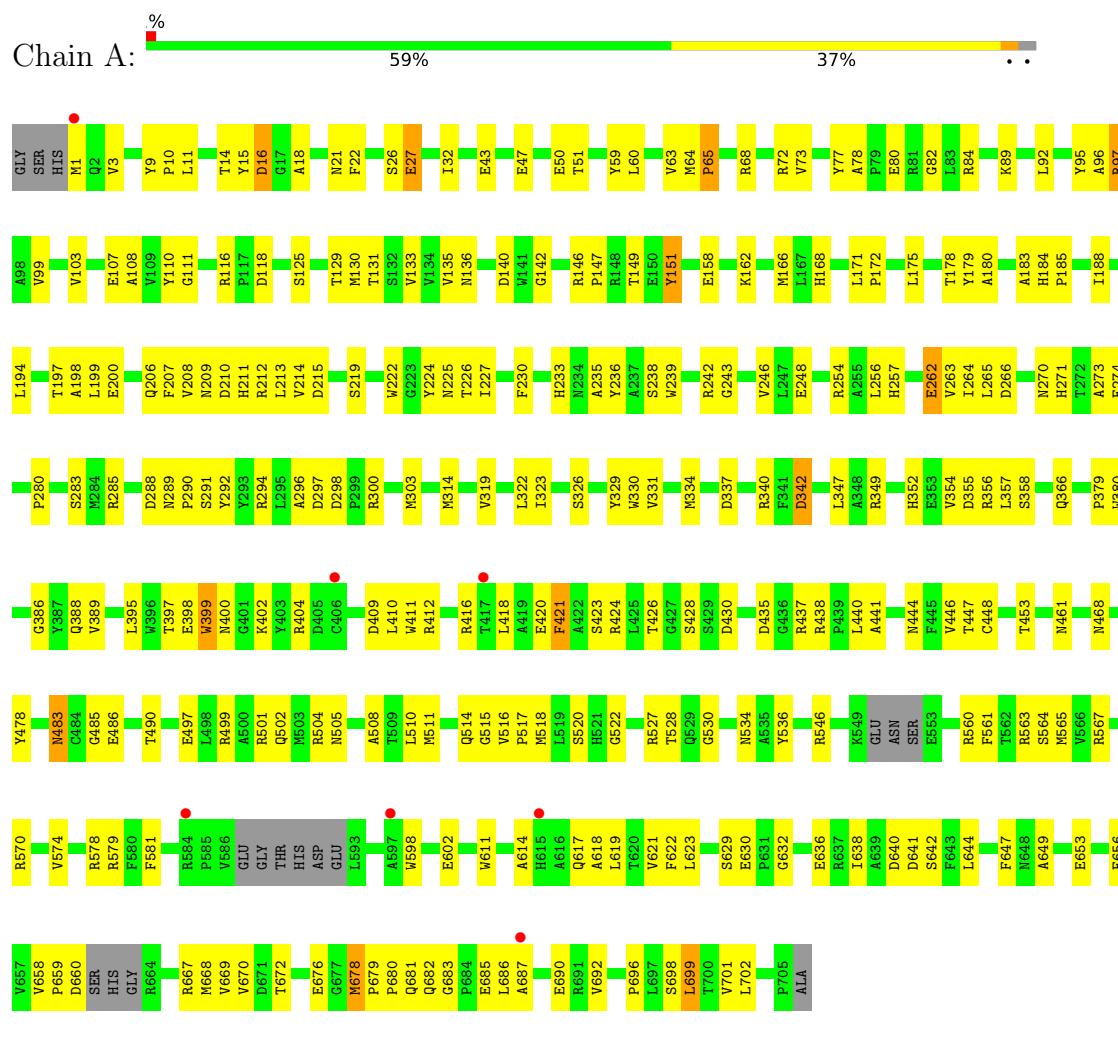
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	D	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

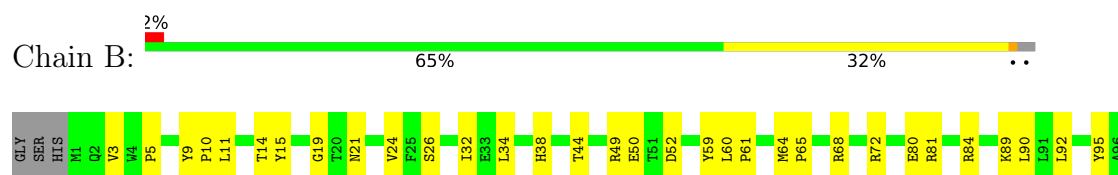
3 Residue-property plots

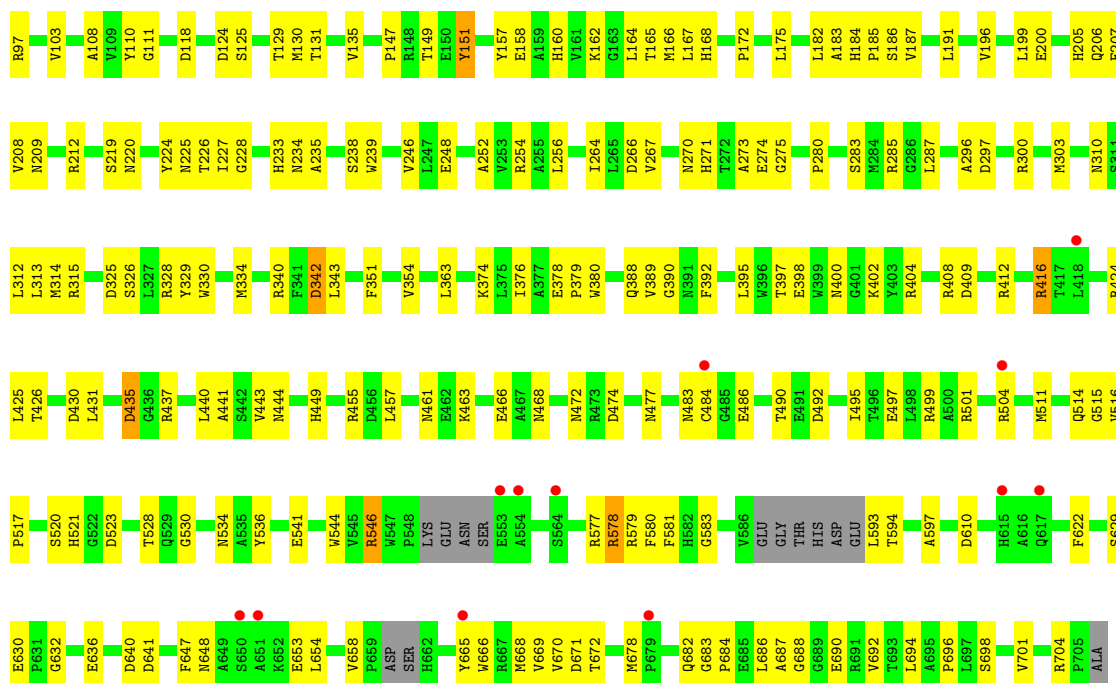
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glycogen debranching enzyme GlgX

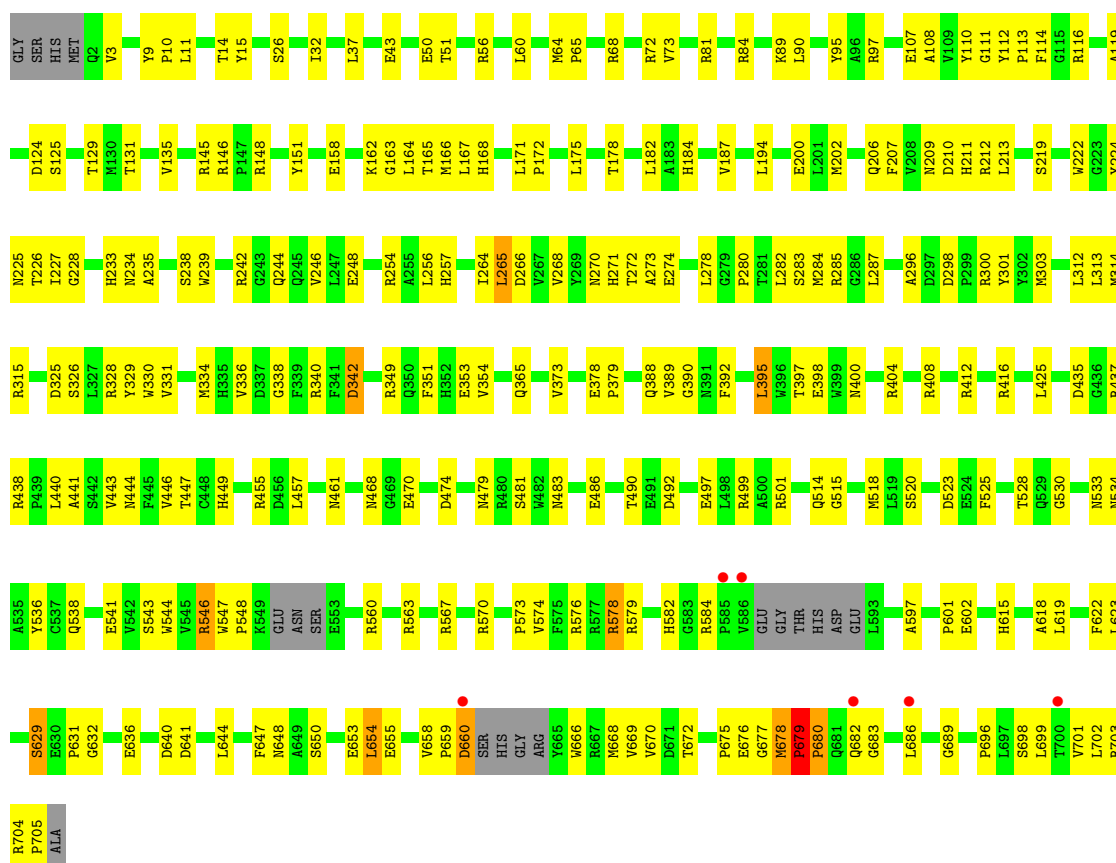


• Molecule 1: Glycogen debranching enzyme GlgX





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ALA	A618	G526	S429	D430	R212	S326	F114	GLY
	F622	P527	L431	L431	L213	Y329	G115	HIS
	L623	T528			D215	W330	R116	MET
	S629	N533	D435	D435	S219	V331	P117	Q2
	P631	A535	R437	R437			D118	W4
G630	N534	R438	R438	N225	M334	H335	D124	P5
G632	Y536	R439	R439	T226	R336	V336	S125	P10
E636	C537	L440	L440	I227	V337		A126	L11
L644	Q538	A441	A441	H233	D337			T14
F647	S543	S442	S442	R242	R340	F341	T129	
N648	R546	V443	V443	V246	N234	A235	M130	
L654	K549	M444	M444	L247	D342	Y236	T131	S26
E655	GLU	R445	R445	E248	L343	A237	S132	E27
V658	ASN	V458	V458	L375	L434	V133	V133	A28
P659	SER			I376	V354		V135	I32
ASP	E553			R356	R242		W141	E33
SER	R560	M461	M461	K374	R247	E248	D144	L34
H662	R563	N465	N465	L375	A252		R146	L37
W666	S564	M468	M468	A377	R253		Y151	E47
R667	W565			E378	R254		E158	E50
M668	V566	D474	D474	W380	A255			T51
V669	L568	Y478	Y478	G386	H257		L167	D52
R569	R570	M479	M479	Q388	L264		L171	R56
D671		R480	R480	V389	L265			L60
T672	V574			G390	D266		L175	
S673		M483	M483	N391	V267			R68
E676	R578	C484	C484	F392			T178	
G677	R579	G485	G485		H271		Y179	R72
M678	F580	E486	E486	L395	T272		A180	
P679	F581			W396	A273		G181	G82
Q682	H582	I495	I495	T397	E274		L182	L83
				E398	G275		A183	R84
				W399	N276		H184	
				N400				K89
	L686	GLU	A500	Y403	P280		L191	L90
A687	G687	GLY	R501	R404				L91
G688	G688	THR	Q502	R408	D288		L194	L92
G689	G689	HIS	M503	D409	N289		G195	D93
E690	E690	ASP	R504	V407	R408		V196	P94
		GLU			P290		L199	A95
T693	L693		M511				E200	A96
L694	A695		S513				L201	R97
P696	P696		Q514					
L697	L697		G515					
S698	P601							
L699	E602							

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.47Å 127.66Å 179.72Å 90.00° 93.73° 90.00°	Depositor
Resolution (Å)	89.67 – 3.34 89.67 – 3.34	Depositor EDS
% Data completeness (in resolution range)	99.5 (89.67-3.34) 99.5 (89.67-3.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.205 , 0.275 0.210 , 0.273	Depositor DCC
R_{free} test set	2000 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.817	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 15.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	22242	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C2E

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	0.50	7/5673 (0.1%)	0.61	3/7715 (0.0%)
1	B	0.26	0/5667	0.49	2/7706 (0.0%)
1	C	0.35	2/5656 (0.0%)	0.53	4/7691 (0.1%)
1	D	0.26	0/5662	0.50	2/7702 (0.0%)
All	All	0.36	9/22658 (0.0%)	0.54	11/30814 (0.0%)

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	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	680	PRO	N-CA	12.94	1.69	1.47
1	A	358	SER	CA-CB	-6.14	1.43	1.52
1	A	291	SER	CA-CB	-5.80	1.44	1.52
1	A	262	GLU	CD-OE1	-5.77	1.19	1.25
1	C	679	PRO	C-N	5.56	1.44	1.34
1	A	399	TRP	C-N	-5.48	1.21	1.34
1	A	262	GLU	CD-OE2	-5.43	1.19	1.25
1	A	65	PRO	N-CD	-5.39	1.40	1.47
1	A	421	PHE	C-N	-5.30	1.21	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	680	PRO	CA-N-CD	-7.02	101.67	111.50
1	C	435	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	435	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	435	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	342	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	342	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	660	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	435	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	660	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	342	ASP	CB-CG-OD2	5.17	122.95	118.30
1	D	342	ASP	CB-CG-OD2	5.15	122.93	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	421	PHE	Mainchain
1	A	678	MET	Peptide

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	5523	0	5230	231	0
1	B	5517	0	5218	163	0
1	C	5507	0	5210	190	0
1	D	5511	0	5209	171	0
2	A	46	0	21	5	0
2	B	46	0	18	2	0
2	C	46	0	19	3	0
2	D	46	0	18	10	0
All	All	22242	0	20943	746	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 17.

All (746) 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:A:486:GLU:OE1	1:A:490:THR:CG2	1.70	1.39
1:C:680:PRO:N	1:C:680:PRO:CA	1.69	1.33
1:C:579:ARG:HG2	2:D:801:C2E:C81	1.60	1.31
1:A:486:GLU:OE1	1:A:490:THR:HG21	1.23	1.22
1:A:246:VAL:HG23	1:A:334:MET:HE3	1.17	1.16
1:D:246:VAL:HG23	1:D:334:MET:HE3	1.19	1.15
1:B:246:VAL:HG23	1:B:334:MET:HE3	1.16	1.10
1:A:561:PHE:CD1	1:A:679:PRO:CD	2.35	1.09
1:C:246:VAL:HG23	1:C:334:MET:HE3	1.32	1.09
1:C:158:GLU:HB2	1:C:518:MET:HE3	1.31	1.08
1:D:296:ALA:HB2	1:D:303:MET:HG2	1.09	1.07
1:A:211:HIS:NE2	1:A:215:ASP:OD2	1.89	1.04
1:D:158:GLU:HB2	1:D:518:MET:HE3	1.34	1.03
1:A:211:HIS:CD2	1:A:215:ASP:OD2	2.12	1.03
1:D:246:VAL:HG23	1:D:334:MET:CE	1.87	1.03
1:A:561:PHE:HD1	1:A:679:PRO:CD	1.70	1.03
1:A:561:PHE:CD1	1:A:679:PRO:HG3	1.97	1.00
1:B:246:VAL:HG23	1:B:334:MET:CE	1.91	0.99
1:A:486:GLU:OE1	1:A:490:THR:HG23	1.58	0.98
1:C:158:GLU:HB2	1:C:518:MET:CE	1.93	0.98
1:C:246:VAL:CG2	1:C:334:MET:HE3	1.94	0.97
1:A:97:ARG:HB3	1:A:135:VAL:HG21	1.46	0.97
1:A:246:VAL:HG23	1:A:334:MET:CE	1.95	0.97
1:A:561:PHE:CD1	1:A:679:PRO:CG	2.47	0.97
1:B:3:VAL:HG13	1:B:60:LEU:CD2	1.93	0.96
1:A:246:VAL:CG2	1:A:334:MET:HE3	1.97	0.95
1:D:158:GLU:HB2	1:D:518:MET:CE	1.97	0.94
1:A:561:PHE:CE1	1:A:679:PRO:HD3	2.02	0.94
1:C:578:ARG:NH2	1:C:631:PRO:O	2.01	0.93
1:C:246:VAL:CG2	1:C:334:MET:CE	2.46	0.92
1:B:246:VAL:CG2	1:B:334:MET:HE3	1.99	0.91
1:A:246:VAL:CG2	1:A:334:MET:CE	2.49	0.91
1:D:296:ALA:HB2	1:D:303:MET:CG	2.00	0.90
1:A:314:MET:HE3	1:A:347:LEU:HD23	1.53	0.90
1:B:246:VAL:CG2	1:B:334:MET:CE	2.49	0.90
1:C:202:MET:CE	1:C:449:HIS:HB3	2.03	0.88
1:A:416:ARG:CG	1:A:614:ALA:HA	1.98	0.88
1:D:296:ALA:CB	1:D:303:MET:HG2	2.00	0.88
1:D:246:VAL:CG2	1:D:334:MET:CE	2.52	0.87
1:C:579:ARG:CG	2:D:801:C2E:C81	2.50	0.87
1:A:561:PHE:HD1	1:A:679:PRO:HD2	1.37	0.87
1:C:579:ARG:HG2	2:D:801:C2E:H81	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:PRO:HG2	1:A:14:THR:HG21	1.57	0.86
1:A:416:ARG:HG3	1:A:614:ALA:O	1.75	0.86
1:A:314:MET:CE	1:A:347:LEU:HD23	2.05	0.85
1:A:15:TYR:CE1	1:A:65:PRO:HD3	2.12	0.85
1:A:565:MET:SD	1:A:679:PRO:HB3	2.18	0.83
1:A:18:ALA:HB3	1:A:59:TYR:OH	1.79	0.82
1:A:416:ARG:CG	1:A:614:ALA:O	2.27	0.82
1:D:84:ARG:HD2	1:D:285:ARG:HD2	1.62	0.81
1:A:561:PHE:CD1	1:A:679:PRO:HD3	2.13	0.81
1:C:202:MET:HE2	1:C:449:HIS:HB3	1.61	0.81
1:C:578:ARG:HH11	1:C:578:ARG:HB2	1.46	0.81
1:A:418:LEU:HD21	1:A:618:ALA:O	1.81	0.81
1:A:158:GLU:HB2	1:A:518:MET:HE3	1.62	0.80
1:C:312:LEU:HB3	1:C:314:MET:HE3	1.63	0.80
1:B:3:VAL:HG13	1:B:60:LEU:HD22	1.63	0.80
1:C:10:PRO:HG2	1:C:14:THR:HG21	1.62	0.79
1:D:504:ARG:NH1	1:D:672:THR:O	2.15	0.79
1:D:146:ARG:NH2	1:D:331:VAL:O	2.15	0.79
1:A:420:GLU:OE2	1:A:424:ARG:NH1	2.15	0.79
1:B:10:PRO:HG2	1:B:14:THR:HG21	1.62	0.79
1:A:678:MET:CE	1:A:683:GLY:HA3	2.14	0.78
1:C:246:VAL:HG23	1:C:334:MET:CE	2.10	0.78
1:A:416:ARG:HG2	1:A:614:ALA:HA	1.65	0.77
1:A:424:ARG:NH2	1:A:430:ASP:OD2	2.18	0.77
1:C:678:MET:CE	1:C:682:GLN:O	2.33	0.77
1:D:72:ARG:NH2	1:D:124:ASP:OD1	2.18	0.77
1:D:658:VAL:HB	1:D:689:GLY:H	1.49	0.77
1:B:72:ARG:NH2	1:B:124:ASP:OD1	2.18	0.77
1:A:89:LYS:NZ	1:A:108:ALA:O	2.17	0.77
1:A:207:PHE:HA	1:A:226:THR:HA	1.66	0.76
1:A:485:GLY:O	1:A:486:GLU:HG3	1.85	0.76
1:A:97:ARG:HB3	1:A:135:VAL:CG2	2.16	0.76
1:A:678:MET:HE1	1:A:683:GLY:HA3	1.66	0.75
1:C:501:ARG:NH2	1:C:696:PRO:O	2.18	0.75
1:C:340:ARG:NH2	1:C:378:GLU:OE1	2.19	0.75
1:D:356:ARG:NH1	1:D:391:ASN:O	2.19	0.74
1:C:365:GLN:HG3	1:C:395:LEU:HD12	1.69	0.73
1:D:511:MET:CE	1:D:566:VAL:HG22	2.17	0.73
1:C:312:LEU:HB3	1:C:314:MET:CE	2.18	0.73
1:A:501:ARG:NH2	1:A:696:PRO:O	2.21	0.73
1:D:10:PRO:HG2	1:D:14:THR:HG21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:ARG:HH11	1:C:578:ARG:CG	2.01	0.73
1:A:227:ILE:HG23	1:A:273:ALA:HB3	1.71	0.72
1:C:578:ARG:HH11	1:C:578:ARG:CB	2.02	0.72
1:B:653:GLU:HG3	1:B:696:PRO:HD3	1.71	0.72
1:C:246:VAL:CG2	1:C:334:MET:HE1	2.19	0.72
1:B:246:VAL:CG2	1:B:334:MET:HE1	2.19	0.72
1:A:579:ARG:NH1	1:A:629:SER:O	2.22	0.72
1:C:461:ASN:OD1	1:C:483:ASN:ND2	2.23	0.72
1:D:632:GLY:HA3	1:D:636:GLU:HG3	1.71	0.72
1:A:158:GLU:HB2	1:A:518:MET:CE	2.20	0.71
1:C:110:TYR:HH	1:C:211:HIS:HD1	1.38	0.71
1:B:501:ARG:NH2	1:B:696:PRO:O	2.23	0.71
1:A:32:ILE:HG12	1:A:73:VAL:HG22	1.73	0.70
1:A:84:ARG:HD2	1:A:285:ARG:HD2	1.73	0.70
1:A:89:LYS:HE3	1:A:111:GLY:HA2	1.73	0.70
1:C:669:VAL:HG13	1:C:670:VAL:HG23	1.73	0.70
1:C:72:ARG:NH2	1:C:124:ASP:OD1	2.25	0.70
1:C:202:MET:HE1	1:C:449:HIS:HB3	1.73	0.70
1:D:227:ILE:HG23	1:D:273:ALA:HB3	1.74	0.70
1:D:246:VAL:CG2	1:D:334:MET:HE1	2.21	0.70
1:C:528:THR:HG22	1:C:530:GLY:H	1.58	0.69
1:D:379:PRO:HG2	1:D:389:VAL:HG22	1.75	0.69
1:B:501:ARG:HH21	1:B:698:SER:HB2	1.58	0.69
1:C:644:LEU:HD21	1:C:659:PRO:HD2	1.74	0.69
1:C:678:MET:HE2	1:C:682:GLN:O	1.93	0.69
1:D:501:ARG:NH2	1:D:696:PRO:O	2.25	0.69
1:B:379:PRO:HG3	1:B:398:GLU:HB3	1.74	0.69
1:D:354:VAL:HG11	1:D:388:GLN:HG3	1.74	0.69
1:B:486:GLU:O	1:B:499:ARG:NH2	2.26	0.69
1:A:567:ARG:HG2	1:A:570:ARG:HH21	1.56	0.69
1:C:32:ILE:HD12	1:C:56:ARG:HG3	1.74	0.69
1:D:68:ARG:HB3	1:D:131:THR:HG21	1.74	0.68
1:A:246:VAL:CG2	1:A:334:MET:HE1	2.24	0.68
1:B:84:ARG:HD2	1:B:285:ARG:HD2	1.74	0.68
1:B:340:ARG:NH2	1:B:378:GLU:OE1	2.26	0.68
1:C:266:ASP:OD2	1:C:340:ARG:NH1	2.27	0.68
1:C:644:LEU:HD23	1:C:702:LEU:HD12	1.74	0.67
1:D:435:ASP:OD1	1:D:435:ASP:O	2.13	0.67
1:A:653:GLU:HG3	1:A:696:PRO:HD3	1.77	0.66
1:D:51:THR:HG23	1:D:56:ARG:HG2	1.76	0.66
1:D:158:GLU:HA	1:D:200:GLU:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:VAL:HG11	1:A:388:GLN:HG3	1.78	0.66
1:A:225:ASN:HD22	1:A:271:HIS:CE1	2.14	0.65
1:B:296:ALA:HB2	1:B:303:MET:HG3	1.78	0.65
1:B:354:VAL:HG11	1:B:388:GLN:HG3	1.78	0.65
1:A:668:MET:HG2	1:A:678:MET:HE2	1.76	0.65
1:A:225:ASN:HD22	1:A:271:HIS:HE1	1.42	0.65
1:D:225:ASN:HD22	1:D:271:HIS:HE1	1.41	0.65
1:A:64:MET:HB3	1:A:65:PRO:CD	2.27	0.65
1:C:274:GLU:O	1:C:285:ARG:NH2	2.29	0.65
1:A:99:VAL:HB	1:A:206:GLN:OE1	1.97	0.65
1:A:379:PRO:HG2	1:A:389:VAL:HG22	1.79	0.64
1:B:68:ARG:HB3	1:B:131:THR:HG21	1.78	0.64
1:C:486:GLU:O	1:C:499:ARG:NH2	2.30	0.64
1:C:679:PRO:N	1:C:680:PRO:CD	2.59	0.64
1:D:182:LEU:HD21	1:D:256:LEU:HD11	1.79	0.64
1:C:110:TYR:OH	1:C:211:HIS:ND1	2.29	0.64
1:A:27:GLU:N	1:A:288:ASP:OD1	2.28	0.64
1:B:669:VAL:HG13	1:B:670:VAL:HG23	1.79	0.64
1:D:5:PRO:HB3	1:D:50:GLU:HG3	1.78	0.64
1:D:486:GLU:O	1:D:499:ARG:NH2	2.31	0.64
1:A:561:PHE:HA	1:A:679:PRO:HG2	1.79	0.64
1:B:511:MET:CE	1:B:517:PRO:HB2	2.28	0.64
1:C:246:VAL:HG22	1:C:334:MET:CE	2.27	0.64
1:A:349:ARG:NH1	1:A:352:HIS:O	2.31	0.64
1:A:400:ASN:ND2	1:A:428:SER:OG	2.30	0.63
1:C:578:ARG:HB2	1:C:578:ARG:NH1	2.12	0.63
1:C:444:ASN:ND2	1:C:514:GLN:O	2.32	0.63
1:B:274:GLU:O	1:B:285:ARG:NH2	2.30	0.63
1:B:501:ARG:HG3	1:B:672:THR:HG22	1.80	0.63
1:C:146:ARG:HH12	1:C:331:VAL:HG13	1.61	0.63
1:C:668:MET:O	1:C:683:GLY:HA3	1.99	0.63
1:A:598:TRP:CE3	1:A:621:VAL:HG22	2.33	0.63
1:A:644:LEU:HB3	1:A:702:LEU:HB2	1.80	0.63
1:A:416:ARG:HG2	1:A:614:ALA:O	1.99	0.62
1:A:561:PHE:HE1	1:A:679:PRO:HD3	1.59	0.62
1:D:511:MET:HE3	1:D:566:VAL:HG22	1.81	0.62
1:A:16:ASP:OD2	1:A:59:TYR:CE1	2.52	0.62
1:A:647:PHE:CE2	1:A:699:LEU:CD1	2.82	0.62
1:C:206:GLN:HG3	1:C:233:HIS:HA	1.81	0.62
1:C:560:ARG:NH2	1:C:676:GLU:O	2.32	0.62
1:B:666:TRP:N	1:B:686:LEU:O	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:ASP:OD2	1:D:340:ARG:NH1	2.32	0.62
1:B:468:ASN:ND2	1:B:534:ASN:O	2.30	0.62
1:C:658:VAL:HB	1:C:689:GLY:H	1.64	0.62
1:A:647:PHE:CD2	1:A:699:LEU:HD12	2.35	0.62
1:C:242:ARG:N	1:C:244:GLN:OE1	2.33	0.61
1:B:511:MET:HE2	1:B:517:PRO:CB	2.31	0.61
1:A:68:ARG:HB3	1:A:131:THR:HG21	1.82	0.61
1:A:678:MET:O	1:A:678:MET:HG2	1.99	0.61
1:C:578:ARG:HH11	1:C:578:ARG:HG3	1.66	0.61
1:A:16:ASP:OD2	1:A:59:TYR:HE1	1.84	0.61
1:A:43:GLU:OE2	1:A:72:ARG:NH2	2.34	0.61
1:B:270:ASN:ND2	1:B:342:ASP:O	2.34	0.61
1:C:354:VAL:HG11	1:C:388:GLN:HG3	1.82	0.61
1:D:397:THR:HG23	1:D:441:ALA:HA	1.83	0.61
1:A:504:ARG:HB2	1:A:672:THR:HG23	1.82	0.61
1:C:632:GLY:HA3	1:C:636:GLU:HG3	1.83	0.60
1:D:578:ARG:HB3	1:D:630:GLU:HG2	1.82	0.60
1:D:207:PHE:HB3	1:D:226:THR:HG22	1.83	0.60
1:A:416:ARG:CG	1:A:614:ALA:CA	2.75	0.60
1:A:668:MET:HG2	1:A:678:MET:CE	2.31	0.60
1:D:207:PHE:HA	1:D:226:THR:HA	1.82	0.60
1:A:397:THR:HG23	1:A:441:ALA:HA	1.84	0.60
1:D:225:ASN:HD22	1:D:271:HIS:CE1	2.18	0.60
1:C:270:ASN:ND2	1:C:342:ASP:O	2.33	0.60
1:C:56:ARG:NH1	2:C:801:C2E:O6	2.31	0.60
1:C:440:LEU:HA	1:C:515:GLY:HA2	1.83	0.60
1:C:679:PRO:N	1:C:680:PRO:HD2	2.16	0.60
1:B:640:ASP:OD2	1:B:641:ASP:N	2.35	0.59
1:A:410:LEU:O	1:A:649:ALA:HB1	2.02	0.59
1:D:340:ARG:NH2	1:D:378:GLU:OE1	2.35	0.59
1:B:206:GLN:NE2	1:B:234:ASN:OD1	2.35	0.59
1:D:399:TRP:HZ2	1:D:518:MET:HE1	1.67	0.59
1:D:167:LEU:HD23	1:D:546:ARG:HD2	1.84	0.59
1:A:486:GLU:O	1:A:499:ARG:NH2	2.36	0.59
1:D:426:THR:HG23	1:D:581:PHE:HD1	1.68	0.59
1:D:468:ASN:ND2	1:D:534:ASN:O	2.36	0.59
1:B:397:THR:HG23	1:B:441:ALA:HA	1.85	0.59
1:D:446:VAL:HG23	1:D:447:THR:HG22	1.84	0.59
1:B:90:LEU:H	1:B:125:SER:HB3	1.66	0.58
1:B:392:PHE:O	1:B:437:ARG:NH2	2.34	0.58
1:C:89:LYS:HE3	1:C:111:GLY:HA2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:ASN:O	1:C:273:ALA:HB2	2.03	0.58
1:A:158:GLU:HA	1:A:200:GLU:HB3	1.86	0.58
1:C:298:ASP:O	1:C:300:ARG:N	2.36	0.58
1:D:538:GLN:O	1:D:543:SER:OG	2.18	0.58
1:B:511:MET:HE1	1:B:517:PRO:HB2	1.85	0.58
1:C:200:GLU:HA	1:C:264:ILE:O	2.03	0.58
1:D:257:HIS:NE2	1:D:337:ASP:OD2	2.36	0.58
1:A:51:THR:O	2:A:801:C2E:N11	2.24	0.58
1:A:194:LEU:HA	1:A:563:ARG:HG2	1.84	0.58
1:C:660:ASP:OD1	1:C:660:ASP:O	2.22	0.58
1:B:130:MET:HE3	1:B:208:VAL:HG22	1.86	0.58
1:D:298:ASP:O	1:D:300:ARG:N	2.37	0.58
1:D:666:TRP:N	1:D:686:LEU:O	2.36	0.58
1:B:665:TYR:HA	1:B:687:ALA:HA	1.86	0.58
1:C:50:GLU:OE1	1:D:438:ARG:NH2	2.33	0.58
1:B:200:GLU:HA	1:B:264:ILE:O	2.03	0.58
1:C:274:GLU:OE2	1:C:283:SER:N	2.35	0.58
1:D:194:LEU:HA	1:D:563:ARG:HG2	1.86	0.58
1:D:440:LEU:HA	1:D:515:GLY:HA2	1.85	0.58
1:A:404:ARG:HG3	1:A:446:VAL:O	2.04	0.57
1:C:408:ARG:O	1:C:412:ARG:HB2	2.04	0.57
1:D:511:MET:HE1	1:D:566:VAL:HG22	1.86	0.57
1:A:50:GLU:OE1	1:B:578:ARG:NH2	2.37	0.57
1:B:167:LEU:HD23	1:B:546:ARG:HD2	1.86	0.57
1:A:97:ARG:HD2	1:A:329:TYR:CZ	2.40	0.57
1:B:379:PRO:HG2	1:B:389:VAL:HG22	1.85	0.57
1:D:520:SER:OG	1:D:523:ASP:OD2	2.22	0.57
1:B:225:ASN:HD22	1:B:271:HIS:HE1	1.52	0.57
1:C:296:ALA:HA	1:C:303:MET:HG2	1.87	0.57
1:D:574:VAL:HG11	1:D:623:LEU:HB3	1.87	0.57
1:C:379:PRO:HG3	1:C:398:GLU:HB3	1.85	0.57
1:A:292:TYR:HA	1:A:319:VAL:CG2	2.34	0.57
1:A:483:ASN:H	1:A:483:ASN:HD22	1.53	0.57
1:C:158:GLU:HA	1:C:200:GLU:HB3	1.86	0.57
1:C:313:LEU:HD22	1:C:315:ARG:HG2	1.87	0.57
1:D:424:ARG:NH2	1:D:430:ASP:OD2	2.38	0.57
1:D:560:ARG:NH2	1:D:676:GLU:O	2.38	0.57
1:A:296:ALA:HA	1:A:303:MET:HG2	1.87	0.57
1:D:89:LYS:HE3	1:D:111:GLY:HA2	1.86	0.57
1:D:130:MET:HE3	1:D:208:VAL:HG22	1.87	0.57
1:B:312:LEU:HB3	1:B:314:MET:CE	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:574:VAL:HG11	1:C:623:LEU:HB3	1.86	0.56
1:D:670:VAL:HG13	1:D:679:PRO:HG3	1.86	0.56
1:C:68:ARG:HB3	1:C:131:THR:HG21	1.87	0.56
1:D:125:SER:O	1:D:129:THR:OG1	2.18	0.56
1:C:238:SER:N	1:C:248:GLU:OE2	2.39	0.56
1:A:270:ASN:ND2	1:A:342:ASP:O	2.39	0.56
1:A:233:HIS:CE1	1:A:235:ALA:HB3	2.41	0.56
1:B:461:ASN:OD1	1:B:483:ASN:ND2	2.39	0.56
1:C:51:THR:C	2:C:801:C2E:HN11	2.08	0.56
1:A:103:VAL:HG23	1:A:130:MET:HE3	1.87	0.56
1:A:198:ALA:HB1	1:A:264:ILE:HG13	1.87	0.56
1:C:340:ARG:HH21	1:C:378:GLU:HB2	1.70	0.56
1:D:579:ARG:HD2	1:D:630:GLU:HG3	1.87	0.56
1:C:26:SER:HB3	1:C:32:ILE:HD11	1.86	0.56
1:D:200:GLU:HA	1:D:264:ILE:O	2.06	0.56
1:A:96:ALA:O	1:A:230:PHE:HB2	2.06	0.55
1:C:644:LEU:HB3	1:C:702:LEU:HB2	1.88	0.55
1:D:103:VAL:HG23	1:D:130:MET:HE3	1.88	0.55
1:C:379:PRO:HG2	1:C:389:VAL:HG22	1.88	0.55
1:A:502:GLN:HA	1:A:505:ASN:HD22	1.72	0.55
1:D:461:ASN:OD1	1:D:483:ASN:ND2	2.40	0.55
1:D:468:ASN:ND2	1:D:474:ASP:OD2	2.25	0.55
1:A:669:VAL:HG13	1:A:670:VAL:HG23	1.87	0.55
1:C:242:ARG:HB2	1:C:244:GLN:HE22	1.71	0.55
1:A:274:GLU:OE2	1:A:283:SER:N	2.32	0.54
1:A:679:PRO:HG2	1:A:680:PRO:HD3	1.89	0.54
1:B:26:SER:HB3	1:B:32:ILE:HD11	1.88	0.54
1:B:297:ASP:OD2	1:B:297:ASP:N	2.39	0.54
1:B:520:SER:OG	1:B:523:ASP:OD2	2.22	0.54
1:A:686:LEU:HD13	1:A:692:VAL:HG21	1.87	0.54
1:C:182:LEU:HD21	1:C:256:LEU:HD11	1.89	0.54
1:B:632:GLY:HA3	1:B:636:GLU:HG3	1.88	0.54
1:A:64:MET:HB3	1:A:65:PRO:HD2	1.88	0.54
1:A:411:TRP:CE2	1:A:505:ASN:HB3	2.42	0.54
1:D:579:ARG:NH1	1:D:629:SER:O	2.40	0.54
1:A:125:SER:O	1:A:129:THR:OG1	2.19	0.54
1:A:206:GLN:HG3	1:A:233:HIS:CD2	2.43	0.54
1:A:314:MET:HE1	1:A:347:LEU:HD23	1.86	0.54
1:C:239:TRP:CD2	1:C:248:GLU:HG2	2.43	0.54
1:D:93:ASP:HB3	1:D:96:ALA:HB2	1.90	0.54
1:A:135:VAL:HG11	1:A:246:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:VAL:HB	1:B:688:GLY:O	2.08	0.54
1:D:47:GLU:OE1	2:D:801:C2E:N1	2.34	0.54
1:D:209:ASN:HD21	1:D:219:SER:HB2	1.73	0.54
1:B:504:ARG:HB2	1:B:672:THR:HG23	1.90	0.53
1:C:135:VAL:HG11	1:C:246:VAL:HG11	1.89	0.53
1:C:207:PHE:HA	1:C:226:THR:HA	1.90	0.53
1:A:26:SER:HB3	1:A:32:ILE:HD11	1.89	0.53
1:D:141:TRP:HB3	1:D:144:ASP:HB2	1.89	0.53
1:D:3:VAL:HG22	1:D:60:LEU:HD22	1.91	0.53
1:A:82:GLY:O	1:A:290:PRO:HG3	2.08	0.53
1:B:541:GLU:HA	1:B:544:TRP:CD1	2.42	0.53
1:A:438:ARG:NH1	1:B:52:ASP:OD1	2.42	0.53
1:A:485:GLY:O	1:A:486:GLU:CG	2.55	0.53
1:A:647:PHE:CD2	1:A:699:LEU:CD1	2.92	0.53
1:B:206:GLN:HG3	1:B:233:HIS:HA	1.90	0.53
1:C:227:ILE:HG23	1:C:273:ALA:HB3	1.89	0.53
1:B:313:LEU:HD22	1:B:315:ARG:HG2	1.91	0.53
1:D:671:ASP:HB3	1:D:678:MET:HG2	1.90	0.53
1:A:212:ARG:NH2	1:A:536:TYR:OH	2.40	0.53
1:B:511:MET:CE	1:B:517:PRO:CB	2.87	0.53
1:C:64:MET:HB3	1:C:65:PRO:HD2	1.91	0.53
1:D:399:TRP:CZ2	1:D:518:MET:HE1	2.44	0.53
1:A:239:TRP:N	1:A:248:GLU:OE2	2.41	0.53
1:A:444:ASN:ND2	1:A:514:GLN:O	2.41	0.53
1:D:212:ARG:NH2	1:D:536:TYR:OH	2.41	0.53
1:D:644:LEU:HD23	1:D:702:LEU:HD12	1.91	0.53
1:A:501:ARG:HA	1:A:504:ARG:HD2	1.90	0.52
1:B:671:ASP:N	1:B:678:MET:HG2	2.25	0.52
1:D:669:VAL:HG13	1:D:670:VAL:HG23	1.92	0.52
1:C:89:LYS:NZ	1:C:108:ALA:O	2.33	0.52
1:C:497:GLU:OE2	1:C:675:PRO:HB3	2.10	0.52
1:A:511:MET:CE	1:A:517:PRO:HB2	2.38	0.52
1:B:444:ASN:ND2	1:B:514:GLN:O	2.43	0.52
1:A:678:MET:CE	1:A:683:GLY:CA	2.88	0.52
1:B:296:ALA:CB	1:B:303:MET:HG3	2.39	0.52
1:D:51:THR:C	2:D:801:C2E:HN11	2.13	0.52
1:A:298:ASP:O	1:A:300:ARG:N	2.42	0.52
1:A:560:ARG:NH2	1:A:676:GLU:O	2.43	0.52
1:D:455:ARG:HD2	1:D:528:THR:OG1	2.09	0.52
1:B:426:THR:HG23	1:B:581:PHE:HD1	1.73	0.52
1:C:116:ARG:HB3	1:C:119:ALA:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ASP:HB2	1:A:213:LEU:HB2	1.91	0.52
1:A:508:ALA:HB3	1:A:699:LEU:HD22	1.91	0.52
1:B:110:TYR:HA	1:B:280:PRO:HA	1.90	0.52
1:B:402:LYS:HD2	1:B:431:LEU:HD11	1.91	0.52
1:B:670:VAL:HB	1:B:701:VAL:HB	1.90	0.52
1:C:408:ARG:NH1	1:C:446:VAL:O	2.42	0.52
1:C:567:ARG:HG3	1:C:570:ARG:HH21	1.75	0.52
1:D:428:SER:HB3	1:D:431:LEU:HB2	1.91	0.52
1:A:238:SER:N	1:A:248:GLU:OE2	2.43	0.52
1:A:257:HIS:NE2	1:A:337:ASP:OD2	2.42	0.51
1:D:238:SER:N	1:D:248:GLU:OE2	2.43	0.51
1:A:147:PRO:O	1:A:149:THR:N	2.41	0.51
1:C:206:GLN:NE2	1:C:234:ASN:OD1	2.43	0.51
1:A:647:PHE:CE2	1:A:699:LEU:HD11	2.44	0.51
1:B:239:TRP:CD2	1:B:248:GLU:HG2	2.46	0.51
1:C:501:ARG:HG3	1:C:672:THR:HG22	1.92	0.51
1:A:206:GLN:HG3	1:A:233:HIS:HD2	1.76	0.51
1:A:416:ARG:HG2	1:A:614:ALA:CA	2.35	0.51
1:B:686:LEU:HB3	1:B:690:GLU:OE1	2.11	0.51
1:C:573:PRO:HA	1:C:576:ARG:HG3	1.92	0.51
1:C:640:ASP:OD2	1:C:641:ASP:N	2.42	0.51
1:D:629:SER:O	1:D:629:SER:OG	2.29	0.51
1:C:455:ARG:HD2	1:C:528:THR:OG1	2.11	0.51
1:B:686:LEU:HD13	1:B:692:VAL:HG21	1.92	0.51
1:A:366:GLN:HG2	1:B:363:LEU:HD21	1.93	0.51
1:B:5:PRO:HB3	1:B:50:GLU:HG3	1.92	0.51
1:B:64:MET:HB3	1:B:65:PRO:HD2	1.92	0.51
1:C:125:SER:O	1:C:129:THR:OG1	2.23	0.51
1:A:511:MET:HE1	1:A:517:PRO:HB2	1.92	0.51
1:B:463:LYS:HE2	1:B:477:ASN:HA	1.93	0.51
1:C:158:GLU:HB2	1:C:518:MET:HE2	1.88	0.51
1:C:158:GLU:OE2	1:C:449:HIS:ND1	2.44	0.51
1:C:171:LEU:HD22	1:C:184:HIS:CG	2.46	0.51
1:A:561:PHE:CE1	1:A:679:PRO:CD	2.74	0.51
1:C:579:ARG:HG2	2:D:801:C2E:N71	2.19	0.51
1:A:678:MET:HE3	1:A:683:GLY:HA3	1.89	0.51
1:B:38:HIS:HE2	1:B:44:THR:HG1	1.58	0.51
1:D:28:ALA:N	1:D:288:ASP:OD1	2.43	0.51
1:D:233:HIS:CD2	1:D:235:ALA:HB3	2.46	0.51
1:A:461:ASN:OD1	1:A:483:ASN:ND2	2.43	0.50
1:C:404:ARG:HG2	1:C:408:ARG:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:MET:HE1	1:A:347:LEU:CD2	2.40	0.50
1:D:144:ASP:OD2	1:D:335:HIS:ND1	2.40	0.50
1:A:440:LEU:HA	1:A:515:GLY:HA2	1.92	0.50
1:B:89:LYS:HE3	1:B:111:GLY:HA2	1.93	0.50
1:B:579:ARG:NH1	1:B:629:SER:O	2.45	0.50
1:D:501:ARG:HH21	1:D:698:SER:HB2	1.74	0.50
1:C:194:LEU:HA	1:C:563:ARG:HG2	1.93	0.50
1:D:92:LEU:HD22	1:D:227:ILE:HD13	1.93	0.50
1:D:135:VAL:HG11	1:D:246:VAL:HG11	1.93	0.50
1:D:26:SER:HB3	1:D:32:ILE:HD11	1.94	0.50
1:B:103:VAL:HG23	1:B:130:MET:HE3	1.93	0.50
1:B:212:ARG:NH2	1:B:536:TYR:OH	2.45	0.50
1:C:84:ARG:HD2	1:C:285:ARG:HD2	1.94	0.50
1:C:325:ASP:OD2	1:C:328:ARG:NH2	2.44	0.50
1:D:500:ALA:O	1:D:504:ARG:HG3	2.12	0.50
1:D:503:MET:HE1	1:D:526:GLY:HA2	1.94	0.50
1:C:270:ASN:OD1	1:C:271:HIS:ND1	2.36	0.50
1:D:205:HIS:CE1	1:D:267:VAL:HG12	2.47	0.50
1:A:314:MET:CE	1:A:347:LEU:CD2	2.85	0.49
1:C:162:LYS:HE2	1:C:166:MET:CE	2.42	0.49
1:D:409:ASP:OD2	1:D:480:ARG:NH1	2.40	0.49
1:A:501:ARG:HH21	1:A:698:SER:HB2	1.77	0.49
1:D:37:LEU:HD11	1:D:90:LEU:HD21	1.94	0.49
1:A:564:SER:O	1:A:567:ARG:HB2	2.13	0.49
1:B:409:ASP:HB3	1:B:416:ARG:HG3	1.92	0.49
1:A:80:GLU:HG3	1:A:300:ARG:HH21	1.76	0.49
1:C:425:LEU:HD11	1:C:647:PHE:CZ	2.48	0.49
1:A:678:MET:HE3	1:A:683:GLY:CA	2.42	0.49
1:B:225:ASN:O	1:B:273:ALA:HB2	2.13	0.49
1:B:340:ARG:HH21	1:B:378:GLU:HB2	1.77	0.49
1:A:426:THR:HG23	1:A:581:PHE:HD1	1.77	0.49
1:B:15:TYR:CE1	1:B:65:PRO:HD3	2.48	0.49
1:B:408:ARG:O	1:B:412:ARG:HB2	2.13	0.49
1:B:490:THR:HG22	1:B:492:ASP:H	1.78	0.49
1:B:668:MET:CE	1:B:684:PRO:HD2	2.41	0.49
1:B:682:GLN:HG2	1:B:683:GLY:H	1.78	0.49
1:D:662:HIS:HA	1:D:688:GLY:O	2.12	0.49
1:C:172:PRO:HG2	1:C:175:LEU:HG	1.94	0.49
1:A:209:ASN:HB3	1:A:214:VAL:HG23	1.94	0.49
1:A:266:ASP:OD2	1:A:340:ARG:NH1	2.32	0.49
1:A:508:ALA:CB	1:A:699:LEU:CD2	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:PRO:O	1:B:149:THR:N	2.44	0.49
1:C:90:LEU:H	1:C:125:SER:HB3	1.78	0.49
1:C:239:TRP:N	1:C:248:GLU:OE2	2.43	0.49
1:C:227:ILE:HD12	1:C:228:GLY:N	2.28	0.49
1:D:175:LEU:HD22	1:D:180:ALA:HB3	1.95	0.48
1:A:51:THR:C	2:A:801:C2E:HN11	2.14	0.48
1:A:103:VAL:HG23	1:A:130:MET:CE	2.43	0.48
1:B:233:HIS:CD2	1:B:235:ALA:HB3	2.48	0.48
1:B:266:ASP:OD2	1:B:340:ARG:NH1	2.43	0.48
1:B:484:CYS:O	1:B:495:ILE:HG22	2.14	0.48
1:C:210:ASP:HB2	1:C:213:LEU:HB2	1.95	0.48
1:C:677:GLY:O	1:C:680:PRO:HD2	2.12	0.48
1:D:68:ARG:HG2	1:D:133:VAL:HG22	1.94	0.48
1:C:648:ASN:ND2	1:C:696:PRO:HA	2.26	0.48
1:A:47:GLU:OE2	2:A:801:C2E:N1	2.42	0.48
1:A:68:ARG:HG2	1:A:133:VAL:HG22	1.96	0.48
1:A:561:PHE:CG	1:A:679:PRO:HG3	2.47	0.48
1:C:51:THR:O	2:C:801:C2E:N11	2.34	0.48
1:C:233:HIS:CD2	1:C:235:ALA:HB3	2.48	0.48
1:D:296:ALA:C	1:D:298:ASP:H	2.17	0.48
1:B:528:THR:HG22	1:B:530:GLY:H	1.78	0.48
1:D:103:VAL:HG23	1:D:130:MET:CE	2.44	0.48
1:A:151:TYR:CE2	1:A:516:VAL:HG21	2.48	0.48
1:B:81:ARG:HG2	1:C:81:ARG:HD2	1.94	0.48
1:C:97:ARG:HD3	1:C:329:TYR:CE1	2.49	0.48
1:A:129:THR:HG22	1:A:130:MET:H	1.79	0.48
1:B:3:VAL:HG13	1:B:60:LEU:HD21	1.90	0.48
1:C:629:SER:O	1:C:629:SER:OG	2.29	0.48
1:D:296:ALA:O	1:D:298:ASP:N	2.46	0.48
1:C:678:MET:HE1	1:C:682:GLN:O	2.11	0.48
1:C:682:GLN:CD	1:C:682:GLN:H	2.17	0.48
1:D:329:TYR:OH	1:D:334:MET:CE	2.61	0.48
1:D:565:MET:HE1	1:D:679:PRO:HG3	1.95	0.48
1:A:92:LEU:HD22	1:A:227:ILE:HD13	1.96	0.47
1:B:19:GLY:HA3	1:B:61:PRO:HA	1.96	0.47
1:B:224:TYR:HH	1:B:449:HIS:CE1	2.31	0.47
1:C:483:ASN:HD22	1:C:483:ASN:H	1.60	0.47
1:A:110:TYR:HA	1:A:280:PRO:HA	1.96	0.47
1:B:125:SER:O	1:B:129:THR:OG1	2.21	0.47
1:B:668:MET:HE3	1:B:684:PRO:HD2	1.96	0.47
1:D:11:LEU:HD12	1:D:95:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:SER:N	1:B:248:GLU:OE2	2.48	0.47
1:C:392:PHE:HB2	1:C:437:ARG:HH22	1.79	0.47
1:C:597:ALA:HB3	1:C:622:PHE:HB3	1.96	0.47
1:A:644:LEU:HD23	1:A:702:LEU:HD12	1.96	0.47
1:B:64:MET:HB3	1:B:65:PRO:CD	2.44	0.47
1:C:438:ARG:NH2	1:D:50:GLU:OE1	2.45	0.47
1:A:574:VAL:HG11	1:A:623:LEU:HB3	1.96	0.47
1:C:601:PRO:HG3	1:C:618:ALA:HB3	1.97	0.47
1:A:560:ARG:O	1:A:564:SER:OG	2.23	0.47
1:B:455:ARG:HD3	1:B:528:THR:OG1	2.14	0.47
1:C:11:LEU:HD12	1:C:95:TYR:CZ	2.49	0.47
1:C:338:GLY:HA2	1:C:373:VAL:HB	1.96	0.47
1:A:329:TYR:OH	1:A:334:MET:HE1	2.14	0.47
1:A:528:THR:HG22	1:A:530:GLY:H	1.80	0.47
1:B:227:ILE:HG23	1:B:273:ALA:HB3	1.95	0.47
1:B:329:TYR:CE2	1:B:334:MET:HE2	2.49	0.47
1:C:315:ARG:HH11	1:C:351:PHE:HD2	1.63	0.47
1:C:446:VAL:HG23	1:C:447:THR:HG22	1.96	0.47
1:C:579:ARG:CG	2:D:801:C2E:N71	2.78	0.47
1:D:158:GLU:CB	1:D:518:MET:CE	2.83	0.47
1:D:296:ALA:HB1	1:D:303:MET:SD	2.55	0.47
1:A:15:TYR:HE1	1:A:64:MET:HA	1.80	0.47
1:A:175:LEU:HD22	1:A:180:ALA:HB3	1.96	0.47
1:B:682:GLN:HG2	1:B:683:GLY:N	2.30	0.47
1:D:72:ARG:HH22	1:D:126:ALA:HB2	1.79	0.47
1:A:399:TRP:CZ2	1:A:518:MET:HE1	2.50	0.47
1:C:666:TRP:O	1:C:686:LEU:N	2.48	0.47
1:C:703:ARG:HD2	1:C:705:PRO:HG3	1.96	0.47
1:D:191:LEU:HD22	1:D:196:VAL:HG21	1.96	0.47
1:D:265:LEU:HG	1:D:336:VAL:HG11	1.97	0.47
1:A:448:CYS:HA	1:A:520:SER:HB3	1.96	0.46
1:A:632:GLY:HA3	1:A:636:GLU:HG3	1.97	0.46
1:B:182:LEU:HD21	1:B:256:LEU:HD11	1.97	0.46
1:B:424:ARG:NH2	1:B:430:ASP:OD2	2.48	0.46
1:B:654:LEU:HD23	1:B:654:LEU:HA	1.81	0.46
1:B:397:THR:HG22	1:B:443:VAL:HG23	1.96	0.46
1:C:9:TYR:CG	1:C:10:PRO:HA	2.49	0.46
1:D:404:ARG:HG2	1:D:408:ARG:HD2	1.98	0.46
1:B:21:ASN:HB2	1:B:59:TYR:HD1	1.79	0.46
1:C:280:PRO:HB2	1:C:282:LEU:HG	1.97	0.46
1:D:420:GLU:OE2	1:D:424:ARG:NH1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:ALA:HB2	1:D:252:ALA:HA	1.97	0.46
1:A:3:VAL:HG22	1:A:60:LEU:HD22	1.97	0.46
1:B:151:TYR:CE2	1:B:516:VAL:HG21	2.51	0.46
1:B:425:LEU:HD11	1:B:647:PHE:CZ	2.50	0.46
1:C:520:SER:OG	1:C:523:ASP:OD2	2.26	0.46
1:D:671:ASP:H	1:D:678:MET:HB3	1.81	0.46
1:B:165:THR:HG22	1:B:187:VAL:HG21	1.98	0.46
1:C:113:PRO:HB2	1:C:116:ARG:HB2	1.97	0.46
1:D:97:ARG:HD3	1:D:329:TYR:CE1	2.51	0.46
1:D:118:ASP:OD1	1:D:300:ARG:HD3	2.16	0.46
1:D:392:PHE:HB2	1:D:437:ARG:HH22	1.81	0.46
1:A:379:PRO:HG3	1:A:398:GLU:HB3	1.96	0.46
1:A:239:TRP:CD2	1:A:248:GLU:HG2	2.51	0.46
1:A:678:MET:HG3	1:A:681:GLN:O	2.15	0.46
1:B:325:ASP:OD2	1:B:328:ARG:NH2	2.47	0.46
1:C:538:GLN:O	1:C:543:SER:OG	2.34	0.46
1:D:158:GLU:HB2	1:D:518:MET:HE2	1.92	0.46
1:D:329:TYR:OH	1:D:334:MET:HE1	2.16	0.46
1:A:168:HIS:HB3	1:A:171:LEU:HG	1.98	0.46
1:C:163:GLY:HA2	1:C:544:TRP:HE3	1.81	0.46
1:C:670:VAL:HB	1:C:701:VAL:HB	1.98	0.46
1:D:82:GLY:CA	1:D:299:PRO:HB2	2.46	0.46
1:A:183:ALA:HA	1:A:188:ILE:HD11	1.98	0.45
1:B:490:THR:HB	1:B:495:ILE:HD11	1.96	0.45
1:D:246:VAL:CG2	1:D:334:MET:HE3	2.07	0.45
1:A:402:LYS:HB3	1:A:424:ARG:NH1	2.31	0.45
1:C:541:GLU:HA	1:C:544:TRP:CD1	2.52	0.45
1:D:146:ARG:NH1	1:D:336:VAL:O	2.48	0.45
1:A:184:HIS:CG	1:A:185:PRO:HD2	2.51	0.45
1:A:243:GLY:O	1:A:246:VAL:HG12	2.16	0.45
1:C:224:TYR:HA	1:C:268:VAL:HG21	1.98	0.45
1:C:246:VAL:HG22	1:C:334:MET:HE1	1.94	0.45
1:C:390:GLY:N	1:C:398:GLU:OE1	2.44	0.45
1:A:146:ARG:NH2	1:A:331:VAL:O	2.50	0.45
1:C:272:THR:HG21	1:C:284:MET:HE2	1.97	0.45
1:D:408:ARG:O	1:D:412:ARG:HB2	2.16	0.45
1:A:15:TYR:CE1	1:A:64:MET:HA	2.52	0.45
1:D:68:ARG:HB3	1:D:131:THR:CG2	2.45	0.45
1:D:209:ASN:ND2	1:D:219:SER:HB2	2.31	0.45
1:A:178:THR:HG21	1:A:238:SER:HB3	1.99	0.45
1:A:483:ASN:H	1:A:483:ASN:ND2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:ARG:HD2	1:C:301:TYR:HE1	1.82	0.45
1:C:654:LEU:HD23	1:C:654:LEU:HA	1.70	0.45
1:D:376:ILE:HG12	1:D:397:THR:HB	1.98	0.45
1:A:468:ASN:ND2	1:A:534:ASN:O	2.37	0.45
1:B:157:TYR:HB2	1:B:196:VAL:HG11	1.99	0.45
1:B:483:ASN:HD22	1:B:483:ASN:H	1.65	0.45
1:A:78:ALA:HA	1:C:416:ARG:NH1	2.32	0.45
1:A:197:THR:O	1:A:262:GLU:HG3	2.17	0.45
1:B:34:LEU:HD23	1:B:60:LEU:HD11	1.99	0.45
1:B:135:VAL:HG11	1:B:246:VAL:HG11	1.98	0.45
1:B:209:ASN:ND2	1:B:219:SER:HB2	2.33	0.45
1:C:265:LEU:HG	1:C:336:VAL:HG11	1.97	0.45
1:A:118:ASP:O	1:C:416:ARG:NH2	2.50	0.44
1:B:207:PHE:HA	1:B:226:THR:HA	1.98	0.44
1:C:578:ARG:CB	1:C:578:ARG:NH1	2.72	0.44
1:D:211:HIS:NE2	1:D:215:ASP:OD2	2.50	0.44
1:D:648:ASN:ND2	1:D:696:PRO:HA	2.32	0.44
1:A:172:PRO:HG2	1:A:175:LEU:HG	1.98	0.44
1:A:296:ALA:C	1:A:298:ASP:H	2.21	0.44
1:B:205:HIS:NE2	1:B:267:VAL:HG12	2.33	0.44
1:D:32:ILE:HD12	1:D:56:ARG:HG3	1.99	0.44
1:A:130:MET:HE3	1:A:208:VAL:HG22	1.98	0.44
1:A:329:TYR:OH	1:A:334:MET:CE	2.65	0.44
1:B:390:GLY:O	1:B:435:ASP:OD2	2.35	0.44
1:C:296:ALA:C	1:C:298:ASP:H	2.21	0.44
1:D:146:ARG:NH2	1:D:335:HIS:HA	2.32	0.44
1:B:9:TYR:CG	1:B:10:PRO:HA	2.52	0.44
1:D:56:ARG:NH1	2:D:801:C2E:O6	2.49	0.44
1:B:312:LEU:CB	1:B:314:MET:HE3	2.47	0.44
1:D:107:GLU:HA	1:D:114:PHE:CZ	2.53	0.44
1:A:522:GLY:C	1:A:527:ARG:HB2	2.38	0.44
1:C:168:HIS:HD2	1:C:187:VAL:HG22	1.82	0.44
1:B:24:VAL:HG11	1:B:32:ILE:HG21	1.99	0.44
1:B:158:GLU:HA	1:B:200:GLU:HB3	2.00	0.44
1:C:73:VAL:HG21	1:C:287:LEU:HD23	1.99	0.44
1:C:158:GLU:CB	1:C:518:MET:CE	2.81	0.44
1:D:182:LEU:HD11	1:D:201:LEU:HD11	2.00	0.44
1:A:256:LEU:HD12	1:A:263:VAL:HG22	2.00	0.44
1:B:376:ILE:HG23	1:B:443:VAL:HG21	2.00	0.44
1:C:64:MET:HB3	1:C:65:PRO:CD	2.48	0.44
1:D:597:ALA:HB3	1:D:622:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:GLN:O	1:A:649:ALA:N	2.50	0.44
1:B:326:SER:O	1:B:330:TRP:HD1	2.00	0.44
1:B:430:ASP:OD1	1:B:431:LEU:N	2.51	0.44
1:B:597:ALA:HB3	1:B:622:PHE:HB3	1.99	0.44
1:D:644:LEU:HB3	1:D:702:LEU:HB2	2.00	0.44
1:B:97:ARG:HD3	1:B:329:TYR:CE1	2.53	0.43
1:D:179:TYR:CZ	1:D:236:TYR:HB2	2.52	0.43
1:D:667:ARG:HH11	1:D:703:ARG:HH21	1.66	0.43
1:A:656:PHE:O	1:A:692:VAL:N	2.44	0.43
1:A:678:MET:O	1:A:678:MET:CG	2.64	0.43
1:C:202:MET:HE1	1:C:449:HIS:CB	2.45	0.43
1:C:349:ARG:HA	1:C:353:GLU:O	2.18	0.43
1:D:89:LYS:HA	1:D:125:SER:HB3	1.99	0.43
1:A:77:TYR:O	1:C:416:ARG:NH1	2.52	0.43
1:A:622:PHE:HE1	1:A:642:SER:HB3	1.83	0.43
1:B:283:SER:O	1:B:287:LEU:HG	2.18	0.43
1:B:330:TRP:HA	1:B:334:MET:HB2	2.00	0.43
1:B:440:LEU:HA	1:B:515:GLY:HA2	2.00	0.43
1:C:164:LEU:HD23	1:C:547:TRP:HZ2	1.84	0.43
1:C:167:LEU:HD23	1:C:546:ARG:HD2	1.99	0.43
1:C:497:GLU:O	1:C:501:ARG:HB3	2.17	0.43
1:D:522:GLY:C	1:D:527:ARG:HB2	2.39	0.43
1:B:583:GLY:O	1:B:594:THR:OG1	2.32	0.43
1:C:68:ARG:HD3	1:C:242:ARG:CZ	2.49	0.43
1:D:397:THR:HG22	1:D:443:VAL:HG23	1.99	0.43
1:B:160:HIS:O	1:B:164:LEU:HB2	2.18	0.43
1:C:209:ASN:ND2	1:C:219:SER:HB2	2.33	0.43
1:C:525:PHE:CD2	1:C:548:PRO:HG3	2.54	0.43
1:D:34:LEU:HD23	1:D:60:LEU:HD11	2.00	0.43
1:A:213:LEU:HD23	1:A:219:SER:C	2.39	0.43
1:A:297:ASP:OD2	1:A:297:ASP:N	2.51	0.43
1:C:165:THR:HG22	1:C:187:VAL:HG21	1.99	0.43
1:C:479:ASN:OD1	1:C:533:ASN:ND2	2.49	0.43
1:D:687:ALA:O	1:D:690:GLU:HG2	2.18	0.43
1:B:157:TYR:CZ	1:B:521:HIS:HA	2.54	0.43
1:D:264:ILE:HD11	1:D:374:LYS:HD2	2.01	0.43
1:A:22:PHE:HZ	1:A:63:VAL:HG11	1.84	0.43
1:A:416:ARG:CG	1:A:614:ALA:C	2.85	0.43
1:D:274:GLU:O	1:D:285:ARG:NH2	2.48	0.43
1:D:296:ALA:CB	1:D:303:MET:CG	2.79	0.43
1:A:129:THR:HG22	1:A:130:MET:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ASP:C	1:A:142:GLY:H	2.21	0.43
2:A:801:C2E:H4A	1:B:580:PHE:HB2	2.01	0.43
1:B:474:ASP:OD1	1:B:474:ASP:N	2.51	0.43
1:C:602:GLU:H	1:C:602:GLU:HG3	1.64	0.43
1:B:227:ILE:HD12	1:B:228:GLY:N	2.34	0.43
1:B:280:PRO:O	1:B:285:ARG:NH2	2.49	0.43
1:D:465:ASN:ND2	1:D:533:ASN:OD1	2.41	0.43
1:D:513:SER:O	1:D:569:ARG:NH2	2.49	0.43
1:A:319:VAL:O	1:A:323:ILE:HG13	2.19	0.42
1:B:49:ARG:NH2	2:B:801:C2E:O11	2.50	0.42
1:B:129:THR:HG22	1:B:130:MET:N	2.34	0.42
1:B:162:LYS:HE2	1:B:166:MET:CE	2.49	0.42
1:B:205:HIS:HE1	1:B:330:TRP:NE1	2.17	0.42
1:C:162:LYS:HE2	1:C:166:MET:HE2	2.00	0.42
1:C:163:GLY:HA2	1:C:544:TRP:CE3	2.54	0.42
1:B:97:ARG:HB2	1:B:135:VAL:HG21	2.00	0.42
1:D:601:PRO:HG3	1:D:618:ALA:HB3	2.02	0.42
1:A:398:GLU:OE2	1:A:437:ARG:NH2	2.50	0.42
1:B:92:LEU:HD11	1:B:130:MET:HB2	2.01	0.42
1:C:647:PHE:CD2	1:C:699:LEU:HD21	2.53	0.42
1:D:125:SER:OG	1:D:129:THR:OG1	2.29	0.42
1:A:567:ARG:HG2	1:A:570:ARG:NH2	2.31	0.42
1:B:172:PRO:HG2	1:B:175:LEU:HG	2.02	0.42
1:C:3:VAL:HG22	1:C:60:LEU:HD22	2.01	0.42
1:B:497:GLU:O	1:B:501:ARG:HB3	2.19	0.42
1:D:483:ASN:OD1	1:D:486:GLU:N	2.53	0.42
1:A:9:TYR:CG	1:A:10:PRO:HA	2.55	0.42
1:A:289:ASN:N	1:A:290:PRO:CD	2.83	0.42
1:A:355:ASP:OD2	1:A:356:ARG:N	2.53	0.42
1:A:440:LEU:HD22	1:A:440:LEU:H	1.84	0.42
1:C:15:TYR:CE1	1:C:65:PRO:HD3	2.54	0.42
1:C:178:THR:HG21	1:C:238:SER:HB3	2.00	0.42
1:A:423:SER:O	1:A:428:SER:N	2.51	0.42
1:A:501:ARG:HG3	1:A:672:THR:HG22	2.01	0.42
1:A:508:ALA:HB1	1:A:699:LEU:CD2	2.49	0.42
1:B:315:ARG:HH11	1:B:351:PHE:HD2	1.67	0.42
2:B:801:C2E:O5'	2:B:801:C2E:H8	2.19	0.42
1:C:227:ILE:CG2	1:C:273:ALA:HB3	2.50	0.42
1:C:272:THR:HG21	1:C:284:MET:CE	2.49	0.42
1:C:490:THR:HG22	1:C:492:ASP:H	1.84	0.42
1:D:567:ARG:HG2	1:D:570:ARG:HH21	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:GLU:HB2	1:A:638:ILE:HD12	2.02	0.42
1:A:670:VAL:HB	1:A:701:VAL:HB	2.01	0.42
1:B:577:ARG:HH21	1:B:630:GLU:HG3	1.85	0.42
1:D:296:ALA:CB	1:D:303:MET:SD	3.08	0.42
1:A:95:TYR:HA	1:A:230:PHE:CD1	2.55	0.42
1:A:409:ASP:HA	1:A:412:ARG:HD3	2.00	0.42
1:A:438:ARG:NH2	1:B:50:GLU:OE1	2.44	0.42
1:D:343:LEU:HA	1:D:380:TRP:O	2.19	0.42
1:D:484:CYS:O	1:D:495:ILE:HG12	2.19	0.42
1:A:68:ARG:HD3	1:A:242:ARG:CZ	2.50	0.41
1:A:640:ASP:OD2	1:A:641:ASP:N	2.53	0.41
1:B:184:HIS:ND1	1:B:186:SER:OG	2.47	0.41
1:B:408:ARG:HH21	1:B:457:LEU:HD13	1.84	0.41
1:C:672:THR:HB	1:C:699:LEU:H	1.85	0.41
1:A:162:LYS:HE2	1:A:166:MET:HE3	2.03	0.41
1:B:408:ARG:HE	1:B:457:LEU:CD1	2.33	0.41
1:C:326:SER:O	1:C:330:TRP:HD1	2.03	0.41
1:D:105:TRP:HH2	1:D:280:PRO:HG3	1.85	0.41
1:D:129:THR:HG22	1:D:130:MET:H	1.84	0.41
1:D:178:THR:HG21	1:D:238:SER:HB3	2.01	0.41
1:D:654:LEU:HD23	1:D:654:LEU:HA	1.93	0.41
1:A:687:ALA:HB3	1:A:690:GLU:HB3	2.01	0.41
1:D:129:THR:HG22	1:D:130:MET:N	2.36	0.41
1:D:444:ASN:ND2	1:D:514:GLN:O	2.54	0.41
1:D:458:VAL:HG11	1:D:502:GLN:HB3	2.02	0.41
1:B:264:ILE:HD11	1:B:374:LYS:HD2	2.02	0.41
1:C:107:GLU:HG2	1:C:114:PHE:CG	2.56	0.41
1:C:112:TYR:CZ	1:C:278:LEU:HA	2.55	0.41
1:C:202:MET:CE	1:C:449:HIS:CB	2.88	0.41
1:C:397:THR:HG23	1:C:441:ALA:HA	2.02	0.41
1:C:397:THR:HG22	1:C:443:VAL:HG23	2.03	0.41
1:C:468:ASN:ND2	1:C:534:ASN:O	2.48	0.41
1:B:466:GLU:HG3	1:B:472:ASN:HB2	2.02	0.41
1:D:51:THR:O	2:D:801:C2E:N11	2.41	0.41
1:D:326:SER:O	1:D:330:TRP:HD1	2.03	0.41
1:A:162:LYS:HE2	1:A:166:MET:CE	2.51	0.41
1:A:486:GLU:CD	1:A:490:THR:HG21	2.21	0.41
1:A:658:VAL:HA	1:A:659:PRO:HD3	1.93	0.41
1:B:80:GLU:CD	1:B:80:GLU:H	2.23	0.41
1:B:118:ASP:CG	1:B:300:ARG:HH22	2.24	0.41
1:D:275:GLY:O	1:D:310:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:TYR:CZ	1:D:407:VAL:HG21	2.56	0.41
1:D:648:ASN:HB3	1:D:694:LEU:HD22	2.02	0.41
1:A:246:VAL:HG21	1:A:334:MET:HE1	2.00	0.41
2:A:801:C2E:O5'	2:A:801:C2E:H8	2.21	0.41
1:A:21:ASN:HB2	1:A:59:TYR:HD1	1.85	0.41
1:A:179:TYR:CZ	1:A:236:TYR:HB2	2.56	0.41
1:A:326:SER:O	1:A:330:TRP:HD1	2.04	0.41
1:A:497:GLU:O	1:A:501:ARG:HB3	2.20	0.41
1:B:89:LYS:NZ	1:B:108:ALA:O	2.43	0.41
1:D:408:ARG:NH1	1:D:446:VAL:O	2.54	0.41
1:A:222:TRP:HB3	1:A:224:TYR:CE1	2.56	0.41
1:A:508:ALA:HB1	1:A:699:LEU:HD21	2.03	0.41
1:A:602:GLU:H	1:A:602:GLU:HG3	1.64	0.41
1:A:644:LEU:HD21	1:A:659:PRO:HD2	2.03	0.41
1:B:184:HIS:CG	1:B:185:PRO:HD2	2.56	0.41
1:B:402:LYS:HD2	1:B:431:LEU:HD21	2.02	0.41
1:C:212:ARG:NH2	1:C:536:TYR:OH	2.53	0.41
1:C:698:SER:OG	1:C:699:LEU:N	2.53	0.41
1:D:380:TRP:HA	1:D:386:GLY:O	2.20	0.41
1:A:264:ILE:O	1:A:264:ILE:HG22	2.20	0.41
1:D:105:TRP:CD1	1:D:214:VAL:HG21	2.55	0.41
1:B:11:LEU:HD12	1:B:95:TYR:CZ	2.56	0.40
1:B:191:LEU:HB3	1:B:196:VAL:HG22	2.03	0.40
1:B:209:ASN:HA	1:B:220:ASN:HB2	2.03	0.40
1:C:457:LEU:HD12	1:C:481:SER:HB3	2.03	0.40
1:D:276:ASN:OD1	1:D:276:ASN:N	2.49	0.40
1:A:329:TYR:CE2	1:A:334:MET:HE2	2.56	0.40
1:A:453:THR:HG21	1:A:527:ARG:HE	1.87	0.40
1:C:222:TRP:HB3	1:C:224:TYR:CE1	2.56	0.40
1:D:655:GLU:HA	1:D:693:THR:HA	2.03	0.40
1:A:11:LEU:HD12	1:A:95:TYR:CZ	2.57	0.40
1:A:78:ALA:HA	1:C:416:ARG:HH11	1.87	0.40
1:B:183:ALA:HB2	1:B:252:ALA:HA	2.03	0.40
1:B:343:LEU:HA	1:B:380:TRP:O	2.22	0.40
1:C:470:GLU:OE1	1:C:474:ASP:HB3	2.21	0.40
1:D:171:LEU:HD22	1:D:184:HIS:CG	2.56	0.40
1:D:289:ASN:N	1:D:290:PRO:HD2	2.36	0.40
1:A:207:PHE:HB2	1:A:225:ASN:O	2.22	0.40
1:A:380:TRP:HA	1:A:386:GLY:O	2.21	0.40
1:B:275:GLY:O	1:B:310:ASN:ND2	2.55	0.40
1:B:648:ASN:HB3	1:B:694:LEU:HD22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:ARG:HD3	1:D:242:ARG:CZ	2.52	0.40
1:A:65:PRO:HG2	1:A:136:ASN:HB2	2.03	0.40
1:A:446:VAL:HG23	1:A:447:THR:H	1.86	0.40
1:A:510:LEU:HG	1:A:511:MET:HE2	2.04	0.40
1:B:89:LYS:HA	1:B:89:LYS:HD3	1.91	0.40
1:C:37:LEU:CD2	1:C:43:GLU:HG3	2.52	0.40
1:C:579:ARG:CG	2:D:801:C2E:H81	2.35	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	685/709 (97%)	628 (92%)	57 (8%)	0	100	100
1	B	685/709 (97%)	642 (94%)	43 (6%)	0	100	100
1	C	683/709 (96%)	632 (92%)	49 (7%)	2 (0%)	41	72
1	D	685/709 (97%)	630 (92%)	55 (8%)	0	100	100
All	All	2738/2836 (96%)	2532 (92%)	204 (8%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	679	PRO
1	C	678	MET

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	575/590 (98%)	551 (96%)	24 (4%)	30	62
1	B	573/590 (97%)	560 (98%)	13 (2%)	50	75
1	C	573/590 (97%)	553 (96%)	20 (4%)	36	66
1	D	572/590 (97%)	555 (97%)	17 (3%)	41	70
All	All	2293/2360 (97%)	2219 (97%)	74 (3%)	39	69

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	16	ASP
1	A	27	GLU
1	A	97	ARG
1	A	107	GLU
1	A	116	ARG
1	A	151	TYR
1	A	199	LEU
1	A	254	ARG
1	A	265	LEU
1	A	294	ARG
1	A	322	LEU
1	A	357	LEU
1	A	395	LEU
1	A	478	TYR
1	A	483	ASN
1	A	546	ARG
1	A	578	ARG
1	A	611	TRP
1	A	619	LEU
1	A	667	ARG
1	A	682	GLN
1	A	685	GLU
1	A	699	LEU
1	B	151	TYR
1	B	168	HIS
1	B	199	LEU
1	B	254	ARG
1	B	395	LEU
1	B	400	ASN

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Mol	Chain	Res	Type
1	B	404	ARG
1	B	416	ARG
1	B	546	ARG
1	B	578	ARG
1	B	593	LEU
1	B	610	ASP
1	B	704	ARG
1	C	145	ARG
1	C	148	ARG
1	C	151	TYR
1	C	254	ARG
1	C	257	HIS
1	C	265	LEU
1	C	395	LEU
1	C	400	ASN
1	C	546	ARG
1	C	578	ARG
1	C	582	HIS
1	C	584	ARG
1	C	615	HIS
1	C	619	LEU
1	C	629	SER
1	C	650	SER
1	C	653	GLU
1	C	654	LEU
1	C	655	GLU
1	C	704	ARG
1	D	52	ASP
1	D	102	ARG
1	D	107	GLU
1	D	116	ARG
1	D	151	TYR
1	D	199	LEU
1	D	254	ARG
1	D	265	LEU
1	D	340	ARG
1	D	395	LEU
1	D	400	ASN
1	D	412	ARG
1	D	478	TYR
1	D	501	ARG
1	D	546	ARG

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Mol	Chain	Res	Type
1	D	699	LEU
1	D	704	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	HIS
1	A	271	HIS
1	A	400	ASN
1	A	461	ASN
1	A	483	ASN
1	A	505	ASN
1	B	206	GLN
1	B	234	ASN
1	B	271	HIS
1	B	483	ASN
1	C	206	GLN
1	C	234	ASN
1	C	461	ASN
1	C	483	ASN
1	C	681	GLN
1	D	205	HIS
1	D	271	HIS
1	D	461	ASN
1	D	483	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 monosaccharides in this entry.

5.6 Ligand geometry

4 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
2	C2E	A	801	-	44,52,52	5.41	33 (75%)	52,82,82	1.65	15 (28%)
2	C2E	D	801	-	44,52,52	5.42	32 (72%)	52,82,82	1.70	16 (30%)
2	C2E	B	801	-	44,52,52	5.42	33 (75%)	52,82,82	1.68	16 (30%)
2	C2E	C	801	-	44,52,52	5.41	33 (75%)	52,82,82	1.66	15 (28%)

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
2	C2E	A	801	-	-	1/22/62/62	0/6/7/7
2	C2E	D	801	-	-	1/22/62/62	0/6/7/7
2	C2E	B	801	-	-	1/22/62/62	0/6/7/7
2	C2E	C	801	-	-	5/22/62/62	0/6/7/7

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	C2E	C2'-C1'	-18.14	1.26	1.53
2	C	801	C2E	C2'-C1'	-18.13	1.26	1.53
2	B	801	C2E	C2'-C1'	-18.10	1.26	1.53
2	A	801	C2E	C2'-C1'	-18.06	1.26	1.53
2	C	801	C2E	C2A-C3A	-13.51	1.22	1.52
2	B	801	C2E	C2A-C3A	-13.48	1.22	1.52
2	A	801	C2E	C2A-C3A	-13.46	1.22	1.52
2	D	801	C2E	C2A-C3A	-13.46	1.22	1.52
2	A	801	C2E	C3'-C4'	-10.95	1.23	1.52
2	B	801	C2E	C3'-C4'	-10.93	1.23	1.52
2	D	801	C2E	C3'-C4'	-10.89	1.23	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	C2E	C3'-C4'	-10.87	1.23	1.52
2	D	801	C2E	O4'-C1'	8.69	1.53	1.41
2	A	801	C2E	O4'-C1'	8.64	1.53	1.41
2	C	801	C2E	O4'-C1'	8.58	1.53	1.41
2	B	801	C2E	O4'-C1'	8.57	1.53	1.41
2	B	801	C2E	O4A-C1A	7.89	1.52	1.41
2	A	801	C2E	O4A-C1A	7.82	1.52	1.41
2	C	801	C2E	O4A-C1A	7.81	1.52	1.41
2	D	801	C2E	O4A-C1A	7.58	1.51	1.41
2	D	801	C2E	O4A-C4A	-6.75	1.29	1.45
2	C	801	C2E	O4A-C4A	-6.60	1.30	1.45
2	B	801	C2E	O4A-C4A	-6.54	1.30	1.45
2	A	801	C2E	O4A-C4A	-6.53	1.30	1.45
2	D	801	C2E	C2A-C1A	6.52	1.63	1.53
2	A	801	C2E	C2'-C3'	6.47	1.67	1.52
2	B	801	C2E	C2'-C3'	6.43	1.67	1.52
2	C	801	C2E	C2'-C3'	6.43	1.67	1.52
2	B	801	C2E	C2A-C1A	6.37	1.63	1.53
2	D	801	C2E	C2'-C3'	6.36	1.67	1.52
2	A	801	C2E	C2A-C1A	6.33	1.63	1.53
2	C	801	C2E	C2A-C1A	6.22	1.63	1.53
2	B	801	C2E	C3A-C4A	5.90	1.68	1.52
2	A	801	C2E	C3A-C4A	5.87	1.68	1.52
2	C	801	C2E	C3A-C4A	5.87	1.68	1.52
2	D	801	C2E	C3A-C4A	5.81	1.68	1.52
2	A	801	C2E	C2-N3	5.75	1.47	1.33
2	C	801	C2E	C2-N3	5.74	1.47	1.33
2	D	801	C2E	C2-N3	5.73	1.47	1.33
2	B	801	C2E	C2-N3	5.73	1.47	1.33
2	B	801	C2E	C21-N31	5.72	1.47	1.33
2	A	801	C2E	O4'-C4'	5.71	1.57	1.45
2	B	801	C2E	O4'-C4'	5.66	1.57	1.45
2	C	801	C2E	O4'-C4'	5.66	1.57	1.45
2	D	801	C2E	O4'-C4'	5.65	1.57	1.45
2	D	801	C2E	C21-N31	5.61	1.46	1.33
2	A	801	C2E	C21-N31	5.58	1.46	1.33
2	C	801	C2E	C21-N31	5.56	1.46	1.33
2	D	801	C2E	C2-N2	5.32	1.46	1.34
2	B	801	C2E	C21-N21	5.31	1.46	1.34
2	C	801	C2E	C21-N21	5.30	1.46	1.34
2	A	801	C2E	C21-N21	5.29	1.46	1.34
2	D	801	C2E	C21-N21	5.29	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	C2E	C2-N2	5.28	1.46	1.34
2	B	801	C2E	C2-N2	5.25	1.46	1.34
2	C	801	C2E	C2-N2	5.24	1.46	1.34
2	A	801	C2E	C4-N3	5.24	1.50	1.37
2	D	801	C2E	C4-N3	5.24	1.50	1.37
2	C	801	C2E	C4-N3	5.23	1.50	1.37
2	B	801	C2E	C4-N3	5.20	1.50	1.37
2	B	801	C2E	C41-N31	5.09	1.49	1.37
2	C	801	C2E	C41-N31	5.09	1.49	1.37
2	A	801	C2E	C41-N31	5.08	1.49	1.37
2	D	801	C2E	C41-N31	5.07	1.49	1.37
2	B	801	C2E	C61-N11	4.06	1.43	1.37
2	C	801	C2E	C6-N1	4.02	1.43	1.37
2	A	801	C2E	C6-N1	3.94	1.43	1.37
2	B	801	C2E	C6-N1	3.93	1.43	1.37
2	D	801	C2E	C6-N1	3.92	1.43	1.37
2	D	801	C2E	C61-N11	3.90	1.43	1.37
2	A	801	C2E	C61-N11	3.79	1.43	1.37
2	C	801	C2E	C61-N11	3.74	1.43	1.37
2	D	801	C2E	C5'-C4'	3.66	1.63	1.51
2	B	801	C2E	O2A-C2A	3.64	1.51	1.43
2	B	801	C2E	C5'-C4'	3.64	1.62	1.51
2	A	801	C2E	C5'-C4'	3.61	1.62	1.51
2	C	801	C2E	C5'-C4'	3.61	1.62	1.51
2	A	801	C2E	O2A-C2A	3.61	1.51	1.43
2	C	801	C2E	O2A-C2A	3.59	1.51	1.43
2	D	801	C2E	O2A-C2A	3.58	1.51	1.43
2	B	801	C2E	C5-C6	3.41	1.54	1.47
2	D	801	C2E	C5-C6	3.40	1.54	1.47
2	C	801	C2E	C5-C6	3.39	1.54	1.47
2	B	801	C2E	C51-C61	3.37	1.54	1.47
2	A	801	C2E	C5-C6	3.35	1.54	1.47
2	A	801	C2E	P1-O3A	3.29	1.69	1.60
2	D	801	C2E	P1-O3A	3.28	1.69	1.60
2	B	801	C2E	P1-O3A	3.27	1.69	1.60
2	D	801	C2E	C51-C61	3.26	1.54	1.47
2	A	801	C2E	C51-C61	3.22	1.53	1.47
2	C	801	C2E	C51-C61	3.22	1.53	1.47
2	C	801	C2E	P1-O3A	3.16	1.68	1.60
2	B	801	C2E	C21-N11	2.96	1.45	1.37
2	B	801	C2E	C2-N1	2.94	1.44	1.37
2	C	801	C2E	C2-N1	2.92	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	C2E	P11-O3'	2.91	1.68	1.60
2	A	801	C2E	P11-O3'	2.88	1.68	1.60
2	D	801	C2E	C2-N1	2.88	1.44	1.37
2	B	801	C2E	P11-O3'	2.86	1.68	1.60
2	A	801	C2E	C2-N1	2.86	1.44	1.37
2	D	801	C2E	C21-N11	2.84	1.44	1.37
2	D	801	C2E	P11-O3'	2.83	1.67	1.60
2	C	801	C2E	C21-N11	2.81	1.44	1.37
2	A	801	C2E	C21-N11	2.80	1.44	1.37
2	D	801	C2E	P1-O5'	2.73	1.70	1.59
2	A	801	C2E	P1-O5'	2.71	1.70	1.59
2	C	801	C2E	P1-O5'	2.70	1.70	1.59
2	B	801	C2E	P1-O5'	2.70	1.70	1.59
2	A	801	C2E	P11-O5A	2.36	1.68	1.59
2	C	801	C2E	P11-O5A	2.36	1.68	1.59
2	D	801	C2E	C51-C41	-2.34	1.37	1.43
2	D	801	C2E	C5-C4	-2.34	1.37	1.43
2	B	801	C2E	P11-O5A	2.33	1.68	1.59
2	C	801	C2E	C5-C4	-2.33	1.37	1.43
2	B	801	C2E	C5-C4	-2.33	1.37	1.43
2	C	801	C2E	C51-C41	-2.31	1.37	1.43
2	A	801	C2E	C5-C4	-2.28	1.37	1.43
2	B	801	C2E	C51-C41	-2.27	1.37	1.43
2	D	801	C2E	P11-O5A	2.26	1.68	1.59
2	A	801	C2E	C51-C41	-2.24	1.37	1.43
2	D	801	C2E	O3A-C3A	2.18	1.52	1.44
2	B	801	C2E	O3A-C3A	2.17	1.52	1.44
2	C	801	C2E	O3'-C3'	2.17	1.52	1.44
2	B	801	C2E	O3'-C3'	2.15	1.51	1.44
2	A	801	C2E	O3A-C3A	2.15	1.51	1.44
2	A	801	C2E	O3'-C3'	2.15	1.51	1.44
2	C	801	C2E	O3A-C3A	2.14	1.51	1.44
2	D	801	C2E	O3'-C3'	2.14	1.51	1.44
2	A	801	C2E	O6-C6	-2.03	1.19	1.23
2	B	801	C2E	O6-C6	-2.02	1.19	1.23
2	C	801	C2E	O6-C6	-2.02	1.19	1.23

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	C2E	C5-C6-N1	3.45	120.04	113.95
2	A	801	C2E	C5-C6-N1	3.44	120.03	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	C2E	C5-C6-N1	3.43	120.01	113.95
2	B	801	C2E	C5-C6-N1	3.43	120.01	113.95
2	B	801	C2E	C51-C61-N11	3.41	119.97	113.95
2	D	801	C2E	C51-C61-N11	3.28	119.74	113.95
2	A	801	C2E	C51-C61-N11	3.18	119.56	113.95
2	C	801	C2E	C51-C61-N11	3.17	119.55	113.95
2	C	801	C2E	P1-O3A-C3A	-3.09	108.17	119.41
2	D	801	C2E	C3'-C2'-C1'	3.04	106.62	99.89
2	D	801	C2E	C81-N71-C51	3.03	108.77	102.99
2	A	801	C2E	C2-N1-C6	-2.99	119.59	125.10
2	C	801	C2E	C2-N1-C6	-2.98	119.61	125.10
2	B	801	C2E	C2-N1-C6	-2.98	119.62	125.10
2	B	801	C2E	C21-N11-C61	-2.94	119.68	125.10
2	D	801	C2E	C2-N1-C6	-2.93	119.70	125.10
2	B	801	C2E	C3'-C2'-C1'	2.92	106.35	99.89
2	A	801	C2E	C3'-C2'-C1'	2.87	106.24	99.89
2	B	801	C2E	C81-N71-C51	2.77	108.26	102.99
2	D	801	C2E	O21-P11-O3'	2.75	117.63	106.78
2	C	801	C2E	O21-P11-O3'	2.71	117.49	106.78
2	A	801	C2E	O21-P11-O3'	2.70	117.45	106.78
2	C	801	C2E	C3'-C2'-C1'	2.70	105.87	99.89
2	D	801	C2E	C8-N7-C5	2.69	108.11	102.99
2	B	801	C2E	O21-P11-O3'	2.69	117.38	106.78
2	C	801	C2E	C8-N7-C5	2.68	108.10	102.99
2	D	801	C2E	C21-N11-C61	-2.65	120.22	125.10
2	B	801	C2E	P1-O3A-C3A	-2.64	109.80	119.41
2	C	801	C2E	C81-N71-C51	2.64	108.02	102.99
2	A	801	C2E	C81-N71-C51	2.63	108.00	102.99
2	A	801	C2E	P1-O3A-C3A	-2.63	109.84	119.41
2	D	801	C2E	P11-O3'-C3'	-2.63	109.84	119.41
2	A	801	C2E	C8-N7-C5	2.63	108.00	102.99
2	B	801	C2E	C8-N7-C5	2.61	107.97	102.99
2	D	801	C2E	P1-O3A-C3A	-2.52	110.23	119.41
2	A	801	C2E	P11-O3'-C3'	-2.50	110.31	119.41
2	A	801	C2E	C21-N11-C61	-2.50	120.50	125.10
2	D	801	C2E	C3A-C2A-C1A	2.48	105.38	99.89
2	C	801	C2E	C21-N11-C61	-2.47	120.54	125.10
2	C	801	C2E	P11-O3'-C3'	-2.43	110.58	119.41
2	B	801	C2E	P11-O3'-C3'	-2.42	110.58	119.41
2	B	801	C2E	C3A-C2A-C1A	2.40	105.21	99.89
2	C	801	C2E	C3A-C2A-C1A	2.32	105.03	99.89
2	A	801	C2E	O6-C6-C5	-2.29	119.91	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	C2E	O6-C6-C5	-2.28	119.91	124.37
2	D	801	C2E	O6-C6-C5	-2.28	119.93	124.37
2	A	801	C2E	C3A-C2A-C1A	2.27	104.92	99.89
2	C	801	C2E	O6-C6-C5	-2.26	119.96	124.37
2	B	801	C2E	O61-C61-C51	-2.20	120.08	124.37
2	A	801	C2E	P11-O5A-C5A	-2.20	108.80	121.68
2	D	801	C2E	O21-P11-O5A	2.17	117.83	107.75
2	C	801	C2E	P11-O5A-C5A	-2.15	109.06	121.68
2	B	801	C2E	P11-O5A-C5A	-2.15	109.07	121.68
2	D	801	C2E	C2'-C3'-C4'	2.10	106.95	103.22
2	B	801	C2E	O21-P11-O5A	2.08	117.42	107.75
2	A	801	C2E	O21-P11-O5A	2.06	117.31	107.75
2	C	801	C2E	O21-P11-O5A	2.05	117.26	107.75
2	C	801	C2E	O61-C61-C51	-2.04	120.39	124.37
2	A	801	C2E	O61-C61-C51	-2.04	120.39	124.37
2	D	801	C2E	O61-C61-C51	-2.03	120.40	124.37
2	D	801	C2E	P11-O5A-C5A	-2.02	109.83	121.68
2	B	801	C2E	C2'-C3'-C4'	2.02	106.80	103.22

There are no chirality outliers.

All (8) torsion outliers are listed below:

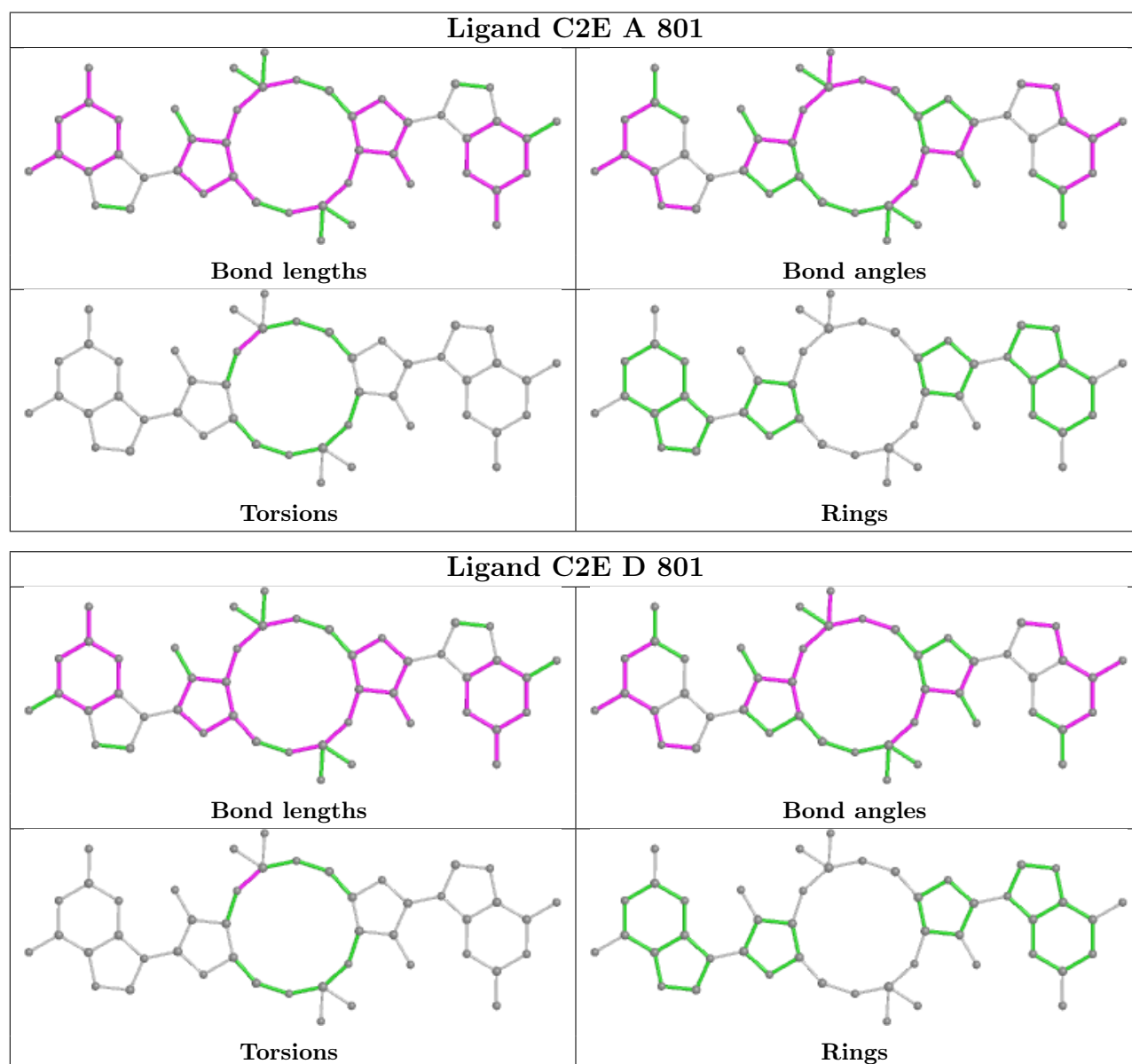
Mol	Chain	Res	Type	Atoms
2	C	801	C2E	C5A-O5A-P11-O3'
2	B	801	C2E	C3'-O3'-P11-O5A
2	A	801	C2E	C3'-O3'-P11-O5A
2	C	801	C2E	C3'-O3'-P11-O5A
2	C	801	C2E	C5'-O5'-P1-O3A
2	C	801	C2E	C5A-O5A-P11-O11
2	D	801	C2E	C3'-O3'-P11-O5A
2	C	801	C2E	C5'-O5'-P1-O1P

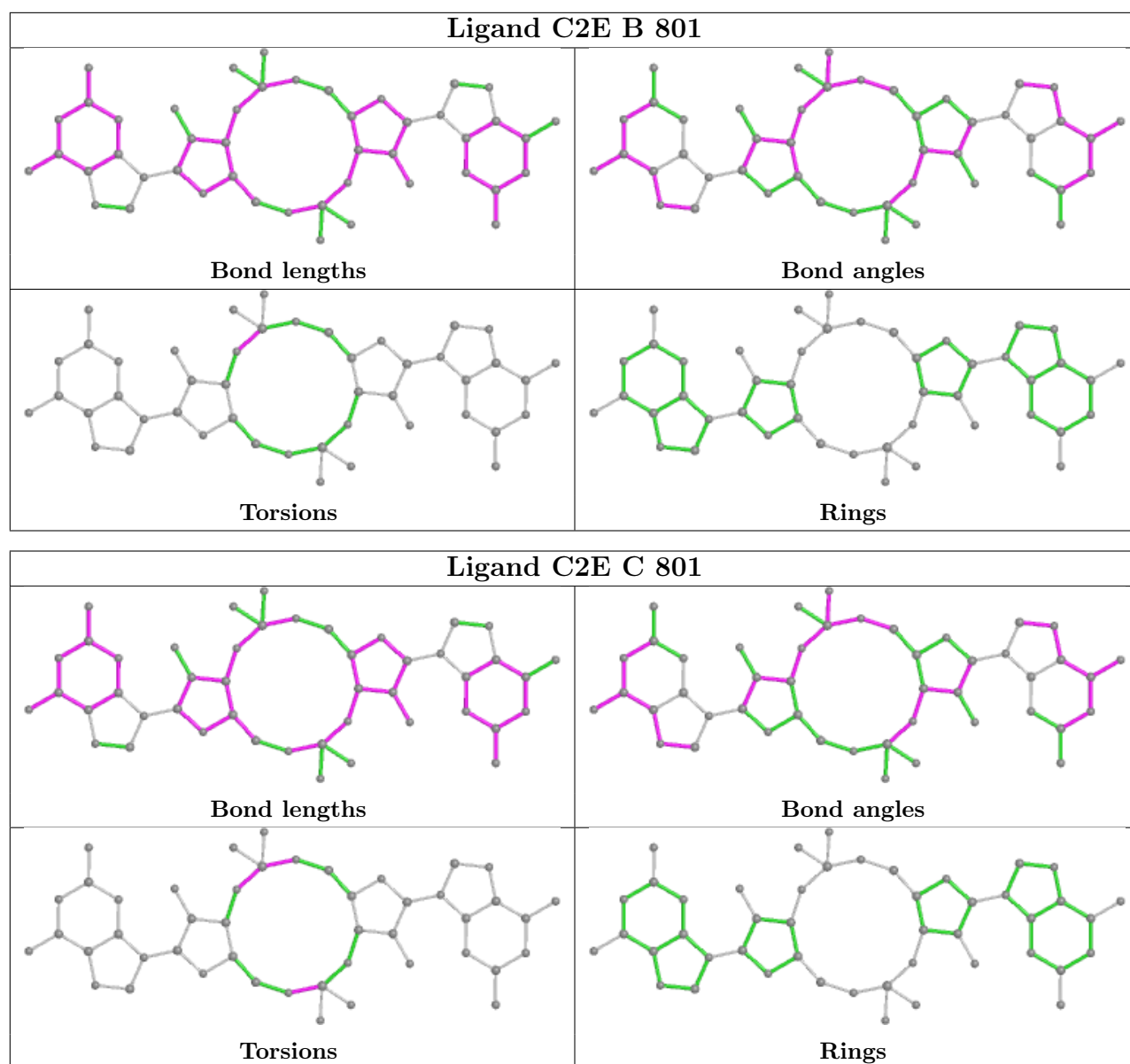
There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	C2E	5	0
2	D	801	C2E	10	0
2	B	801	C2E	2	0
2	C	801	C2E	3	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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	693/709 (97%)	0.17	7 (1%) 82 83	16, 31, 59, 95	0
1	B	693/709 (97%)	0.13	12 (1%) 70 69	16, 32, 68, 99	0
1	C	691/709 (97%)	0.10	6 (0%) 84 85	16, 33, 64, 88	0
1	D	693/709 (97%)	0.28	15 (2%) 62 61	18, 36, 67, 97	0
All	All	2770/2836 (97%)	0.17	40 (1%) 75 75	16, 33, 65, 99	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	682	GLN	3.4
1	B	615	HIS	3.3
1	D	602	GLU	3.3
1	C	700	THR	3.0
1	A	615	HIS	3.0
1	A	687	ALA	3.0
1	D	617	GLN	2.7
1	C	660	ASP	2.6
1	C	586	VAL	2.6
1	A	584	ARG	2.6
1	B	650	SER	2.6
1	D	705	PRO	2.5
1	B	553	GLU	2.5
1	D	582	HIS	2.5
1	A	1	MET	2.4
1	B	617	GLN	2.4
1	B	484	CYS	2.4
1	D	682	GLN	2.4
1	B	679	PRO	2.4
1	C	686	LEU	2.4
1	B	651	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	623	LEU	2.3
1	C	585	PRO	2.3
1	D	673	SER	2.3
1	D	647	PHE	2.3
1	D	654	LEU	2.3
1	D	687	ALA	2.2
1	D	693	THR	2.2
1	B	564	SER	2.2
1	D	608	SER	2.2
1	D	593	LEU	2.2
1	A	406	CYS	2.1
1	A	597	ALA	2.1
1	B	665	TYR	2.1
1	B	554	ALA	2.1
1	D	615	HIS	2.1
1	D	662	HIS	2.1
1	B	418	LEU	2.0
1	A	417	THR	2.0
1	B	504	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

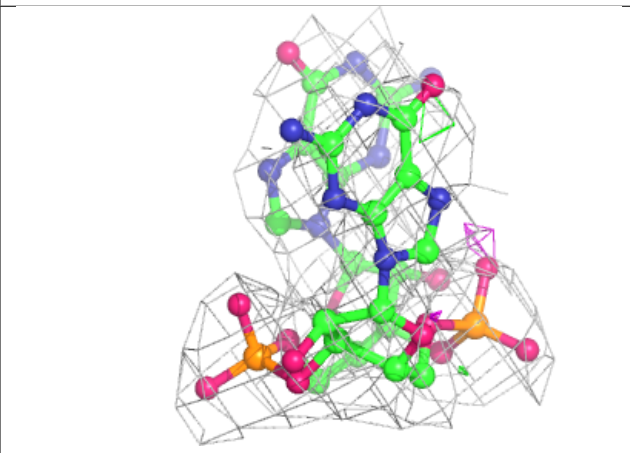
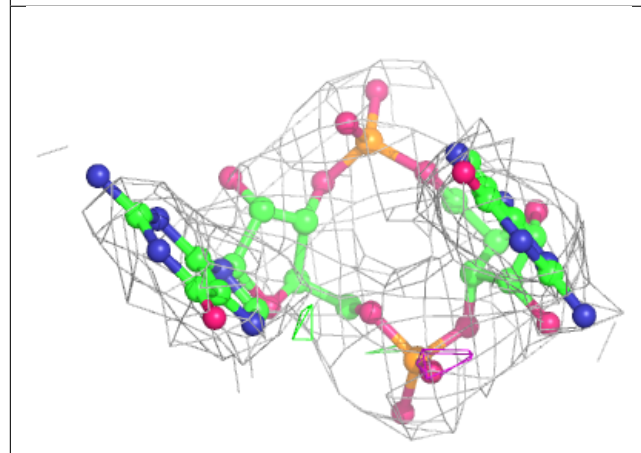
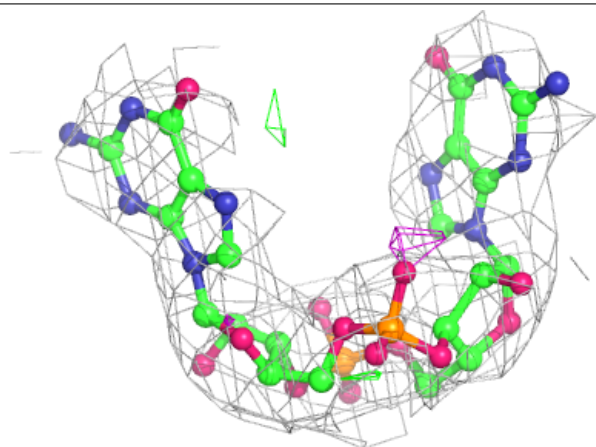
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	C2E	D	801	46/46	0.90	0.22	37,47,59,63	0
2	C2E	C	801	46/46	0.92	0.20	26,38,47,58	0
2	C2E	A	801	46/46	0.93	0.18	39,44,51,59	0
2	C2E	B	801	46/46	0.93	0.23	36,46,58,83	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.

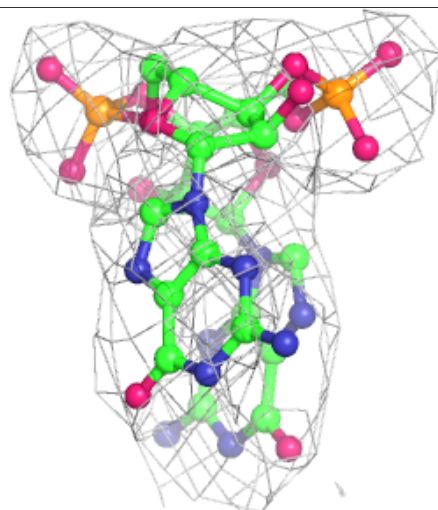
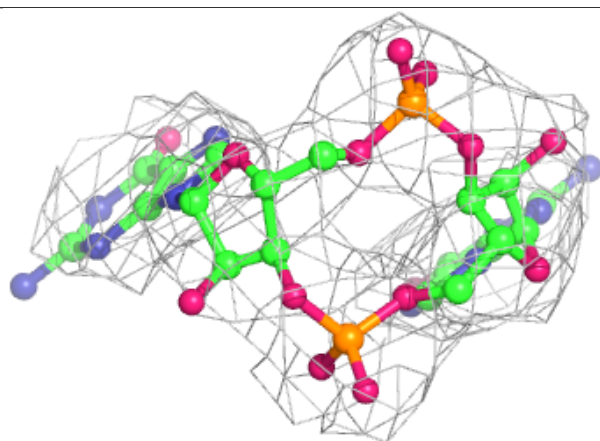
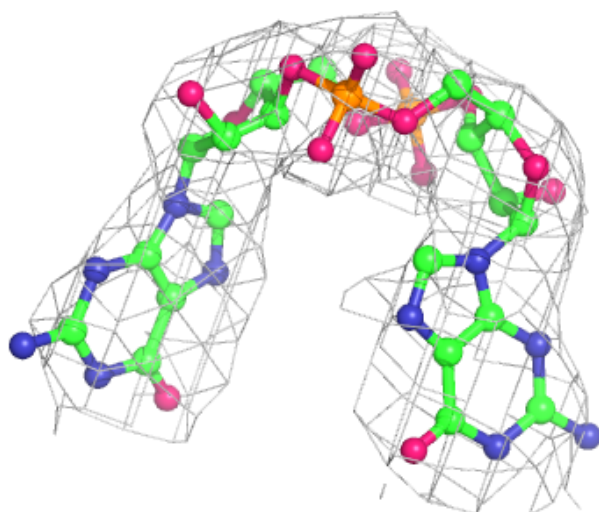
Electron density around C2E D 801:

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



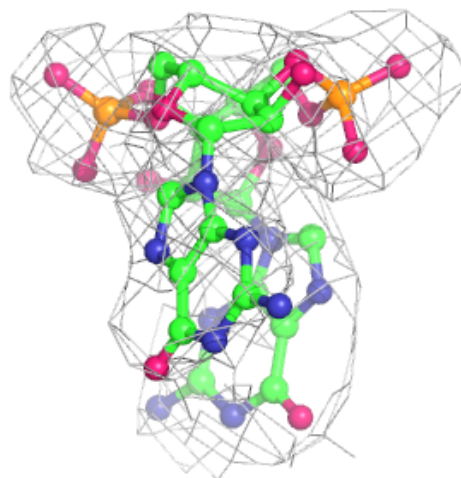
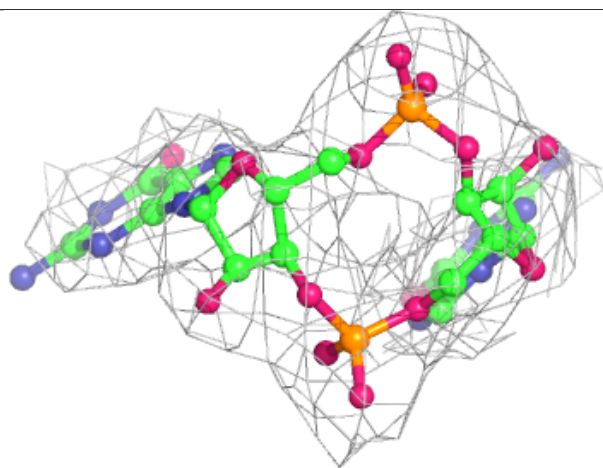
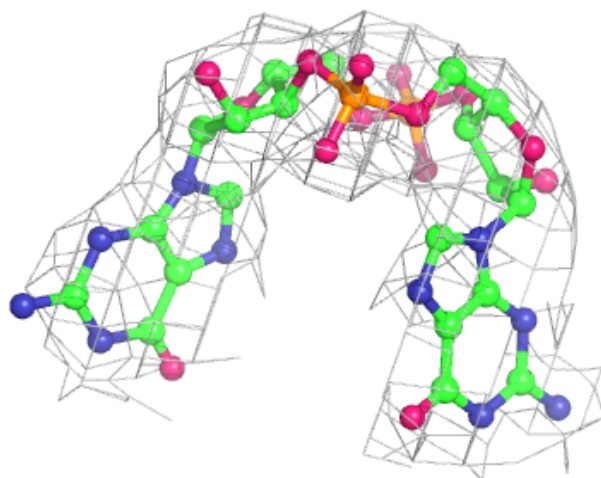
Electron density around C2E C 801:

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



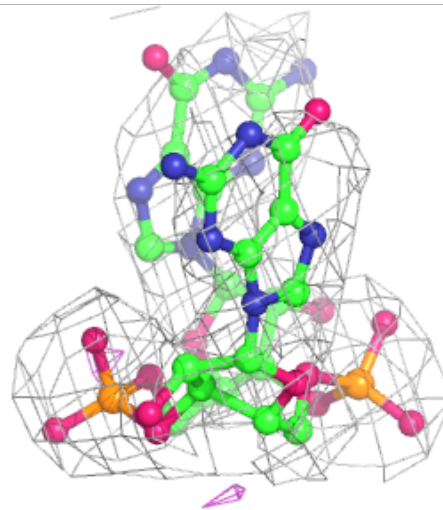
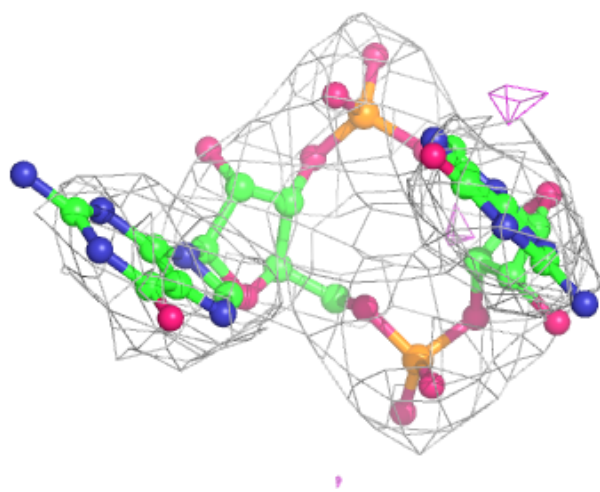
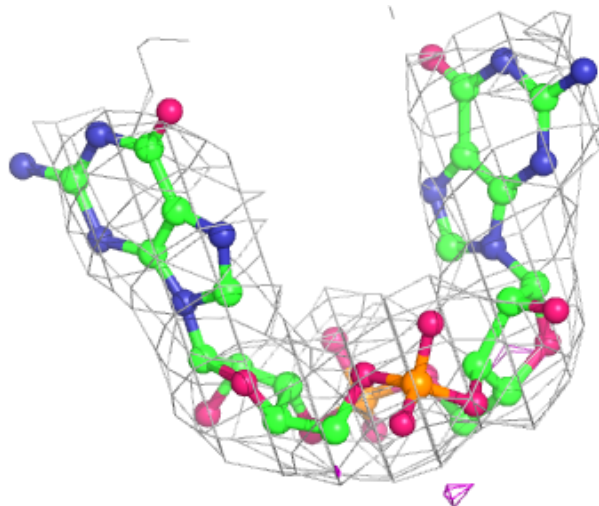
Electron density around C2E A 801:

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



Electron density around C2E B 801:

$2mF_o-DF_c$ (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.