



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 11:27 am BST

PDB ID : 2GLX
Title : Crystal Structure Analysis of bacterial 1,5-AF Reductase
Authors : Dambe, T.R.; Scheidig, A.J.
Deposited on : 2006-04-05
Resolution : 2.20 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 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 : 2.11
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) : 2.11

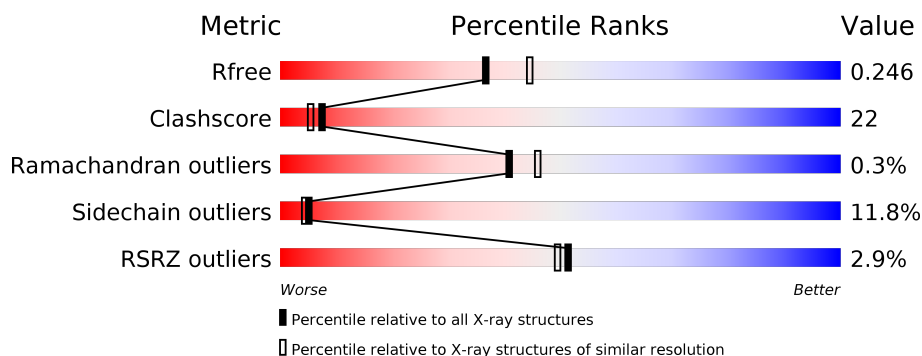
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	332	<div> <div>8%</div> <div>79%</div> <div>18%</div> <div>•</div> </div>
1	B	332	<div> <div>70%</div> <div>26%</div> <div>5%</div> </div>
1	C	332	<div> <div>72%</div> <div>25%</div> <div>•</div> </div>
1	D	332	<div> <div>8%</div> <div>57%</div> <div>37%</div> <div>6%</div> <div>•</div> </div>
1	E	332	<div> <div>67%</div> <div>27%</div> <div>6%</div> </div>
1	F	332	<div> <div>6%</div> <div>57%</div> <div>35%</div> <div>7%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	1502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16352 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 1,5-anhydro-D-fructose reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2456	1525	446	476	9			
1	B	332	Total	C	N	O	S	0	0	0
			2456	1525	446	476	9			
1	C	332	Total	C	N	O	S	0	0	0
			2456	1525	446	476	9			
1	D	332	Total	C	N	O	S	0	0	0
			2456	1525	446	476	9			
1	E	332	Total	C	N	O	S	0	0	0
			2456	1525	446	476	9			
1	F	332	Total	C	N	O	S	0	0	0
			2456	1525	446	476	9			

There are 12 discrepancies between the modelled and reference sequences:

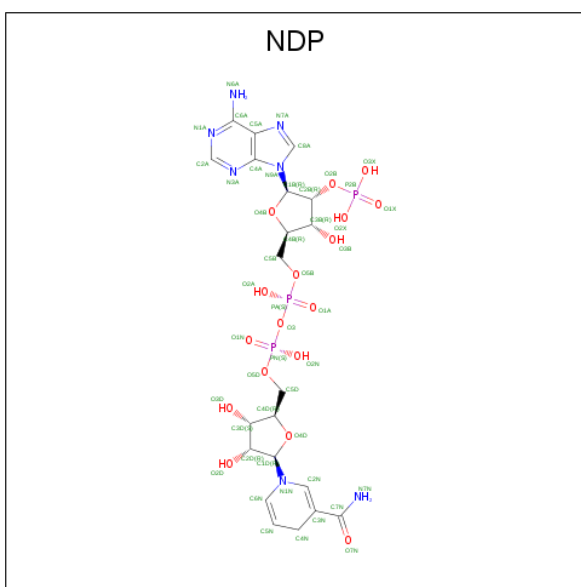
Chain	Residue	Modelled	Actual	Comment	Reference
A	217	VAL	GLY	CONFLICT	UNP Q2I8V6
A	218	LEU	VAL	CONFLICT	UNP Q2I8V6
B	217	VAL	GLY	CONFLICT	UNP Q2I8V6
B	218	LEU	VAL	CONFLICT	UNP Q2I8V6
C	217	VAL	GLY	CONFLICT	UNP Q2I8V6
C	218	LEU	VAL	CONFLICT	UNP Q2I8V6
D	217	VAL	GLY	CONFLICT	UNP Q2I8V6
D	218	LEU	VAL	CONFLICT	UNP Q2I8V6
E	217	VAL	GLY	CONFLICT	UNP Q2I8V6
E	218	LEU	VAL	CONFLICT	UNP Q2I8V6
F	217	VAL	GLY	CONFLICT	UNP Q2I8V6
F	218	LEU	VAL	CONFLICT	UNP Q2I8V6

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	D	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	E	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	F	1	Total 48	C 21	N 7	O 17	P 3	0	0

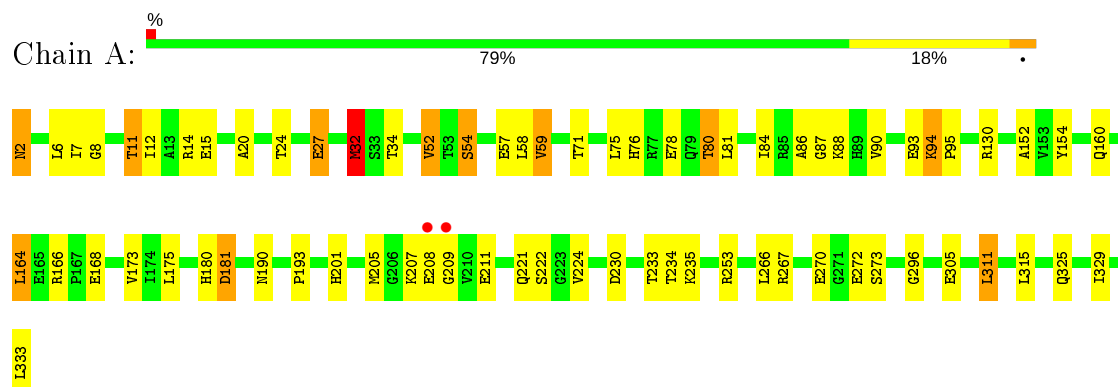
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	349	Total O 349 349	0	0
4	B	271	Total O 271 271	0	0
4	C	211	Total O 211 211	0	0
4	D	102	Total O 102 102	0	0
4	E	242	Total O 242 242	0	0
4	F	129	Total O 129 129	0	0

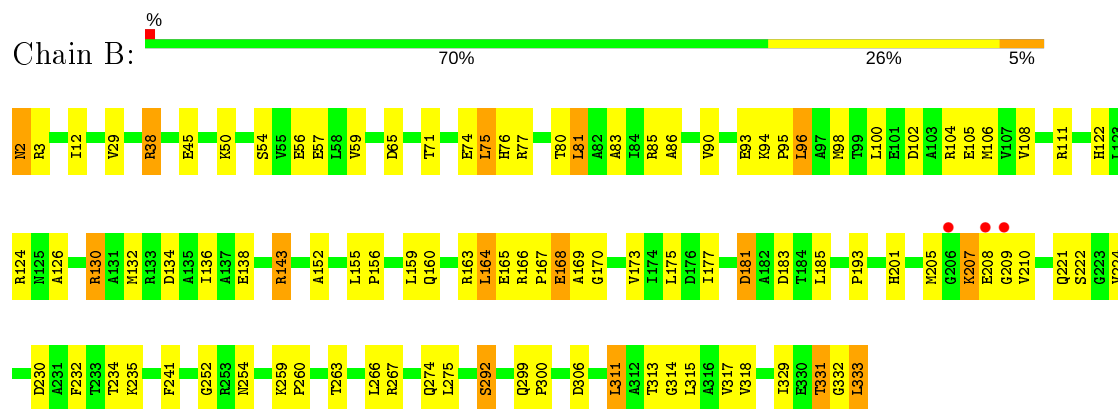
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

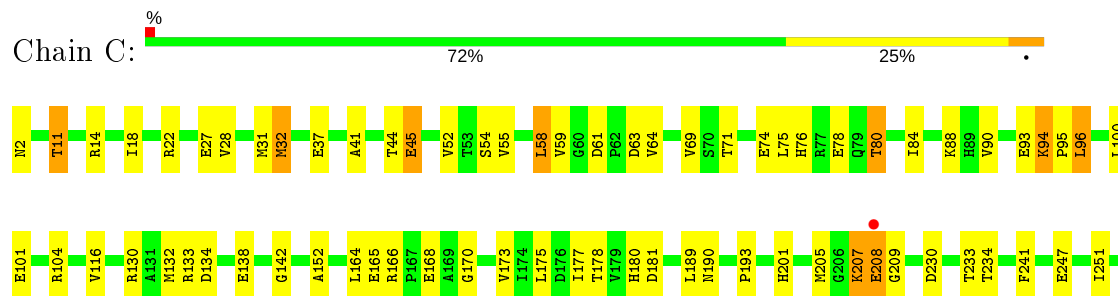
- Molecule 1: 1,5-anhydro-D-fructose reductase



- Molecule 1: 1,5-anhydro-D-fructose reductase

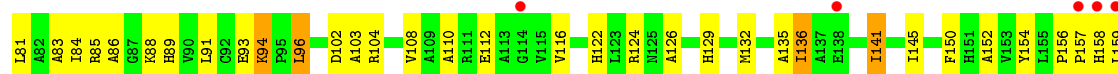


- Molecule 1: 1,5-anhydro-D-fructose reductase

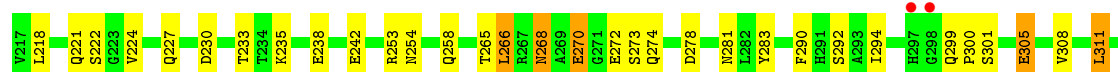
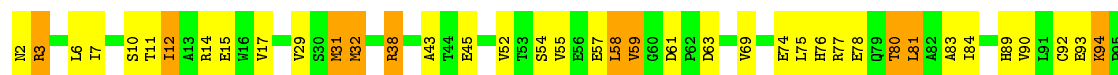




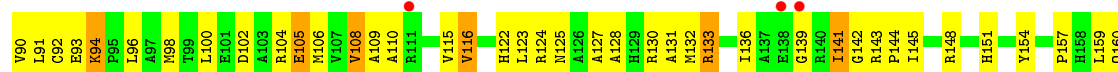
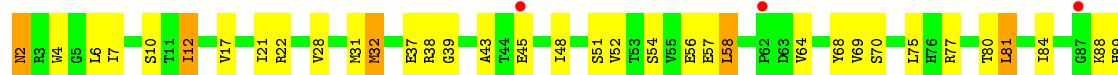
- Molecule 1: 1,5-anhydro-D-fructose reductase

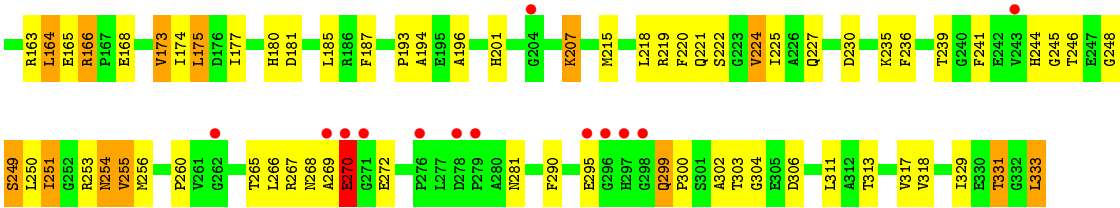


- Molecule 1: 1,5-anhydro-D-fructose reductase



- Molecule 1: 1,5-anhydro-D-fructose reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.19 Å 84.90 Å 150.94 Å 90.00° 96.30° 90.00°	Depositor
Resolution (Å)	19.00 – 2.20 19.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.00-2.20) 99.3 (19.96-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.19 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.190 , 0.251 0.191 , 0.246	Depositor DCC
R_{free} test set	6156 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16352	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: NDP, ACT

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	0.84	0/2499	0.88	3/3395 (0.1%)
1	B	0.73	0/2499	0.82	2/3395 (0.1%)
1	C	0.63	0/2499	0.74	1/3395 (0.0%)
1	D	0.52	0/2499	0.64	2/3395 (0.1%)
1	E	0.70	0/2499	0.80	3/3395 (0.1%)
1	F	0.53	0/2499	0.63	0/3395
All	All	0.67	0/14994	0.76	11/20370 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	143	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	32	MET	CA-CB-CG	6.34	124.08	113.30
1	E	140	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	E	140	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	181	ASP	CB-CG-OD1	5.41	123.17	118.30
1	D	38	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	C	58	LEU	CA-CB-CG	-5.14	103.47	115.30
1	D	58	LEU	CA-CB-CG	-5.11	103.55	115.30
1	A	181	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	32	MET	CB-CG-SD	5.04	127.53	112.40
1	E	58	LEU	CA-CB-CG	-5.03	103.73	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2456	0	2414	62	0
1	B	2456	0	2414	115	0
1	C	2456	0	2414	77	0
1	D	2456	0	2414	156	0
1	E	2456	0	2414	101	0
1	F	2456	0	2414	166	0
2	A	4	0	3	4	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
2	E	4	0	3	1	0
2	F	4	0	3	1	0
3	A	48	0	26	7	0
3	B	48	0	24	3	0
3	C	48	0	24	3	0
3	D	48	0	24	5	0
3	E	48	0	26	6	0
3	F	48	0	26	3	0
4	A	349	0	0	17	0
4	B	271	0	0	22	0
4	C	211	0	0	14	0
4	D	102	0	0	21	0
4	E	242	0	0	26	0
4	F	129	0	0	22	0
All	All	16352	0	14652	659	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 22.

All (659) 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:D:141:ILE:HG22	4:D:4506:HOH:O	1.28	1.31
1:D:222:SER:OG	1:D:224:VAL:HG13	1.38	1.23
1:D:255:VAL:HB	4:D:4546:HOH:O	1.42	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:LYS:HE3	4:B:2659:HOH:O	1.44	1.15
1:B:130:ARG:HD2	4:B:2702:HOH:O	1.46	1.15
1:A:94:LYS:HD3	1:A:180:HIS:CE1	1.83	1.12
1:B:38:ARG:CG	1:B:38:ARG:HH11	1.63	1.12
1:B:38:ARG:HD3	4:B:2764:HOH:O	1.48	1.11
1:A:270:GLU:HB2	4:A:1559:HOH:O	1.51	1.10
1:D:281:ASN:HB3	1:D:284:GLU:HG3	1.23	1.10
1:B:38:ARG:HH11	1:B:38:ARG:HG3	1.06	1.08
1:F:93:GLU:OE1	3:F:6500:NDP:H2N	1.52	1.07
1:E:76:HIS:O	1:E:80:THR:HG23	1.50	1.07
1:B:143:ARG:HB2	4:B:2682:HOH:O	1.56	1.06
1:C:278:ASP:HB2	4:C:3594:HOH:O	1.52	1.06
1:B:254:ASN:HB2	4:B:2533:HOH:O	1.58	1.04
1:D:281:ASN:CB	1:D:284:GLU:HG3	1.90	1.01
1:B:54:SER:HB3	1:B:57:GLU:HB2	1.43	1.01
1:D:225:ILE:HB	1:F:215:MET:CE	1.93	0.99
1:D:305:GLU:HA	1:D:308:VAL:HG12	1.40	0.99
1:A:94:LYS:HD3	1:A:180:HIS:NE2	1.77	0.98
1:D:17:VAL:O	1:D:21:ILE:HG13	1.64	0.98
1:D:225:ILE:HD12	1:F:215:MET:HE2	1.46	0.97
1:C:76:HIS:O	1:C:80:THR:HG23	1.65	0.97
1:B:85:ARG:HH11	1:B:85:ARG:HG3	1.30	0.95
1:D:257:THR:HG22	4:D:4575:HOH:O	1.66	0.95
1:F:165:GLU:HG2	1:F:166:ARG:N	1.79	0.95
1:E:31:MET:HE1	1:E:43:ALA:HA	1.50	0.94
1:B:331:THR:CG2	1:B:333:LEU:H	1.79	0.94
1:E:12:ILE:HG12	3:E:5500:NDP:H41N	1.46	0.94
1:C:265:THR:HG21	1:C:272:GLU:OE2	1.68	0.93
1:D:281:ASN:HB3	1:D:284:GLU:CG	1.99	0.93
1:A:205:MET:HE3	1:A:233:THR:HG22	1.50	0.93
1:F:139:GLY:HA2	4:F:6584:HOH:O	1.70	0.92
1:B:331:THR:HG23	1:B:333:LEU:H	1.34	0.92
1:E:31:MET:HE1	1:E:43:ALA:CA	2.01	0.91
1:E:305:GLU:HG2	4:E:5517:HOH:O	1.71	0.91
1:D:136:ILE:CD1	1:D:250:LEU:CD1	2.50	0.90
1:F:6:LEU:CD1	1:F:28:VAL:CG1	2.52	0.88
1:C:251:ILE:HD11	1:C:267:ARG:HD3	1.55	0.88
1:C:134:ASP:O	1:C:138:GLU:HG3	1.74	0.87
1:B:38:ARG:NH1	1:B:38:ARG:HG3	1.89	0.87
1:B:98:MET:HE3	1:B:170:GLY:HA2	1.54	0.87
1:C:2:ASN:N	4:C:3692:HOH:O	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:64:VAL:O	1:F:88:LYS:NZ	2.08	0.86
1:E:274:GLN:HG2	4:E:5529:HOH:O	1.76	0.85
1:F:6:LEU:CD1	1:F:28:VAL:HG11	2.06	0.85
1:B:98:MET:CE	1:B:170:GLY:HA2	2.07	0.84
1:D:279:PRO:HB2	4:D:4601:HOH:O	1.78	0.84
1:D:225:ILE:HB	1:F:215:MET:HE2	1.58	0.83
1:F:6:LEU:HD11	1:F:28:VAL:HG11	1.57	0.83
1:B:59:VAL:CG1	1:B:83:ALA:HA	2.10	0.82
1:F:94:LYS:HD2	1:F:94:LYS:C	1.99	0.82
1:B:38:ARG:CG	1:B:38:ARG:NH1	2.35	0.81
1:D:305:GLU:HA	1:D:308:VAL:CG1	2.10	0.81
1:D:331:THR:CG2	1:D:332:GLY:N	2.42	0.81
1:D:6:LEU:HD11	1:D:8:GLY:O	1.80	0.81
1:C:93:GLU:OE1	3:C:3500:NDP:H2N	1.80	0.81
1:F:52:VAL:HG21	1:F:57:GLU:HB3	1.60	0.81
1:D:217:VAL:HG13	1:F:215:MET:HE3	1.64	0.80
1:F:102:ASP:O	1:F:106:MET:HG3	1.81	0.80
1:F:94:LYS:HD2	1:F:94:LYS:O	1.81	0.80
1:A:173:VAL:HG12	1:A:211:GLU:HG2	1.63	0.80
1:E:122:HIS:CD2	1:E:122:HIS:H	1.95	0.80
1:F:12:ILE:HD13	1:F:70:SER:HB2	1.64	0.80
1:C:142:GLY:HA3	1:C:247:GLU:HG3	1.63	0.79
1:D:64:VAL:O	1:D:88:LYS:NZ	2.13	0.78
1:D:225:ILE:HB	1:F:215:MET:HE1	1.63	0.78
1:D:278:ASP:HB2	4:D:4587:HOH:O	1.83	0.78
1:F:157:PRO:HA	1:F:160:GLN:HG3	1.65	0.78
1:A:32:MET:HB2	1:A:52:VAL:HG12	1.66	0.78
1:C:80:THR:HB	1:C:90:VAL:HG11	1.63	0.78
1:D:222:SER:HG	1:D:224:VAL:HG13	1.50	0.77
1:A:11:THR:CG2	3:A:1500:NDP:O2A	2.32	0.77
1:F:132:MET:O	1:F:136:ILE:HG12	1.84	0.77
1:E:2:ASN:N	4:E:5723:HOH:O	2.16	0.77
1:E:59:VAL:CG2	1:E:83:ALA:HA	2.15	0.77
1:E:89:HIS:ND1	1:E:116:VAL:HG13	1.98	0.77
1:A:2:ASN:HB2	4:A:1575:HOH:O	1.84	0.77
1:E:31:MET:CE	1:E:43:ALA:HB2	2.16	0.76
1:D:258:GLN:HG2	1:D:283:TYR:OH	1.86	0.76
1:D:225:ILE:CD1	1:F:215:MET:HE2	2.16	0.76
1:F:6:LEU:HD11	1:F:28:VAL:CG1	2.16	0.76
1:B:306:ASP:OD2	4:B:2758:HOH:O	2.04	0.75
1:E:270:GLU:HG2	4:E:5711:HOH:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:VAL:CG1	1:F:215:MET:HE3	2.17	0.75
1:A:11:THR:HG22	3:A:1500:NDP:O2A	1.87	0.75
1:F:104:ARG:O	1:F:108:VAL:HG13	1.86	0.75
1:D:240:GLY:HA2	1:D:255:VAL:HG12	1.67	0.74
1:F:12:ILE:CD1	1:F:70:SER:HB2	2.17	0.74
1:D:331:THR:HG22	1:D:332:GLY:H	1.51	0.74
1:D:331:THR:HG23	1:D:332:GLY:N	2.03	0.74
1:E:80:THR:HB	1:E:90:VAL:HG11	1.67	0.74
1:A:76:HIS:O	1:A:80:THR:CG2	2.35	0.74
1:B:331:THR:HG23	1:B:333:LEU:N	2.03	0.74
1:D:2:ASN:N	4:D:4590:HOH:O	2.21	0.73
1:F:136:ILE:HD11	1:F:250:LEU:CD1	2.19	0.73
1:F:52:VAL:HG23	1:F:57:GLU:OE1	1.89	0.73
1:B:2:ASN:ND2	4:B:2759:HOH:O	2.20	0.73
1:D:136:ILE:HD11	1:D:250:LEU:CD1	2.18	0.73
1:D:331:THR:CG2	1:D:332:GLY:H	1.99	0.73
1:F:222:SER:OG	1:F:224:VAL:CG1	2.38	0.72
1:E:69:VAL:HG21	1:E:80:THR:HG22	1.70	0.72
1:B:38:ARG:NH1	1:B:38:ARG:CB	2.53	0.71
1:F:239:THR:HB	1:F:256:MET:HB2	1.72	0.71
1:B:59:VAL:HG11	1:B:83:ALA:HA	1.72	0.71
1:F:136:ILE:HD11	1:F:250:LEU:HD12	1.73	0.71
1:F:6:LEU:CD1	1:F:28:VAL:HG13	2.20	0.71
1:D:281:ASN:CG	1:D:284:GLU:HG3	2.10	0.70
1:A:93:GLU:OE1	3:A:1500:NDP:H2N	1.91	0.70
1:D:136:ILE:CD1	1:D:250:LEU:HD11	2.22	0.70
1:E:31:MET:HE1	1:E:43:ALA:CB	2.22	0.70
1:A:94:LYS:HE3	1:A:94:LYS:O	1.92	0.69
1:D:277:LEU:O	1:D:279:PRO:HD3	1.91	0.69
1:B:173:VAL:HG23	1:B:177:ILE:HD12	1.74	0.69
1:A:296:GLY:HA3	4:A:1622:HOH:O	1.91	0.69
1:F:6:LEU:HD13	1:F:28:VAL:CG1	2.22	0.69
1:C:207:LYS:HE2	4:C:3706:HOH:O	1.91	0.69
1:B:85:ARG:CG	1:B:85:ARG:HH11	2.04	0.68
1:F:331:THR:CG2	1:F:333:LEU:HB2	2.23	0.68
1:C:142:GLY:CA	1:C:247:GLU:HG3	2.22	0.68
1:E:134:ASP:OD2	4:E:5614:HOH:O	2.11	0.68
1:F:194:ALA:HB2	1:F:221:GLN:HG2	1.76	0.68
1:C:74:GLU:N	1:C:74:GLU:OE1	2.25	0.68
1:F:159:LEU:HD22	1:F:163:ARG:NH1	2.08	0.68
1:F:165:GLU:HG2	1:F:166:ARG:H	1.52	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:GLY:HA3	1:C:247:GLU:CG	2.24	0.68
1:D:122:HIS:CD2	1:D:122:HIS:H	2.11	0.68
1:F:181:ASP:OD2	1:F:230:ASP:OD1	2.12	0.68
1:D:225:ILE:C	1:F:215:MET:HE1	2.15	0.68
1:F:222:SER:OG	1:F:224:VAL:HG12	1.94	0.68
1:D:236:PHE:HB2	1:F:249:SER:HB2	1.75	0.67
1:B:38:ARG:CB	1:B:38:ARG:HH11	2.06	0.67
1:B:59:VAL:HG13	1:B:83:ALA:HA	1.74	0.67
1:D:222:SER:OG	1:D:224:VAL:CG1	2.30	0.67
1:A:76:HIS:O	1:A:80:THR:HG23	1.95	0.67
1:C:100:LEU:HD21	1:C:312:ALA:HB2	1.76	0.67
1:C:193:PRO:HB2	1:C:329:ILE:HD13	1.76	0.67
1:D:173:VAL:HG23	1:D:177:ILE:HD12	1.76	0.67
1:D:89:HIS:NE2	1:D:294:ILE:HG23	2.09	0.67
1:F:2:ASN:N	4:F:6614:HOH:O	2.26	0.67
1:B:85:ARG:NH1	1:B:85:ARG:HG3	2.05	0.67
1:D:124:ARG:HD2	1:D:183:ASP:OD2	1.95	0.67
1:D:31:MET:CE	1:D:48:ILE:HD12	2.25	0.67
1:E:140:ARG:HD2	4:E:5617:HOH:O	1.95	0.67
1:A:130:ARG:HD2	4:A:1678:HOH:O	1.93	0.67
1:B:331:THR:CG2	1:B:333:LEU:HB2	2.25	0.67
1:C:173:VAL:HG23	1:C:177:ILE:HD12	1.76	0.66
1:D:68:TYR:CD1	1:D:91:LEU:HD23	2.30	0.66
1:B:56:GLU:OE1	4:B:2635:HOH:O	2.12	0.66
1:C:251:ILE:CD1	1:C:267:ARG:HD3	2.26	0.66
1:F:130:ARG:HH11	1:F:130:ARG:HG2	1.59	0.66
1:F:94:LYS:HE2	1:F:180:HIS:NE2	2.11	0.66
1:A:15:GLU:OE2	4:A:1712:HOH:O	2.13	0.66
1:C:2:ASN:OD1	4:C:3603:HOH:O	2.12	0.66
1:E:122:HIS:H	1:E:122:HIS:HD2	1.44	0.66
4:E:5716:HOH:O	1:F:207:LYS:HE2	1.95	0.66
1:E:59:VAL:HG21	1:E:83:ALA:HA	1.77	0.66
1:D:3:ARG:HG2	1:D:29:VAL:CG1	2.26	0.66
1:A:208:GLU:HG3	1:A:209:GLY:H	1.62	0.65
1:E:31:MET:HE3	1:E:43:ALA:HB2	1.78	0.65
1:D:4:TRP:CD1	1:D:21:ILE:HG21	2.32	0.65
1:B:299:GLN:HB3	1:B:300:PRO:HD2	1.78	0.65
1:B:143:ARG:NH1	4:B:2535:HOH:O	2.30	0.65
1:D:136:ILE:HD11	1:D:250:LEU:HD12	1.77	0.65
1:B:164:LEU:HD21	1:B:205:MET:HE3	1.78	0.64
1:B:38:ARG:HB2	1:B:38:ARG:NH1	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:VAL:O	1:C:59:VAL:HG13	1.97	0.64
1:F:136:ILE:CD1	1:F:250:LEU:CD1	2.76	0.64
2:A:1502:ACT:OXT	4:A:1846:HOH:O	2.14	0.64
1:E:78:GLU:OE2	4:E:5714:HOH:O	2.15	0.64
1:C:164:LEU:HD11	1:C:205:MET:HE3	1.77	0.64
1:B:311:LEU:HD22	1:B:315:LEU:HG	1.80	0.64
1:E:59:VAL:HG22	1:E:83:ALA:HA	1.79	0.64
1:A:2:ASN:CB	4:A:1575:HOH:O	2.43	0.64
1:C:76:HIS:O	1:C:80:THR:CG2	2.41	0.64
1:E:93:GLU:OE1	3:E:5500:NDP:H2N	1.98	0.64
1:C:58:LEU:HG	1:C:58:LEU:O	1.98	0.64
1:E:299:GLN:HG3	4:E:5582:HOH:O	1.98	0.64
1:C:164:LEU:HD11	1:C:205:MET:CE	2.27	0.63
1:F:116:VAL:CG2	1:F:290:PHE:CZ	2.80	0.63
1:D:84:ILE:HD11	1:D:110:ALA:HB2	1.80	0.63
1:D:150:PHE:HB3	1:F:148:ARG:NH2	2.14	0.63
1:F:130:ARG:HD2	4:F:6625:HOH:O	1.99	0.63
1:B:331:THR:HG22	1:B:333:LEU:H	1.64	0.63
1:D:77:ARG:HD2	1:D:102:ASP:CG	2.19	0.62
1:A:222:SER:OG	1:A:224:VAL:HG13	2.00	0.62
1:C:132:MET:HE1	1:C:241:PHE:CD1	2.34	0.62
1:E:32:MET:HE2	1:E:55:VAL:HG22	1.80	0.62
1:D:251:ILE:HD11	1:D:267:ARG:HD3	1.82	0.62
1:E:96:LEU:HD22	1:E:106:MET:HE1	1.79	0.62
1:E:311:LEU:HD22	1:E:315:LEU:HG	1.82	0.62
1:A:80:THR:HB	1:A:90:VAL:HG11	1.79	0.62
1:B:331:THR:HG21	1:B:333:LEU:HB2	1.81	0.62
1:E:133:ARG:NH2	4:E:5738:HOH:O	2.31	0.62
1:C:276:PRO:HG3	4:C:3700:HOH:O	2.00	0.62
1:D:331:THR:HG23	1:D:333:LEU:H	1.65	0.62
1:C:94:LYS:C	1:C:94:LYS:HD2	2.20	0.62
1:E:77:ARG:HG2	1:E:81:LEU:HD22	1.81	0.62
1:F:84:ILE:HG22	4:F:6516:HOH:O	2.00	0.62
1:A:267:ARG:NH1	1:A:272:GLU:OE2	2.33	0.61
1:D:17:VAL:O	1:D:21:ILE:CG1	2.46	0.61
1:D:253:ARG:HG2	4:D:4603:HOH:O	1.99	0.61
1:B:193:PRO:HB2	1:B:329:ILE:HD13	1.82	0.61
1:C:27:GLU:OE1	1:C:28:VAL:N	2.28	0.61
1:F:193:PRO:HB2	1:F:329:ILE:HD12	1.83	0.61
1:B:122:HIS:CD2	1:B:122:HIS:H	2.18	0.61
1:E:2:ASN:ND2	4:E:5509:HOH:O	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:GLU:HG3	4:A:1550:HOH:O	1.99	0.61
1:B:93:GLU:OE1	3:B:2500:NDP:H2N	2.00	0.61
1:F:130:ARG:HG2	1:F:130:ARG:NH1	2.14	0.61
1:F:239:THR:CB	1:F:256:MET:HB2	2.31	0.61
1:C:11:THR:HG23	3:C:3500:NDP:O2A	2.01	0.61
1:D:27:GLU:OE1	1:D:28:VAL:N	2.34	0.61
1:E:331:THR:OG1	1:E:333:LEU:HB2	2.01	0.60
1:A:11:THR:HG23	3:A:1500:NDP:O2A	2.01	0.60
1:B:159:LEU:HD22	1:B:163:ARG:NH1	2.15	0.60
1:D:244:HIS:HD2	1:D:249:SER:OG	1.85	0.60
1:C:132:MET:HE1	1:C:241:PHE:HD1	1.65	0.60
1:A:76:HIS:O	1:A:80:THR:HG22	2.00	0.60
1:C:265:THR:CG2	1:C:272:GLU:OE2	2.46	0.60
1:D:59:VAL:HG13	1:D:86:ALA:CB	2.32	0.60
1:B:221:GLN:HG2	4:B:2762:HOH:O	2.02	0.60
1:E:61:ASP:C	1:E:61:ASP:OD1	2.39	0.60
1:D:173:VAL:CG2	1:D:177:ILE:HD12	2.31	0.60
1:D:221:GLN:HA	1:D:221:GLN:NE2	2.17	0.59
1:D:305:GLU:CA	1:D:308:VAL:HG12	2.24	0.59
1:F:331:THR:CG2	1:F:333:LEU:H	2.16	0.59
1:F:244:HIS:HD2	1:F:249:SER:OG	1.86	0.59
1:C:94:LYS:HD2	1:C:94:LYS:O	2.02	0.59
1:B:98:MET:HE3	1:B:170:GLY:CA	2.30	0.59
1:C:101:GLU:HB2	4:C:3612:HOH:O	2.02	0.59
1:C:173:VAL:CG2	1:C:177:ILE:HD12	2.32	0.59
1:E:31:MET:HE1	1:E:43:ALA:HB2	1.82	0.59
1:E:268:ASN:C	1:E:268:ASN:HD22	2.05	0.59
1:A:94:LYS:CD	1:A:180:HIS:CE1	2.73	0.59
1:B:59:VAL:HG12	1:B:86:ALA:CB	2.32	0.59
1:D:84:ILE:CD1	1:D:110:ALA:HB2	2.33	0.59
1:D:154:TYR:O	1:D:156:PRO:HD3	2.03	0.59
1:B:98:MET:CE	1:B:170:GLY:CA	2.81	0.59
1:D:136:ILE:HD12	1:D:250:LEU:HD11	1.83	0.59
1:F:196:ALA:HB2	1:F:218:LEU:HD23	1.83	0.58
1:C:331:THR:OG1	1:C:333:LEU:HB2	2.04	0.58
1:D:275:LEU:HB3	1:D:276:PRO:HD2	1.84	0.58
1:F:52:VAL:CG2	1:F:57:GLU:OE1	2.51	0.58
1:E:31:MET:CE	1:E:43:ALA:CB	2.81	0.58
1:D:225:ILE:CB	1:F:215:MET:CE	2.77	0.58
1:B:177:ILE:HG12	4:B:2670:HOH:O	2.03	0.57
1:D:3:ARG:HG2	1:D:29:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:ALA:O	1:D:45:GLU:HB2	2.04	0.57
1:F:128:ALA:HB1	1:F:255:VAL:CG2	2.34	0.57
1:B:160:GLN:HG2	1:B:164:LEU:CD2	2.35	0.57
1:F:299:GLN:CB	1:F:300:PRO:HD2	2.35	0.57
1:D:331:THR:CG2	1:D:333:LEU:H	2.17	0.57
4:E:5716:HOH:O	1:F:207:LYS:CE	2.51	0.57
1:B:76:HIS:HD2	1:B:95:PRO:O	1.88	0.57
1:C:193:PRO:HD2	1:C:309:TRP:CZ3	2.40	0.57
1:E:308:VAL:HG11	1:E:333:LEU:HD13	1.84	0.57
1:F:108:VAL:CG2	1:F:109:ALA:N	2.67	0.57
1:B:124:ARG:HH21	1:B:183:ASP:CG	2.08	0.57
1:E:96:LEU:HD22	1:E:106:MET:CE	2.34	0.57
1:E:31:MET:O	1:E:31:MET:HG2	2.03	0.57
1:F:306:ASP:OD2	4:F:6601:HOH:O	2.17	0.57
1:A:208:GLU:CG	1:A:209:GLY:N	2.66	0.57
1:D:126:ALA:HB3	1:D:129:HIS:HD2	1.70	0.57
1:C:41:ALA:O	1:C:45:GLU:HB2	2.05	0.57
1:D:103:ALA:HB2	1:D:311:LEU:HD12	1.86	0.57
1:E:111:ARG:NH2	4:E:5604:HOH:O	2.37	0.57
1:B:181:ASP:OD2	1:B:230:ASP:OD1	2.23	0.56
1:D:132:MET:O	1:D:136:ILE:HD13	2.05	0.56
1:E:305:GLU:CG	4:E:5517:HOH:O	2.38	0.56
1:B:74:GLU:HG2	1:B:75:LEU:HD13	1.87	0.56
1:E:94:LYS:HD3	1:E:94:LYS:O	2.06	0.56
1:F:98:MET:HG3	4:F:6574:HOH:O	2.04	0.56
1:E:12:ILE:HG12	3:E:5500:NDP:C4N	2.29	0.56
1:F:157:PRO:CA	1:F:160:GLN:HG3	2.36	0.56
1:C:208:GLU:CG	1:C:209:GLY:H	2.18	0.56
1:F:124:ARG:HD2	1:F:302:ALA:HB2	1.87	0.56
1:F:260:PRO:HG3	1:F:281:ASN:HA	1.88	0.56
1:E:59:VAL:HG21	1:E:83:ALA:CA	2.36	0.56
1:C:11:THR:CG2	3:C:3500:NDP:O2A	2.53	0.56
1:E:3:ARG:HG2	1:E:29:VAL:HG11	1.87	0.56
1:D:211:GLU:O	1:D:211:GLU:HG2	2.06	0.56
1:E:235:LYS:NZ	4:E:5561:HOH:O	2.35	0.56
1:F:116:VAL:HG23	1:F:290:PHE:CZ	2.41	0.55
1:D:331:THR:HG23	1:D:333:LEU:N	2.20	0.55
1:F:219:ARG:HD2	4:F:6524:HOH:O	2.04	0.55
1:B:122:HIS:HE1	4:B:2511:HOH:O	1.90	0.55
1:E:130:ARG:HD2	4:E:5547:HOH:O	2.06	0.55
1:D:225:ILE:CB	1:F:215:MET:HE2	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6:LEU:N	1:F:6:LEU:HD12	2.22	0.55
1:F:6:LEU:HD13	1:F:28:VAL:HG11	1.83	0.55
1:C:278:ASP:CB	4:C:3594:HOH:O	2.28	0.55
1:B:235:LYS:HG3	4:B:2557:HOH:O	2.06	0.55
1:E:32:MET:HE2	1:E:55:VAL:CG2	2.37	0.55
1:A:2:ASN:N	4:A:1822:HOH:O	2.40	0.55
1:B:71:THR:O	1:B:76:HIS:HE1	1.89	0.55
1:D:268:ASN:OD1	1:D:270:GLU:HB3	2.06	0.55
1:E:148:ARG:HD2	1:E:242:GLU:OE1	2.06	0.55
1:C:330:GLU:N	1:C:330:GLU:OE1	2.33	0.55
1:B:104:ARG:O	1:B:108:VAL:HG13	2.06	0.55
1:B:221:GLN:CG	4:B:2762:HOH:O	2.54	0.55
1:D:157:PRO:C	1:D:159:LEU:H	2.10	0.55
1:B:126:ALA:O	1:B:130:ARG:HG3	2.07	0.55
1:D:279:PRO:HG2	4:D:4601:HOH:O	2.07	0.55
1:B:132:MET:O	1:B:136:ILE:HG13	2.07	0.54
1:F:105:GLU:HG2	4:F:6585:HOH:O	2.06	0.54
1:F:159:LEU:HD22	1:F:163:ARG:HH12	1.71	0.54
1:A:80:THR:O	1:A:84:ILE:HG13	2.07	0.54
1:A:152:ALA:HB1	1:A:234:THR:OG1	2.07	0.54
1:B:222:SER:OG	1:B:224:VAL:HG23	2.08	0.54
1:D:4:TRP:HE1	1:D:291:HIS:HE1	1.54	0.54
1:F:142:GLY:O	1:F:144:PRO:HD3	2.08	0.54
1:D:94:LYS:CE	3:D:4500:NDP:O2D	2.56	0.54
1:E:98:MET:CE	1:E:98:MET:HA	2.38	0.54
1:A:160:GLN:HA	1:A:164:LEU:HD22	1.90	0.54
1:D:94:LYS:HG2	1:D:180:HIS:CE1	2.42	0.54
1:A:193:PRO:HB2	1:A:329:ILE:HD13	1.89	0.54
1:B:124:ARG:NH2	1:B:183:ASP:OD1	2.41	0.54
1:C:251:ILE:CD1	1:C:267:ARG:CD	2.86	0.54
1:D:236:PHE:O	1:F:267:ARG:NH1	2.41	0.54
1:D:217:VAL:HG13	1:F:215:MET:CE	2.35	0.54
1:A:57:GLU:HG2	4:A:1814:HOH:O	2.08	0.54
1:F:123:LEU:C	1:F:125:ASN:H	2.11	0.54
1:F:160:GLN:HB3	1:F:164:LEU:HD22	1.89	0.54
1:D:152:ALA:HB1	1:D:234:THR:OG1	2.07	0.53
1:D:122:HIS:H	1:D:122:HIS:HD2	1.55	0.53
1:E:253:ARG:HD3	4:E:5631:HOH:O	2.07	0.53
2:E:5502:ACT:C	3:E:5500:NDP:H42N	2.39	0.53
1:F:17:VAL:HG21	1:F:68:TYR:OH	2.08	0.53
1:D:275:LEU:HB3	1:D:276:PRO:CD	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ASN:ND2	4:A:1761:HOH:O	2.41	0.53
1:F:151:HIS:HB3	1:F:230:ASP:OD1	2.09	0.53
1:C:170:GLY:HA2	4:C:3703:HOH:O	2.07	0.53
1:D:204:GLY:CA	4:D:4516:HOH:O	2.56	0.53
1:C:80:THR:O	1:C:84:ILE:HG13	2.08	0.53
1:F:38:ARG:HH11	1:F:38:ARG:HG3	1.73	0.53
1:B:331:THR:CG2	1:B:332:GLY:N	2.71	0.53
1:B:54:SER:HB3	1:B:57:GLU:CB	2.29	0.53
1:E:77:ARG:HD2	1:E:102:ASP:CG	2.29	0.53
1:F:77:ARG:HD3	4:F:6547:HOH:O	2.07	0.53
1:E:324:GLY:HA2	4:E:5564:HOH:O	2.09	0.53
1:F:4:TRP:CD1	1:F:21:ILE:HG21	2.44	0.53
1:D:24:THR:O	4:D:4604:HOH:O	2.19	0.53
1:E:54:SER:HB3	1:E:57:GLU:HG3	1.91	0.53
1:C:170:GLY:CA	4:C:3703:HOH:O	2.57	0.53
1:F:128:ALA:HB1	1:F:255:VAL:HG21	1.89	0.52
1:D:12:ILE:HG22	3:D:4500:NDP:O1N	2.10	0.52
1:A:76:HIS:HD2	1:A:95:PRO:O	1.92	0.52
1:C:44:THR:HG21	4:C:3555:HOH:O	2.09	0.52
1:B:210:VAL:HG23	4:B:2703:HOH:O	2.09	0.52
1:D:93:GLU:OE1	3:D:4500:NDP:H2N	2.10	0.52
1:E:222:SER:OG	1:E:224:VAL:HG13	2.10	0.52
1:F:304:GLY:HA3	4:F:6622:HOH:O	2.09	0.52
1:B:3:ARG:HG2	1:B:29:VAL:HG11	1.92	0.52
1:C:64:VAL:O	1:C:88:LYS:NZ	2.37	0.52
1:D:325:GLN:O	1:D:326:ALA:C	2.47	0.52
1:F:173:VAL:HG22	1:F:177:ILE:HD12	1.90	0.52
1:F:2:ASN:N	4:F:6609:HOH:O	2.43	0.52
1:A:208:GLU:HG3	1:A:209:GLY:N	2.24	0.52
1:B:155:LEU:HD12	1:B:156:PRO:HD2	1.91	0.52
1:B:85:ARG:CG	1:B:85:ARG:NH1	2.64	0.52
1:F:122:HIS:O	1:F:125:ASN:HB2	2.10	0.52
1:B:122:HIS:CE1	4:B:2511:HOH:O	2.60	0.52
1:B:98:MET:HE1	1:B:170:GLY:HA2	1.88	0.52
1:E:108:VAL:CG2	4:E:5623:HOH:O	2.57	0.52
1:D:150:PHE:HD2	1:F:148:ARG:CZ	2.23	0.52
1:F:244:HIS:CD2	1:F:249:SER:OG	2.63	0.52
1:D:145:ILE:HD11	1:D:246:THR:CG2	2.41	0.51
1:C:61:ASP:OD1	1:C:63:ASP:HB2	2.10	0.51
1:D:150:PHE:HB3	1:F:148:ARG:HH22	1.75	0.51
1:B:80:THR:HG21	1:B:106:MET:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:GLU:HG3	1:E:270:GLU:O	2.09	0.51
1:F:173:VAL:CG2	1:F:177:ILE:HD12	2.40	0.51
1:B:331:THR:HG22	1:B:332:GLY:N	2.25	0.51
1:D:6:LEU:CD1	1:D:8:GLY:O	2.55	0.51
1:E:14:ARG:HD3	4:E:5728:HOH:O	2.10	0.51
1:A:12:ILE:HD13	3:A:1500:NDP:H41N	1.92	0.51
1:A:7:ILE:HG12	1:A:58:LEU:HD22	1.92	0.51
1:F:136:ILE:CD1	1:F:250:LEU:HD12	2.40	0.51
1:D:174:ILE:O	1:D:178:THR:HB	2.10	0.51
1:D:200:SER:HB3	1:D:214:VAL:HG23	1.92	0.51
1:F:22:ARG:O	4:F:6557:HOH:O	2.19	0.51
1:D:27:GLU:OE1	1:D:27:GLU:HA	2.11	0.50
1:D:104:ARG:O	1:D:108:VAL:HG22	2.11	0.50
1:D:135:ALA:CB	1:D:250:LEU:HD21	2.41	0.50
1:F:37:GLU:HB3	4:F:6615:HOH:O	2.10	0.50
1:C:11:THR:HB	1:C:14:ARG:NH2	2.26	0.50
1:D:157:PRO:O	1:D:159:LEU:N	2.44	0.50
1:E:12:ILE:O	1:E:12:ILE:HD12	2.11	0.50
1:F:10:SER:OG	1:F:12:ILE:HD12	2.11	0.50
1:E:89:HIS:ND1	1:E:116:VAL:CG1	2.70	0.50
1:F:130:ARG:HB3	4:F:6621:HOH:O	2.11	0.50
1:F:133:ARG:CD	4:F:6610:HOH:O	2.59	0.50
1:D:225:ILE:CB	1:F:215:MET:HE1	2.38	0.50
1:F:84:ILE:CD1	1:F:110:ALA:HB2	2.42	0.50
1:F:4:TRP:CD1	1:F:21:ILE:CG2	2.95	0.50
1:F:32:MET:SD	1:F:32:MET:C	2.90	0.50
1:D:181:ASP:OD2	1:D:230:ASP:OD1	2.30	0.50
1:F:331:THR:HG22	1:F:333:LEU:H	1.76	0.50
1:E:181:ASP:OD2	1:E:230:ASP:OD1	2.29	0.50
1:E:238:GLU:HB3	1:E:254:ASN:OD1	2.12	0.50
1:B:71:THR:O	1:B:76:HIS:CE1	2.65	0.49
1:F:17:VAL:HG21	1:F:68:TYR:CZ	2.47	0.49
1:B:102:ASP:O	1:B:106:MET:HG3	2.12	0.49
1:F:154:TYR:HB2	1:F:235:LYS:HA	1.93	0.49
1:F:174:ILE:HG21	1:F:318:VAL:HG23	1.95	0.49
1:E:80:THR:HG21	1:E:92:CYS:SG	2.52	0.49
1:E:104:ARG:NH1	1:E:331:THR:O	2.36	0.49
1:F:157:PRO:HA	1:F:160:GLN:CG	2.39	0.49
1:C:208:GLU:CG	1:C:209:GLY:N	2.76	0.49
1:B:93:GLU:HA	1:B:93:GLU:OE1	2.13	0.49
1:D:44:THR:O	1:D:46:ASN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:ASP:HA	4:D:4504:HOH:O	2.12	0.48
1:D:255:VAL:HG22	1:D:255:VAL:O	2.12	0.48
1:F:160:GLN:HB3	1:F:164:LEU:CD2	2.43	0.48
1:B:314:GLY:O	1:B:318:VAL:HG23	2.12	0.48
1:F:133:ARG:HD3	4:F:6610:HOH:O	2.13	0.48
1:D:168:GLU:HB3	4:D:4535:HOH:O	2.12	0.48
1:F:196:ALA:HB2	1:F:218:LEU:CD2	2.43	0.48
1:E:299:GLN:HB2	1:E:300:PRO:HD2	1.94	0.48
1:D:217:VAL:HG11	1:F:215:MET:HE3	1.96	0.48
1:A:59:VAL:HG13	1:A:86:ALA:CB	2.44	0.48
1:E:266:LEU:HD13	4:E:5721:HOH:O	2.13	0.48
1:A:20:ALA:O	1:A:24:THR:HG23	2.13	0.48
1:A:52:VAL:HG13	1:A:54:SER:H	1.79	0.48
1:B:205:MET:HB3	1:B:205:MET:HE3	1.63	0.48
1:B:313:THR:O	1:B:317:VAL:HG23	2.14	0.48
1:C:133:ARG:HD3	4:C:3529:HOH:O	2.14	0.48
1:D:13:ALA:HB2	1:D:68:TYR:HE2	1.79	0.48
1:E:290:PHE:O	1:E:294:ILE:HG13	2.13	0.47
1:F:141:ILE:HG12	1:F:245:GLY:HA3	1.96	0.47
1:F:128:ALA:CB	1:F:255:VAL:CG2	2.92	0.47
1:A:181:ASP:OD2	1:A:230:ASP:OD1	2.32	0.47
1:B:3:ARG:NH1	1:B:65:ASP:OD2	2.47	0.47
1:D:204:GLY:N	4:D:4516:HOH:O	2.26	0.47
1:D:225:ILE:CG1	1:F:215:MET:HE2	2.44	0.47
1:D:260:PRO:HG3	1:D:281:ASN:HA	1.96	0.47
1:D:3:ARG:HH21	1:D:63:ASP:HA	1.79	0.47
1:C:2:ASN:HA	4:C:3693:HOH:O	2.15	0.47
1:D:32:MET:HE2	4:D:4548:HOH:O	2.14	0.47
1:D:36:ALA:HA	4:D:4519:HOH:O	2.13	0.47
1:D:74:GLU:HG2	1:D:75:LEU:HD13	1.96	0.47
1:D:75:LEU:O	1:D:79:GLN:HG3	2.15	0.47
1:F:270:GLU:HG2	4:F:6612:HOH:O	2.14	0.47
1:F:313:THR:O	1:F:317:VAL:HG23	2.14	0.47
1:A:2:ASN:O	1:A:27:GLU:N	2.44	0.47
1:B:100:LEU:HA	1:B:100:LEU:HD23	1.74	0.47
1:C:94:LYS:HE2	1:C:180:HIS:NE2	2.30	0.47
1:E:14:ARG:NE	4:E:5728:HOH:O	2.48	0.47
2:A:1502:ACT:C	4:A:1738:HOH:O	2.62	0.47
1:D:59:VAL:HG22	1:D:83:ALA:HA	1.95	0.47
1:A:205:MET:HE3	1:A:233:THR:CG2	2.32	0.47
1:A:71:THR:O	1:A:76:HIS:HE1	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:THR:CG2	1:B:333:LEU:HD22	2.45	0.47
1:D:331:THR:HG23	1:D:333:LEU:HG	1.97	0.47
1:D:59:VAL:HG13	1:D:86:ALA:HB3	1.97	0.47
1:F:148:ARG:HD2	1:F:244:HIS:HE1	1.79	0.47
1:B:102:ASP:O	1:B:105:GLU:HB3	2.14	0.47
1:B:122:HIS:HD2	1:B:122:HIS:H	1.60	0.47
1:B:185:LEU:HD23	1:B:241:PHE:CZ	2.50	0.46
1:C:133:ARG:CD	4:C:3529:HOH:O	2.62	0.46
1:C:265:THR:HG23	1:C:272:GLU:HG3	1.96	0.46
1:D:96:LEU:HA	1:D:96:LEU:HD23	1.66	0.46
1:F:94:LYS:C	1:F:94:LYS:CD	2.79	0.46
1:B:166:ARG:HB2	4:B:2673:HOH:O	2.14	0.46
1:B:207:LYS:O	1:B:210:VAL:HG23	2.15	0.46
1:F:80:THR:HG22	1:F:90:VAL:HG11	1.97	0.46
2:A:1502:ACT:C	3:A:1500:NDP:H42N	2.44	0.46
1:F:123:LEU:C	1:F:125:ASN:N	2.68	0.46
1:F:128:ALA:O	1:F:131:ALA:HB3	2.16	0.46
1:B:80:THR:HG23	1:B:90:VAL:HG11	1.96	0.46
1:C:165:GLU:O	1:C:166:ARG:C	2.52	0.46
1:E:11:THR:O	1:E:15:GLU:HG3	2.14	0.46
1:E:125:ASN:HD21	1:E:301:SER:CB	2.27	0.46
1:B:143:ARG:HD3	4:B:2682:HOH:O	2.16	0.46
1:B:93:GLU:HG3	3:B:2500:NDP:O4D	2.16	0.46
1:B:96:LEU:HA	1:B:96:LEU:HD23	1.68	0.46
1:C:32:MET:HB2	1:C:52:VAL:HG23	1.98	0.46
1:D:4:TRP:HE1	1:D:291:HIS:CE1	2.32	0.46
1:E:281:ASN:C	1:E:281:ASN:OD1	2.54	0.46
1:C:152:ALA:HB1	1:C:234:THR:OG1	2.16	0.46
1:D:145:ILE:HD11	1:D:246:THR:HG23	1.98	0.46
1:D:3:ARG:HD3	4:D:4573:HOH:O	2.15	0.46
1:F:89:HIS:HB3	1:F:116:VAL:HG22	1.98	0.46
1:B:45:GLU:HG2	4:B:2621:HOH:O	2.16	0.46
1:D:136:ILE:HD12	1:D:250:LEU:CD1	2.41	0.46
1:D:94:LYS:HE2	3:D:4500:NDP:O2D	2.15	0.46
1:F:299:GLN:NE2	4:F:6619:HOH:O	2.43	0.46
1:C:71:THR:O	1:C:76:HIS:NE2	2.49	0.45
1:E:32:MET:HB2	1:E:52:VAL:HG12	1.99	0.45
1:E:61:ASP:OD1	1:E:63:ASP:N	2.46	0.45
1:F:7:ILE:HG12	1:F:58:LEU:HD22	1.99	0.45
1:F:81:LEU:HA	1:F:81:LEU:HD12	1.65	0.45
1:B:134:ASP:O	1:B:138:GLU:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:ILE:HD11	1:D:267:ARG:CD	2.46	0.45
1:F:227:GLN:NE2	4:F:6608:HOH:O	2.30	0.45
1:F:39:GLY:HA3	4:F:6552:HOH:O	2.15	0.45
1:A:94:LYS:HG3	1:A:94:LYS:H	1.65	0.45
1:E:94:LYS:HG2	1:E:180:HIS:CE1	2.51	0.45
1:E:173:VAL:HG12	1:E:211:GLU:HG2	1.99	0.45
1:D:4:TRP:CD1	1:D:21:ILE:CG2	3.00	0.45
1:F:239:THR:HB	1:F:256:MET:CB	2.45	0.45
1:F:299:GLN:HB3	1:F:300:PRO:HD2	1.97	0.45
1:E:38:ARG:HG3	1:E:38:ARG:HH11	1.80	0.45
1:F:141:ILE:HG13	1:F:248:GLY:O	2.16	0.45
1:E:32:MET:CE	1:E:55:VAL:HG22	2.46	0.45
1:D:290:PHE:O	1:D:293:ALA:HB3	2.16	0.45
1:D:191:ASP:OD2	1:D:220:PHE:HB3	2.17	0.45
1:C:314:GLY:O	1:C:318:VAL:HG23	2.17	0.45
1:F:6:LEU:N	1:F:6:LEU:CD1	2.80	0.45
1:E:108:VAL:CG2	1:E:109:ALA:N	2.80	0.45
1:F:123:LEU:O	1:F:125:ASN:N	2.51	0.44
1:F:68:TYR:CD1	1:F:91:LEU:HD23	2.52	0.44
1:D:255:VAL:CB	4:D:4546:HOH:O	2.26	0.44
1:E:174:ILE:HG21	1:E:318:VAL:HG23	1.98	0.44
1:E:59:VAL:CG2	1:E:83:ALA:CA	2.90	0.44
1:A:221:GLN:NE2	4:A:1661:HOH:O	2.50	0.44
1:A:311:LEU:HD22	1:A:315:LEU:HG	1.99	0.44
1:C:205:MET:HG3	1:C:233:THR:HG22	2.00	0.44
1:D:214:VAL:HG12	1:D:230:ASP:HB2	1.99	0.44
1:D:275:LEU:CB	1:D:276:PRO:CD	2.94	0.44
3:F:6500:NDP:H6N	3:F:6500:NDP:O5D	2.17	0.44
1:B:167:PRO:C	1:B:169:ALA:H	2.20	0.44
1:B:77:ARG:HD2	1:B:102:ASP:HB3	1.99	0.44
1:C:100:LEU:O	1:C:104:ARG:HG3	2.18	0.44
1:C:207:LYS:O	1:C:208:GLU:C	2.54	0.44
1:D:229:HIS:HE1	4:F:6623:HOH:O	2.00	0.44
1:D:259:LYS:HB2	4:D:4600:HOH:O	2.15	0.44
1:F:108:VAL:HG22	1:F:109:ALA:N	2.32	0.44
1:F:175:LEU:HA	1:F:175:LEU:HD12	1.84	0.44
1:D:221:GLN:CA	1:D:221:GLN:NE2	2.80	0.44
1:F:133:ARG:HE	1:F:133:ARG:HB3	1.35	0.44
1:C:330:GLU:CD	1:C:330:GLU:H	2.19	0.44
1:A:8:GLY:HA2	3:A:1500:NDP:O2X	2.18	0.44
1:C:94:LYS:HG2	1:C:180:HIS:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:VAL:CG1	1:B:86:ALA:HB3	2.48	0.44
1:D:37:GLU:HB2	4:D:4540:HOH:O	2.17	0.44
1:F:84:ILE:HD11	1:F:110:ALA:HB2	2.00	0.44
1:F:331:THR:HG23	1:F:333:LEU:HB2	1.98	0.44
1:D:59:VAL:HG22	1:D:83:ALA:CB	2.47	0.44
1:F:133:ARG:HG3	1:F:187:PHE:O	2.18	0.44
1:D:203:ALA:O	1:F:143:ARG:NH2	2.51	0.44
1:F:331:THR:HG23	1:F:333:LEU:H	1.81	0.44
1:D:152:ALA:O	1:D:237:ALA:HB3	2.16	0.43
1:E:305:GLU:H	1:E:305:GLU:HG2	1.52	0.43
1:F:239:THR:O	1:F:254:ASN:N	2.50	0.43
1:B:152:ALA:HB1	1:B:234:THR:OG1	2.18	0.43
1:A:78:GLU:OE2	4:A:1830:HOH:O	2.21	0.43
1:D:307:GLY:O	1:D:311:LEU:HB2	2.19	0.43
1:D:71:THR:O	1:D:76:HIS:NE2	2.48	0.43
1:D:59:VAL:HG13	1:D:86:ALA:HB2	2.00	0.43
1:A:207:LYS:O	1:A:208:GLU:HG2	2.18	0.43
1:A:333:LEU:HA	1:A:333:LEU:HD23	1.69	0.43
1:E:265:THR:CG2	1:E:272:GLU:HB3	2.49	0.43
1:A:87:GLY:C	1:A:88:LYS:HD3	2.39	0.43
1:B:168:GLU:HG2	1:B:168:GLU:O	2.18	0.43
1:B:12:ILE:HD13	3:B:2500:NDP:C4N	2.48	0.43
1:C:181:ASP:OD2	1:C:230:ASP:OD1	2.37	0.43
1:C:18:ILE:O	1:C:22:ARG:HG3	2.18	0.43
1:E:140:ARG:CG	4:E:5617:HOH:O	2.66	0.43
1:E:258:GLN:HG2	1:E:283:TYR:OH	2.18	0.43
1:E:10:SER:HB2	3:E:5500:NDP:O1N	2.18	0.43
1:F:267:ARG:HD2	1:F:272:GLU:OE2	2.19	0.43
1:A:2:ASN:CG	4:A:1761:HOH:O	2.57	0.43
1:F:136:ILE:HD13	1:F:250:LEU:CD1	2.49	0.43
1:C:78:GLU:HB3	1:F:56:GLU:HG3	1.99	0.43
2:F:6502:ACT:C	3:F:6500:NDP:H42N	2.48	0.43
1:B:259:LYS:HB3	1:B:260:PRO:HD2	2.00	0.43
1:B:54:SER:CB	1:B:57:GLU:HB2	2.31	0.43
1:C:69:VAL:HG21	1:C:80:THR:HG22	2.00	0.43
1:D:275:LEU:CB	1:D:276:PRO:HD2	2.48	0.43
1:D:31:MET:HE3	1:D:48:ILE:HD12	2.00	0.43
1:F:136:ILE:HD13	1:F:250:LEU:HD11	1.99	0.43
1:F:265:THR:HG22	1:F:267:ARG:HG3	2.01	0.43
1:F:94:LYS:HE2	1:F:180:HIS:HE2	1.83	0.43
1:C:178:THR:O	1:C:181:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:MET:CE	1:E:55:VAL:CG2	2.97	0.43
1:F:268:ASN:HB2	1:F:269:ALA:H	1.66	0.43
1:F:69:VAL:HG21	1:F:80:THR:HG22	2.01	0.43
1:A:14:ARG:HH11	1:A:14:ARG:HG2	1.84	0.43
1:F:127:ALA:O	1:F:128:ALA:C	2.56	0.43
1:F:331:THR:HG23	1:F:333:LEU:HD22	2.00	0.42
1:B:155:LEU:HB2	1:B:232:PHE:HB3	2.00	0.42
1:B:263:THR:HB	1:B:274:GLN:HE22	1.83	0.42
1:B:299:GLN:HB2	1:B:299:GLN:HE21	1.63	0.42
1:D:157:PRO:C	1:D:159:LEU:N	2.73	0.42
1:E:52:VAL:HG13	1:E:54:SER:H	1.84	0.42
1:B:122:HIS:CD2	1:B:122:HIS:N	2.84	0.42
1:D:165:GLU:HB2	4:D:4596:HOH:O	2.19	0.42
1:A:59:VAL:HG13	1:A:86:ALA:HB3	2.01	0.42
1:D:94:LYS:HE3	3:D:4500:NDP:O2D	2.20	0.42
1:A:154:TYR:HB2	1:A:235:LYS:HA	2.01	0.42
1:D:61:ASP:OD1	1:D:61:ASP:C	2.58	0.42
1:E:17:VAL:O	1:E:17:VAL:HG12	2.20	0.42
1:F:80:THR:HG21	1:F:92:CYS:HB2	2.01	0.42
1:F:94:LYS:HG2	1:F:180:HIS:CE1	2.54	0.42
1:C:299:GLN:HB3	1:C:300:PRO:HD2	2.00	0.42
1:E:205:MET:HG3	1:E:233:THR:HG22	2.01	0.42
1:B:164:LEU:C	1:B:165:GLU:HG3	2.39	0.42
1:B:252:GLY:HA2	1:B:263:THR:O	2.19	0.42
1:D:266:LEU:HA	1:D:266:LEU:HD23	1.91	0.42
1:F:38:ARG:HH11	1:F:38:ARG:CG	2.33	0.42
1:B:331:THR:OG1	1:B:333:LEU:HD22	2.20	0.42
1:B:50:LYS:HE3	1:B:50:LYS:HB2	1.63	0.42
1:F:175:LEU:HB2	4:F:6503:HOH:O	2.19	0.42
1:C:305:GLU:HB3	1:C:333:LEU:HD21	2.02	0.42
1:F:225:ILE:HG13	1:F:225:ILE:O	2.20	0.42
1:B:259:LYS:CE	4:B:2659:HOH:O	2.28	0.42
1:B:292:SER:HB3	4:B:2581:HOH:O	2.19	0.41
1:C:32:MET:SD	1:C:32:MET:C	2.98	0.41
1:D:279:PRO:CG	4:D:4601:HOH:O	2.64	0.41
1:E:98:MET:HA	1:E:98:MET:HE2	2.02	0.41
1:A:208:GLU:CG	1:A:209:GLY:H	2.21	0.41
1:B:311:LEU:CD2	1:B:315:LEU:HG	2.48	0.41
1:E:169:ALA:O	4:E:5634:HOH:O	2.22	0.41
1:E:207:LYS:N	1:E:207:LYS:HD3	2.35	0.41
1:E:274:GLN:CG	4:E:5529:HOH:O	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:LEU:HB3	1:F:220:PHE:CZ	2.55	0.41
1:F:77:ARG:O	1:F:81:LEU:HB2	2.20	0.41
1:A:94:LYS:HE3	1:A:94:LYS:C	2.40	0.41
1:B:209:GLY:N	4:B:2703:HOH:O	2.52	0.41
1:C:266:LEU:HB2	1:C:275:LEU:HD21	2.02	0.41
1:C:294:ILE:O	1:C:294:ILE:HG22	2.19	0.41
1:C:189:LEU:HD23	1:C:189:LEU:HA	1.83	0.41
1:D:7:ILE:HG13	1:D:58:LEU:HD22	2.02	0.41
1:E:207:LYS:O	1:E:208:GLU:C	2.58	0.41
2:A:1502:ACT:H3	4:A:1738:HOH:O	2.21	0.41
1:A:71:THR:O	1:A:76:HIS:CE1	2.74	0.41
1:A:78:GLU:HB3	1:B:56:GLU:HG3	2.02	0.41
1:E:130:ARG:HH11	1:E:130:ARG:HG2	1.85	0.41
1:E:143:ARG:HA	1:E:144:PRO:HD3	1.95	0.41
1:E:224:VAL:HG13	4:E:5659:HOH:O	2.20	0.41
1:D:150:PHE:CD2	1:F:148:ARG:CZ	3.04	0.41
1:C:95:PRO:O	1:C:96:LEU:C	2.59	0.41
1:D:248:GLY:HA2	1:F:236:PHE:CD2	2.56	0.41
1:D:258:GLN:NE2	1:D:283:TYR:OH	2.46	0.41
1:F:145:ILE:HD11	1:F:246:THR:HG22	2.03	0.41
1:F:43:ALA:O	1:F:48:ILE:N	2.50	0.41
1:B:77:ARG:HG3	1:B:81:LEU:HD22	2.03	0.41
1:E:216:GLY:O	1:E:227:GLN:HA	2.21	0.41
1:B:173:VAL:CG2	1:B:177:ILE:HD12	2.48	0.40
1:B:98:MET:HE1	1:B:170:GLY:CA	2.49	0.40
1:E:84:ILE:HG12	1:E:115:VAL:HG21	2.04	0.40
1:E:93:GLU:HG3	3:E:5500:NDP:O4D	2.21	0.40
1:A:273:SER:HB3	4:C:3697:HOH:O	2.19	0.40
1:C:132:MET:CE	1:C:241:PHE:CD1	3.02	0.40
1:E:151:HIS:CE1	1:E:177:ILE:HG23	2.56	0.40
1:A:253:ARG:NH1	4:A:1523:HOH:O	2.38	0.40
1:B:155:LEU:HB3	1:B:205:MET:HE1	2.03	0.40
1:F:165:GLU:CG	1:F:166:ARG:N	2.64	0.40
1:D:217:VAL:CG1	1:F:215:MET:CE	2.94	0.40
1:E:108:VAL:HG23	1:E:109:ALA:N	2.37	0.40
1:F:185:LEU:HD23	1:F:241:PHE:CZ	2.57	0.40
1:B:165:GLU:O	1:B:166:ARG:C	2.60	0.40
1:B:98:MET:HE1	1:B:170:GLY:N	2.37	0.40
1:D:260:PRO:CB	1:D:280:ALA:O	2.69	0.40
1:D:28:VAL:HG11	1:D:48:ILE:HD13	2.03	0.40
1:F:251:ILE:HD11	1:F:253:ARG:NE	2.36	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	330/332 (99%)	319 (97%)	10 (3%)	1 (0%)	41	46
1	B	330/332 (99%)	321 (97%)	9 (3%)	0	100	100
1	C	330/332 (99%)	315 (96%)	15 (4%)	0	100	100
1	D	330/332 (99%)	297 (90%)	31 (9%)	2 (1%)	25	26
1	E	330/332 (99%)	319 (97%)	11 (3%)	0	100	100
1	F	330/332 (99%)	297 (90%)	31 (9%)	2 (1%)	25	26
All	All	1980/1992 (99%)	1868 (94%)	107 (5%)	5 (0%)	41	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	45	GLU
1	F	270	GLU
1	D	158	HIS
1	A	34	THR
1	F	166	ARG

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	246/246 (100%)	225 (92%)	21 (8%)	10	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	246/246 (100%)	225 (92%)	21 (8%)	10	10
1	C	246/246 (100%)	221 (90%)	25 (10%)	7	6
1	D	246/246 (100%)	211 (86%)	35 (14%)	3	2
1	E	246/246 (100%)	212 (86%)	34 (14%)	3	3
1	F	246/246 (100%)	208 (85%)	38 (15%)	2	2
All	All	1476/1476 (100%)	1302 (88%)	174 (12%)	5	4

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	6	LEU
1	A	11	THR
1	A	27	GLU
1	A	32	MET
1	A	52	VAL
1	A	54	SER
1	A	59	VAL
1	A	75	LEU
1	A	80	THR
1	A	81	LEU
1	A	94	LYS
1	A	164	LEU
1	A	166	ARG
1	A	168	GLU
1	A	175	LEU
1	A	190	ASN
1	A	201	HIS
1	A	266	LEU
1	A	311	LEU
1	A	325	GLN
1	B	2	ASN
1	B	38	ARG
1	B	75	LEU
1	B	81	LEU
1	B	94	LYS
1	B	96	LEU
1	B	111	ARG
1	B	130	ARG
1	B	164	LEU

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Mol	Chain	Res	Type
1	B	168	GLU
1	B	175	LEU
1	B	201	HIS
1	B	207	LYS
1	B	208	GLU
1	B	266	LEU
1	B	267	ARG
1	B	275	LEU
1	B	292	SER
1	B	311	LEU
1	B	331	THR
1	B	333	LEU
1	C	11	THR
1	C	31	MET
1	C	32	MET
1	C	37	GLU
1	C	45	GLU
1	C	54	SER
1	C	75	LEU
1	C	80	THR
1	C	94	LYS
1	C	96	LEU
1	C	116	VAL
1	C	130	ARG
1	C	168	GLU
1	C	175	LEU
1	C	190	ASN
1	C	201	HIS
1	C	207	LYS
1	C	208	GLU
1	C	265	THR
1	C	266	LEU
1	C	292	SER
1	C	311	LEU
1	C	325	GLN
1	C	328	GLU
1	C	330	GLU
1	D	3	ARG
1	D	6	LEU
1	D	27	GLU
1	D	31	MET
1	D	32	MET

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Mol	Chain	Res	Type
1	D	35	SER
1	D	45	GLU
1	D	48	ILE
1	D	53	THR
1	D	58	LEU
1	D	59	VAL
1	D	75	LEU
1	D	77	ARG
1	D	81	LEU
1	D	85	ARG
1	D	94	LYS
1	D	96	LEU
1	D	112	GLU
1	D	116	VAL
1	D	136	ILE
1	D	141	ILE
1	D	164	LEU
1	D	168	GLU
1	D	175	LEU
1	D	201	HIS
1	D	207	LYS
1	D	224	VAL
1	D	254	ASN
1	D	266	LEU
1	D	275	LEU
1	D	278	ASP
1	D	292	SER
1	D	303	THR
1	D	311	LEU
1	D	331	THR
1	E	3	ARG
1	E	6	LEU
1	E	7	ILE
1	E	12	ILE
1	E	31	MET
1	E	32	MET
1	E	38	ARG
1	E	45	GLU
1	E	58	LEU
1	E	59	VAL
1	E	74	GLU
1	E	75	LEU

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Mol	Chain	Res	Type
1	E	80	THR
1	E	81	LEU
1	E	94	LYS
1	E	96	LEU
1	E	116	VAL
1	E	140	ARG
1	E	164	LEU
1	E	168	GLU
1	E	175	LEU
1	E	201	HIS
1	E	207	LYS
1	E	208	GLU
1	E	218	LEU
1	E	221	GLN
1	E	266	LEU
1	E	268	ASN
1	E	270	GLU
1	E	273	SER
1	E	278	ASP
1	E	292	SER
1	E	305	GLU
1	E	311	LEU
1	F	2	ASN
1	F	12	ILE
1	F	31	MET
1	F	32	MET
1	F	45	GLU
1	F	51	SER
1	F	54	SER
1	F	58	LEU
1	F	75	LEU
1	F	81	LEU
1	F	94	LYS
1	F	96	LEU
1	F	100	LEU
1	F	105	GLU
1	F	108	VAL
1	F	115	VAL
1	F	116	VAL
1	F	133	ARG
1	F	141	ILE
1	F	164	LEU

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Mol	Chain	Res	Type
1	F	168	GLU
1	F	173	VAL
1	F	175	LEU
1	F	201	HIS
1	F	207	LYS
1	F	224	VAL
1	F	249	SER
1	F	251	ILE
1	F	254	ASN
1	F	255	VAL
1	F	266	LEU
1	F	270	GLU
1	F	295	GLU
1	F	299	GLN
1	F	303	THR
1	F	311	LEU
1	F	331	THR
1	F	333	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	120	ASN
1	A	190	ASN
1	A	221	GLN
1	A	254	ASN
1	A	274	GLN
1	B	76	HIS
1	B	122	HIS
1	B	125	ASN
1	B	160	GLN
1	B	190	ASN
1	B	274	GLN
1	B	299	GLN
1	C	2	ASN
1	C	190	ASN
1	C	221	GLN
1	C	254	ASN
1	D	2	ASN
1	D	122	HIS
1	D	129	HIS

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Mol	Chain	Res	Type
1	D	160	GLN
1	D	190	ASN
1	D	221	GLN
1	D	244	HIS
1	D	254	ASN
1	D	258	GLN
1	D	274	GLN
1	D	291	HIS
1	D	299	GLN
1	E	120	ASN
1	E	122	HIS
1	E	125	ASN
1	E	190	ASN
1	E	258	GLN
1	E	268	ASN
1	F	190	ASN
1	F	244	HIS
1	F	325	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	ACT	A	1502	-	1,3,3	2.34	1 (100%)	0,3,3	0.00	-
2	ACT	F	6502	-	1,3,3	1.99	0	0,3,3	0.00	-
3	NDP	C	3500	-	45,52,52	2.12	4 (8%)	53,80,80	1.18	5 (9%)
3	NDP	F	6500	-	45,52,52	2.09	4 (8%)	53,80,80	1.39	7 (13%)
2	ACT	D	4502	-	1,3,3	1.81	0	0,3,3	0.00	-
2	ACT	C	3502	-	1,3,3	1.75	0	0,3,3	0.00	-
3	NDP	A	1500	-	45,52,52	2.15	4 (8%)	53,80,80	1.30	6 (11%)
3	NDP	D	4500	-	45,52,52	2.11	4 (8%)	53,80,80	1.33	6 (11%)
2	ACT	E	5502	-	1,3,3	2.20	1 (100%)	0,3,3	0.00	-
2	ACT	B	2502	-	1,3,3	2.94	1 (100%)	0,3,3	0.00	-
3	NDP	B	2500	-	45,52,52	2.18	5 (11%)	53,80,80	1.42	6 (11%)
3	NDP	E	5500	-	45,52,52	2.08	3 (6%)	53,80,80	1.29	3 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	D	4500	-	-	4/30/77/77	0/5/5/5
3	NDP	C	3500	-	-	5/30/77/77	0/5/5/5
3	NDP	F	6500	-	-	6/30/77/77	0/5/5/5
3	NDP	A	1500	-	-	3/30/77/77	0/5/5/5
3	NDP	B	2500	-	-	4/30/77/77	0/5/5/5
3	NDP	E	5500	-	-	4/30/77/77	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5500	NDP	C4N-C3N	-10.37	1.29	1.49
3	B	2500	NDP	C4N-C3N	-10.22	1.29	1.49
3	C	3500	NDP	C4N-C3N	-10.09	1.30	1.49
3	D	4500	NDP	C4N-C3N	-10.06	1.30	1.49
3	F	6500	NDP	C4N-C3N	-9.97	1.30	1.49
3	A	1500	NDP	C4N-C3N	-9.80	1.30	1.49
3	B	2500	NDP	C4N-C5N	-7.49	1.29	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4500	NDP	C4N-C5N	-7.45	1.29	1.48
3	C	3500	NDP	C4N-C5N	-7.43	1.29	1.48
3	A	1500	NDP	C4N-C5N	-7.28	1.29	1.48
3	F	6500	NDP	C4N-C5N	-7.01	1.30	1.48
3	E	5500	NDP	C4N-C5N	-6.85	1.31	1.48
3	A	1500	NDP	C6N-C5N	4.47	1.41	1.33
3	F	6500	NDP	C6N-C5N	4.16	1.40	1.33
3	E	5500	NDP	C6N-C5N	3.68	1.39	1.33
3	B	2500	NDP	C6N-C5N	3.53	1.39	1.33
3	D	4500	NDP	C6N-C5N	3.42	1.39	1.33
3	C	3500	NDP	C6N-C5N	3.21	1.39	1.33
2	B	2502	ACT	CH3-C	2.94	1.52	1.48
3	B	2500	NDP	C2A-N3A	2.56	1.36	1.32
3	A	1500	NDP	C2A-N3A	2.44	1.36	1.32
2	A	1502	ACT	CH3-C	2.34	1.51	1.48
3	D	4500	NDP	O4B-C1B	2.22	1.44	1.41
2	E	5502	ACT	CH3-C	2.20	1.51	1.48
3	F	6500	NDP	C2A-N3A	2.19	1.35	1.32
3	B	2500	NDP	O7N-C7N	-2.10	1.19	1.24
3	C	3500	NDP	C2N-C3N	2.03	1.40	1.34

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5500	NDP	N3A-C2A-N1A	-4.69	121.34	128.68
3	F	6500	NDP	N3A-C2A-N1A	-4.47	121.69	128.68
3	A	1500	NDP	N3A-C2A-N1A	-4.39	121.82	128.68
3	C	3500	NDP	N3A-C2A-N1A	-4.31	121.94	128.68
3	F	6500	NDP	O3D-C3D-C4D	-4.08	99.27	111.05
3	D	4500	NDP	N3A-C2A-N1A	-4.04	122.36	128.68
3	B	2500	NDP	N3A-C2A-N1A	-3.95	122.50	128.68
3	D	4500	NDP	C3N-C2N-N1N	-3.87	117.57	123.10
3	E	5500	NDP	C3N-C2N-N1N	-3.75	117.75	123.10
3	B	2500	NDP	C3N-C7N-N7N	3.45	123.79	117.67
3	B	2500	NDP	O2B-C2B-C1B	-3.01	99.25	110.10
3	C	3500	NDP	N6A-C6A-N1A	2.98	124.77	118.57
3	B	2500	NDP	N6A-C6A-N1A	2.78	124.34	118.57
3	A	1500	NDP	O3X-P2B-O1X	2.69	121.21	110.68
3	D	4500	NDP	C1D-N1N-C2N	-2.58	116.81	121.11
3	B	2500	NDP	C1D-N1N-C2N	-2.53	116.89	121.11
3	C	3500	NDP	C5A-C6A-N6A	-2.52	116.53	120.35
3	C	3500	NDP	C3N-C2N-N1N	-2.48	119.56	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4500	NDP	O2B-P2B-O1X	-2.43	100.00	109.39
3	D	4500	NDP	C1B-N9A-C4A	-2.35	122.51	126.64
3	F	6500	NDP	C3N-C2N-N1N	-2.26	119.88	123.10
3	B	2500	NDP	O7N-C7N-N7N	-2.19	117.77	122.88
3	F	6500	NDP	PN-O3-PA	-2.18	125.35	132.83
3	F	6500	NDP	O3X-P2B-O1X	2.18	119.21	110.68
3	F	6500	NDP	N6A-C6A-N1A	2.15	123.03	118.57
3	A	1500	NDP	C3N-C2N-N1N	-2.13	120.06	123.10
3	A	1500	NDP	O2A-PA-O1A	2.08	122.55	112.24
3	A	1500	NDP	O3D-C3D-C4D	-2.06	105.10	111.05
3	A	1500	NDP	N6A-C6A-N1A	2.04	122.81	118.57
3	E	5500	NDP	PN-O3-PA	-2.03	125.87	132.83
3	D	4500	NDP	C2B-C3B-C4B	2.01	106.37	101.99
3	C	3500	NDP	O2B-P2B-O1X	-2.01	101.64	109.39
3	F	6500	NDP	O3D-C3D-C2D	-2.00	105.35	111.82

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	6500	NDP	C5D-O5D-PN-O1N
3	D	4500	NDP	C4B-C5B-O5B-PA
3	F	6500	NDP	C5D-O5D-PN-O3
3	F	6500	NDP	PN-O3-PA-O2A
3	D	4500	NDP	C2D-C1D-N1N-C2N
3	B	2500	NDP	O4D-C1D-N1N-C2N
3	C	3500	NDP	C4B-C5B-O5B-PA
3	D	4500	NDP	O4D-C1D-N1N-C2N
3	E	5500	NDP	O4D-C1D-N1N-C2N
3	A	1500	NDP	O4D-C1D-N1N-C2N
3	C	3500	NDP	O4D-C1D-N1N-C2N
3	A	1500	NDP	C2D-C1D-N1N-C2N
3	E	5500	NDP	C2D-C1D-N1N-C2N
3	F	6500	NDP	O4D-C1D-N1N-C2N
3	C	3500	NDP	C2D-C1D-N1N-C2N
3	F	6500	NDP	C2D-C1D-N1N-C2N
3	E	5500	NDP	C4B-C5B-O5B-PA
3	B	2500	NDP	C2D-C1D-N1N-C2N
3	F	6500	NDP	PN-O3-PA-O1A
3	C	3500	NDP	PA-O3-PN-O2N
3	B	2500	NDP	PN-O3-PA-O2A
3	A	1500	NDP	C4B-C5B-O5B-PA

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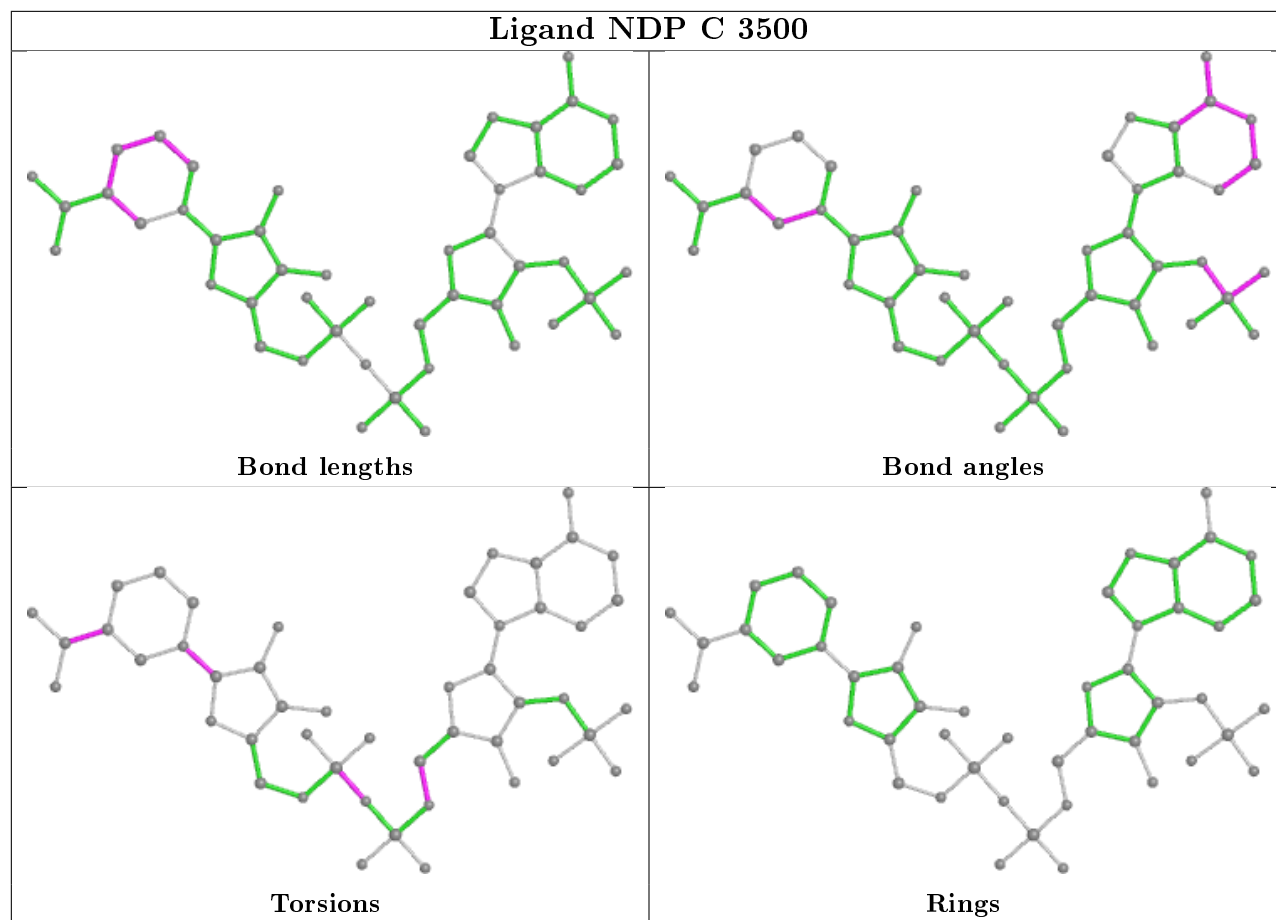
Mol	Chain	Res	Type	Atoms
3	C	3500	NDP	C2N-C3N-C7N-N7N
3	E	5500	NDP	C2N-C3N-C7N-N7N
3	D	4500	NDP	C2D-C1D-N1N-C6N
3	B	2500	NDP	C4B-C5B-O5B-PA

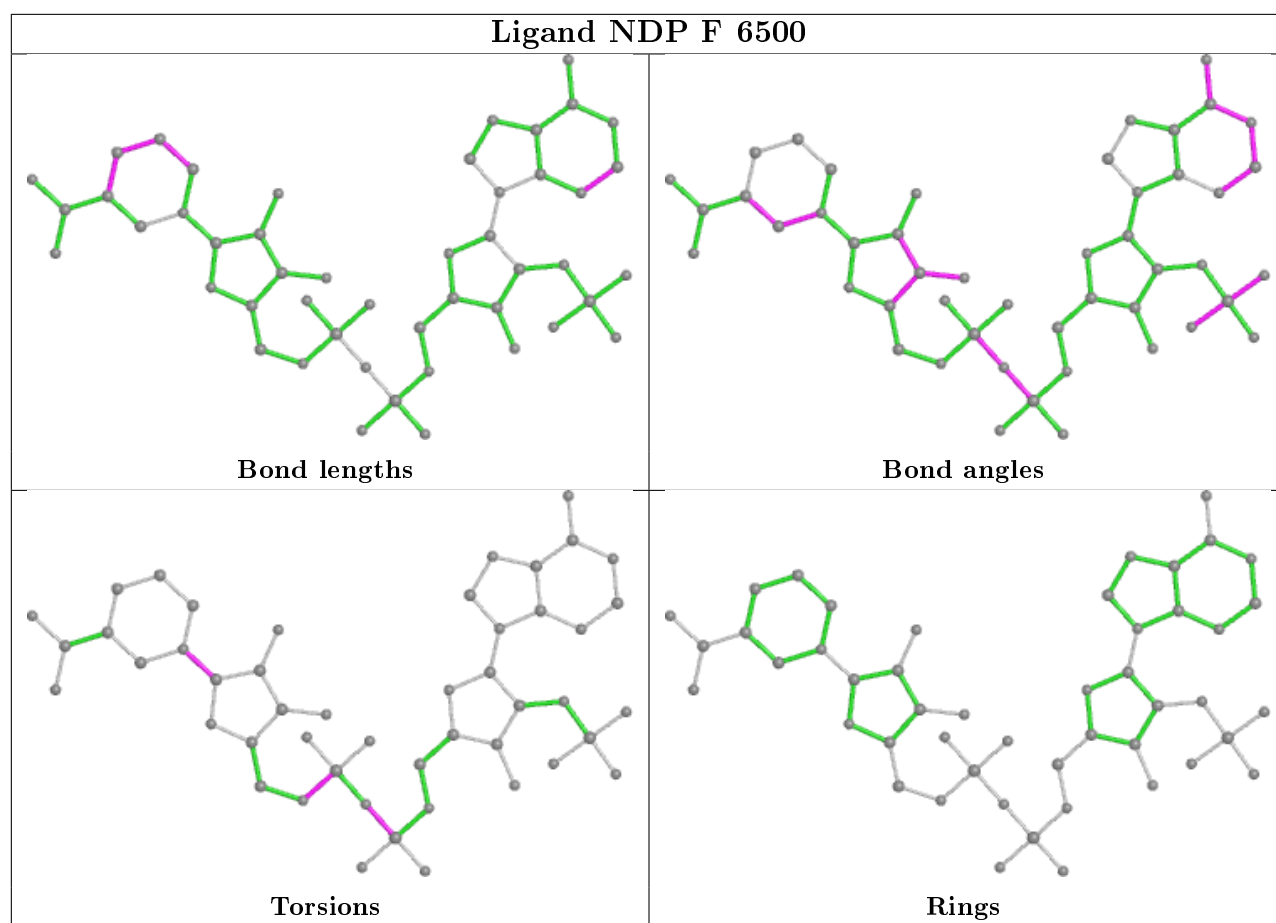
There are no ring outliers.

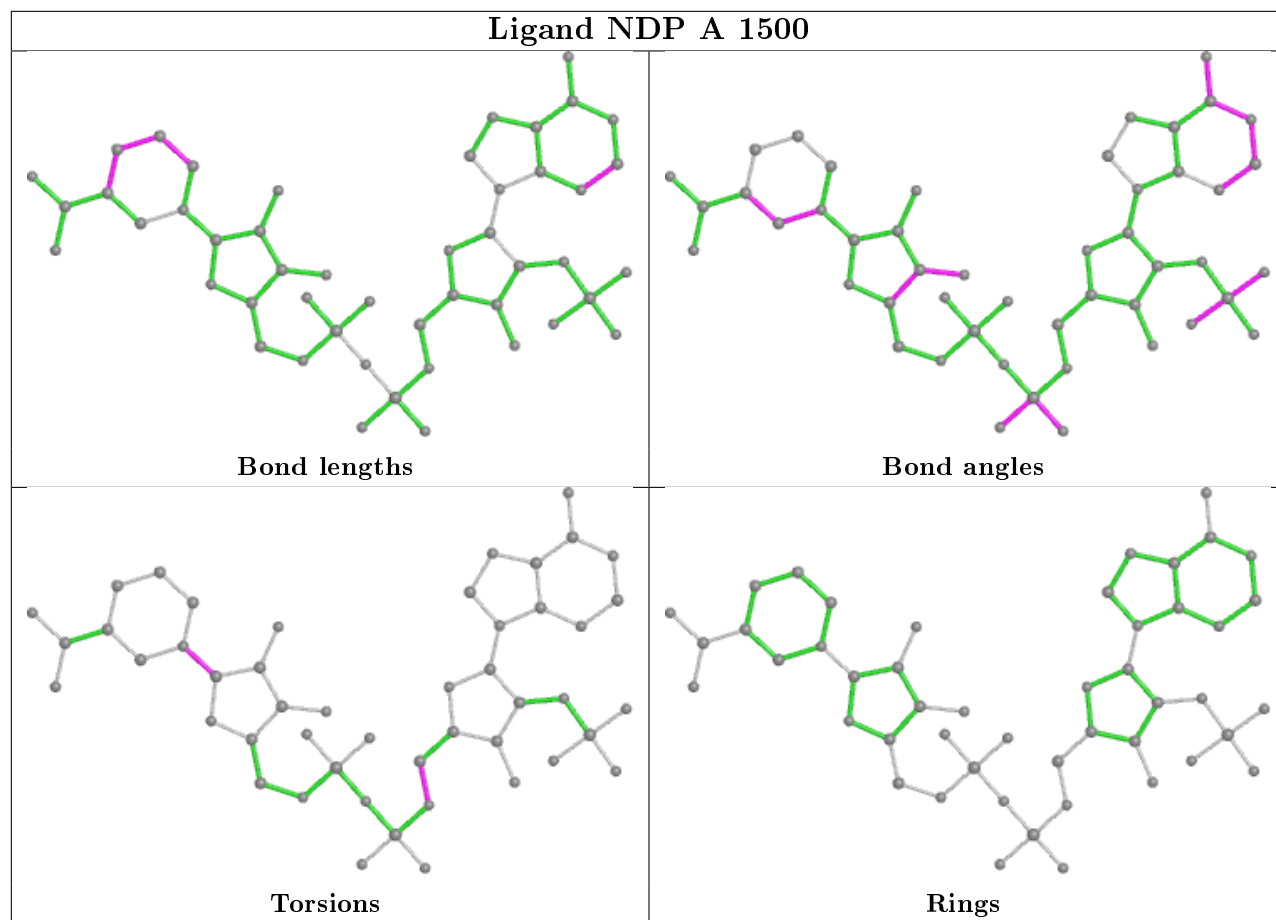
9 monomers are involved in 30 short contacts:

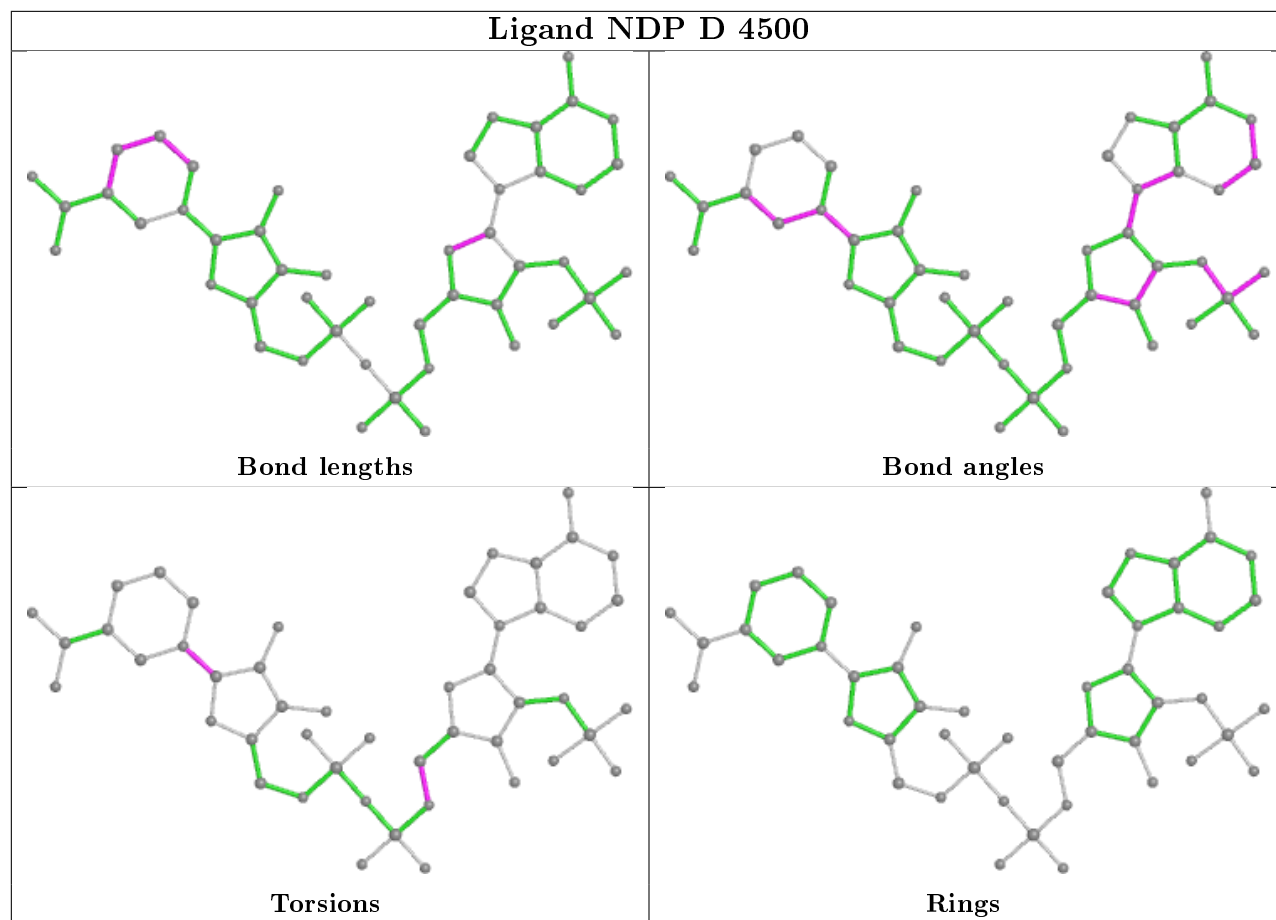
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1502	ACT	4	0
2	F	6502	ACT	1	0
3	C	3500	NDP	3	0
3	F	6500	NDP	3	0
3	A	1500	NDP	7	0
3	D	4500	NDP	5	0
2	E	5502	ACT	1	0
3	B	2500	NDP	3	0
3	E	5500	NDP	6	0

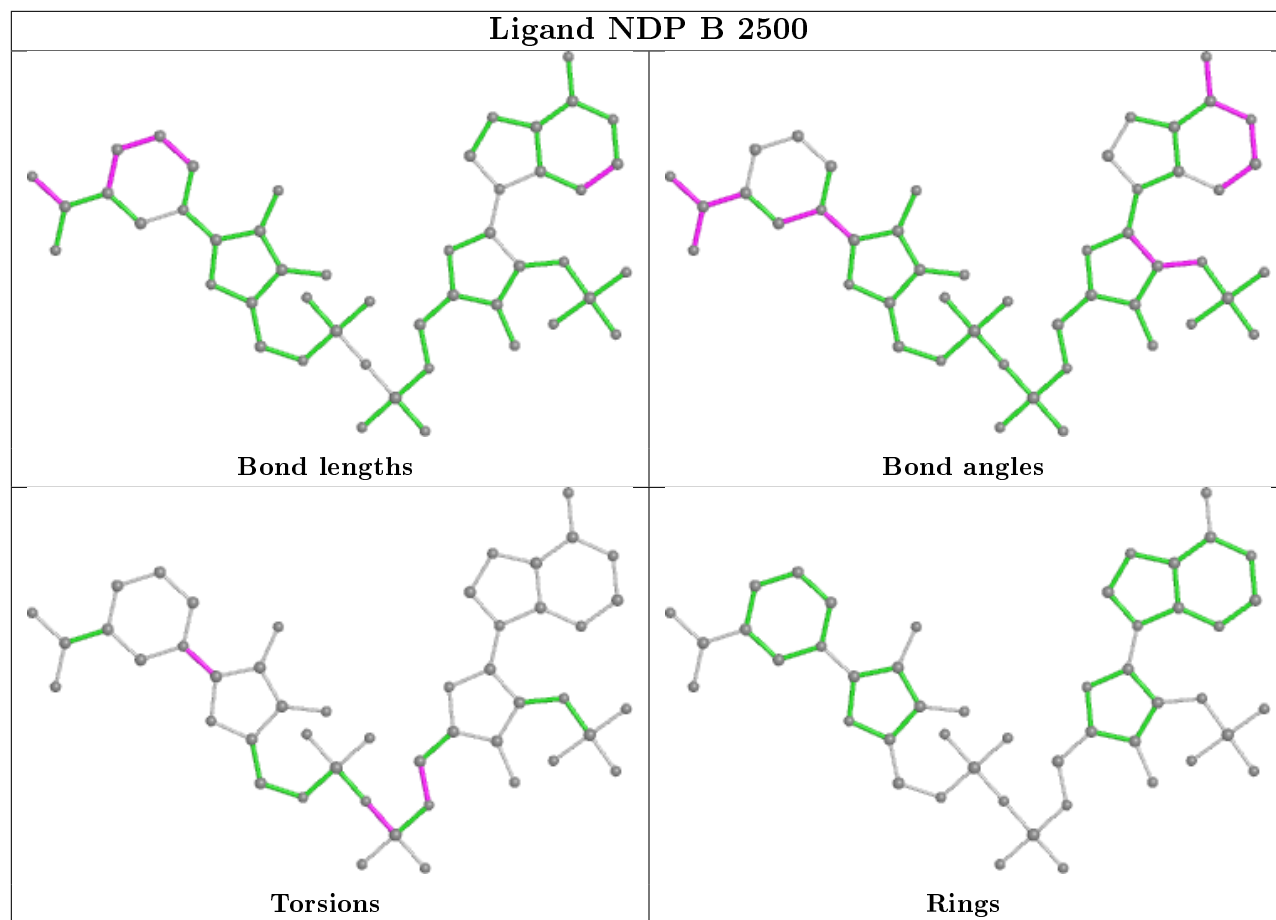
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

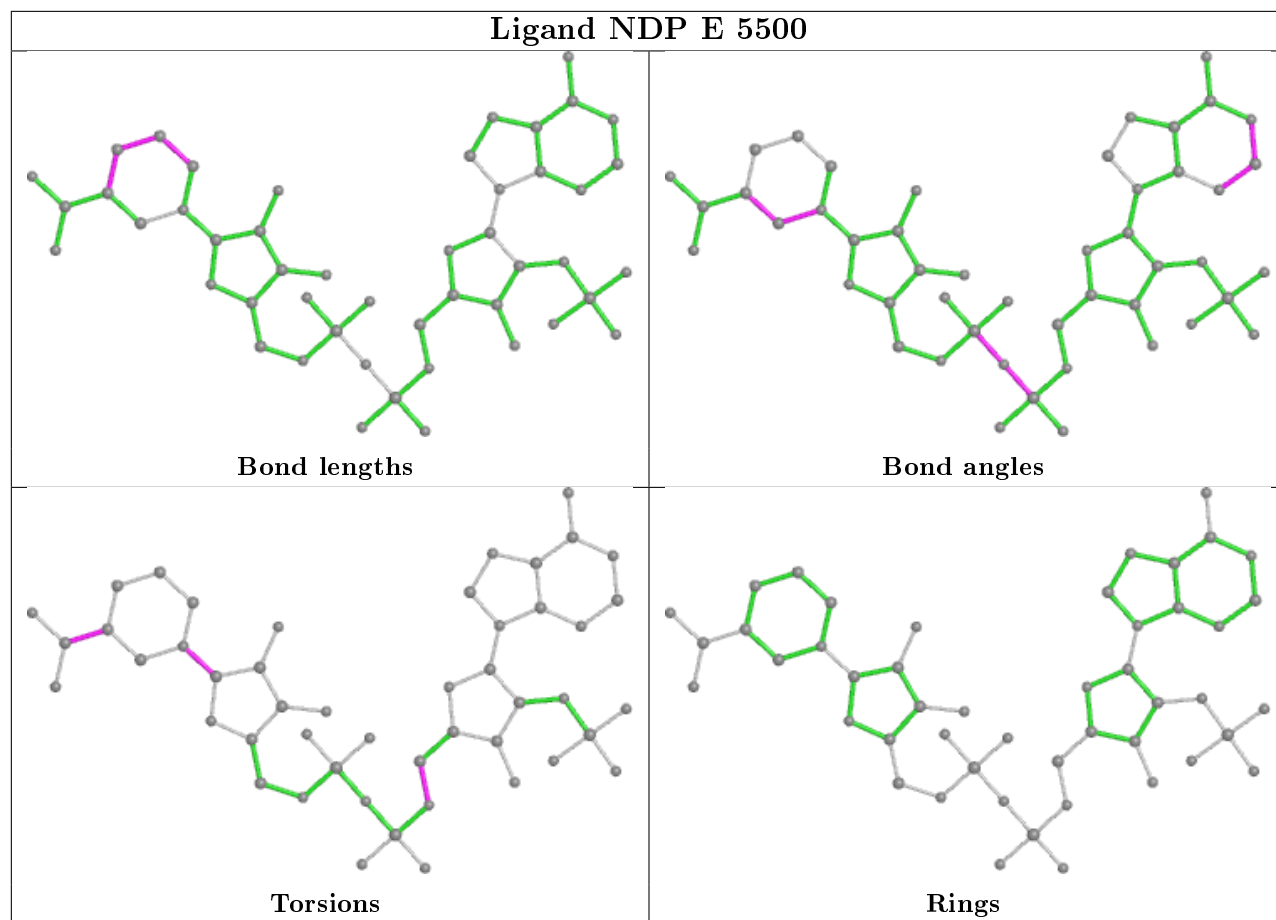












5.7 Other polymers [i](#)

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	332/332 (100%)	-0.54	2 (0%) 89 88	14, 25, 44, 67	0
1	B	332/332 (100%)	-0.42	3 (0%) 84 83	14, 30, 54, 75	0
1	C	332/332 (100%)	-0.32	3 (0%) 84 83	19, 37, 59, 75	0
1	D	332/332 (100%)	0.29	27 (8%) 12 10	33, 54, 74, 75	0
1	E	332/332 (100%)	-0.35	3 (0%) 84 83	16, 34, 54, 68	0
1	F	332/332 (100%)	0.26	19 (5%) 23 22	34, 54, 74, 75	0
All	All	1992/1992 (100%)	-0.18	57 (2%) 51 49	14, 39, 67, 75	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	269	ALA	6.3
1	D	278	ASP	5.0
1	F	296	GLY	4.8
1	F	297	HIS	4.6
1	C	333	LEU	4.1
1	D	209	GLY	4.1
1	D	295	GLU	4.1
1	B	209	GLY	4.0
1	F	298	GLY	3.8
1	D	279	PRO	3.8
1	B	208	GLU	3.8
1	F	278	ASP	3.8
1	F	271	GLY	3.7
1	D	269	ALA	3.7
1	F	262	GLY	3.6
1	D	270	GLU	3.6
1	D	138	GLU	3.3
1	D	297	HIS	3.3
1	F	139	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	271	GLY	3.2
1	F	270	GLU	3.2
1	D	158	HIS	3.1
1	A	209	GLY	3.1
1	D	159	LEU	3.0
1	F	295	GLU	2.8
1	F	45	GLU	2.7
1	D	333	LEU	2.6
1	D	208	GLU	2.6
1	A	208	GLU	2.6
1	D	296	GLY	2.6
1	F	276	PRO	2.5
1	D	280	ALA	2.5
1	C	208	GLU	2.5
1	E	298	GLY	2.5
1	F	138	GLU	2.4
1	D	207	LYS	2.4
1	F	243	VAL	2.4
1	F	62	PRO	2.3
1	D	157	PRO	2.3
1	D	277	LEU	2.3
1	D	276	PRO	2.3
1	B	206	GLY	2.2
1	E	297	HIS	2.2
1	D	274	GLN	2.2
1	F	111	ARG	2.2
1	D	6	LEU	2.2
1	F	279	PRO	2.2
1	D	168	GLU	2.2
1	D	273	SER	2.2
1	F	87	GLY	2.2
1	D	23	ALA	2.1
1	F	204	GLY	2.1
1	D	25	GLY	2.1
1	D	250	LEU	2.0
1	D	114	GLY	2.0
1	E	208	GLU	2.0
1	C	278	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

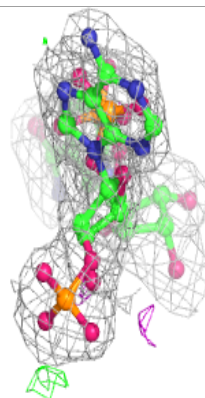
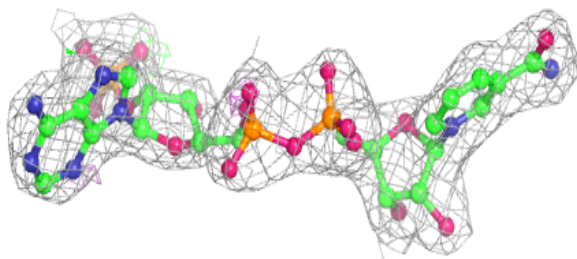
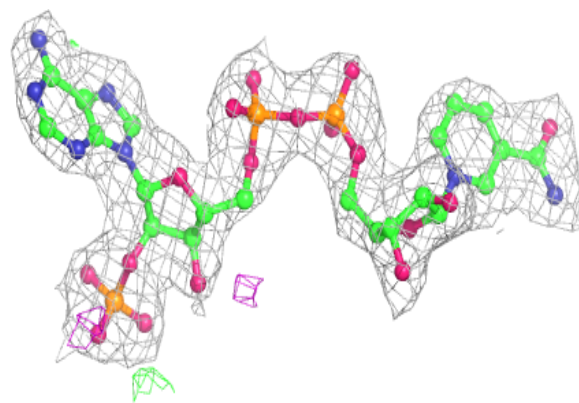
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ACT	F	6502	4/4	0.88	0.25	64,66,68,68	0
2	ACT	B	2502	4/4	0.93	0.15	37,41,43,44	0
2	ACT	D	4502	4/4	0.94	0.13	57,57,59,61	0
2	ACT	E	5502	4/4	0.95	0.12	33,36,37,37	0
3	NDP	D	4500	48/48	0.95	0.11	32,45,55,56	0
3	NDP	F	6500	48/48	0.96	0.10	27,48,55,58	0
2	ACT	A	1502	4/4	0.96	0.12	30,31,31,36	0
2	ACT	C	3502	4/4	0.96	0.13	51,52,54,58	0
3	NDP	A	1500	48/48	0.97	0.10	15,26,37,39	0
3	NDP	C	3500	48/48	0.97	0.08	24,33,41,44	0
3	NDP	B	2500	48/48	0.98	0.08	16,27,36,43	0
3	NDP	E	5500	48/48	0.98	0.08	20,31,41,46	0

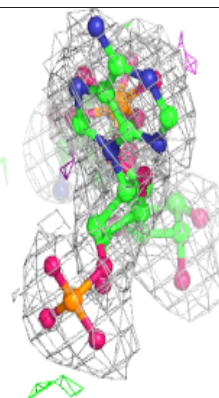
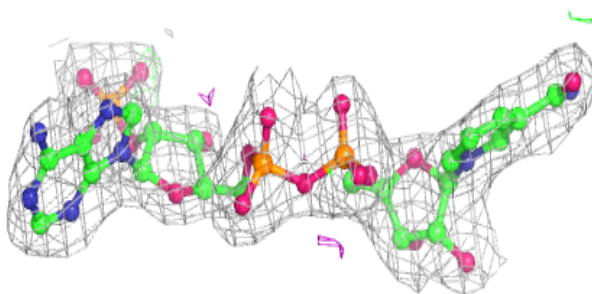
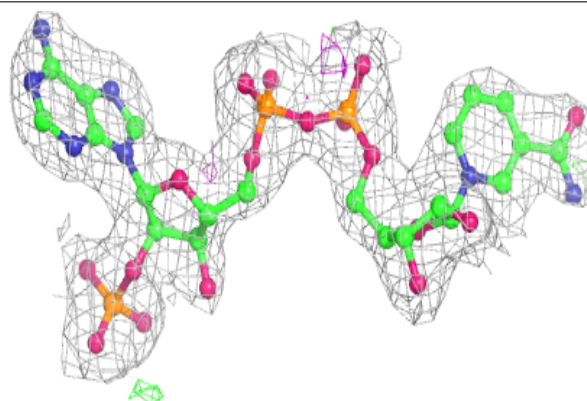
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP D 4500:

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

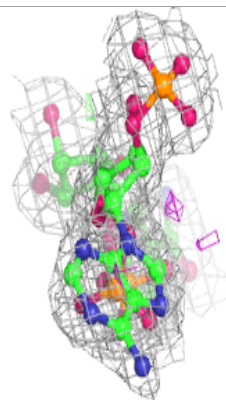
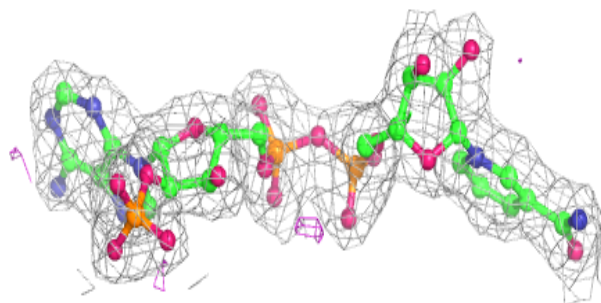
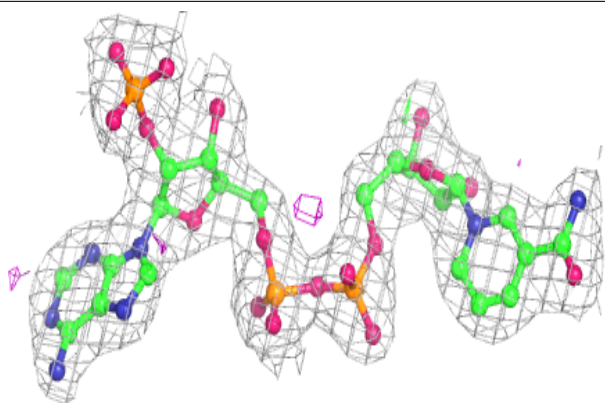
**Electron density around NDP F 6500:**

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

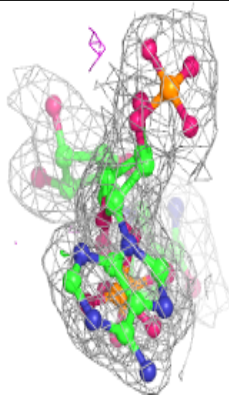
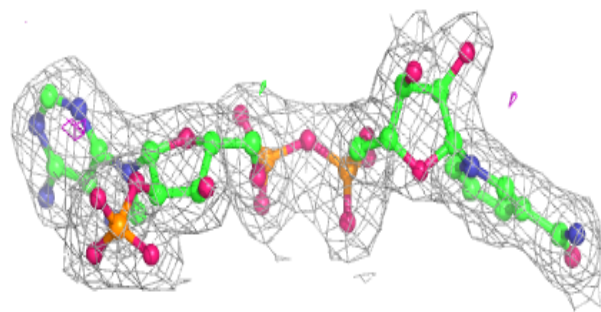
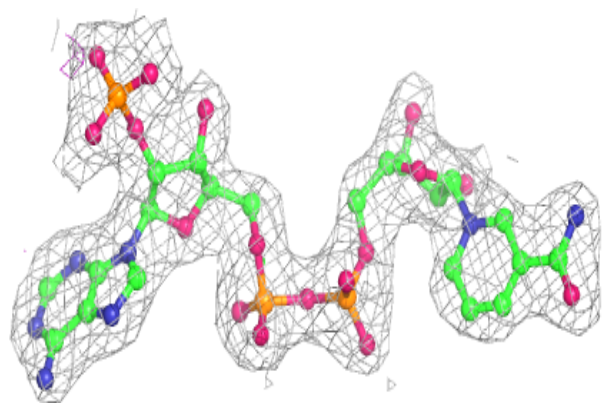


Electron density around NDP A 1500:

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

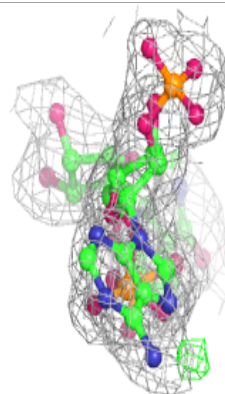
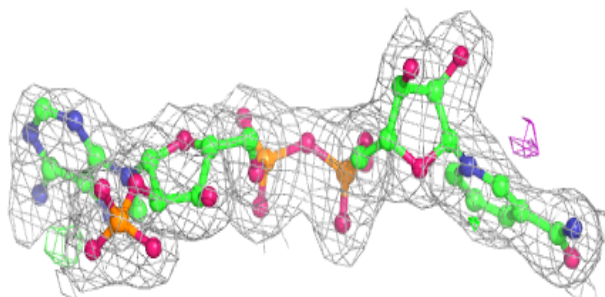
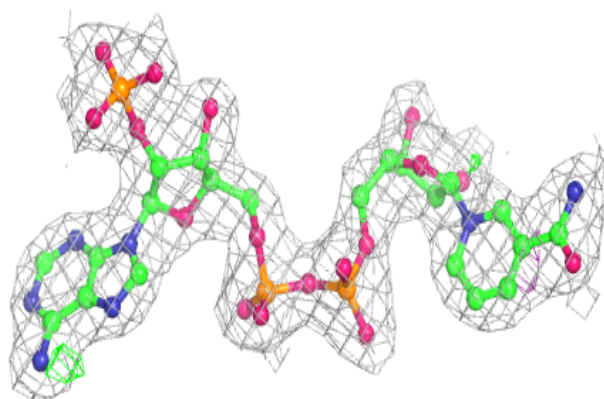
**Electron density around NDP C 3500:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

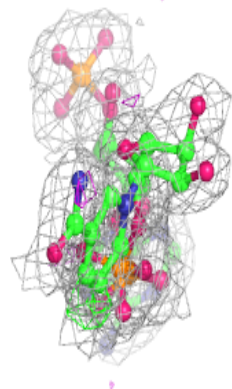
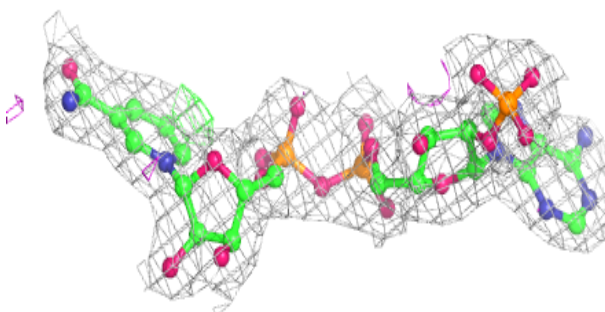
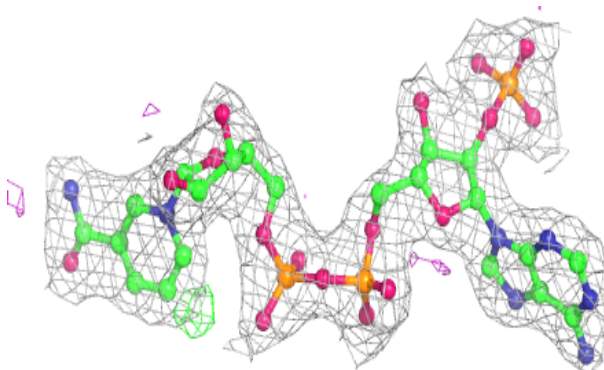


Electron density around NDP B 2500:

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

**Electron density around NDP E 5500:**

$2mF_o-DF_c$ (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.