



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 10:45 AM EDT

PDB ID : 3PRJ
Title : Role of Packing Defects in the Evolution of Allostery and Induced Fit in Human UDP-Glucose Dehydrogenase.
Authors : Kadirvelraj, R.; Wood, Z.A.
Deposited on : unknown
Resolution : 3.10 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

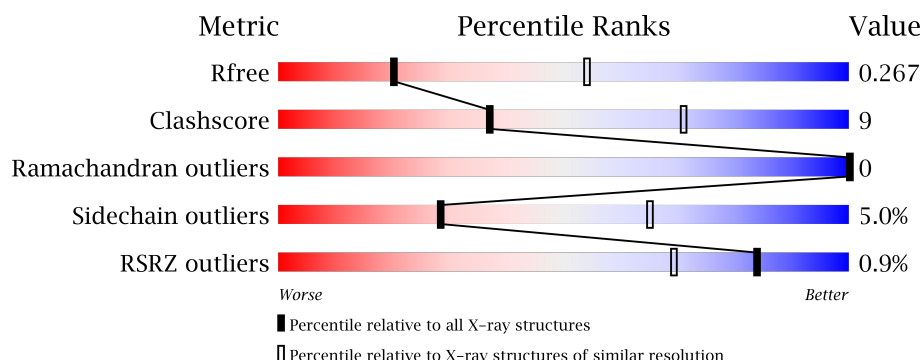
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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. 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	494	
1	B	494	
1	C	494	
1	D	494	
1	E	494	

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Mol	Chain	Length	Quality of chain
1	F	494	<div><div><div>%</div><div><div></div></div><div>81%</div><div>10%</div><div>• 7%</div></div></div>

2 Entry composition [i](#)

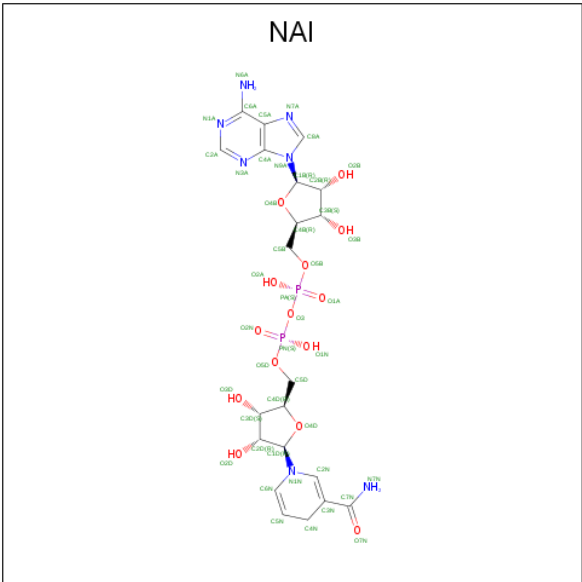
There are 4 unique types of molecules in this entry. The entry contains 22209 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-glucose 6-dehydrogenase.

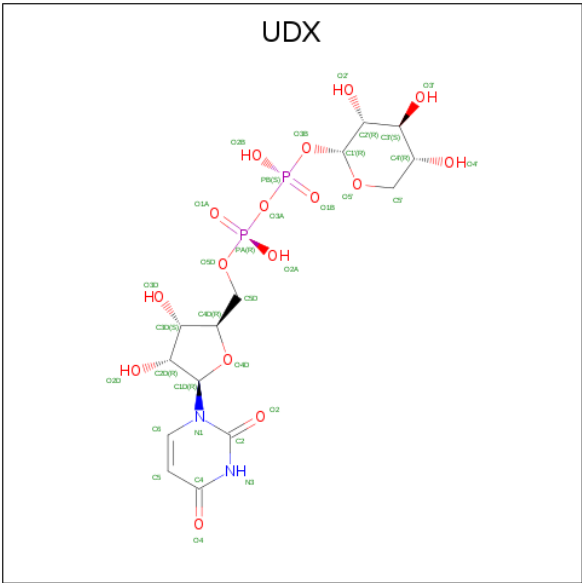
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	1	0
			3600	2278	621	681	20			
1	B	459	Total	C	N	O	S	0	1	0
			3600	2278	621	681	20			
1	C	459	Total	C	N	O	S	0	1	0
			3600	2278	621	681	20			
1	D	458	Total	C	N	O	S	0	1	0
			3593	2273	620	680	20			
1	E	459	Total	C	N	O	S	0	1	0
			3600	2278	621	681	20			
1	F	459	Total	C	N	O	S	0	1	0
			3600	2278	621	681	20			

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-XYLOPYRANOSE (three-letter code: UDX) (formula: C₁₄H₂₂N₂O₁₆P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
3	B	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
3	C	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
3	D	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
3	E	1	Total	C	N	O	P	0	0
			34	14	2	16	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			34	14	2	16	2		

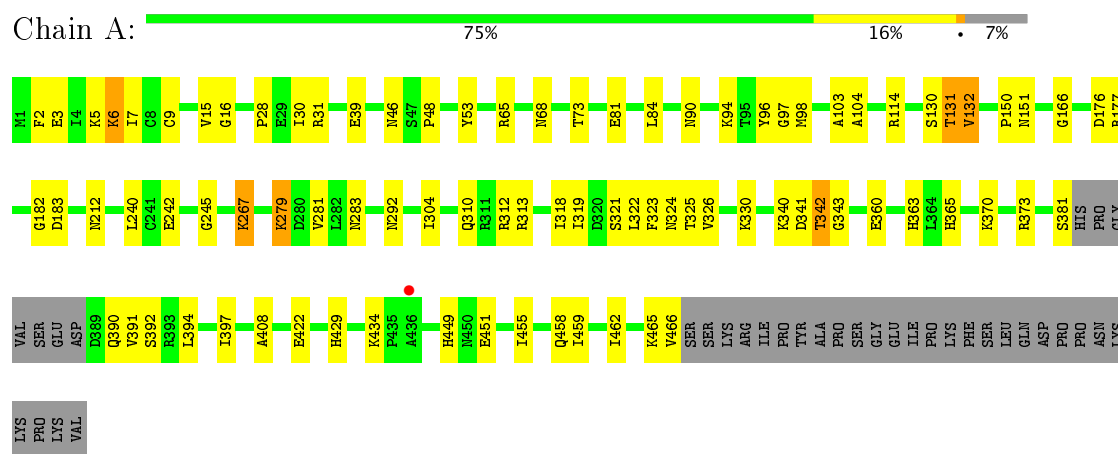
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total	O	0	0
			36	36		
4	B	32	Total	O	0	0
			32	32		
4	C	13	Total	O	0	0
			13	13		
4	D	23	Total	O	0	0
			23	23		
4	E	28	Total	O	0	0
			28	28		
4	F	16	Total	O	0	0
			16	16		

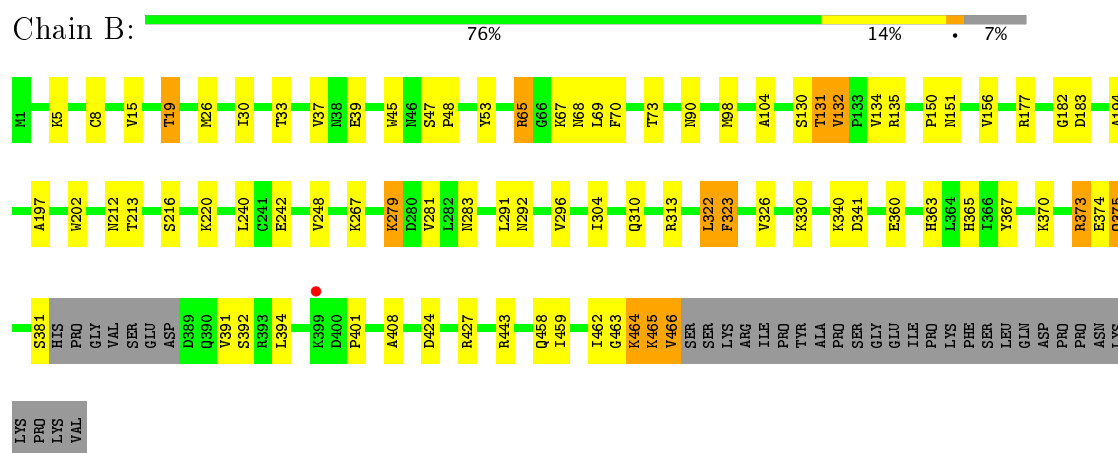
3 Residue-property plots

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.

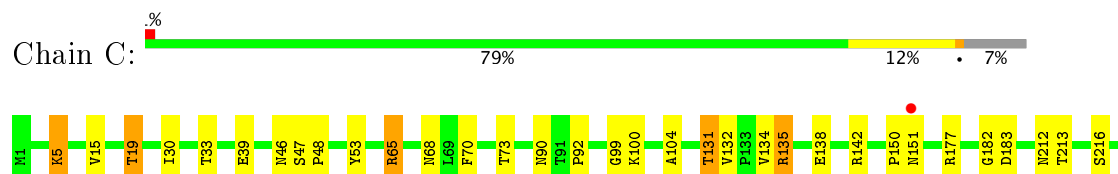
• Molecule 1: UDP-glucose 6-dehydrogenase

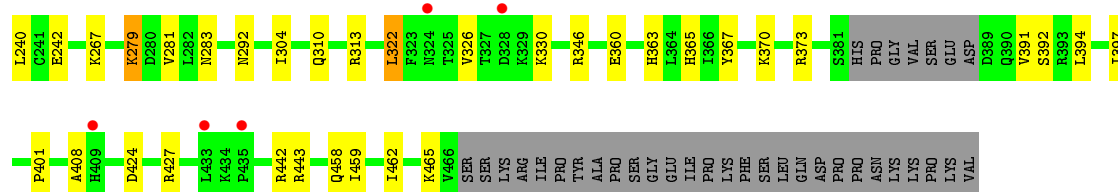


• Molecule 1: UDP-glucose 6-dehydrogenase

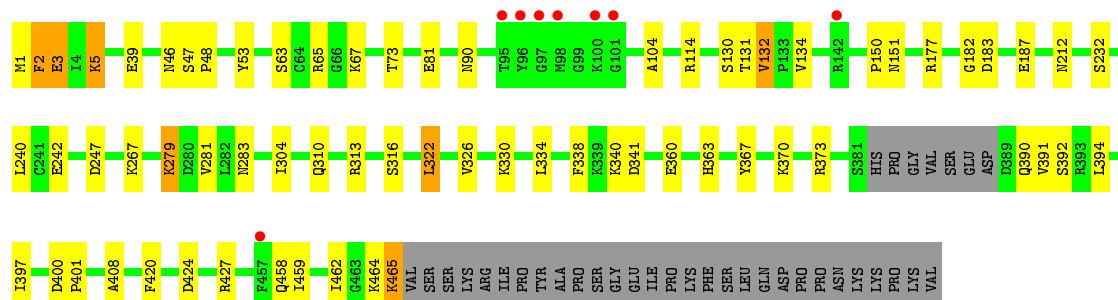
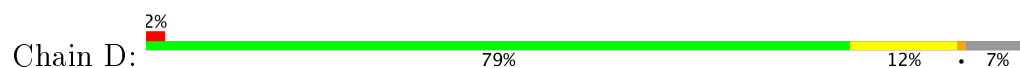


• Molecule 1: UDP-glucose 6-dehydrogenase

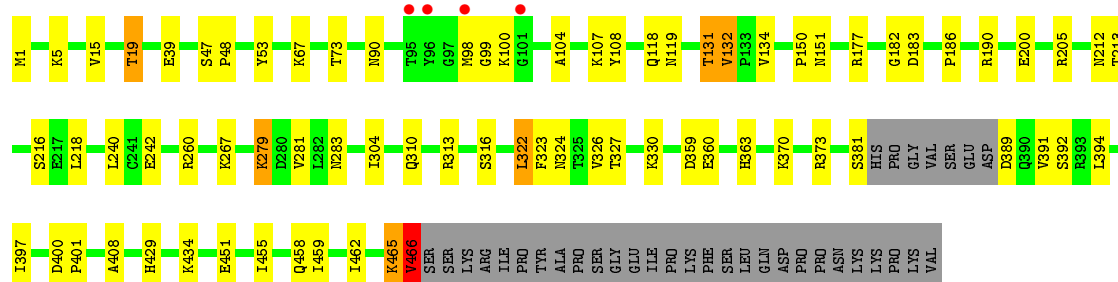
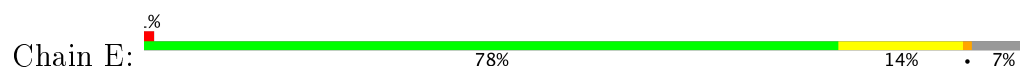




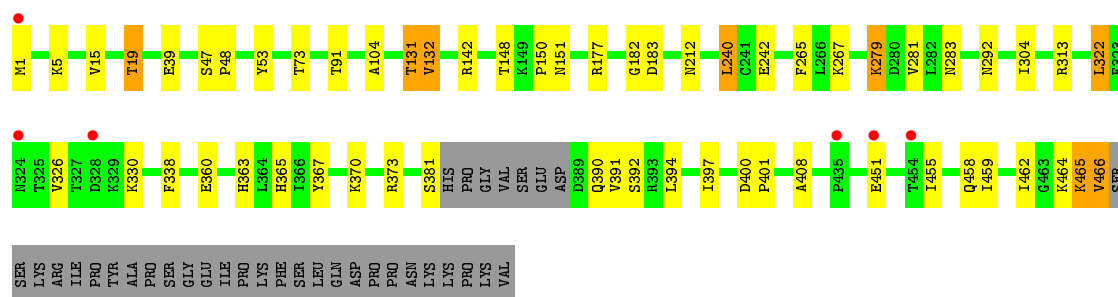
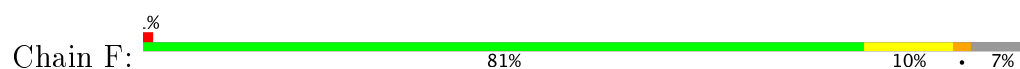
• Molecule 1: UDP-glucose 6-dehydrogenase



• Molecule 1: UDP-glucose 6-dehydrogenase



• Molecule 1: UDP-glucose 6-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.79Å 160.64Å 205.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.29 – 3.10 48.29 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.9 (48.29-3.10) 96.9 (48.29-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.01 (at 3.12Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.228 , 0.273 0.225 , 0.267	Depositor DCC
R_{free} test set	3314 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	59.3	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	22209	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.69	2/3668 (0.1%)	0.68	0/4963
1	B	0.69	1/3668 (0.0%)	0.65	0/4963
1	C	0.69	0/3668	0.65	0/4963
1	D	0.68	0/3661	0.66	0/4953
1	E	0.67	2/3668 (0.1%)	0.66	1/4963 (0.0%)
1	F	0.66	0/3668	0.65	0/4963
All	All	0.68	5/22001 (0.0%)	0.66	1/29768 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	CYS	CB-SG	-5.55	1.72	1.81
1	B	323	PHE	CE1-CZ	5.44	1.47	1.37
1	E	466	VAL	CA-CB	5.41	1.66	1.54
1	A	466	VAL	CA-CB	5.12	1.65	1.54
1	E	323	PHE	CE1-CZ	5.07	1.47	1.37

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	465	LYS	N-CA-C	5.53	125.93	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3600	0	3622	103	0
1	B	3600	0	3622	71	0
1	C	3600	0	3622	56	0
1	D	3593	0	3613	61	0
1	E	3600	0	3622	79	0
1	F	3600	0	3622	59	0
2	A	44	0	27	16	0
2	B	44	0	27	10	0
2	C	44	0	27	13	0
2	D	44	0	27	15	0
2	E	44	0	27	16	0
2	F	44	0	27	12	0
3	A	34	0	20	2	0
3	B	34	0	20	1	0
3	C	34	0	20	0	0
3	D	34	0	20	1	0
3	E	34	0	20	0	0
3	F	34	0	20	1	0
4	A	36	0	0	8	0
4	B	32	0	0	5	0
4	C	13	0	0	1	0
4	D	23	0	0	6	0
4	E	28	0	0	6	0
4	F	16	0	0	1	0
All	All	22209	0	22005	393	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 9.

All (393) 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:279:LYS:NZ	2:C:500:NAI:H6N	1.60	1.15
1:F:465:LYS:H	1:F:465:LYS:HD3	0.97	1.13
1:C:279:LYS:HZ2	2:C:500:NAI:H6N	1.10	1.11
1:A:98:MET:SD	1:E:316:SER:HB3	1.92	1.09
1:A:422:GLU:HG3	4:A:505:HOH:O	1.49	1.09
1:E:205:ARG:HG2	4:E:495:HOH:O	1.49	1.09
1:F:465:LYS:CD	1:F:465:LYS:H	1.66	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:GLN:HA	1:B:375:GLN:HE21	1.17	1.02
1:E:98:MET:HB2	4:E:503:HOH:O	1.59	1.01
1:D:2:PHE:CD2	1:D:3:GLU:N	2.30	1.00
1:A:46:ASN:HA	1:A:65:ARG:NH1	1.78	0.98
1:A:46:ASN:HA	1:A:65:ARG:HH11	1.26	0.97
1:B:375:GLN:CA	1:B:375:GLN:HE21	1.69	0.97
1:F:15:VAL:O	1:F:19:THR:HG22	1.66	0.94
1:F:465:LYS:HD3	1:F:465:LYS:N	1.68	0.93
1:D:2:PHE:C	1:D:2:PHE:HD2	1.71	0.92
1:A:96:TYR:OH	1:E:327:THR:HG23	1.69	0.92
1:A:279:LYS:HZ2	2:A:500:NAI:H6N	1.34	0.91
1:E:15:VAL:O	1:E:19:THR:HG22	1.70	0.91
1:A:322:LEU:HD23	1:A:326:VAL:HG12	1.52	0.90
1:D:2:PHE:C	1:D:2:PHE:CD2	2.40	0.90
1:F:279:LYS:HE3	2:F:500:NAI:C5N	2.03	0.89
1:C:15:VAL:O	1:C:19:THR:HG22	1.73	0.89
1:F:279:LYS:HE3	2:F:500:NAI:C6N	2.01	0.88
1:A:131:THR:HG22	2:A:500:NAI:H4D	1.56	0.88
1:B:15:VAL:O	1:B:19:THR:CG2	2.23	0.85
1:E:15:VAL:O	1:E:19:THR:CG2	2.24	0.85
1:F:15:VAL:O	1:F:19:THR:CG2	2.24	0.85
1:A:2:PHE:CD2	1:A:2:PHE:O	2.30	0.85
1:B:375:GLN:HA	1:B:375:GLN:NE2	1.87	0.84
1:A:325:THR:HG23	1:A:325:THR:O	1.77	0.83
1:D:2:PHE:HD2	1:D:3:GLU:N	1.70	0.83
1:E:389:ASP:HB2	4:E:517:HOH:O	1.78	0.83
1:A:96:TYR:OH	1:E:327:THR:CG2	2.28	0.82
1:B:323:PHE:HZ	1:F:142:ARG:HB3	1.42	0.82
1:B:15:VAL:O	1:B:19:THR:HG22	1.77	0.82
1:C:15:VAL:O	1:C:19:THR:CG2	2.28	0.80
1:E:90:ASN:HB2	2:E:500:NAI:H71N	1.46	0.80
1:F:465:LYS:CD	1:F:465:LYS:N	2.30	0.80
1:C:279:LYS:HE3	2:C:500:NAI:H5N	1.64	0.79
1:E:279:LYS:NZ	2:E:500:NAI:C6N	2.46	0.79
1:B:323:PHE:CZ	1:F:142:ARG:HB3	2.19	0.78
1:C:46:ASN:HA	1:C:65:ARG:HH11	1.50	0.77
1:C:279:LYS:CE	2:C:500:NAI:H6N	2.15	0.77
1:C:92:PRO:HA	2:C:500:NAI:H4N	1.67	0.77
1:A:97:GLY:HA3	1:E:360:GLU:CD	2.06	0.76
1:F:279:LYS:CE	2:F:500:NAI:C6N	2.65	0.74
1:C:279:LYS:NZ	2:C:500:NAI:C6N	2.47	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ASN:CA	1:A:65:ARG:NH1	2.50	0.74
1:A:46:ASN:C	1:A:65:ARG:HH12	1.91	0.73
1:C:142:ARG:NH1	4:C:503:HOH:O	2.23	0.72
1:C:279:LYS:HE3	2:C:500:NAI:C5N	2.20	0.72
1:E:279:LYS:HZ2	2:E:500:NAI:H6N	1.54	0.72
1:A:98:MET:CE	1:E:316:SER:HB3	2.20	0.71
1:B:375:GLN:CA	1:B:375:GLN:NE2	2.45	0.71
1:B:323:PHE:HZ	1:F:142:ARG:CB	2.04	0.71
1:A:279:LYS:NZ	2:A:500:NAI:H6N	2.04	0.71
1:E:279:LYS:HE3	2:E:500:NAI:C5N	2.20	0.71
1:A:98:MET:N	1:E:360:GLU:OE2	2.24	0.70
1:A:267:LYS:HG3	4:A:497:HOH:O	1.89	0.70
1:A:323:PHE:HE2	1:C:142:ARG:CZ	2.06	0.69
1:C:30:ILE:O	1:C:68:ASN:HB2	1.92	0.69
1:F:131:THR:HG22	2:F:500:NAI:H4D	1.73	0.69
1:B:465:LYS:O	1:B:466:VAL:HB	1.92	0.69
1:A:96:TYR:HE2	1:E:360:GLU:O	1.76	0.68
1:D:326:VAL:HG22	1:D:360:GLU:HB3	1.74	0.68
1:F:279:LYS:NZ	2:F:500:NAI:C6N	2.57	0.67
1:B:98:MET:SD	1:D:316:SER:HB3	2.35	0.67
1:D:3:GLU:HG2	1:D:5:LYS:HD3	1.77	0.67
1:E:242:GLU:CD	1:E:313:ARG:HH12	1.98	0.66
1:A:279:LYS:HE3	2:A:500:NAI:C5N	2.25	0.66
1:B:90:ASN:HB2	2:B:500:NAI:H71N	1.59	0.66
1:B:326:VAL:HG22	1:B:360:GLU:HB3	1.77	0.66
1:B:37:VAL:HG13	2:B:500:NAI:C2A	2.26	0.66
1:C:242:GLU:CD	1:C:313:ARG:HH12	1.99	0.66
1:A:98:MET:SD	1:E:316:SER:CB	2.80	0.66
1:B:242:GLU:CD	1:B:313:ARG:HH12	2.00	0.66
1:A:94:LYS:HD2	1:E:324:ASN:O	1.96	0.65
1:F:279:LYS:NZ	2:F:500:NAI:H6N	2.12	0.65
1:A:68:ASN:N	1:A:68:ASN:OD1	2.30	0.65
1:A:131:THR:CG2	2:A:500:NAI:H4D	2.26	0.65
1:B:322:LEU:HD23	1:B:326:VAL:HG12	1.79	0.65
1:F:326:VAL:HG22	1:F:360:GLU:HB3	1.79	0.64
1:E:326:VAL:HG22	1:E:360:GLU:HB3	1.79	0.64
1:B:30:ILE:O	1:B:68:ASN:HB2	1.97	0.64
1:A:322:LEU:HD12	1:A:322:LEU:N	2.11	0.64
1:D:326:VAL:CG2	1:D:360:GLU:HB3	2.27	0.64
1:A:326:VAL:HG22	1:A:360:GLU:HB3	1.80	0.64
1:F:279:LYS:HZ2	2:F:500:NAI:H6N	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ALA:H	1:C:283:ASN:HD21	1.45	0.63
1:F:279:LYS:HG2	2:F:500:NAI:H6N	1.78	0.63
1:C:326:VAL:HG22	1:C:360:GLU:HB3	1.80	0.63
1:E:326:VAL:CG2	1:E:360:GLU:HB3	2.28	0.63
1:B:374:GLU:N	1:B:374:GLU:OE1	2.29	0.63
1:B:374:GLU:CD	1:B:374:GLU:H	2.00	0.63
1:A:97:GLY:CA	1:E:360:GLU:OE2	2.47	0.63
1:B:326:VAL:CG2	1:B:360:GLU:HB3	2.29	0.63
1:A:242:GLU:CD	1:A:313:ARG:HH12	2.00	0.62
1:A:342:THR:OG1	1:A:343:GLY:N	2.33	0.62
1:D:3:GLU:HG2	1:D:5:LYS:CD	2.29	0.62
1:A:279:LYS:NZ	2:A:500:NAI:C6N	2.63	0.62
1:B:340:LYS:O	1:B:341:ASP:HB2	2.00	0.62
1:B:292:ASN:ND2	1:C:292:ASN:HB2	2.15	0.61
1:C:279:LYS:HE3	2:C:500:NAI:C6N	2.31	0.61
1:E:118:GLN:HB3	4:E:515:HOH:O	1.99	0.61
1:D:322:LEU:HD23	1:D:326:VAL:HG12	1.80	0.61
1:E:279:LYS:HZ2	2:E:500:NAI:C6N	2.12	0.61
3:A:501:UDX:O2A	3:A:501:UDX:H1'	1.99	0.61
1:B:15:VAL:O	1:B:19:THR:HG23	2.00	0.61
1:A:310:GLN:OE1	1:A:313:ARG:NH2	2.31	0.61
1:F:242:GLU:CD	1:F:313:ARG:HH12	2.04	0.61
1:E:131:THR:HG22	2:E:500:NAI:H4D	1.83	0.61
1:B:65:ARG:HA	1:B:69:LEU:HB3	1.82	0.60
1:A:319:ILE:HG22	1:A:324:ASN:HA	1.83	0.60
1:F:91:THR:H	2:F:500:NAI:H2D	1.67	0.60
1:D:3:GLU:CG	1:D:5:LYS:HD3	2.31	0.59
1:A:48:PRO:HG2	4:A:514:HOH:O	2.02	0.59
1:B:466:VAL:HG12	4:B:517:HOH:O	2.00	0.59
1:A:46:ASN:C	1:A:65:ARG:NH1	2.56	0.59
1:D:279:LYS:HE3	2:D:500:NAI:C6N	2.33	0.59
1:A:326:VAL:CG2	1:A:360:GLU:HB3	2.33	0.59
1:D:279:LYS:NZ	2:D:500:NAI:H1D	2.18	0.59
1:E:104:ALA:H	1:E:283:ASN:HD21	1.51	0.59
1:E:322:LEU:HD23	1:E:326:VAL:HG12	1.85	0.59
1:D:242:GLU:CD	1:D:313:ARG:HH12	2.06	0.58
1:C:326:VAL:CG2	1:C:360:GLU:HB3	2.32	0.58
1:D:104:ALA:H	1:D:283:ASN:HD21	1.51	0.58
1:D:340:LYS:O	1:D:341:ASP:HB2	2.02	0.58
1:C:53:TYR:CD1	1:C:370:LYS:HE2	2.38	0.58
1:F:465:LYS:HD3	1:F:465:LYS:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ARG:NH1	1:E:434:LYS:O	2.32	0.58
1:E:279:LYS:NZ	2:E:500:NAI:H1D	2.19	0.58
1:D:130:SER:HB2	2:D:500:NAI:O3D	2.03	0.57
1:A:323:PHE:CE2	1:C:142:ARG:CZ	2.87	0.57
1:E:330:LYS:HB3	1:E:408:ALA:HA	1.86	0.57
1:F:326:VAL:CG2	1:F:360:GLU:HB3	2.33	0.57
1:D:279:LYS:NZ	2:D:500:NAI:H6N	2.20	0.57
1:B:39:GLU:HG3	1:B:73:THR:HG21	1.86	0.57
1:F:39:GLU:HG3	1:F:73:THR:HG21	1.85	0.57
1:A:322:LEU:CD2	1:A:326:VAL:HG12	2.31	0.57
1:C:39:GLU:HG3	1:C:73:THR:HG21	1.86	0.57
1:A:94:LYS:NZ	1:E:324:ASN:O	2.37	0.57
1:A:325:THR:CG2	1:A:325:THR:O	2.49	0.56
1:C:279:LYS:CE	2:C:500:NAI:C6N	2.83	0.56
1:C:281:VAL:HB	1:C:304:ILE:HD11	1.86	0.56
1:E:279:LYS:HG2	2:E:500:NAI:H6N	1.86	0.56
1:C:330:LYS:HB3	1:C:408:ALA:HA	1.86	0.56
1:A:96:TYR:CE2	1:E:360:GLU:O	2.56	0.56
1:C:46:ASN:HA	1:C:65:ARG:NH1	2.20	0.56
1:C:150:PRO:O	1:C:151:ASN:HB2	2.05	0.56
1:B:279:LYS:NZ	2:B:500:NAI:C6N	2.69	0.56
1:B:90:ASN:HB2	2:B:500:NAI:N7N	2.20	0.56
1:D:279:LYS:HZ2	2:D:500:NAI:H6N	1.71	0.56
1:A:94:LYS:CE	1:E:324:ASN:O	2.54	0.56
1:A:97:GLY:HA3	1:E:360:GLU:OE1	2.06	0.56
1:F:330:LYS:HB3	1:F:408:ALA:HA	1.88	0.55
1:D:187:GLU:HB2	4:D:495:HOH:O	2.05	0.55
1:D:39:GLU:HG3	1:D:73:THR:HG21	1.87	0.55
1:A:176:ASP:HB2	4:A:506:HOH:O	2.05	0.55
1:F:279:LYS:NZ	2:F:500:NAI:H1D	2.21	0.55
1:F:281:VAL:HB	1:F:304:ILE:HD11	1.88	0.55
1:A:340:LYS:O	1:A:341:ASP:HB2	2.05	0.55
1:A:279:LYS:HE3	2:A:500:NAI:C6N	2.37	0.55
1:E:150:PRO:O	1:E:151:ASN:HB2	2.06	0.55
1:E:279:LYS:CE	2:E:500:NAI:C6N	2.85	0.55
1:F:322:LEU:HD23	1:F:326:VAL:HG12	1.89	0.55
1:E:279:LYS:HE3	2:E:500:NAI:C6N	2.37	0.55
1:F:104:ALA:H	1:F:283:ASN:HD21	1.52	0.55
1:C:322:LEU:HD23	1:C:326:VAL:HG12	1.88	0.54
1:A:322:LEU:N	1:A:322:LEU:CD1	2.69	0.54
1:C:182:GLY:O	1:C:212:ASN:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:ASN:HA	2:C:500:NAI:H2D	1.89	0.54
1:E:279:LYS:HZ1	2:E:500:NAI:H1D	1.73	0.54
1:D:281:VAL:HB	1:D:304:ILE:HD11	1.90	0.54
1:B:465:LYS:O	1:B:466:VAL:CB	2.54	0.54
1:A:292:ASN:ND2	1:F:292:ASN:HB2	2.23	0.54
1:B:373:ARG:HG2	1:B:374:GLU:N	2.22	0.54
1:E:131:THR:HG22	2:E:500:NAI:O4D	2.07	0.54
1:B:150:PRO:O	1:B:151:ASN:HB2	2.08	0.53
1:E:326:VAL:CG2	1:E:360:GLU:CB	2.85	0.53
1:C:326:VAL:CG2	1:C:360:GLU:CB	2.87	0.53
1:B:220:LYS:NZ	3:B:501:UDX:O4'	2.41	0.53
1:D:326:VAL:CG2	1:D:360:GLU:CB	2.87	0.53
1:E:465:LYS:HG2	1:E:465:LYS:O	2.08	0.53
1:B:182:GLY:O	1:B:212:ASN:HA	2.09	0.53
1:B:281:VAL:HB	1:B:304:ILE:HD11	1.91	0.53
1:B:330:LYS:HB3	1:B:408:ALA:HA	1.90	0.53
1:B:375:GLN:C	1:B:375:GLN:HE21	2.10	0.53
1:C:442:ARG:O	1:C:443:ARG:HB2	2.09	0.53
1:D:330:LYS:HB3	1:D:408:ALA:HA	1.91	0.53
1:A:373:ARG:HB3	1:A:397:ILE:HG21	1.90	0.53
1:F:279:LYS:CE	2:F:500:NAI:H6N	2.38	0.53
1:E:131:THR:HG22	2:E:500:NAI:C4D	2.40	0.52
1:A:312:ARG:HD2	4:A:507:HOH:O	2.09	0.52
1:B:104:ALA:H	1:B:283:ASN:HD21	1.58	0.52
1:B:326:VAL:CG2	1:B:360:GLU:CB	2.87	0.52
1:F:330:LYS:HE2	1:F:365:HIS:NE2	2.23	0.52
1:B:466:VAL:CG1	4:B:517:HOH:O	2.56	0.52
1:B:45:TRP:O	1:B:65:ARG:NH1	2.43	0.52
1:D:232:SER:HA	4:D:506:HOH:O	2.09	0.52
1:C:131:THR:HG22	2:C:500:NAI:O3D	2.10	0.52
1:B:213:THR:N	4:B:523:HOH:O	2.42	0.51
1:B:296:VAL:HG23	4:B:528:HOH:O	2.10	0.51
1:B:279:LYS:HZ2	2:B:500:NAI:H6N	1.74	0.51
1:F:373:ARG:HB3	1:F:397:ILE:HG21	1.91	0.51
1:A:97:GLY:CA	1:E:360:GLU:CD	2.79	0.51
1:A:104:ALA:H	1:A:283:ASN:HD21	1.58	0.51
1:D:182:GLY:O	1:D:212:ASN:HA	2.11	0.51
1:A:2:PHE:CG	1:A:2:PHE:O	2.56	0.51
1:A:323:PHE:HE2	1:C:142:ARG:NH1	2.09	0.51
1:D:279:LYS:NZ	2:D:500:NAI:C6N	2.73	0.51
1:A:323:PHE:HZ	1:C:138:GLU:HG2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:VAL:O	1:F:132:VAL:HG22	2.11	0.51
1:A:279:LYS:HZ2	2:A:500:NAI:C6N	2.11	0.51
1:C:279:LYS:HE3	2:C:500:NAI:H6N	1.89	0.51
1:A:96:TYR:HB2	1:E:359:ASP:O	2.11	0.50
1:A:98:MET:O	1:E:324:ASN:OD1	2.28	0.50
1:F:150:PRO:O	1:F:151:ASN:HB2	2.11	0.50
1:D:53:TYR:CD1	1:D:370:LYS:HE2	2.47	0.50
1:E:281:VAL:HB	1:E:304:ILE:HD11	1.94	0.50
1:A:324:ASN:O	1:A:324:ASN:OD1	2.30	0.50
1:F:465:LYS:O	1:F:466:VAL:O	2.30	0.50
1:A:39:GLU:HG3	1:A:73:THR:HG21	1.94	0.50
1:D:90:ASN:HA	2:D:500:NAI:H2D	1.93	0.50
1:E:1:MET:HG3	1:E:190:ARG:HH11	1.76	0.50
1:E:182:GLY:O	1:E:212:ASN:HA	2.12	0.50
1:B:464:LYS:C	1:B:465:LYS:HG3	2.32	0.49
1:A:323:PHE:CE2	1:C:142:ARG:NH1	2.80	0.49
1:E:373:ARG:HB3	1:E:397:ILE:HG21	1.95	0.49
1:F:53:TYR:CD1	1:F:370:LYS:HE2	2.48	0.49
1:A:103:ALA:HB1	4:A:495:HOH:O	2.10	0.49
1:A:318:ILE:O	1:A:322:LEU:HD13	2.12	0.49
1:B:53:TYR:CD1	1:B:370:LYS:HE2	2.48	0.49
1:A:94:LYS:CD	1:E:324:ASN:O	2.61	0.49
1:E:400:ASP:HB2	1:E:401:PRO:HD2	1.95	0.49
1:C:346:ARG:NH1	2:C:500:NAI:O1N	2.35	0.48
1:D:132:VAL:O	1:D:132:VAL:HG22	2.13	0.48
1:E:39:GLU:HG3	1:E:73:THR:HG21	1.95	0.48
1:A:150:PRO:O	1:A:151:ASN:HB2	2.12	0.48
1:E:242:GLU:HB3	1:E:466:VAL:HB	1.94	0.48
1:A:326:VAL:CG2	1:A:360:GLU:CB	2.91	0.48
1:E:131:THR:CG2	2:E:500:NAI:H4D	2.42	0.48
1:A:330:LYS:HB3	1:A:408:ALA:HA	1.95	0.48
1:A:53:TYR:CD1	1:A:370:LYS:HE2	2.49	0.48
1:B:465:LYS:HB2	1:B:466:VAL:H	1.48	0.48
1:C:330:LYS:HE2	1:C:365:HIS:NE2	2.28	0.48
1:D:114:ARG:HD2	4:D:515:HOH:O	2.14	0.48
1:D:424:ASP:OD2	1:D:427:ARG:HB2	2.14	0.48
1:E:279:LYS:HZ1	2:E:500:NAI:C6N	2.26	0.48
1:A:28:PRO:HA	1:A:68:ASN:ND2	2.28	0.48
1:A:130:SER:HB2	2:A:500:NAI:O3D	2.14	0.48
1:C:330:LYS:HE2	1:C:365:HIS:CE1	2.48	0.48
1:D:373:ARG:HB3	1:D:397:ILE:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:VAL:O	1:E:132:VAL:HG22	2.14	0.48
1:C:367:TYR:CE2	1:C:401:PRO:HD3	2.49	0.47
1:B:90:ASN:HA	2:B:500:NAI:H2D	1.97	0.47
1:C:373:ARG:HB3	1:C:397:ILE:HG21	1.95	0.47
1:C:15:VAL:O	1:C:19:THR:HG23	2.14	0.47
1:F:326:VAL:CG2	1:F:360:GLU:CB	2.93	0.47
1:B:363:HIS:HD2	1:B:394:LEU:HD23	1.79	0.47
1:C:363:HIS:HD2	1:C:394:LEU:HD23	1.79	0.47
1:A:279:LYS:CE	2:A:500:NAI:C6N	2.92	0.47
1:B:90:ASN:CB	2:B:500:NAI:H71N	2.23	0.47
1:D:150:PRO:O	1:D:151:ASN:HB2	2.15	0.47
1:F:330:LYS:HE2	1:F:365:HIS:CE1	2.49	0.47
1:D:81:GLU:CB	4:D:518:HOH:O	2.62	0.47
1:A:90:ASN:HA	2:A:500:NAI:H2D	1.97	0.47
1:A:132:VAL:HG22	1:A:132:VAL:O	2.15	0.47
1:A:281:VAL:HB	1:A:304:ILE:HD11	1.96	0.46
1:B:65:ARG:HE	1:B:65:ARG:HB3	1.51	0.46
1:D:279:LYS:CE	2:D:500:NAI:C6N	2.94	0.46
1:A:7:ILE:HD13	1:A:84:LEU:HD23	1.96	0.46
1:F:330:LYS:HE2	1:F:365:HIS:CD2	2.51	0.46
1:D:310:GLN:OE1	1:D:313:ARG:NH2	2.40	0.46
1:E:15:VAL:O	1:E:19:THR:HG23	2.10	0.46
1:A:16:GLY:N	4:A:499:HOH:O	2.39	0.46
1:A:30:ILE:O	1:A:68:ASN:HB2	2.16	0.46
1:A:2:PHE:O	1:A:2:PHE:HD2	1.96	0.45
1:A:451:GLU:O	1:A:455:ILE:HG13	2.16	0.45
1:F:338:PHE:HE1	3:F:501:UDX:H5A2	1.81	0.45
1:A:330:LYS:HE2	1:A:365:HIS:CE1	2.51	0.45
1:D:47:SER:HB2	1:D:48:PRO:HD2	1.97	0.45
1:F:363:HIS:HD2	1:F:394:LEU:HD23	1.81	0.45
1:D:267:LYS:HE3	4:D:509:HOH:O	2.17	0.45
1:B:248:VAL:HG12	1:B:463:GLY:HA3	1.98	0.45
1:D:279:LYS:HG2	2:D:500:NAI:H6N	1.99	0.45
1:A:292:ASN:CG	1:F:292:ASN:ND2	2.70	0.45
1:A:131:THR:HG23	1:A:132:VAL:HG12	1.97	0.45
1:D:400:ASP:HB2	1:D:401:PRO:HD2	1.99	0.45
1:D:46:ASN:HA	1:D:65:ARG:HH11	1.81	0.45
1:B:367:TYR:CE2	1:B:401:PRO:HD3	2.52	0.45
1:C:424:ASP:OD2	1:C:427:ARG:HB2	2.17	0.45
1:B:323:PHE:CZ	1:F:142:ARG:CB	2.89	0.45
1:F:451:GLU:O	1:F:455:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:HIS:CE1	1:A:434:LYS:HE3	2.52	0.45
3:A:501:UDX:C1'	3:A:501:UDX:O2A	2.65	0.45
1:B:291:LEU:O	1:B:292:ASN:HB3	2.17	0.45
1:B:424:ASP:OD2	1:B:427:ARG:HB2	2.16	0.45
1:D:90:ASN:HB2	2:D:500:NAI:H71N	1.82	0.45
1:B:292:ASN:HD21	1:C:292:ASN:HB2	1.81	0.44
1:D:63:SER:O	1:D:67:LYS:HE3	2.18	0.44
1:D:2:PHE:CE2	1:D:3:GLU:C	2.90	0.44
1:E:90:ASN:HB2	2:E:500:NAI:N7N	2.23	0.44
1:F:182:GLY:O	1:F:212:ASN:HA	2.17	0.44
1:E:119:ASN:ND2	4:E:515:HOH:O	2.49	0.44
1:E:53:TYR:CD1	1:E:370:LYS:HE2	2.53	0.44
1:D:465:LYS:HA	1:D:465:LYS:HD3	1.72	0.43
1:D:90:ASN:CB	2:D:500:NAI:H71N	2.31	0.43
1:E:131:THR:HG23	1:E:132:VAL:HG12	2.00	0.43
1:F:400:ASP:HB2	1:F:401:PRO:HD2	2.00	0.43
1:F:148:THR:HG22	4:F:502:HOH:O	2.17	0.43
1:A:321:SER:C	1:A:322:LEU:HD12	2.39	0.43
1:B:279:LYS:HE3	2:B:500:NAI:C5N	2.48	0.43
1:A:6:LYS:HE2	1:A:31:ARG:HD3	1.99	0.43
1:D:279:LYS:HE3	2:D:500:NAI:C5N	2.47	0.43
1:F:279:LYS:HZ1	2:F:500:NAI:H1D	1.84	0.43
1:A:97:GLY:HA3	1:E:360:GLU:OE2	2.13	0.43
1:A:182:GLY:O	1:A:212:ASN:HA	2.18	0.43
1:A:279:LYS:HE3	2:A:500:NAI:H5N	1.99	0.43
1:A:397:ILE:N	1:A:397:ILE:HD12	2.33	0.43
1:F:363:HIS:CD2	1:F:394:LEU:HD23	2.54	0.43
1:A:15:VAL:HG21	2:A:500:NAI:C5D	2.49	0.43
1:A:245:GLY:HA2	1:A:465:LYS:HB2	2.00	0.43
1:D:338:PHE:HE1	3:D:501:UDX:H5A2	1.84	0.43
1:C:363:HIS:CD2	1:C:394:LEU:HD23	2.54	0.42
1:D:279:LYS:HZ1	2:D:500:NAI:H1D	1.84	0.42
1:A:96:TYR:HH	1:E:327:THR:HG23	1.78	0.42
1:F:15:VAL:O	1:F:19:THR:HG23	2.13	0.42
1:F:47:SER:HB2	1:F:48:PRO:HD2	2.01	0.42
1:A:15:VAL:CG2	2:A:500:NAI:H51N	2.49	0.42
1:B:47:SER:HB2	1:B:48:PRO:HD2	2.01	0.42
1:E:99:GLY:O	1:E:100:LYS:C	2.58	0.42
1:E:310:GLN:OE1	1:E:313:ARG:NH2	2.38	0.42
1:A:449:HIS:CD2	4:A:508:HOH:O	2.73	0.42
1:F:390:GLN:HG2	1:F:394:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ARG:HB3	1:D:65:ARG:HE	1.64	0.42
1:E:429:HIS:CE1	1:E:434:LYS:HE3	2.55	0.42
1:A:279:LYS:HG2	2:A:500:NAI:H6N	2.01	0.42
1:B:330:LYS:HE2	1:B:365:HIS:NE2	2.34	0.42
1:D:279:LYS:HZ2	2:D:500:NAI:H1D	1.84	0.42
1:C:310:GLN:OE1	1:C:313:ARG:NH2	2.39	0.42
1:D:367:TYR:CE2	1:D:401:PRO:HD3	2.55	0.42
1:B:156:VAL:HG23	4:B:526:HOH:O	2.20	0.42
1:D:279:LYS:CE	2:D:500:NAI:H6N	2.49	0.42
1:D:81:GLU:HB3	4:D:518:HOH:O	2.20	0.42
1:E:465:LYS:O	1:E:465:LYS:CG	2.67	0.42
1:F:367:TYR:CE2	1:F:401:PRO:HD3	2.54	0.42
1:B:310:GLN:OE1	1:B:313:ARG:NH2	2.39	0.42
1:E:186:PRO:HG2	4:E:499:HOH:O	2.20	0.41
1:D:390:GLN:HG2	1:D:394:LEU:HD12	2.02	0.41
1:B:330:LYS:HE2	1:B:365:HIS:CD2	2.56	0.41
1:B:26:MET:HG3	1:B:202:TRP:CG	2.55	0.41
1:C:330:LYS:HE2	1:C:365:HIS:CD2	2.55	0.41
1:E:242:GLU:OE1	1:E:313:ARG:NH1	2.53	0.41
1:A:390:GLN:HG2	1:A:394:LEU:HD12	2.02	0.41
1:B:131:THR:HG23	1:B:132:VAL:HG12	2.02	0.41
1:A:292:ASN:HD21	1:F:292:ASN:HB2	1.84	0.41
1:A:279:LYS:CE	2:A:500:NAI:H6N	2.50	0.41
1:C:242:GLU:OE1	1:C:313:ARG:NH1	2.53	0.41
1:D:1:MET:HE2	1:D:1:MET:HB3	1.67	0.41
1:D:247:ASP:C	1:D:247:ASP:OD2	2.58	0.41
1:E:200:GLU:OE1	1:E:205:ARG:HD3	2.20	0.41
1:E:213:THR:O	1:E:216:SER:HB3	2.20	0.41
1:B:130:SER:HB2	2:B:500:NAI:O3D	2.20	0.41
1:B:363:HIS:CD2	1:B:394:LEU:HD23	2.54	0.41
1:B:443:ARG:HA	1:B:443:ARG:HD2	1.90	0.41
1:D:363:HIS:HD2	1:D:394:LEU:HD23	1.85	0.41
1:C:213:THR:O	1:C:216:SER:HB3	2.20	0.41
1:D:1:MET:HE3	1:D:1:MET:CA	2.51	0.41
1:E:451:GLU:O	1:E:455:ILE:HG13	2.20	0.41
1:B:194:ALA:O	1:B:197:ALA:HB3	2.21	0.41
1:D:334:LEU:HB3	1:D:420:PHE:CZ	2.56	0.41
1:E:218:LEU:HD11	1:F:240:LEU:HD13	2.03	0.41
1:E:260:ARG:HD2	1:F:265:PHE:CE1	2.56	0.41
1:E:363:HIS:HD2	1:E:394:LEU:HD23	1.85	0.41
1:F:131:THR:HG23	1:F:132:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:397:ILE:N	1:F:397:ILE:HD12	2.36	0.41
1:A:363:HIS:HD2	1:A:394:LEU:HD23	1.86	0.41
1:B:33:THR:HG23	1:B:70:PHE:HB2	2.02	0.41
1:C:99:GLY:O	1:C:100:LYS:C	2.59	0.41
1:A:46:ASN:O	1:A:65:ARG:NH1	2.54	0.40
1:A:6:LYS:NZ	1:A:81:GLU:OE1	2.45	0.40
1:E:107:LYS:HE3	1:E:108:TYR:CZ	2.56	0.40
1:F:465:LYS:HD2	1:F:465:LYS:N	2.30	0.40
1:B:279:LYS:HG2	2:B:500:NAI:H6N	2.02	0.40
1:E:47:SER:HB2	1:E:48:PRO:HD2	2.03	0.40
1:B:213:THR:O	1:B:216:SER:HB3	2.22	0.40
1:C:135:ARG:NH1	1:C:138:GLU:OE1	2.54	0.40
1:C:5:LYS:HB2	1:C:5:LYS:HE3	1.95	0.40
1:C:33:THR:HG23	1:C:70:PHE:HB2	2.04	0.40
1:E:397:ILE:N	1:E:397:ILE:HD12	2.36	0.40
1:A:166:GLY:HA2	1:A:341:ASP:O	2.21	0.40
1:C:47:SER:HB2	1:C:48:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	456/494 (92%)	433 (95%)	23 (5%)	0	100	100
1	B	456/494 (92%)	428 (94%)	28 (6%)	0	100	100
1	C	456/494 (92%)	435 (95%)	21 (5%)	0	100	100
1	D	455/494 (92%)	428 (94%)	27 (6%)	0	100	100
1	E	456/494 (92%)	431 (94%)	25 (6%)	0	100	100
1	F	456/494 (92%)	432 (95%)	24 (5%)	0	100	100
All	All	2735/2964 (92%)	2587 (95%)	148 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	395/426 (93%)	378 (96%)	17 (4%)	33	70
1	B	395/426 (93%)	369 (93%)	26 (7%)	19	54
1	C	395/426 (93%)	376 (95%)	19 (5%)	30	67
1	D	394/426 (92%)	376 (95%)	18 (5%)	31	68
1	E	395/426 (93%)	376 (95%)	19 (5%)	30	67
1	F	395/426 (93%)	375 (95%)	20 (5%)	28	64
All	All	2369/2556 (93%)	2250 (95%)	119 (5%)	28	65

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	5	LYS
1	A	6	LYS
1	A	131	THR
1	A	132	VAL
1	A	177	ARG
1	A	183	ASP
1	A	240	LEU
1	A	267	LYS
1	A	279	LYS
1	A	342	THR
1	A	381	SER
1	A	391	VAL
1	A	392	SER
1	A	458	GLN
1	A	459	ILE
1	A	462	ILE
1	B	5	LYS
1	B	8	CYS

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Mol	Chain	Res	Type
1	B	19	THR
1	B	65	ARG
1	B	67	LYS
1	B	131	THR
1	B	132	VAL
1	B	134	VAL
1	B	135	ARG
1	B	177	ARG
1	B	183	ASP
1	B	240	LEU
1	B	267	LYS
1	B	279	LYS
1	B	322	LEU
1	B	373	ARG
1	B	375	GLN
1	B	381	SER
1	B	391	VAL
1	B	392	SER
1	B	458	GLN
1	B	459	ILE
1	B	462	ILE
1	B	464	LYS
1	B	465	LYS
1	B	466	VAL
1	C	5	LYS
1	C	19	THR
1	C	65	ARG
1	C	131	THR
1	C	132	VAL
1	C	134	VAL
1	C	135	ARG
1	C	177	ARG
1	C	183	ASP
1	C	240	LEU
1	C	267	LYS
1	C	279	LYS
1	C	322	LEU
1	C	391	VAL
1	C	392	SER
1	C	458	GLN
1	C	459	ILE
1	C	462	ILE

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Mol	Chain	Res	Type
1	C	465	LYS
1	D	2	PHE
1	D	3	GLU
1	D	5	LYS
1	D	131	THR
1	D	132	VAL
1	D	134	VAL
1	D	177	ARG
1	D	183	ASP
1	D	240	LEU
1	D	279	LYS
1	D	322	LEU
1	D	391	VAL
1	D	392	SER
1	D	458	GLN
1	D	459	ILE
1	D	462	ILE
1	D	464	LYS
1	D	465	LYS
1	E	5	LYS
1	E	19	THR
1	E	67	LYS
1	E	131	THR
1	E	132	VAL
1	E	134	VAL
1	E	177	ARG
1	E	183	ASP
1	E	240	LEU
1	E	267	LYS
1	E	279	LYS
1	E	322	LEU
1	E	381	SER
1	E	391	VAL
1	E	392	SER
1	E	458	GLN
1	E	459	ILE
1	E	462	ILE
1	E	466	VAL
1	F	1	MET
1	F	5	LYS
1	F	19	THR
1	F	131	THR

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Mol	Chain	Res	Type
1	F	132	VAL
1	F	177	ARG
1	F	183	ASP
1	F	240	LEU
1	F	267	LYS
1	F	279	LYS
1	F	322	LEU
1	F	381	SER
1	F	391	VAL
1	F	392	SER
1	F	458	GLN
1	F	459	ILE
1	F	462	ILE
1	F	464	LYS
1	F	465	LYS
1	F	466	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	ASN
1	A	292	ASN
1	A	363	HIS
1	B	229	GLN
1	B	283	ASN
1	B	292	ASN
1	B	375	GLN
1	C	25	HIS
1	C	151	ASN
1	C	283	ASN
1	C	292	ASN
1	C	363	HIS
1	C	429	HIS
1	D	283	ASN
1	D	363	HIS
1	E	153	ASN
1	E	155	GLN
1	E	229	GLN
1	E	283	ASN
1	E	363	HIS
1	F	283	ASN
1	F	292	ASN

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Mol	Chain	Res	Type
1	F	363	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	NAI	A	500	-	40,48,48	1.83	8 (20%)	41,73,73	1.93	9 (21%)
3	UDX	A	501	-	29,36,36	1.44	3 (10%)	37,55,55	2.05	7 (18%)
2	NAI	B	500	-	40,48,48	1.53	6 (15%)	41,73,73	1.83	7 (17%)
3	UDX	B	501	-	29,36,36	1.36	4 (13%)	37,55,55	2.30	7 (18%)
2	NAI	C	500	-	40,48,48	1.67	6 (15%)	41,73,73	2.12	9 (21%)
3	UDX	C	501	-	29,36,36	1.54	5 (17%)	37,55,55	1.79	8 (21%)
2	NAI	D	500	-	40,48,48	1.48	6 (15%)	41,73,73	1.89	6 (14%)
3	UDX	D	501	-	29,36,36	1.20	3 (10%)	37,55,55	1.64	6 (16%)
2	NAI	E	500	-	40,48,48	1.85	6 (15%)	41,73,73	2.42	11 (26%)
3	UDX	E	501	-	29,36,36	1.23	3 (10%)	37,55,55	2.13	9 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAI	F	500	-	40,48,48	1.58	8 (20%)	41,73,73	1.99	6 (14%)
3	UDX	F	501	-	29,36,36	1.24	2 (6%)	37,55,55	1.71	7 (18%)

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	NAI	A	500	-	-	0/25/72/72	0/5/5/5
3	UDX	A	501	-	-	0/17/54/54	0/3/3/3
2	NAI	B	500	-	-	0/25/72/72	0/5/5/5
3	UDX	B	501	-	-	0/17/54/54	0/3/3/3
2	NAI	C	500	-	-	0/25/72/72	0/5/5/5
3	UDX	C	501	-	-	0/17/54/54	0/3/3/3
2	NAI	D	500	-	-	0/25/72/72	0/5/5/5
3	UDX	D	501	-	-	0/17/54/54	0/3/3/3
2	NAI	E	500	-	-	0/25/72/72	0/5/5/5
3	UDX	E	501	-	-	0/17/54/54	0/3/3/3
2	NAI	F	500	-	-	0/25/72/72	0/5/5/5
3	UDX	F	501	-	-	0/17/54/54	0/3/3/3

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	NAI	C4N-C5N	-4.30	1.39	1.49
2	D	500	NAI	C4N-C5N	-4.28	1.39	1.49
2	F	500	NAI	C4N-C5N	-4.16	1.40	1.49
2	C	500	NAI	C4N-C5N	-4.14	1.40	1.49
2	E	500	NAI	C4N-C5N	-3.87	1.40	1.49
2	B	500	NAI	C4N-C5N	-3.86	1.40	1.49
3	E	501	UDX	C2D-C1D	-2.24	1.50	1.53
2	A	500	NAI	C5A-N7A	-2.13	1.32	1.39
3	A	501	UDX	PB-O3B	-2.09	1.55	1.60
3	C	501	UDX	PB-O3B	-2.06	1.55	1.60
2	A	500	NAI	C6N-N1N	2.04	1.43	1.37
2	B	500	NAI	PA-O2A	2.05	1.65	1.55
2	D	500	NAI	C6N-N1N	2.10	1.43	1.37
2	A	500	NAI	C2N-C3N	2.16	1.41	1.34
2	F	500	NAI	C6N-N1N	2.21	1.43	1.37
3	B	501	UDX	C6-N1	2.29	1.38	1.35
3	D	501	UDX	C6-N1	2.30	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	NAI	PA-O2A	2.33	1.66	1.55
2	F	500	NAI	O4B-C1B	2.34	1.44	1.41
3	C	501	UDX	C2-N3	2.43	1.43	1.38
2	B	500	NAI	C2N-C3N	2.48	1.41	1.34
2	C	500	NAI	C2N-C3N	2.52	1.42	1.34
2	D	500	NAI	C1D-N1N	2.54	1.53	1.46
2	D	500	NAI	C2N-C3N	2.56	1.42	1.34
2	F	500	NAI	PA-O2A	2.67	1.68	1.55
2	F	500	NAI	O4D-C1D	2.72	1.48	1.42
3	C	501	UDX	O4D-C1D	2.72	1.45	1.41
2	B	500	NAI	C1D-N1N	2.86	1.54	1.46
2	F	500	NAI	C1D-N1N	2.98	1.55	1.46
2	F	500	NAI	C2N-C3N	3.00	1.43	1.34
3	D	501	UDX	O4D-C1D	3.01	1.45	1.41
3	F	501	UDX	C4-N3	3.01	1.38	1.33
2	E	500	NAI	C6N-N1N	3.03	1.45	1.37
3	B	501	UDX	O5'-C1'	3.18	1.48	1.41
3	E	501	UDX	C4-N3	3.38	1.39	1.33
2	D	500	NAI	O4D-C1D	3.41	1.50	1.42
3	D	501	UDX	C4-N3	3.48	1.39	1.33
2	C	500	NAI	C1D-N1N	3.50	1.56	1.46
3	B	501	UDX	C4-N3	3.55	1.39	1.33
2	E	500	NAI	C2N-C3N	3.63	1.45	1.34
3	B	501	UDX	O4D-C1D	3.64	1.46	1.41
3	E	501	UDX	C6-N1	3.72	1.40	1.35
2	A	500	NAI	O4D-C1D	3.78	1.51	1.42
2	B	500	NAI	O4D-C1D	3.85	1.51	1.42
2	A	500	NAI	C1D-N1N	3.86	1.57	1.46
2	C	500	NAI	C6N-C5N	3.92	1.40	1.33
3	C	501	UDX	C6-N1	3.98	1.41	1.35
3	C	501	UDX	C4-N3	4.26	1.40	1.33
3	A	501	UDX	C4-N3	4.33	1.40	1.33
2	E	500	NAI	C1D-N1N	4.53	1.59	1.46
2	D	500	NAI	C6N-C5N	4.62	1.41	1.33
2	B	500	NAI	C6N-C5N	4.63	1.41	1.33
2	A	500	NAI	C6N-C5N	4.66	1.41	1.33
2	F	500	NAI	C6N-C5N	4.71	1.42	1.33
3	F	501	UDX	C6-N1	4.84	1.42	1.35
3	A	501	UDX	C6-N1	5.03	1.42	1.35
2	E	500	NAI	C6N-C5N	5.08	1.42	1.33
2	E	500	NAI	O4D-C1D	5.09	1.54	1.42
2	A	500	NAI	O4B-C1B	5.44	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	NAI	O4D-C1D	5.90	1.56	1.42

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	UDX	O5'-C5'-C4'	-8.04	98.20	110.79
2	E	500	NAI	N3A-C2A-N1A	-7.76	122.10	128.86
2	D	500	NAI	N3A-C2A-N1A	-7.67	122.18	128.86
2	C	500	NAI	N3A-C2A-N1A	-7.43	122.38	128.86
2	F	500	NAI	N3A-C2A-N1A	-7.35	122.45	128.86
2	B	500	NAI	N3A-C2A-N1A	-7.31	122.49	128.86
3	A	501	UDX	O5'-C1'-O3B	-7.15	102.02	111.36
3	E	501	UDX	O5'-C1'-C2'	-6.63	100.02	110.00
2	D	500	NAI	C4B-O4B-C1B	-6.47	102.89	109.77
2	A	500	NAI	N3A-C2A-N1A	-6.36	123.32	128.86
2	C	500	NAI	C4B-O4B-C1B	-5.52	103.89	109.77
3	E	501	UDX	O5'-C1'-O3B	-4.43	105.57	111.36
3	A	501	UDX	O5'-C5'-C4'	-4.36	103.95	110.79
3	D	501	UDX	O5'-C1'-O3B	-4.30	105.74	111.36
2	A	500	NAI	O4D-C1D-C2D	-4.00	97.78	106.64
2	E	500	NAI	C4B-O4B-C1B	-3.91	105.61	109.77
2	F	500	NAI	C4B-O4B-C1B	-3.87	105.65	109.77
2	A	500	NAI	C4B-O4B-C1B	-3.86	105.66	109.77
2	B	500	NAI	C4B-O4B-C1B	-3.84	105.68	109.77
2	A	500	NAI	C4A-C5A-N7A	-3.20	106.31	109.41
3	C	501	UDX	O4D-C1D-N1	-3.18	101.70	108.08
2	E	500	NAI	C5D-C4D-C3D	-3.17	103.21	115.29
3	F	501	UDX	O5'-C1'-O3B	-3.14	107.26	111.36
3	D	501	UDX	C4D-O4D-C1D	-3.14	106.43	109.77
2	A	500	NAI	O4B-C4B-C5B	-3.09	98.98	109.40
2	B	500	NAI	C5D-C4D-C3D	-3.04	103.71	115.29
2	E	500	NAI	O4D-C1D-C2D	-3.04	99.92	106.64
2	C	500	NAI	C4A-C5A-N7A	-2.99	106.53	109.41
2	B	500	NAI	C4A-C5A-N7A	-2.95	106.56	109.41
3	D	501	UDX	O5'-C5'-C4'	-2.84	106.34	110.79
3	C	501	UDX	O5'-C5'-C4'	-2.62	106.68	110.79
2	C	500	NAI	C5D-C4D-C3D	-2.57	105.51	115.29
3	E	501	UDX	O5'-C5'-C4'	-2.45	106.96	110.79
3	E	501	UDX	O3'-C3'-C4'	-2.42	105.62	110.02
2	A	500	NAI	O3D-C3D-C4D	-2.34	104.25	111.09
3	A	501	UDX	C5D-C4D-C3D	-2.34	106.36	115.29
2	C	500	NAI	C5B-C4B-C3B	-2.33	106.39	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	UDX	O4D-C4D-C5D	-2.33	101.53	109.40
3	C	501	UDX	C5'-C4'-C3'	-2.32	106.71	109.65
3	B	501	UDX	C5-C4-N3	-2.28	117.69	123.12
3	B	501	UDX	O3B-C1'-C2'	-2.27	104.23	108.38
2	F	500	NAI	O3D-C3D-C4D	-2.26	104.50	111.09
2	B	500	NAI	O4D-C1D-C2D	-2.21	101.74	106.64
3	A	501	UDX	C4'-C3'-C2'	-2.17	107.09	110.88
2	D	500	NAI	C3N-C2N-N1N	-2.16	119.94	123.08
2	E	500	NAI	O3D-C3D-C4D	-2.15	104.79	111.09
3	C	501	UDX	C4D-O4D-C1D	-2.09	107.54	109.77
2	E	500	NAI	O1N-PN-O5D	-2.05	98.47	108.14
3	D	501	UDX	C5'-O5'-C1'	-2.04	108.20	112.36
2	D	500	NAI	O3D-C3D-C4D	-2.03	105.16	111.09
3	C	501	UDX	O3D-C3D-C4D	-2.02	105.19	111.09
3	E	501	UDX	C1'-C2'-C3'	2.02	113.74	109.98
2	B	500	NAI	O4D-C1D-N1N	2.03	112.15	108.07
3	A	501	UDX	O3B-PB-O1B	2.10	117.73	109.46
2	A	500	NAI	C2D-C1D-N1N	2.13	118.80	113.32
2	D	500	NAI	C1D-N1N-C2N	2.14	124.72	121.09
3	E	501	UDX	O2B-PB-O3B	2.15	115.14	106.49
3	E	501	UDX	C5'-C4'-C3'	2.19	112.43	109.65
3	D	501	UDX	O5'-C1'-C2'	2.21	113.33	110.00
3	F	501	UDX	C5'-O5'-C1'	2.30	117.06	112.36
3	B	501	UDX	O3B-PB-O1B	2.36	118.73	109.46
2	C	500	NAI	O4D-C4D-C5D	2.38	117.44	109.40
3	F	501	UDX	O3A-PB-O3B	2.44	106.41	102.05
2	A	500	NAI	O4D-C4D-C5D	2.53	117.93	109.40
2	F	500	NAI	C3D-C2D-C1D	2.58	106.38	101.43
2	C	500	NAI	C2D-C1D-N1N	2.65	120.15	113.32
3	F	501	UDX	O3B-C1'-C2'	2.70	113.33	108.38
3	C	501	UDX	O3A-PB-O3B	2.74	106.94	102.05
2	E	500	NAI	O4D-C1D-N1N	2.81	113.73	108.07
2	E	500	NAI	C3D-C2D-C1D	2.84	106.87	101.43
3	F	501	UDX	O5'-C5'-C4'	2.85	115.26	110.79
2	E	500	NAI	O4D-C4D-C5D	2.95	119.35	109.40
2	F	500	NAI	C1D-N1N-C2N	3.02	126.20	121.09
3	C	501	UDX	O3B-PB-O1B	3.02	121.35	109.46
2	C	500	NAI	C1D-N1N-C2N	3.06	126.28	121.09
2	D	500	NAI	C2D-C1D-N1N	3.33	121.88	113.32
2	B	500	NAI	C2D-C1D-N1N	3.63	122.67	113.32
3	A	501	UDX	O5'-C1'-C2'	3.82	115.76	110.00
3	F	501	UDX	O4D-C1D-N1	3.99	116.06	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	501	UDX	C4-N3-C2	4.32	117.84	114.13
2	E	500	NAI	C1D-N1N-C2N	4.41	128.56	121.09
3	B	501	UDX	O5'-C1'-C2'	4.49	116.77	110.00
2	A	500	NAI	O4D-C1D-N1N	5.03	118.19	108.07
3	D	501	UDX	C4-N3-C2	5.35	118.73	114.13
3	A	501	UDX	C4-N3-C2	5.90	119.20	114.13
3	F	501	UDX	C4-N3-C2	6.02	119.30	114.13
2	C	500	NAI	O4D-C1D-N1N	6.08	120.32	108.07
2	F	500	NAI	C2D-C1D-N1N	6.27	129.44	113.32
3	C	501	UDX	C4-N3-C2	6.53	119.74	114.13
3	E	501	UDX	O3B-C1'-C2'	6.67	120.60	108.38
2	E	500	NAI	C2D-C1D-N1N	7.53	132.71	113.32
3	B	501	UDX	C4-N3-C2	7.98	120.99	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	NAI	16	0
3	A	501	UDX	2	0
2	B	500	NAI	10	0
3	B	501	UDX	1	0
2	C	500	NAI	13	0
2	D	500	NAI	15	0
3	D	501	UDX	1	0
2	E	500	NAI	16	0
2	F	500	NAI	12	0
3	F	501	UDX	1	0

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	459/494 (92%)	-0.05	1 (0%)	94 89	24, 55, 70, 80	0
1	B	459/494 (92%)	-0.16	1 (0%)	94 89	34, 55, 70, 83	0
1	C	459/494 (92%)	-0.02	6 (1%)	77 59	34, 55, 70, 83	0
1	D	458/494 (92%)	-0.05	8 (1%)	70 49	34, 55, 70, 78	0
1	E	459/494 (92%)	-0.11	4 (0%)	84 69	34, 55, 70, 78	0
1	F	459/494 (92%)	0.01	6 (1%)	77 59	34, 55, 70, 83	0
All	All	2753/2964 (92%)	-0.06	26 (0%)	84 69	24, 55, 70, 83	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	324	ASN	5.1
1	E	95	THR	4.9
1	D	98	MET	4.1
1	D	95	THR	3.6
1	E	101	GLY	3.5
1	F	324	ASN	3.4
1	C	435	PRO	3.0
1	D	96	TYR	2.9
1	F	328	ASP	2.8
1	F	1	MET	2.7
1	D	457	PHE	2.7
1	D	101	GLY	2.7
1	C	151	ASN	2.5
1	F	435	PRO	2.5
1	E	98	MET	2.3
1	D	97	GLY	2.3
1	F	451	GLU	2.2
1	C	328	ASP	2.2
1	F	454	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	100	LYS	2.2
1	E	96	TYR	2.2
1	B	399	LYS	2.1
1	C	409	HIS	2.1
1	C	433	LEU	2.1
1	D	142	ARG	2.0
1	A	436	ALA	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	NAI	B	500	44/44	0.95	0.21	0.85	43,51,91,95	0
3	UDX	C	501	34/34	0.97	0.22	0.75	36,45,52,53	0
2	NAI	F	500	44/44	0.93	0.21	0.47	46,54,86,87	0
2	NAI	E	500	44/44	0.94	0.21	0.17	35,46,75,76	0
2	NAI	D	500	44/44	0.95	0.20	0.10	53,58,90,91	0
2	NAI	C	500	44/44	0.93	0.20	0.05	46,53,86,86	0
3	UDX	D	501	34/34	0.98	0.17	-0.46	25,36,42,44	0
3	UDX	F	501	34/34	0.98	0.18	-0.47	25,32,36,38	0
2	NAI	A	500	44/44	0.96	0.19	-0.54	35,47,80,82	0
3	UDX	B	501	34/34	0.97	0.15	-0.79	35,44,48,48	0
3	UDX	A	501	34/34	0.97	0.16	-1.06	33,37,39,43	0
3	UDX	E	501	34/34	0.98	0.15	-1.51	23,26,29,31	0

6.5 Other polymers

There are no such residues in this entry.