



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 09:02 PM EDT

PDB ID : 4TYS
Title : Crystal structure of Canavalia maritima lectin (ConM) complexed with a dinucleotide
Authors : Vieira, D.B.H.A.; Delatorre, P.; Silva-Filho, J.C.; Nobrega, R.B.; Cavada, B.S.; Rocha, B.A.M.; Lima, E.M.; Teixeira, C.S.
Deposited on : 2014-07-09
Resolution : 3.25 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	:	2.37.1
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)	:	2.37.1

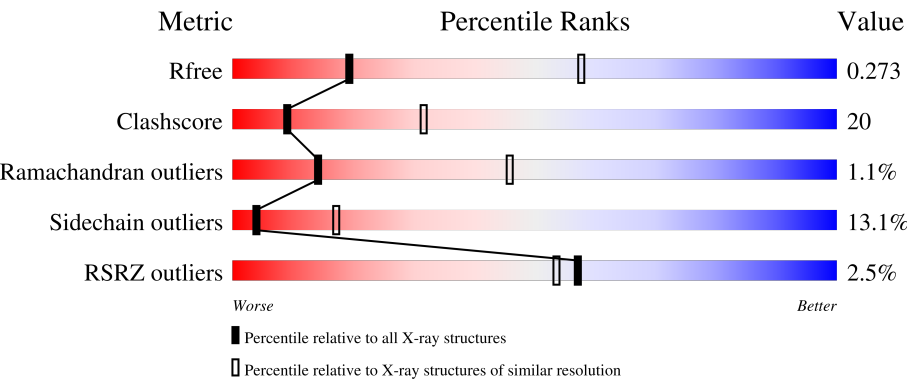
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	237	<div><div>3%</div><div>61%</div><div>30%</div><div>7%</div><div>.</div></div>
1	B	237	<div><div>3%</div><div>57%</div><div>30%</div><div>10%</div><div>..</div></div>
1	C	237	<div><div>3%</div><div>61%</div><div>30%</div><div>6%</div><div>..</div></div>
1	D	237	<div><div>3%</div><div>63%</div><div>29%</div><div>5%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
1	E	237	
1	F	237	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10750 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.

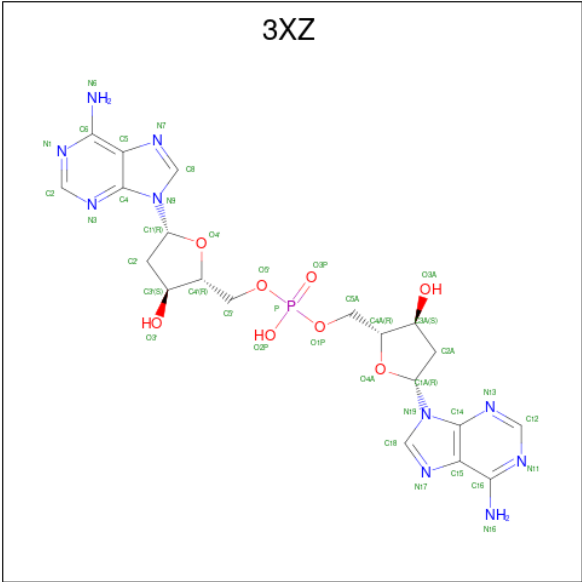
- Molecule 1 is a protein called Concanavalin-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1761	1113	294	353	1			
1	B	232	Total	C	N	O	S	0	0	0
			1761	1113	294	353	1			
1	C	233	Total	C	N	O	S	0	0	0
			1770	1118	295	356	1			
1	D	232	Total	C	N	O	S	0	0	0
			1761	1113	294	353	1			
1	E	232	Total	C	N	O	S	0	0	0
			1761	1113	294	353	1			
1	F	232	Total	C	N	O	S	0	0	0
			1761	1113	294	353	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	SER	ASN	conflict	UNP P81460
B	168	SER	ASN	conflict	UNP P81460
C	168	SER	ASN	conflict	UNP P81460
D	168	SER	ASN	conflict	UNP P81460
E	168	SER	ASN	conflict	UNP P81460
F	168	SER	ASN	conflict	UNP P81460

- Molecule 2 is bis{[(2R,3S,5R)-5-(6-amino-9H-purin-9-yl)-3-hydroxytetrahydrofuran-2-yl]methyl} hydrogen phosphate (three-letter code: 3XZ) (formula: C₂₀H₂₅N₁₀O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			39	20	10	8	1		

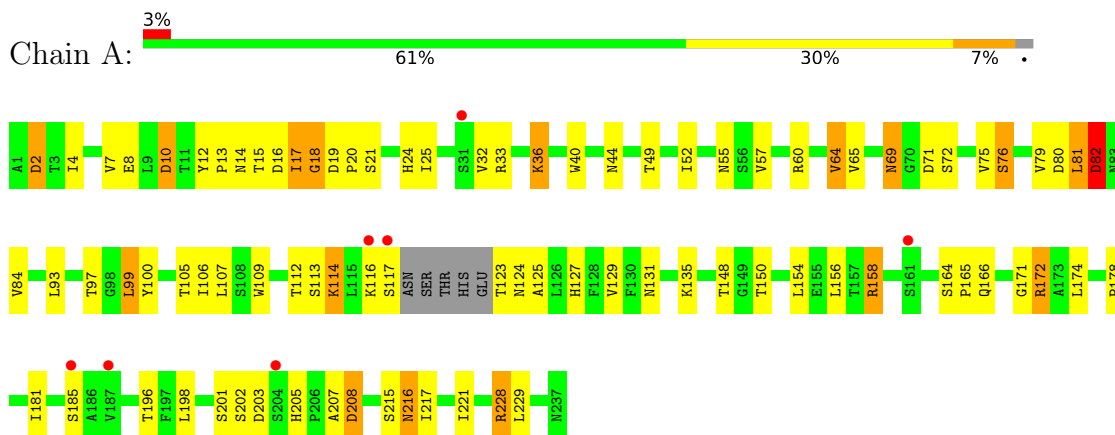
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	25	Total O	0	0
			25 25		
3	B	21	Total O	0	0
			21 21		
3	C	24	Total O	0	0
			24 24		
3	D	19	Total O	0	0
			19 19		
3	E	25	Total O	0	0
			25 25		
3	F	22	Total O	0	0
			22 22		

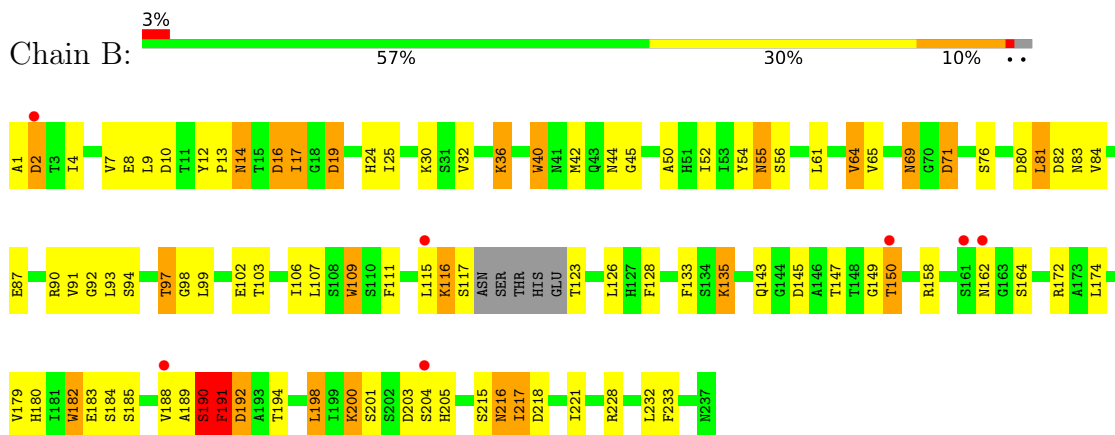
3 Residue-property plots [i](#)

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

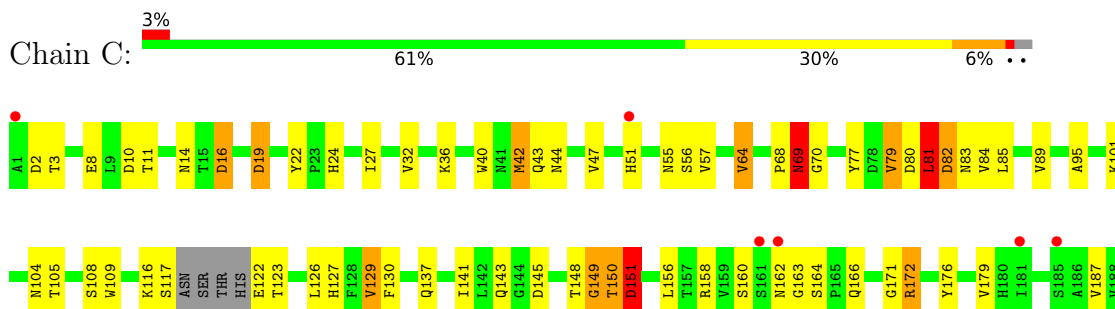
• Molecule 1: Concanavalin-A

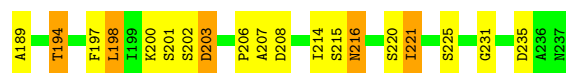


• Molecule 1: Concanavalin-A

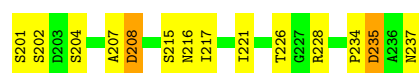


• Molecule 1: Concanavalin-A

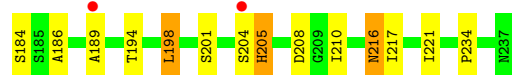




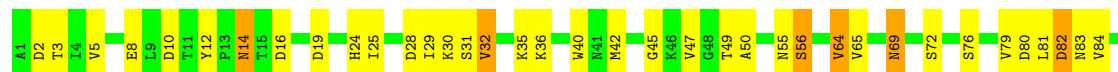
• Molecule 1: Concanavalin-A



• Molecule 1: Concanavalin-A



• Molecule 1: Concanavalin-A



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	140.69Å 140.57Å 199.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.29 – 3.25 38.28 – 3.25	Depositor EDS
% Data completeness (in resolution range)	98.7 (38.29-3.25) 99.0 (38.28-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.216 , 0.267 0.218 , 0.273	Depositor DCC
R_{free} test set	1570 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 26.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.399 for $-1/2^*h+1/2^*k+1/2^*l, 1/2^*h-1/2^*k+1/2^*l, h+k$ 0.408 for $-1/2^*h+1/2^*k-1/2^*l, 1/2^*h-1/2^*k-1/2^*l, -h-k$ 0.408 for $k, h, -l$ 0.400 for $-1/2^*h-1/2^*k-1/2^*l, -1/2^*h-1/2^*k+1/2^*l, -h+k$ 0.397 for $-1/2^*h-1/2^*k+1/2^*l, -1/2^*h-1/2^*k-1/2^*l, h-k$	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	10750	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: 3XZ

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	0.74	3/1800 (0.2%)	0.93	7/2450 (0.3%)
1	B	0.72	5/1800 (0.3%)	0.91	11/2450 (0.4%)
1	C	0.78	5/1809 (0.3%)	0.98	14/2462 (0.6%)
1	D	0.75	5/1800 (0.3%)	0.90	7/2450 (0.3%)
1	E	0.70	3/1800 (0.2%)	0.90	8/2450 (0.3%)
1	F	0.68	2/1800 (0.1%)	0.86	4/2450 (0.2%)
All	All	0.73	23/10809 (0.2%)	0.91	51/14712 (0.3%)

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	B	0	4
1	C	0	3
1	E	0	1
All	All	0	8

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	PRO	N-CD	11.10	1.63	1.47
1	C	151	ASP	C-N	9.25	1.49	1.33
1	D	151	ASP	C-N	9.03	1.49	1.33
1	C	81	LEU	C-N	8.61	1.53	1.34
1	C	149	GLY	C-N	8.49	1.53	1.34
1	E	81	LEU	C-N	7.22	1.50	1.34
1	B	98	GLY	C-N	7.12	1.50	1.34
1	D	148	THR	C-N	-6.79	1.20	1.33
1	C	148	THR	C-N	-6.60	1.21	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	97	THR	C-N	5.91	1.43	1.33
1	B	109	TRP	CD2-CE2	5.88	1.48	1.41
1	D	109	TRP	CD2-CE2	5.63	1.48	1.41
1	E	109	TRP	CD2-CE2	5.62	1.48	1.41
1	B	40	TRP	CD2-CE2	5.57	1.48	1.41
1	D	182	TRP	CD2-CE2	5.50	1.48	1.41
1	F	182	TRP	CD2-CE2	5.41	1.47	1.41
1	A	109	TRP	CD2-CE2	5.41	1.47	1.41
1	C	109	TRP	CD2-CE2	5.34	1.47	1.41
1	E	182	TRP	CD2-CE2	5.34	1.47	1.41
1	D	40	TRP	CD2-CE2	5.29	1.47	1.41
1	F	109	TRP	CD2-CE2	5.27	1.47	1.41
1	A	40	TRP	CD2-CE2	5.15	1.47	1.41
1	B	182	TRP	CD2-CE2	5.05	1.47	1.41

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	GLY	O-C-N	-14.51	99.49	122.70
1	A	81	LEU	O-C-N	12.02	141.94	122.70
1	A	82	ASP	O-C-N	-11.77	103.86	122.70
1	E	82	ASP	O-C-N	11.20	140.61	122.70
1	A	81	LEU	CA-C-N	-10.21	94.73	117.20
1	E	82	ASP	CA-C-N	-9.58	96.13	117.20
1	F	207	ALA	CB-CA-C	9.32	124.08	110.10
1	B	191	PHE	N-CA-C	9.02	135.34	111.00
1	B	99	LEU	N-CA-C	-8.89	86.99	111.00
1	D	235	ASP	N-CA-CB	8.79	126.42	110.60
1	C	151	ASP	N-CA-CB	8.69	126.24	110.60
1	B	191	PHE	CB-CA-C	-8.30	93.80	110.40
1	A	82	ASP	CA-C-N	7.69	134.12	117.20
1	A	82	ASP	C-N-CA	7.38	140.14	121.70
1	B	190	SER	C-N-CA	7.30	139.96	121.70
1	C	151	ASP	N-CA-C	-7.16	91.68	111.00
1	E	19	ASP	CB-CG-OD1	7.12	124.71	118.30
1	C	150	THR	C-N-CA	-7.12	103.91	121.70
1	C	203	ASP	N-CA-C	-7.03	92.01	111.00
1	C	149	GLY	CA-C-N	6.88	132.35	117.20
1	F	208	ASP	N-CA-CB	6.85	122.93	110.60
1	C	19	ASP	CB-CG-OD1	6.71	124.34	118.30
1	C	149	GLY	C-N-CA	6.67	138.37	121.70
1	C	203	ASP	CB-CA-C	6.56	123.51	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	149	GLY	C-N-CA	6.50	137.96	121.70
1	E	205	HIS	N-CA-C	-6.46	93.56	111.00
1	B	191	PHE	C-N-CA	6.40	137.69	121.70
1	C	82	ASP	N-CA-C	-6.38	93.77	111.00
1	B	97	THR	C-N-CA	-6.32	109.03	122.30
1	B	117	SER	N-CA-CB	6.21	119.82	110.50
1	A	81	LEU	C-N-CA	-6.19	106.22	121.70
1	C	150	THR	O-C-N	6.05	132.37	122.70
1	D	149	GLY	O-C-N	-5.95	113.19	122.70
1	B	19	ASP	CB-CG-OD1	5.93	123.63	118.30
1	C	151	ASP	O-C-N	5.71	132.91	123.20
1	A	17	ILE	N-CA-C	-5.56	95.98	111.00
1	D	202	SER	O-C-N	5.56	131.59	122.70
1	F	150	THR	CB-CA-C	5.51	126.48	111.60
1	D	202	SER	CA-C-N	-5.51	105.08	117.20
1	E	204	SER	CB-CA-C	-5.50	99.64	110.10
1	D	151	ASP	N-CA-C	5.49	125.82	111.00
1	D	234	PRO	CB-CA-C	-5.44	98.39	112.00
1	F	205	HIS	N-CA-C	-5.42	96.38	111.00
1	C	151	ASP	CA-C-N	-5.41	105.38	116.20
1	B	192	ASP	N-CA-C	5.41	125.61	111.00
1	E	198	LEU	CA-CB-CG	5.38	127.69	115.30
1	E	37	THR	N-CA-CB	5.29	120.34	110.30
1	E	36	LYS	CB-CA-C	5.17	120.74	110.40
1	B	116	LYS	CB-CA-C	5.09	120.58	110.40
1	C	150	THR	N-CA-C	5.03	124.58	111.00
1	B	116	LYS	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	190	SER	Peptide
1	B	191	PHE	Peptide
1	B	81	LEU	Peptide
1	B	97	THR	Mainchain
1	C	149	GLY	Peptide,Mainchain
1	C	81	LEU	Peptide
1	E	127	HIS	Mainchain

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	1761	0	1715	74	2
1	B	1761	0	1716	74	1
1	C	1770	0	1722	79	3
1	D	1761	0	1715	75	2
1	E	1761	0	1716	68	5
1	F	1761	0	1716	71	3
2	E	39	0	24	18	0
3	A	25	0	0	6	0
3	B	21	0	0	5	0
3	C	24	0	0	6	0
3	D	19	0	0	13	0
3	E	25	0	0	2	0
3	F	22	0	0	5	0
All	All	10750	0	10324	420	8

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 20.

All (420) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:VAL:CG2	3:D:314:HOH:O	1.69	1.34
1:A:15:THR:HG22	1:A:19:ASP:O	1.28	1.29
1:F:200:LYS:HE2	3:F:316:HOH:O	1.06	1.21
1:B:1:ALA:HB1	3:B:319:HOH:O	1.48	1.12
1:A:216:ASN:OD1	3:A:305:HOH:O	1.65	1.12
1:C:187:VAL:HG21	3:D:314:HOH:O	1.25	1.11
1:B:80:ASP:O	1:B:82:ASP:O	1.75	1.05
1:B:44:ASN:HD21	1:B:201:SER:H	1.04	0.98
1:A:131:ASN:OD1	3:A:308:HOH:O	1.81	0.97
2:E:601:3XZ:H5	2:E:601:3XZ:H15	1.48	0.94
1:D:194:THR:CG2	3:D:311:HOH:O	2.17	0.92
1:D:80:ASP:CG	1:D:82:ASP:HB2	1.91	0.90
1:F:94:SER:HB2	1:F:213:PHE:HE1	1.37	0.90
1:F:117:SER:HA	1:F:186:ALA:HA	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:200:LYS:CE	3:F:316:HOH:O	1.75	0.88
1:C:80:ASP:O	1:C:82:ASP:O	1.90	0.88
1:A:4:ILE:HD13	1:A:215:SER:HB3	1.54	0.88
1:A:16:ASP:OD2	1:B:80:ASP:OD2	1.92	0.88
1:C:44:ASN:ND2	1:C:200:LYS:HA	1.88	0.87
1:C:216:ASN:H	1:C:216:ASN:HD22	1.23	0.87
1:B:82:ASP:O	1:B:83:ASN:HB2	1.75	0.86
2:E:601:3XZ:H5	2:E:601:3XZ:C5A	2.04	0.86
1:E:112:THR:HG1	1:E:127:HIS:HD1	1.21	0.86
1:B:191:PHE:CG	1:B:191:PHE:O	2.29	0.86
1:E:160:SER:HB3	1:E:166:GLN:NE2	1.91	0.85
1:E:184:SER:HA	3:E:724:HOH:O	1.74	0.85
1:F:80:ASP:CG	1:F:82:ASP:HB2	1.97	0.84
1:E:137:GLN:NE2	3:E:703:HOH:O	2.10	0.84
1:A:49:THR:HG22	1:A:196:THR:HG22	1.60	0.83
1:A:16:ASP:OD2	1:B:82:ASP:OD2	1.96	0.83
1:A:127:HIS:NE2	2:E:601:3XZ:C5	2.41	0.83
1:A:127:HIS:NE2	2:E:601:3XZ:C6	2.43	0.82
1:F:94:SER:HB2	1:F:213:PHE:CE1	2.15	0.81
1:B:191:PHE:O	1:B:191:PHE:CD1	2.35	0.80
1:B:80:ASP:CG	1:B:82:ASP:HB3	2.02	0.79
1:E:216:ASN:H	1:E:216:ASN:HD22	1.31	0.79
1:A:8:GLU:OE1	1:A:10:ASP:OD2	2.01	0.79
1:C:143:GLN:HE22	1:C:220:SER:HA	1.49	0.78
1:A:148:THR:HG22	1:A:154:LEU:HA	1.65	0.77
1:B:9:LEU:HD11	1:B:65:VAL:HG21	1.65	0.77
1:E:127:HIS:NE2	2:E:601:3XZ:N13	2.33	0.77
1:A:123:THR:N	3:A:320:HOH:O	2.18	0.76
1:C:187:VAL:HG22	3:D:314:HOH:O	1.52	0.76
1:F:135:LYS:HD2	3:F:305:HOH:O	1.85	0.76
1:E:2:ASP:HB2	1:E:216:ASN:HD21	1.51	0.75
1:E:44:ASN:HD21	1:E:201:SER:H	1.34	0.75
1:C:123:THR:H	1:E:131:ASN:HD22	1.35	0.75
1:D:10:ASP:OD2	1:D:19:ASP:OD1	2.05	0.75
1:E:25:ILE:HG21	1:E:65:VAL:HG21	1.67	0.75
1:B:44:ASN:HD21	1:B:201:SER:N	1.82	0.74
1:A:99:LEU:HD11	1:B:185:SER:HB2	1.70	0.74
1:F:80:ASP:OD2	1:F:82:ASP:HB2	1.88	0.74
1:C:44:ASN:HD21	1:C:200:LYS:HA	1.51	0.73
1:D:36:LYS:HG3	1:D:75:VAL:HG23	1.70	0.73
1:A:15:THR:CG2	1:A:19:ASP:O	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LYS:HG2	1:B:149:GLY:HA2	1.71	0.73
1:E:160:SER:HB3	1:E:166:GLN:HE21	1.51	0.72
1:C:19:ASP:CG	1:C:24:HIS:CE1	2.62	0.72
1:D:16:ASP:OD2	1:F:82:ASP:OD2	2.08	0.72
1:C:101:LYS:HD2	3:C:319:HOH:O	1.88	0.72
1:C:80:ASP:OD2	1:C:82:ASP:OD2	2.08	0.71
1:A:125:ALA:HB1	2:E:601:3XZ:O3P	1.90	0.71
1:B:80:ASP:C	1:B:82:ASP:O	2.27	0.71
1:A:216:ASN:HD22	1:A:216:ASN:H	1.38	0.71
1:B:54:TYR:O	1:B:190:SER:HB3	1.89	0.71
1:B:87:GLU:HG3	1:B:182:TRP:O	1.89	0.71
1:B:172:ARG:HD2	1:B:221:ILE:HG12	1.73	0.71
1:E:129:VAL:HG21	2:E:601:3XZ:N16	2.06	0.71
1:D:16:ASP:OD2	1:F:80:ASP:OD2	2.08	0.70
1:F:8:GLU:OE1	1:F:10:ASP:OD2	2.09	0.70
1:E:216:ASN:H	1:E:216:ASN:ND2	1.90	0.70
1:C:80:ASP:OD1	1:C:82:ASP:HB3	1.90	0.70
1:A:80:ASP:CG	1:A:82:ASP:HB3	2.12	0.70
1:D:8:GLU:OE1	1:D:10:ASP:OD2	2.10	0.70
1:D:10:ASP:HB3	1:D:24:HIS:CE1	2.27	0.70
1:B:143:GLN:HB2	1:B:172:ARG:HB2	1.73	0.69
1:F:81:LEU:HA	1:F:84:VAL:HG12	1.75	0.69
1:E:112:THR:OG1	1:E:127:HIS:ND1	2.19	0.68
1:A:17:ILE:HD13	1:A:228:ARG:HD2	1.76	0.68
1:D:190:SER:O	3:D:313:HOH:O	2.12	0.67
1:D:66:SER:CB	3:D:314:HOH:O	2.42	0.67
1:F:156:LEU:O	1:F:171:GLY:HA3	1.94	0.67
1:B:19:ASP:OD1	1:B:24:HIS:NE2	2.28	0.67
1:A:19:ASP:HB3	1:A:24:HIS:CE1	2.30	0.66
1:C:81:LEU:HA	1:C:84:VAL:HG12	1.77	0.66
1:B:162:ASN:HD21	1:B:164:SER:HB2	1.62	0.65
1:C:143:GLN:HB3	1:C:221:ILE:HD11	1.77	0.65
1:F:132:GLN:HA	1:F:132:GLN:OE1	1.94	0.65
1:D:127:HIS:CD2	2:E:601:3XZ:O2P	2.50	0.65
1:A:17:ILE:HG13	1:A:18:GLY:H	1.62	0.65
1:E:129:VAL:HG21	2:E:601:3XZ:H25	1.60	0.65
1:B:126:LEU:HD12	3:B:304:HOH:O	1.95	0.65
1:B:90:ARG:HD3	1:B:174:LEU:HD23	1.79	0.64
1:C:80:ASP:CG	1:C:82:ASP:HB3	2.17	0.64
1:B:9:LEU:HD11	1:B:65:VAL:CG2	2.27	0.64
1:E:2:ASP:CB	1:E:216:ASN:HD21	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ASP:OD2	1:B:4:ILE:HD11	1.98	0.63
1:D:69:ASN:ND2	1:D:71:ASP:H	1.96	0.63
1:E:135:LYS:HA	1:E:149:GLY:HA3	1.79	0.63
1:F:200:LYS:CD	3:F:316:HOH:O	2.26	0.63
1:A:17:ILE:O	1:A:33:ARG:NH1	2.32	0.63
1:B:32:VAL:HG21	3:B:318:HOH:O	1.98	0.63
1:F:160:SER:HB3	1:F:166:GLN:NE2	2.15	0.62
1:C:216:ASN:H	1:C:216:ASN:ND2	1.97	0.62
1:D:194:THR:HG22	3:D:311:HOH:O	1.93	0.62
1:F:10:ASP:OD2	1:F:19:ASP:OD1	2.16	0.62
1:D:28:ASP:HB3	1:D:31:SER:O	1.98	0.62
1:D:69:ASN:ND2	1:D:70:GLY:H	1.97	0.62
1:B:93:LEU:HD13	1:B:106:ILE:HG13	1.81	0.61
1:F:220:SER:O	1:F:222:PRO:HD3	2.00	0.61
1:A:158:ARG:HG2	1:A:166:GLN:HG3	1.82	0.61
1:D:194:THR:HB	3:D:311:HOH:O	1.99	0.61
1:E:44:ASN:HD21	1:E:201:SER:N	1.98	0.61
2:E:601:3XZ:H5	2:E:601:3XZ:C4A	2.31	0.61
1:A:201:SER:OG	1:A:202:SER:N	2.33	0.61
1:D:80:ASP:CG	1:D:82:ASP:CB	2.69	0.60
1:D:36:LYS:CG	1:D:75:VAL:HG23	2.30	0.60
1:C:19:ASP:HB3	1:C:24:HIS:CE1	2.36	0.60
1:D:117:SER:HA	1:D:186:ALA:HA	1.83	0.60
1:D:237:ASN:OD1	1:F:30:LYS:NZ	2.34	0.60
1:A:178:PRO:HB3	1:A:217:ILE:HG22	1.85	0.59
1:B:10:ASP:OD2	1:B:19:ASP:OD1	2.21	0.59
1:B:180:HIS:NE2	1:B:183:GLU:HG2	2.18	0.59
1:A:123:THR:N	3:A:319:HOH:O	2.35	0.59
1:D:156:LEU:O	1:D:171:GLY:HA3	2.03	0.58
1:B:54:TYR:HB2	1:B:61:LEU:HD12	1.85	0.58
1:C:56:SER:HB3	1:C:189:ALA:O	2.04	0.58
1:C:225:SER:OG	1:C:231:GLY:HA2	2.04	0.58
1:C:8:GLU:OE1	1:C:10:ASP:OD2	2.21	0.58
1:D:145:ASP:HA	1:D:158:ARG:HH21	1.68	0.58
1:D:16:ASP:OD2	1:F:82:ASP:CB	2.52	0.58
1:D:80:ASP:OD2	1:D:82:ASP:CB	2.51	0.58
1:B:7:VAL:HG21	1:B:52:ILE:HG12	1.86	0.58
1:C:176:TYR:HD1	1:E:177:ALA:HA	1.68	0.58
1:E:10:ASP:OD2	1:E:19:ASP:OD1	2.21	0.57
1:C:19:ASP:OD1	1:C:24:HIS:NE2	2.36	0.57
1:D:115:LEU:HD22	1:D:183:GLU:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ILE:CG1	1:A:18:GLY:H	2.16	0.57
1:C:216:ASN:HD22	1:C:216:ASN:N	1.98	0.57
1:E:56:SER:HB3	1:E:189:ALA:O	2.03	0.57
1:C:123:THR:N	1:E:131:ASN:HD22	2.00	0.57
1:F:216:ASN:HD22	1:F:216:ASN:H	1.53	0.56
1:C:43:GLN:HE22	1:C:69:ASN:ND2	2.03	0.56
1:A:216:ASN:HD22	1:A:216:ASN:N	2.01	0.56
1:B:8:GLU:OE1	1:B:10:ASP:OD2	2.24	0.56
1:D:80:ASP:OD1	1:D:82:ASP:HB2	2.05	0.56
1:E:82:ASP:HB3	1:E:83:ASN:OD1	2.05	0.56
1:A:114:LYS:HZ2	1:A:116:LYS:HE2	1.71	0.56
1:F:116:LYS:HA	1:F:123:THR:HG22	1.87	0.56
1:A:7:VAL:HG21	1:A:52:ILE:HG12	1.87	0.56
1:C:69:ASN:HD22	1:C:69:ASN:H	1.54	0.56
1:D:226:THR:HG21	3:D:302:HOH:O	2.05	0.56
1:A:25:ILE:HG21	1:A:65:VAL:HG21	1.88	0.56
1:E:15:THR:HG22	1:E:19:ASP:O	2.05	0.56
1:A:114:LYS:NZ	1:A:116:LYS:HE2	2.21	0.55
1:F:49:THR:HG23	1:F:196:THR:HG22	1.87	0.55
1:B:40:TRP:CH2	1:B:42:MET:HG2	2.42	0.55
1:B:69:ASN:ND2	1:B:71:ASP:H	2.04	0.55
1:E:14:ASN:O	1:E:19:ASP:HB2	2.07	0.55
1:D:2:ASP:CB	1:D:216:ASN:HD21	2.21	0.54
1:E:8:GLU:OE1	1:E:10:ASP:OD2	2.25	0.54
1:E:145:ASP:HA	1:E:158:ARG:HH21	1.72	0.54
2:E:601:3XZ:H5	2:E:601:3XZ:H16	1.89	0.54
1:A:36:LYS:NZ	3:A:314:HOH:O	2.40	0.54
1:C:116:LYS:HD3	1:D:51:HIS:CE1	2.42	0.54
1:F:81:LEU:C	1:F:83:ASN:H	2.12	0.53
1:A:14:ASN:HB2	1:A:17:ILE:HD11	1.90	0.53
1:A:80:ASP:C	1:A:82:ASP:N	2.58	0.53
1:D:3:THR:H	1:D:216:ASN:ND2	2.05	0.53
1:F:12:TYR:HD1	1:F:207:ALA:HB2	1.73	0.53
1:A:4:ILE:HD13	1:A:215:SER:CB	2.35	0.53
1:E:127:HIS:NE2	2:E:601:3XZ:C14	2.72	0.53
1:A:17:ILE:HG13	1:A:18:GLY:N	2.23	0.53
1:B:44:ASN:ND2	1:B:201:SER:H	1.88	0.52
1:C:19:ASP:CB	1:C:24:HIS:CE1	2.92	0.52
1:B:44:ASN:ND2	1:B:200:LYS:HA	2.25	0.52
1:D:127:HIS:HD2	2:E:601:3XZ:O2P	1.92	0.52
1:E:10:ASP:HB3	1:E:24:HIS:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:SER:HB3	1:F:189:ALA:O	2.08	0.52
1:E:126:LEU:HD23	1:E:179:VAL:HG22	1.89	0.52
1:A:19:ASP:HB3	1:A:24:HIS:HE1	1.74	0.52
1:F:40:TRP:CH2	1:F:42:MET:HG2	2.44	0.52
1:B:216:ASN:H	1:B:216:ASN:ND2	2.06	0.52
1:B:45:GLY:HA2	1:B:200:LYS:HB2	1.91	0.52
1:D:172:ARG:HD3	1:D:221:ILE:HG12	1.91	0.52
1:F:12:TYR:CD1	1:F:207:ALA:HB2	2.44	0.52
1:C:216:ASN:ND2	1:C:216:ASN:N	2.57	0.51
1:D:69:ASN:ND2	1:D:70:GLY:N	2.57	0.51
1:F:28:ASP:HB3	1:F:31:SER:O	2.10	0.51
1:B:145:ASP:HA	1:B:158:ARG:HH21	1.75	0.51
1:D:3:THR:O	1:D:215:SER:HB2	2.11	0.51
1:F:29:ILE:HG23	1:F:84:VAL:HG21	1.91	0.51
1:C:158:ARG:HG2	1:C:166:GLN:HG3	1.92	0.51
1:E:69:ASN:C	1:E:69:ASN:HD22	2.15	0.51
1:B:135:LYS:HG2	1:B:149:GLY:CA	2.40	0.51
1:E:156:LEU:O	1:E:171:GLY:HA3	2.10	0.51
1:F:201:SER:OG	1:F:202:SER:N	2.43	0.51
1:C:126:LEU:HD23	1:C:179:VAL:HG22	1.93	0.51
1:D:69:ASN:HD21	1:D:71:ASP:H	1.59	0.51
1:B:36:LYS:NZ	3:B:314:HOH:O	2.44	0.50
1:C:3:THR:O	1:C:215:SER:CB	2.58	0.50
1:D:10:ASP:HB3	1:D:24:HIS:NE2	2.26	0.50
1:D:66:SER:HB2	3:D:314:HOH:O	2.08	0.50
1:A:205:HIS:CE1	3:A:315:HOH:O	2.63	0.50
1:F:25:ILE:HG21	1:F:65:VAL:HG21	1.94	0.50
1:F:101:LYS:HE3	1:F:167:GLY:N	2.27	0.50
1:F:213:PHE:CD1	1:F:232:LEU:HD21	2.47	0.50
1:E:87:GLU:OE1	1:E:183:GLU:OE1	2.29	0.50
1:D:51:HIS:CD2	3:D:312:HOH:O	2.65	0.49
1:A:123:THR:O	1:D:131:ASN:HB2	2.12	0.49
1:C:69:ASN:HD22	1:C:69:ASN:N	2.09	0.49
1:C:201:SER:OG	1:C:202:SER:N	2.45	0.49
1:F:80:ASP:OD2	1:F:82:ASP:CB	2.59	0.49
1:C:27:ILE:HD13	1:C:77:TYR:HB2	1.94	0.49
1:E:19:ASP:CG	1:E:24:HIS:CE1	2.86	0.49
1:F:126:LEU:HD23	1:F:179:VAL:HG22	1.94	0.49
1:D:16:ASP:OD2	1:F:82:ASP:HB3	2.12	0.49
1:A:10:ASP:OD2	1:A:19:ASP:OD2	2.29	0.49
1:B:162:ASN:HB3	3:B:310:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ASP:HB3	1:C:216:ASN:HD21	1.78	0.49
1:E:81:LEU:HA	1:E:84:VAL:HG12	1.93	0.49
1:F:170:VAL:HB	1:F:226:THR:HG22	1.95	0.49
1:A:123:THR:HG22	1:A:124:ASN:N	2.28	0.49
1:D:80:ASP:C	1:D:82:ASP:N	2.66	0.49
1:A:60:ARG:HE	1:E:60:ARG:HE	1.59	0.48
1:B:162:ASN:HD21	1:B:164:SER:CB	2.26	0.48
1:A:97:THR:HG22	1:A:207:ALA:O	2.12	0.48
1:D:113:SER:O	1:D:125:ALA:HA	2.12	0.48
1:A:57:VAL:HG11	1:E:64:VAL:HG22	1.95	0.48
1:E:22:TYR:CD1	1:E:39:LYS:HD2	2.48	0.48
1:E:34:SER:HB2	1:E:37:THR:HG22	1.96	0.48
1:D:19:ASP:OD1	1:D:24:HIS:NE2	2.47	0.48
1:F:81:LEU:C	1:F:83:ASN:N	2.64	0.48
1:E:115:LEU:HD22	1:E:186:ALA:HB2	1.96	0.48
1:B:191:PHE:CD1	1:B:191:PHE:C	2.85	0.48
1:C:108:SER:HB2	3:C:322:HOH:O	2.12	0.48
1:F:69:ASN:C	1:F:69:ASN:ND2	2.67	0.48
1:F:87:GLU:HG2	1:F:182:TRP:O	2.14	0.48
1:C:19:ASP:CG	1:C:24:HIS:HE1	2.13	0.48
1:B:102:GLU:HA	1:B:201:SER:HB2	1.96	0.48
1:F:12:TYR:HB2	1:F:207:ALA:CB	2.44	0.48
1:A:178:PRO:HB3	1:A:217:ILE:CG2	2.43	0.48
1:B:45:GLY:HA2	1:B:198:LEU:HD11	1.96	0.48
1:C:162:ASN:O	1:C:164:SER:N	2.47	0.48
1:C:143:GLN:HB2	1:C:172:ARG:HB2	1.96	0.47
1:F:69:ASN:C	1:F:69:ASN:HD22	2.18	0.47
1:A:17:ILE:CG1	1:A:18:GLY:N	2.77	0.47
1:B:92:GLY:HA2	1:B:109:TRP:CH2	2.49	0.47
1:F:90:ARG:HD2	1:F:217:ILE:O	2.15	0.47
1:B:25:ILE:O	1:B:25:ILE:HG13	2.15	0.47
1:D:99:LEU:HD13	1:F:184:SER:HB2	1.95	0.47
1:E:95:ALA:HB2	1:E:210:ILE:HG12	1.96	0.47
1:A:116:LYS:HB3	1:E:51:HIS:CE1	2.50	0.47
1:B:10:ASP:OD2	1:B:19:ASP:CG	2.53	0.47
1:F:50:ALA:HA	1:F:64:VAL:O	2.15	0.47
1:A:127:HIS:CE1	2:E:601:3XZ:C6	2.98	0.47
1:F:126:LEU:HD12	1:F:127:HIS:N	2.30	0.47
1:C:172:ARG:HD2	1:C:221:ILE:HG23	1.97	0.46
1:F:45:GLY:HA2	1:F:200:LYS:HB2	1.97	0.46
1:E:19:ASP:OD1	1:E:24:HIS:NE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:320:HOH:O	1:E:124:ASN:ND2	2.47	0.46
1:D:10:ASP:CB	1:D:24:HIS:CE1	2.98	0.46
1:A:80:ASP:OD2	1:A:82:ASP:OD2	2.33	0.46
1:B:10:ASP:OD2	1:B:19:ASP:OD2	2.34	0.46
1:A:93:LEU:HD13	1:A:106:ILE:HG13	1.96	0.46
1:B:217:ILE:HG13	1:B:218:ASP:N	2.28	0.46
1:A:2:ASP:HB3	1:A:216:ASN:HD21	1.80	0.46
1:A:207:ALA:HB1	1:A:208:ASP:OD1	2.15	0.46
1:F:96:SER:OG	1:F:230:LEU:HA	2.15	0.46
1:A:156:LEU:O	1:A:171:GLY:HA3	2.15	0.46
1:B:50:ALA:O	1:B:194:THR:HA	2.15	0.46
1:C:127:HIS:HB3	1:E:127:HIS:HB3	1.98	0.46
1:A:100:TYR:HD1	1:A:203:ASP:HB3	1.81	0.46
1:B:32:VAL:HB	1:B:233:PHE:CD2	2.51	0.46
1:E:101:LYS:HD3	1:E:165:PRO:O	2.16	0.46
1:B:19:ASP:CG	1:B:24:HIS:CE1	2.90	0.46
1:C:81:LEU:C	1:C:82:ASP:O	2.53	0.46
1:C:137:GLN:N	3:C:318:HOH:O	2.49	0.46
1:E:143:GLN:HB2	1:E:172:ARG:HB2	1.97	0.46
1:B:14:ASN:O	1:B:17:ILE:HG13	2.16	0.45
1:C:108:SER:HA	1:C:130:PHE:O	2.16	0.45
1:E:129:VAL:HG11	2:E:601:3XZ:C16	2.46	0.45
1:E:216:ASN:ND2	1:E:216:ASN:N	2.62	0.45
1:A:80:ASP:CG	1:A:82:ASP:CB	2.84	0.45
1:C:207:ALA:HA	1:C:208:ASP:HA	1.79	0.45
1:F:80:ASP:C	1:F:82:ASP:N	2.68	0.45
1:A:12:TYR:HA	1:A:13:PRO:HD3	1.78	0.45
1:C:77:TYR:HD2	1:C:79:VAL:CG1	2.29	0.45
1:D:55:ASN:HD22	1:D:55:ASN:H	1.62	0.45
1:A:207:ALA:HA	1:A:208:ASP:HA	1.80	0.45
1:C:89:VAL:HG21	1:C:214:ILE:CG2	2.46	0.45
1:E:19:ASP:CG	1:E:24:HIS:HE1	2.19	0.45
1:C:80:ASP:C	1:C:82:ASP:O	2.54	0.45
1:F:19:ASP:HB3	1:F:24:HIS:HE1	1.81	0.45
1:C:129:VAL:CG1	1:E:125:ALA:HB3	2.47	0.45
1:A:44:ASN:HD21	1:A:201:SER:H	1.64	0.45
1:C:77:TYR:CD2	1:C:79:VAL:HG12	2.52	0.45
1:C:151:ASP:O	3:C:321:HOH:O	2.21	0.45
1:F:50:ALA:O	1:F:194:THR:HA	2.16	0.45
1:A:93:LEU:O	1:A:172:ARG:HA	2.17	0.44
1:D:14:ASN:ND2	1:D:228:ARG:HB3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:ILE:HD12	1:D:75:VAL:HG22	1.98	0.44
1:F:143:GLN:HB3	1:F:221:ILE:HD11	1.98	0.44
1:F:158:ARG:HG2	1:F:166:GLN:CG	2.45	0.44
1:A:216:ASN:N	1:A:216:ASN:ND2	2.64	0.44
1:C:3:THR:O	1:C:215:SER:HB3	2.18	0.44
1:F:29:ILE:HB	1:F:35:LYS:HE3	1.99	0.44
1:F:111:PHE:C	1:F:111:PHE:CD2	2.90	0.44
1:D:172:ARG:CD	1:D:221:ILE:HG12	2.48	0.44
1:E:7:VAL:HG21	1:E:52:ILE:HG12	1.99	0.44
1:E:81:LEU:HA	1:E:84:VAL:CG1	2.48	0.44
1:B:45:GLY:CA	1:B:200:LYS:HB2	2.48	0.44
1:A:69:ASN:ND2	1:A:71:ASP:H	2.16	0.44
1:C:40:TRP:CH2	1:C:42:MET:HG2	2.53	0.44
1:D:56:SER:HB3	1:D:189:ALA:O	2.18	0.44
1:F:19:ASP:OD1	1:F:24:HIS:NE2	2.49	0.44
1:F:216:ASN:H	1:F:216:ASN:ND2	2.14	0.44
1:B:80:ASP:OD1	1:B:82:ASP:CB	2.66	0.44
1:A:181:ILE:HD12	1:A:181:ILE:HA	1.87	0.44
1:B:81:LEU:HA	1:B:84:VAL:HG12	2.00	0.44
1:B:94:SER:HB3	1:B:232:LEU:HD21	1.99	0.44
1:E:14:ASN:OD1	1:E:19:ASP:OD2	2.36	0.44
1:B:80:ASP:OD2	1:B:82:ASP:OD2	2.35	0.44
1:C:11:THR:HG22	1:C:40:TRP:HZ3	1.82	0.43
1:C:47:VAL:HG22	1:C:198:LEU:HD22	1.99	0.43
1:C:160:SER:HB3	1:C:166:GLN:HE21	1.84	0.43
1:D:141:ILE:HB	1:D:174:LEU:HB2	2.00	0.43
1:E:9:LEU:HA	1:E:25:ILE:HG22	2.00	0.43
1:A:4:ILE:CD1	1:A:215:SER:HB3	2.38	0.43
1:C:57:VAL:HG11	1:D:64:VAL:HG22	2.01	0.43
1:D:10:ASP:CB	1:D:24:HIS:NE2	2.82	0.43
1:A:17:ILE:H	1:A:17:ILE:HG12	1.69	0.43
1:A:60:ARG:HH21	1:E:60:ARG:HH21	1.66	0.43
1:E:25:ILE:HD13	1:E:65:VAL:HG23	2.00	0.43
1:F:200:LYS:CG	3:F:316:HOH:O	2.61	0.43
1:C:81:LEU:HA	1:C:84:VAL:CG1	2.46	0.43
1:D:69:ASN:HD22	1:D:70:GLY:H	1.66	0.43
1:E:87:GLU:OE1	1:E:183:GLU:HG2	2.19	0.43
1:D:12:TYR:HA	1:D:13:PRO:HD3	1.77	0.43
1:D:33:ARG:HD3	3:D:316:HOH:O	2.18	0.43
1:F:19:ASP:HB3	1:F:24:HIS:CE1	2.53	0.43
1:B:12:TYR:HA	1:B:13:PRO:HD3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:THR:H	1:C:216:ASN:ND2	2.17	0.43
1:F:25:ILE:HD13	1:F:65:VAL:HG23	2.01	0.43
1:A:60:ARG:HD3	1:A:76:SER:OG	2.19	0.43
1:B:10:ASP:OD2	1:B:24:HIS:NE2	2.51	0.43
1:C:10:ASP:OD2	1:C:24:HIS:NE2	2.52	0.43
1:C:105:THR:O	1:C:197:PHE:HA	2.19	0.43
1:C:201:SER:CB	1:C:206:PRO:HB3	2.49	0.43
1:D:80:ASP:OD2	1:D:82:ASP:OD2	2.36	0.43
1:C:11:THR:HG22	1:C:40:TRP:CZ3	2.53	0.43
1:D:100:TYR:N	1:D:100:TYR:CD2	2.87	0.43
1:D:126:LEU:HD23	1:D:179:VAL:HG22	2.01	0.43
1:E:181:ILE:HG23	1:E:182:TRP:CD1	2.54	0.42
1:D:93:LEU:HD13	1:D:106:ILE:HG13	2.01	0.42
1:D:99:LEU:HD11	1:F:185:SER:HB2	2.01	0.42
1:B:111:PHE:HB3	1:B:128:PHE:CZ	2.53	0.42
1:C:47:VAL:HA	1:C:197:PHE:O	2.19	0.42
1:B:116:LYS:HB2	1:B:188:VAL:HB	2.02	0.42
1:E:81:LEU:C	1:E:83:ASN:H	2.23	0.42
1:F:100:TYR:HB2	1:F:207:ALA:HB3	2.02	0.42
1:A:164:SER:HA	1:A:165:PRO:HD2	1.72	0.42
1:F:14:ASN:OD1	1:F:19:ASP:OD2	2.37	0.42
1:C:81:LEU:HB3	1:C:85:LEU:HD12	2.01	0.42
1:D:137:GLN:HG2	1:D:140:LEU:HD12	2.02	0.42
1:D:194:THR:HG21	3:D:311:HOH:O	1.99	0.42
1:E:90:ARG:NH1	1:E:217:ILE:O	2.50	0.42
1:B:80:ASP:OD1	1:B:82:ASP:HB3	2.19	0.42
1:B:115:LEU:O	1:B:116:LYS:C	2.57	0.42
1:D:115:LEU:HB3	1:D:186:ALA:HB2	2.02	0.42
1:F:5:VAL:HG13	1:F:29:ILE:CD1	2.50	0.42
1:C:95:ALA:HB1	1:C:104:ASN:OD1	2.20	0.42
1:C:130:PHE:HE1	3:C:312:HOH:O	2.00	0.42
1:C:207:ALA:HB1	1:C:208:ASP:CG	2.40	0.42
1:D:145:ASP:HB3	1:D:158:ARG:NE	2.35	0.42
1:D:33:ARG:HH22	1:F:83:ASN:ND2	2.18	0.41
1:D:207:ALA:HA	1:D:208:ASP:HA	1.84	0.41
1:F:32:VAL:HG23	1:F:233:PHE:CD2	2.55	0.41
1:C:51:HIS:ND1	1:C:194:THR:OG1	2.53	0.41
1:D:216:ASN:HD22	1:D:216:ASN:H	1.67	0.41
1:F:158:ARG:HG2	1:F:166:GLN:HG2	2.02	0.41
1:A:64:VAL:HG22	1:E:57:VAL:HG11	2.02	0.41
1:B:50:ALA:HA	1:B:64:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LEU:HD23	1:B:179:VAL:HG22	2.02	0.41
1:D:10:ASP:CG	1:D:24:HIS:CE1	2.93	0.41
1:D:14:ASN:O	1:D:17:ILE:HG13	2.20	0.41
1:E:1:ALA:N	1:E:234:PRO:HG3	2.36	0.41
1:A:25:ILE:HD12	1:A:75:VAL:HG12	2.03	0.41
1:A:112:THR:HG21	2:E:601:3XZ:H4	2.02	0.41
1:B:61:LEU:HD13	1:B:81:LEU:HD11	2.03	0.41
2:E:601:3XZ:H16	2:E:601:3XZ:C4'	2.50	0.41
1:B:10:ASP:HB3	1:B:24:HIS:CE1	2.56	0.41
1:C:156:LEU:O	1:C:171:GLY:HA3	2.21	0.41
1:D:132:GLN:HA	1:D:132:GLN:OE1	2.21	0.41
1:D:216:ASN:ND2	1:D:216:ASN:H	2.19	0.41
1:B:80:ASP:CG	1:B:82:ASP:CB	2.82	0.41
1:C:51:HIS:HB2	1:C:64:VAL:HG23	2.03	0.41
1:C:145:ASP:HA	1:C:158:ARG:HH21	1.86	0.41
1:E:127:HIS:CE1	2:E:601:3XZ:N13	2.88	0.41
1:A:113:SER:O	1:A:125:ALA:HA	2.21	0.41
1:B:180:HIS:CE1	1:B:183:GLU:HG2	2.56	0.41
1:C:68:PRO:C	1:C:70:GLY:H	2.25	0.41
1:E:80:ASP:OD2	1:E:82:ASP:OD2	2.39	0.41
1:A:32:VAL:HG21	1:A:229:LEU:HD23	2.02	0.40
1:C:77:TYR:CD2	1:C:79:VAL:CG1	3.04	0.40
1:D:16:ASP:OD2	1:F:82:ASP:CG	2.60	0.40
1:A:112:THR:OG1	1:A:127:HIS:ND1	2.54	0.40
1:B:55:ASN:ND2	1:B:55:ASN:O	2.55	0.40
1:B:56:SER:HB3	1:B:189:ALA:O	2.21	0.40
1:C:44:ASN:HD22	1:C:200:LYS:HA	1.77	0.40
1:D:114:LYS:HA	1:D:124:ASN:O	2.21	0.40
1:F:160:SER:HB3	1:F:166:GLN:HE22	1.86	0.40
1:A:81:LEU:HA	1:A:84:VAL:HG12	2.02	0.40
1:D:3:THR:O	1:D:215:SER:CB	2.69	0.40
1:F:80:ASP:O	1:F:83:ASN:HB2	2.22	0.40
1:B:81:LEU:HA	1:B:84:VAL:CG1	2.51	0.40
1:C:176:TYR:CD1	1:E:178:PRO:HD3	2.56	0.40
1:E:12:TYR:HA	1:E:13:PRO:HD3	1.88	0.40
1:C:145:ASP:CG	1:C:158:ARG:HE	2.25	0.40
1:E:29:ILE:O	1:E:31:SER:N	2.55	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:ASP:OD2	1:F:16:ASP:OD2[8_455]	1.03	1.17
1:B:16:ASP:OD2	1:C:82:ASP:OD2[7_545]	1.60	0.60
1:D:80:ASP:OD2	1:E:16:ASP:OD2[8_555]	1.70	0.50
1:A:80:ASP:OD2	1:C:16:ASP:OD2[7_545]	1.80	0.40
1:D:82:ASP:OD2	1:E:16:ASP:OD2[8_555]	1.84	0.36
1:A:82:ASP:OD2	1:C:16:ASP:OD2[7_545]	1.91	0.29
1:E:82:ASP:OD2	1:F:16:ASP:CG[8_455]	2.16	0.04
1:E:82:ASP:CG	1:F:16:ASP:OD2[8_455]	2.16	0.04

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	228/237 (96%)	197 (86%)	27 (12%)	4 (2%)	8	35
1	B	228/237 (96%)	193 (85%)	31 (14%)	4 (2%)	8	35
1	C	229/237 (97%)	200 (87%)	26 (11%)	3 (1%)	12	41
1	D	228/237 (96%)	199 (87%)	28 (12%)	1 (0%)	34	67
1	E	228/237 (96%)	197 (86%)	30 (13%)	1 (0%)	34	67
1	F	228/237 (96%)	208 (91%)	18 (8%)	2 (1%)	17	50
All	All	1369/1422 (96%)	1194 (87%)	160 (12%)	15 (1%)	14	46

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	82	ASP
1	F	82	ASP
1	F	225	SER
1	A	228	ARG
1	B	30	LYS
1	B	204	SER
1	C	69	ASN

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Mol	Chain	Res	Type
1	D	82	ASP
1	E	81	LEU
1	A	18	GLY
1	B	150	THR
1	C	163	GLY
1	B	228	ARG
1	C	141	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/202 (98%)	172 (87%)	25 (13%)	4	18
1	B	197/202 (98%)	169 (86%)	28 (14%)	3	15
1	C	198/202 (98%)	175 (88%)	23 (12%)	5	22
1	D	197/202 (98%)	174 (88%)	23 (12%)	5	21
1	E	197/202 (98%)	172 (87%)	25 (13%)	4	18
1	F	197/202 (98%)	166 (84%)	31 (16%)	2	11
All	All	1183/1212 (98%)	1028 (87%)	155 (13%)	4	17

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	10	ASP
1	A	36	LYS
1	A	55	ASN
1	A	64	VAL
1	A	69	ASN
1	A	72	SER
1	A	76	SER
1	A	79	VAL
1	A	99	LEU
1	A	105	THR

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Mol	Chain	Res	Type
1	A	107	LEU
1	A	114	LYS
1	A	117	SER
1	A	129	VAL
1	A	135	LYS
1	A	150	THR
1	A	158	ARG
1	A	172	ARG
1	A	174	LEU
1	A	185	SER
1	A	198	LEU
1	A	208	ASP
1	A	216	ASN
1	A	221	ILE
1	B	2	ASP
1	B	14	ASN
1	B	16	ASP
1	B	17	ILE
1	B	36	LYS
1	B	55	ASN
1	B	64	VAL
1	B	69	ASN
1	B	71	ASP
1	B	76	SER
1	B	91	VAL
1	B	103	THR
1	B	107	LEU
1	B	123	THR
1	B	133	PHE
1	B	135	LYS
1	B	147	THR
1	B	150	THR
1	B	184	SER
1	B	190	SER
1	B	192	ASP
1	B	198	LEU
1	B	200	LYS
1	B	203	ASP
1	B	205	HIS
1	B	215	SER
1	B	216	ASN
1	B	217	ILE

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Mol	Chain	Res	Type
1	C	14	ASN
1	C	16	ASP
1	C	22	TYR
1	C	32	VAL
1	C	36	LYS
1	C	42	MET
1	C	55	ASN
1	C	64	VAL
1	C	69	ASN
1	C	79	VAL
1	C	83	ASN
1	C	117	SER
1	C	122	GLU
1	C	129	VAL
1	C	150	THR
1	C	151	ASP
1	C	172	ARG
1	C	194	THR
1	C	198	LEU
1	C	203	ASP
1	C	216	ASN
1	C	221	ILE
1	C	235	ASP
1	D	2	ASP
1	D	3	THR
1	D	14	ASN
1	D	16	ASP
1	D	28	ASP
1	D	55	ASN
1	D	64	VAL
1	D	69	ASN
1	D	71	ASP
1	D	76	SER
1	D	78	ASP
1	D	82	ASP
1	D	135	LYS
1	D	137	GLN
1	D	150	THR
1	D	180	HIS
1	D	183	GLU
1	D	184	SER
1	D	201	SER

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Mol	Chain	Res	Type
1	D	204	SER
1	D	208	ASP
1	D	217	ILE
1	D	235	ASP
1	E	2	ASP
1	E	3	THR
1	E	14	ASN
1	E	39	LYS
1	E	55	ASN
1	E	56	SER
1	E	64	VAL
1	E	69	ASN
1	E	72	SER
1	E	79	VAL
1	E	84	VAL
1	E	101	LYS
1	E	113	SER
1	E	117	SER
1	E	135	LYS
1	E	136	ASP
1	E	150	THR
1	E	180	HIS
1	E	183	GLU
1	E	194	THR
1	E	198	LEU
1	E	205	HIS
1	E	208	ASP
1	E	216	ASN
1	E	221	ILE
1	F	2	ASP
1	F	3	THR
1	F	14	ASN
1	F	32	VAL
1	F	36	LYS
1	F	47	VAL
1	F	55	ASN
1	F	56	SER
1	F	64	VAL
1	F	69	ASN
1	F	72	SER
1	F	76	SER
1	F	79	VAL

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Mol	Chain	Res	Type
1	F	99	LEU
1	F	101	LYS
1	F	117	SER
1	F	129	VAL
1	F	147	THR
1	F	161	SER
1	F	168	SER
1	F	172	ARG
1	F	174	LEU
1	F	180	HIS
1	F	183	GLU
1	F	198	LEU
1	F	200	LYS
1	F	208	ASP
1	F	216	ASN
1	F	217	ILE
1	F	221	ILE
1	F	223	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	44	ASN
1	A	69	ASN
1	A	131	ASN
1	A	180	HIS
1	A	205	HIS
1	A	216	ASN
1	B	14	ASN
1	B	43	GLN
1	B	44	ASN
1	B	69	ASN
1	B	83	ASN
1	B	216	ASN
1	B	237	ASN
1	C	14	ASN
1	C	44	ASN
1	C	69	ASN
1	C	216	ASN
1	C	237	ASN
1	D	14	ASN

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Mol	Chain	Res	Type
1	D	55	ASN
1	D	69	ASN
1	D	153	ASN
1	D	216	ASN
1	E	14	ASN
1	E	43	GLN
1	E	44	ASN
1	E	69	ASN
1	E	131	ASN
1	E	166	GLN
1	E	216	ASN
1	E	237	ASN
1	F	14	ASN
1	F	43	GLN
1	F	69	ASN
1	F	83	ASN
1	F	166	GLN
1	F	216	ASN
1	F	237	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 ⓘ

1 ligand is 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	3XZ	E	601	-	40,44,44	2.28	7 (17%)	41,66,66	2.03	11 (26%)

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	3XZ	E	601	-	-	8/12/53/53	0/6/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	3XZ	C1A-N19	-11.83	1.14	1.49
2	E	601	3XZ	P-O5'	-3.86	1.43	1.59
2	E	601	3XZ	O1P-C5A	2.67	1.55	1.44
2	E	601	3XZ	C1'-N9	-2.61	1.41	1.49
2	E	601	3XZ	C15-C14	2.43	1.47	1.40
2	E	601	3XZ	C5-C4	2.43	1.47	1.40
2	E	601	3XZ	C2-N3	2.37	1.35	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	3XZ	O5'-P-O3P	-5.04	89.37	109.07
2	E	601	3XZ	C2A-C1A-N19	4.85	125.46	114.27
2	E	601	3XZ	P-O5'-C5'	4.22	146.44	121.68
2	E	601	3XZ	N3-C2-N1	-3.45	123.28	128.68
2	E	601	3XZ	N13-C12-N11	-3.17	123.73	128.68
2	E	601	3XZ	O1P-C5A-C4A	3.15	119.84	108.99
2	E	601	3XZ	C2'-C1'-N9	2.90	120.97	114.27
2	E	601	3XZ	O1P-P-O3P	2.64	119.40	109.07
2	E	601	3XZ	C14-C15-N17	-2.64	106.65	109.40
2	E	601	3XZ	O2P-P-O1P	2.52	119.43	107.75
2	E	601	3XZ	O2P-P-O5'	2.33	118.56	107.75

There are no chirality outliers.

All (8) torsion outliers are listed below:

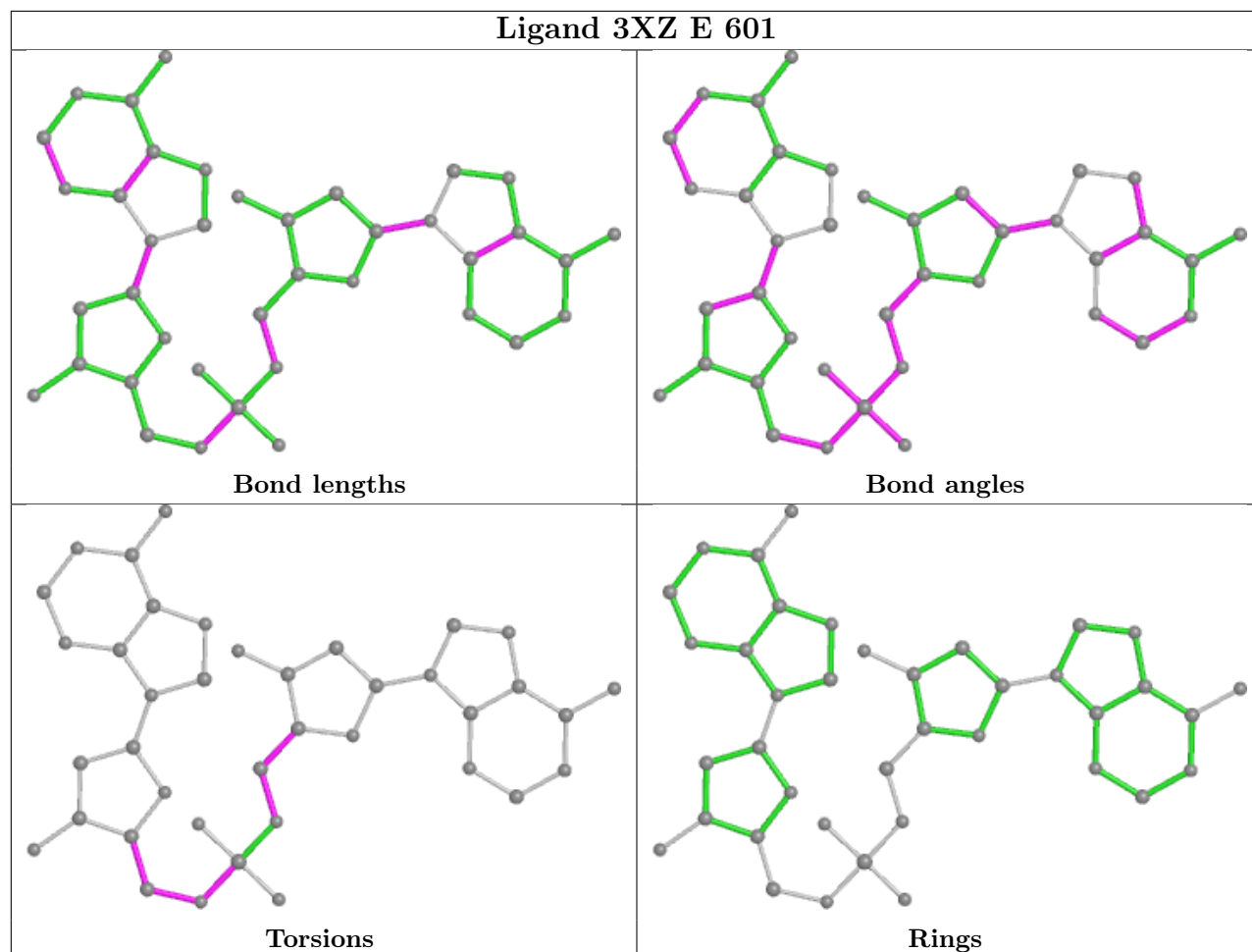
Mol	Chain	Res	Type	Atoms
2	E	601	3XZ	C5'-O5'-P-O3P
2	E	601	3XZ	C5'-O5'-P-O1P
2	E	601	3XZ	C5'-O5'-P-O2P
2	E	601	3XZ	C4A-C5A-O1P-P
2	E	601	3XZ	C4'-C5'-O5'-P
2	E	601	3XZ	C3'-C4'-C5'-O5'
2	E	601	3XZ	O4'-C4'-C5'-O5'
2	E	601	3XZ	O4A-C4A-C5A-O1P

There are no ring outliers.

1 monomer is involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	601	3XZ	18	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	232/237 (97%)	0.54	7 (3%)	50	48	9, 17, 32, 50	0
1	B	232/237 (97%)	0.53	7 (3%)	50	48	10, 17, 34, 61	0
1	C	233/237 (98%)	0.58	6 (2%)	56	52	11, 18, 38, 54	0
1	D	232/237 (97%)	0.59	6 (2%)	56	52	11, 18, 35, 45	0
1	E	232/237 (97%)	0.56	4 (1%)	70	67	11, 17, 33, 57	0
1	F	232/237 (97%)	0.55	5 (2%)	62	59	10, 16, 35, 56	0
All	All	1393/1422 (97%)	0.56	35 (2%)	57	53	9, 17, 35, 61	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	204	SER	4.4
1	B	204	SER	3.7
1	F	204	SER	3.2
1	C	185	SER	3.0
1	B	161	SER	2.8
1	C	161	SER	2.8
1	B	150	THR	2.7
1	F	105	THR	2.7
1	A	187	VAL	2.6
1	A	185	SER	2.5
1	B	188	VAL	2.5
1	C	1	ALA	2.4
1	D	149	GLY	2.4
1	C	181	ILE	2.4
1	C	51	HIS	2.4
1	B	2	ASP	2.4
1	B	115	LEU	2.4
1	E	161	SER	2.3
1	A	117	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	150	THR	2.3
1	C	162	ASN	2.2
1	B	162	ASN	2.2
1	F	186	ALA	2.2
1	D	105	THR	2.2
1	A	116	LYS	2.2
1	D	187	VAL	2.2
1	F	185	SER	2.1
1	A	204	SER	2.1
1	F	150	THR	2.1
1	E	189	ALA	2.1
1	A	31	SER	2.0
1	A	161	SER	2.0
1	E	31	SER	2.0
1	D	41	ASN	2.0
1	D	185	SER	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](#)

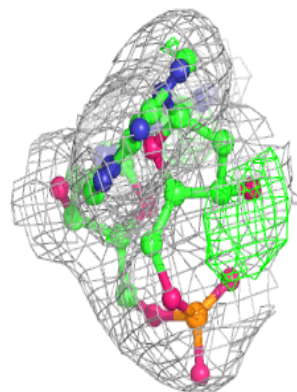
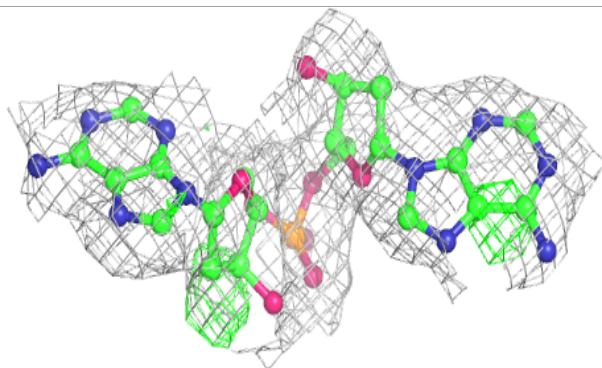
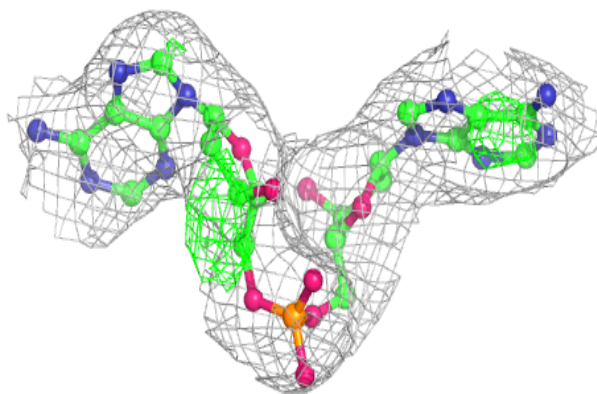
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	3XZ	E	601	39/39	0.93	0.18	19,25,29,32	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 3XZ E 601:

$2mF_o - DF_c$ (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.