



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 11:15 AM GMT

PDB ID : 3V4T
Title : E. cloacae C115D MURA liganded with UNAG
Authors : Zhu, J.-Y.; Yang, Y.; Schonbrunn, E.
Deposited on : 2011-12-15
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

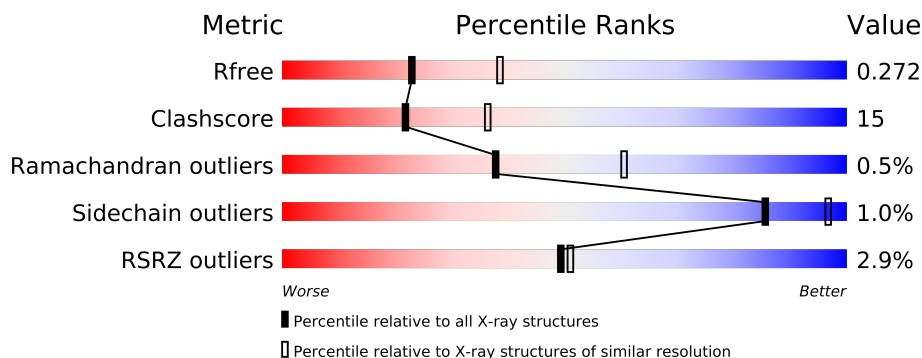
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	419	
1	B	419	
1	C	419	
1	D	419	
1	E	419	
1	F	419	
1	G	419	
1	H	419	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	ACT	A	502	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	ACT	A	503	-	X
3	ACT	A	505	-	X
3	ACT	B	502	-	X
3	ACT	C	502	-	X
3	ACT	C	503	-	X
3	ACT	E	503	-	X
3	ACT	F	502	-	X
3	ACT	F	503	-	X
3	ACT	H	502	-	X
3	ACT	H	503	-	X
3	ACT	H	505	-	X
4	EDO	A	507	-	X
4	EDO	A	509	-	X
4	EDO	B	505	-	X
4	EDO	C	506	-	X
4	EDO	C	507	-	X
4	EDO	D	506	-	X
4	EDO	E	506	-	X
4	EDO	E	507	-	X
4	EDO	E	510	-	X
4	EDO	F	508	-	X
4	EDO	F	509	-	X
4	EDO	G	504	-	X
4	EDO	G	505	-	X
4	EDO	G	507	-	X
4	EDO	H	509	-	X
4	EDO	H	510	-	X
4	EDO	H	513	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26190 atoms, of which 0 are hydrogen and 0 are deuterium.

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-N-acetylglucosamine1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	B	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	C	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	D	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	E	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	F	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	G	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	H	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			

There are 16 discrepancies between the modelled and reference sequences:

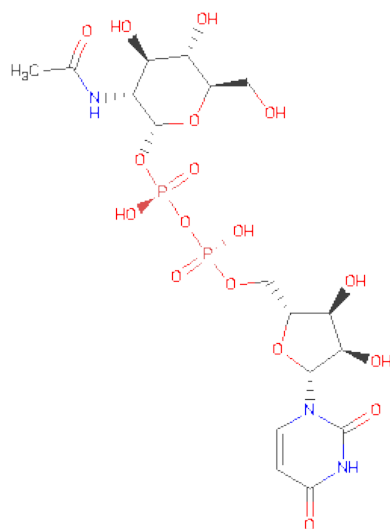
Chain	Residue	Modelled	Actual	Comment	Reference
A	67	IAS	ASN	SEE REMARK 999	UNP P33038
A	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038
B	67	IAS	ASN	SEE REMARK 999	UNP P33038
B	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038
C	67	IAS	ASN	SEE REMARK 999	UNP P33038
C	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038
D	67	IAS	ASN	SEE REMARK 999	UNP P33038
D	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038
E	67	IAS	ASN	SEE REMARK 999	UNP P33038
E	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038
F	67	IAS	ASN	SEE REMARK 999	UNP P33038
F	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038
G	67	IAS	ASN	SEE REMARK 999	UNP P33038

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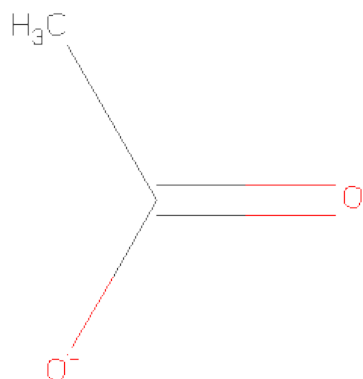
Chain	Residue	Modelled	Actual	Comment	Reference
G	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038
H	67	IAS	ASN	SEE REMARK 999	UNP P33038
H	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038

- Molecule 2 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	C	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	D	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	E	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	F	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	G	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	H	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



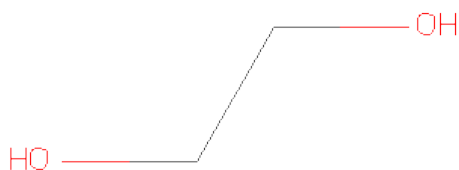
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	67	Total O 67 67	0	0

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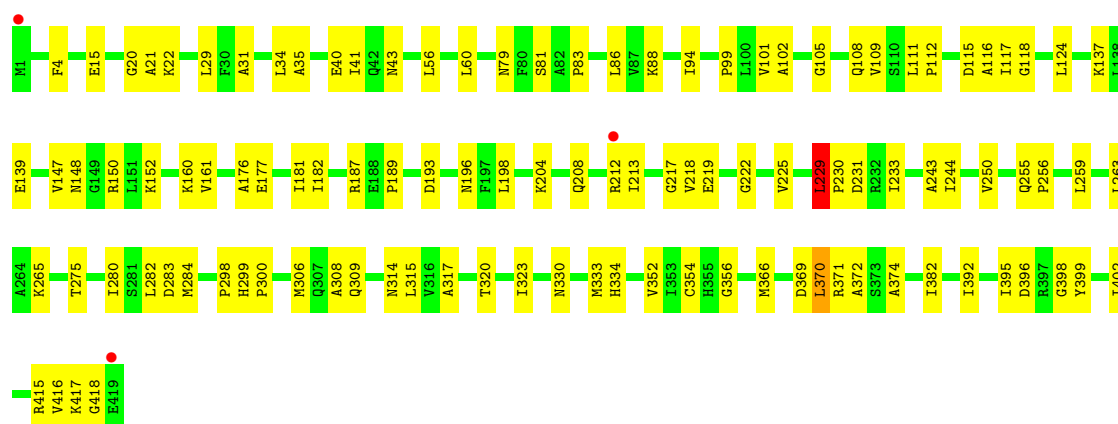
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	33	Total 33	O 33	0	0
5	C	53	Total 53	O 53	0	0
5	D	61	Total 61	O 61	0	0
5	E	66	Total 66	O 66	0	0
5	F	60	Total 60	O 60	0	0
5	G	67	Total 67	O 67	0	0
5	H	63	Total 63	O 63	0	0

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 errors 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.

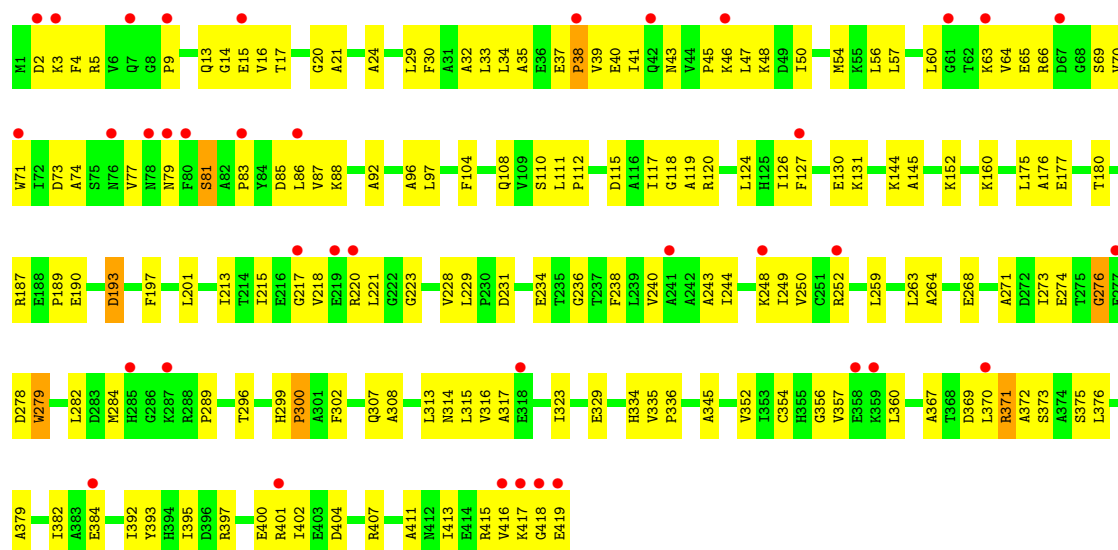
- Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain A: 



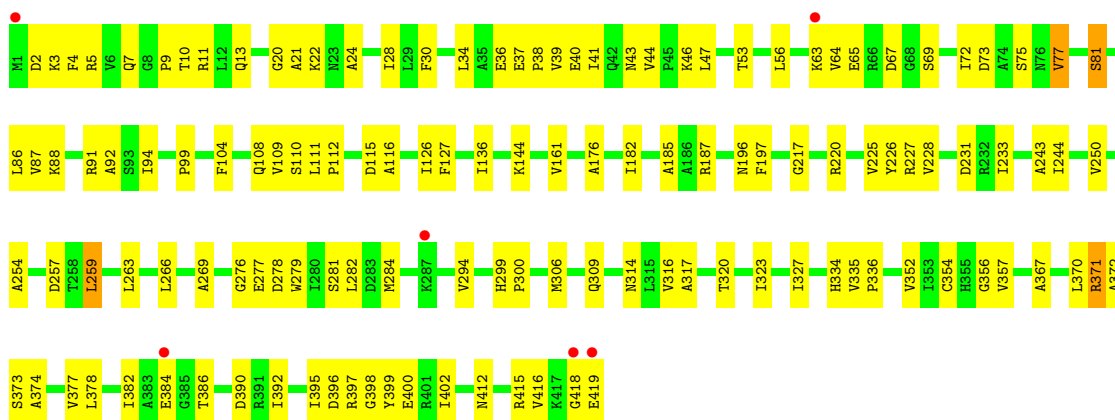
- Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain B: 



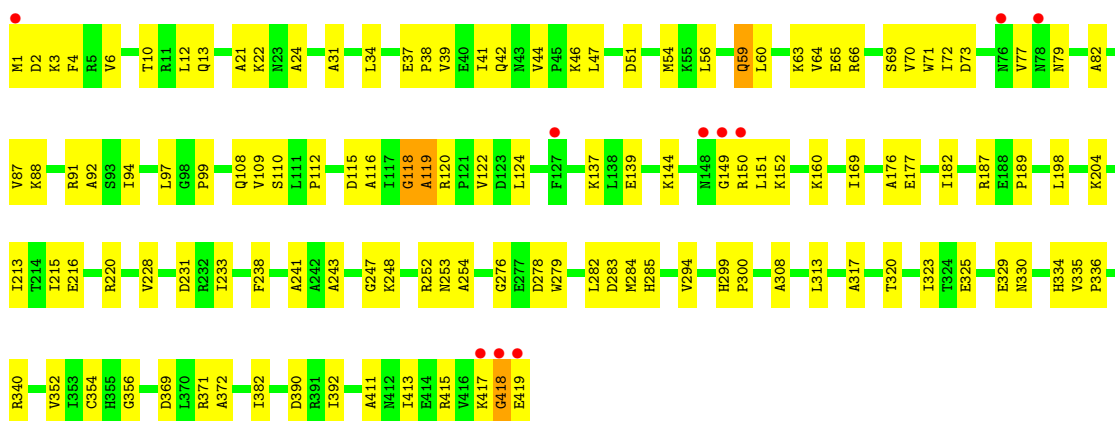
- Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain C: 



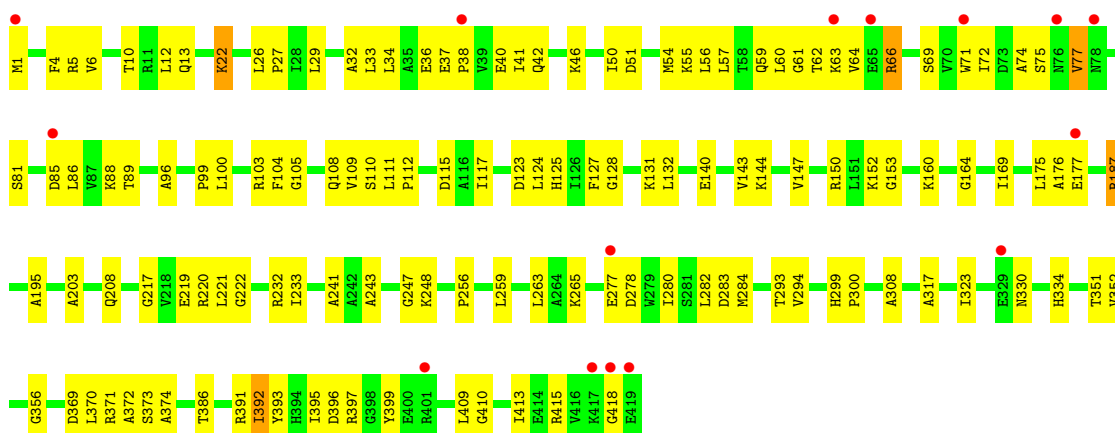
• Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain D:



• Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

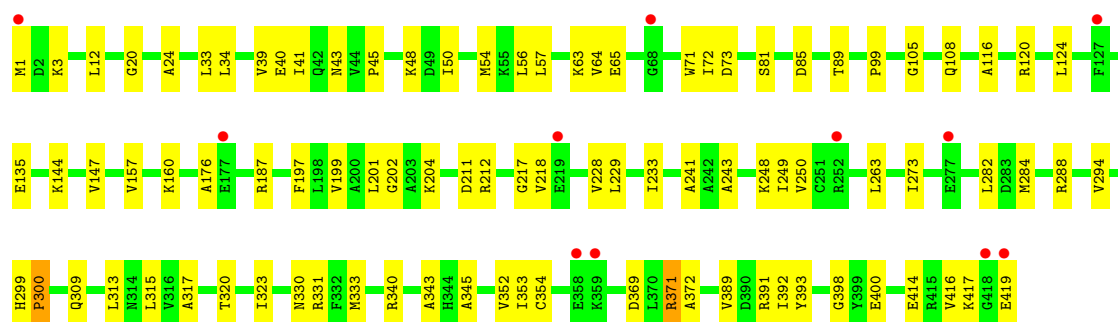
Chain E:



• Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

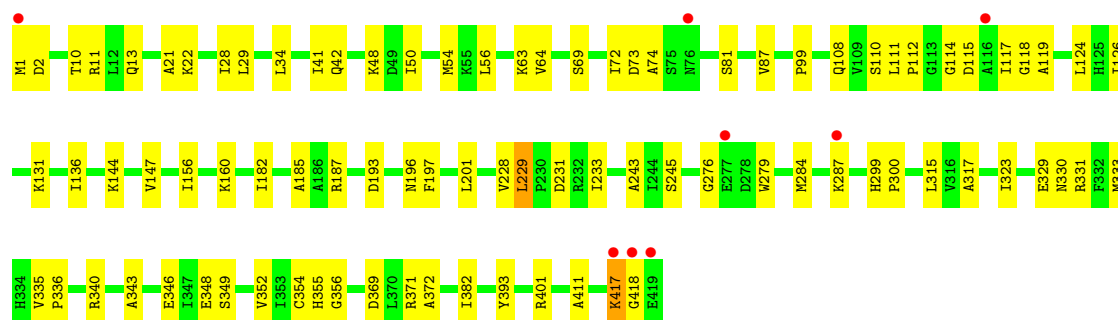
Chain F:





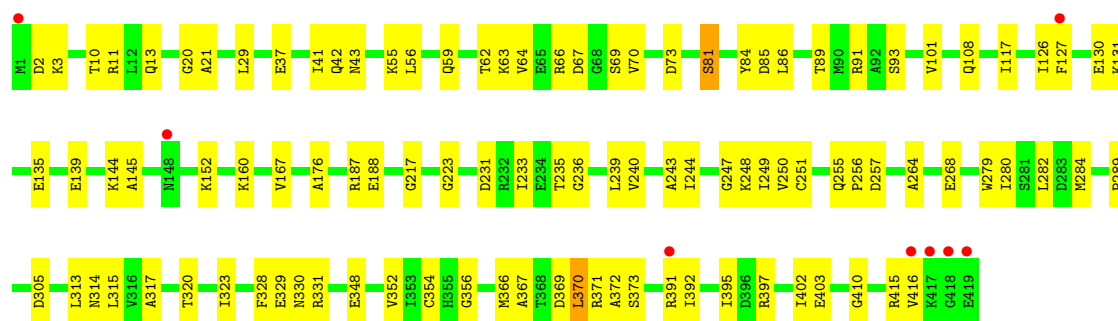
• Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain G:



• Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.05Å 153.14Å 131.68Å 90.00° 102.36° 90.00°	Depositor
Resolution (Å)	19.77 – 2.50 19.77 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.77-2.50) 99.7 (19.77-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.46 (at 2.50Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.208 , 0.271 0.209 , 0.272	Depositor DCC
R_{free} test set	1216 reflections (1.10%)	DCC
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 36.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 110457 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26190	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UD1, EDO, IAS, 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	0.56	1/3180 (0.0%)	0.91	1/4308 (0.0%)
1	B	0.53	3/3180 (0.1%)	0.89	2/4308 (0.0%)
1	C	0.49	0/3180	0.88	1/4308 (0.0%)
1	D	0.49	0/3180	0.90	0/4308
1	E	0.50	1/3180 (0.0%)	0.89	1/4308 (0.0%)
1	F	0.51	1/3180 (0.0%)	0.89	0/4308
1	G	0.52	0/3180	0.89	2/4308 (0.0%)
1	H	0.49	0/3180	0.89	2/4308 (0.0%)
All	All	0.51	6/25440 (0.0%)	0.89	9/34464 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	300	PRO	N-CD	-12.67	1.30	1.47
1	B	300	PRO	N-CD	-12.44	1.30	1.47
1	F	300	PRO	N-CD	-11.88	1.31	1.47
1	B	38	PRO	N-CD	-10.56	1.33	1.47
1	E	277	GLU	CG-CD	5.46	1.60	1.51
1	B	279	TRP	NE1-CE2	-5.03	1.31	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	370	LEU	CA-CB-CG	8.73	135.39	115.30
1	A	229	LEU	CA-CB-CG	6.67	130.64	115.30
1	B	81	SER	N-CA-C	5.83	126.74	111.00
1	G	287	LYS	N-CA-C	5.79	126.63	111.00
1	B	276	GLY	N-CA-C	-5.43	99.53	113.10
1	C	81	SER	N-CA-C	5.19	125.02	111.00
1	G	417	LYS	N-CA-C	5.19	125.02	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	247	GLY	N-CA-C	5.18	126.05	113.10
1	H	81	SER	N-CA-C	5.10	124.77	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3144	0	3215	92	0
1	B	3144	0	3215	136	1
1	C	3144	0	3215	108	0
1	D	3144	0	3215	95	0
1	E	3144	0	3215	112	0
1	F	3144	0	3215	74	0
1	G	3144	0	3215	76	0
1	H	3144	0	3215	99	1
2	A	39	0	25	1	0
2	B	39	0	25	0	0
2	C	39	0	25	0	0
2	D	39	0	25	0	0
2	E	39	0	25	0	0
2	F	39	0	25	0	0
2	G	39	0	25	0	0
2	H	39	0	25	0	0
3	A	16	0	12	0	0
3	B	4	0	3	0	0
3	C	8	0	6	4	0
3	D	8	0	6	0	0
3	E	12	0	9	2	0
3	F	12	0	9	3	0
3	H	20	0	15	2	0
4	A	16	0	24	2	0
4	B	12	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	16	0	24	0	0
4	D	28	0	42	7	0
4	E	28	0	42	1	0
4	F	20	0	30	1	0
4	G	28	0	42	1	0
4	H	28	0	42	3	0
5	A	67	0	0	0	0
5	B	33	0	0	1	0
5	C	53	0	0	4	0
5	D	61	0	0	1	0
5	E	66	0	0	3	0
5	F	60	0	0	2	0
5	G	67	0	0	5	0
5	H	63	0	0	4	0
All	All	26190	0	26244	784	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (784) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:1:MET:O	1:G:418:GLY:HA2	1.20	1.28
1:B:418:GLY:O	1:B:419:GLU:HG3	1.11	1.24
1:A:395:ILE:CD1	1:A:402:ILE:HG21	1.66	1.24
1:C:418:GLY:CA	1:C:419:GLU:O	1.83	1.24
1:A:395:ILE:HD11	1:A:402:ILE:CG2	1.69	1.23
1:C:392:ILE:O	1:C:395:ILE:HG22	1.11	1.22
1:C:418:GLY:HA3	1:C:419:GLU:O	1.40	1.21
1:G:1:MET:O	1:G:418:GLY:CA	1.90	1.20
1:B:418:GLY:O	1:B:419:GLU:CG	1.93	1.16
1:C:392:ILE:O	1:C:395:ILE:CG2	2.03	1.05
1:A:392:ILE:O	1:A:395:ILE:HG22	1.56	1.05
1:C:395:ILE:HD11	1:C:402:ILE:HG21	1.04	1.03
1:B:81:SER:HB3	1:B:108:GLN:HG3	1.42	1.02
1:C:418:GLY:HA2	1:C:419:GLU:O	1.58	1.01
1:D:120:ARG:HH22	4:D:510:EDO:H12	1.26	1.01
1:C:395:ILE:CD1	1:C:402:ILE:HG21	1.92	0.98
1:B:15:GLU:HG2	1:B:250:VAL:HB	1.40	0.98
1:F:108:GLN:HG2	1:F:144:LYS:HG2	1.47	0.97
1:G:118:GLY:HA3	1:G:329:GLU:OE1	1.63	0.97
1:E:34:LEU:HD21	1:E:99:PRO:HA	1.46	0.96
1:C:56:LEU:HB2	1:C:86:LEU:HD13	1.48	0.95

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:233:ILE:HG21	1:D:371:ARG:HD2	1.48	0.94
1:C:395:ILE:HD11	1:C:402:ILE:CG2	1.97	0.93
1:G:108:GLN:HG2	1:G:144:LYS:HG2	1.51	0.93
1:H:108:GLN:HG2	1:H:144:LYS:HG2	1.51	0.93
1:C:4:PHE:HE2	1:C:395:ILE:HD13	1.34	0.92
1:H:370:LEU:HD12	1:H:397:ARG:HD3	1.51	0.91
1:H:2:ASP:HB3	1:H:392:ILE:HD11	1.53	0.90
1:H:370:LEU:CD1	1:H:397:ARG:HD3	2.03	0.89
1:C:63:LYS:HB3	1:C:73:ASP:HB3	1.55	0.88
1:G:323:ILE:HB	1:G:352:VAL:HG12	1.54	0.87
1:D:369:ASP:HB3	1:D:372:ALA:HB3	1.55	0.87
1:D:94:ILE:HA	1:D:109:VAL:HG11	1.58	0.85
1:D:177:GLU:HG2	4:D:508:EDO:H21	1.58	0.84
1:G:2:ASP:OD1	1:G:417:LYS:HG2	1.78	0.83
1:F:331:ARG:H	3:F:503:ACT:H2	1.43	0.83
1:A:259:LEU:HD12	1:A:263:LEU:HG	1.61	0.82
1:D:41:ILE:O	1:D:69:SER:HB2	1.79	0.82
1:F:369:ASP:HB3	1:F:372:ALA:HB3	1.62	0.82
1:G:1:MET:O	1:G:418:GLY:N	2.12	0.81
1:A:306:MET:HE1	1:A:309:GLN:NE2	1.96	0.81
1:H:42:GLN:HA	1:H:69:SER:HB3	1.62	0.80
1:G:118:GLY:CA	1:G:329:GLU:OE1	2.28	0.80
1:C:367:ALA:HB1	1:C:373:SER:HB3	1.62	0.80
1:B:64:VAL:O	1:B:65:GLU:HG3	1.84	0.77
1:G:243:ALA:HA	1:G:284:MET:HG3	1.67	0.77
1:G:81:SER:HB3	1:G:108:GLN:HB2	1.66	0.77
1:E:243:ALA:HA	1:E:284:MET:CG	2.14	0.77
1:B:47:LEU:HB2	1:B:50:ILE:HG12	1.65	0.77
1:F:212:ARG:HD2	5:F:660:HOH:O	1.83	0.77
1:H:243:ALA:HA	1:H:284:MET:CG	2.15	0.76
1:C:4:PHE:CE2	1:C:395:ILE:HD13	2.20	0.76
1:B:4:PHE:CD1	1:B:392:ILE:HD13	2.20	0.76
1:D:108:GLN:HG2	1:D:144:LYS:HG2	1.69	0.75
1:E:34:LEU:HD21	1:E:99:PRO:CA	2.17	0.75
1:H:108:GLN:CG	1:H:144:LYS:HG2	2.17	0.75
1:B:244:ILE:HD12	1:B:382:ILE:HD13	1.68	0.74
1:C:418:GLY:CA	1:C:419:GLU:C	2.52	0.74
1:E:55:LYS:HE3	1:E:86:LEU:HD21	1.69	0.74
1:C:370:LEU:HG	1:C:371:ARG:HG2	1.70	0.74
1:E:36:GLU:HG2	1:E:103:ARG:HH21	1.53	0.73
1:E:36:GLU:O	1:E:75:SER:HB3	1.89	0.73
1:C:41:ILE:HG22	1:C:44:VAL:CG2	2.19	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:233:ILE:HG21	1:G:371:ARG:HD2	1.71	0.72
1:E:1:MET:N	1:E:418:GLY:HA2	2.04	0.72
1:F:48:LYS:NZ	1:F:393:TYR:HB2	2.03	0.72
1:D:91:ARG:NH2	1:D:120:ARG:O	2.22	0.72
1:C:257:ASP:HB3	3:C:502:ACT:H1	1.72	0.72
1:D:323:ILE:HB	1:D:352:VAL:CG1	2.20	0.72
1:G:323:ILE:HB	1:G:352:VAL:CG1	2.18	0.71
1:B:37:GLU:HB2	1:B:223:GLY:H	1.55	0.71
1:A:259:LEU:CD1	1:A:263:LEU:HG	2.20	0.71
1:G:48:LYS:NZ	1:G:393:TYR:HB2	2.06	0.71
1:C:3:LYS:HD3	1:C:390:ASP:OD1	1.89	0.71
1:B:259:LEU:HD12	1:B:263:LEU:HG	1.70	0.71
1:E:127:PHE:CZ	1:E:131:LYS:HE2	2.24	0.71
1:A:181:ILE:HG21	1:A:212:ARG:HD2	1.72	0.71
1:F:331:ARG:N	3:F:503:ACT:H2	2.05	0.71
1:B:63:LYS:HB3	1:B:73:ASP:HB3	1.72	0.71
1:F:33:LEU:HD21	1:F:57:LEU:HD22	1.73	0.71
1:H:243:ALA:HA	1:H:284:MET:HG2	1.73	0.70
1:A:29:LEU:HD23	1:A:41:ILE:CD1	2.21	0.70
1:H:315:LEU:HD23	1:H:354:CYS:HB3	1.72	0.70
1:C:9:PRO:HD3	1:C:384:GLU:HG3	1.73	0.70
1:C:108:GLN:HG2	1:C:144:LYS:HG2	1.74	0.70
1:A:334:HIS:HB3	1:A:372:ALA:HB1	1.73	0.70
1:G:10:THR:HG21	1:G:411:ALA:HA	1.71	0.70
1:C:327:ILE:HD12	3:C:503:ACT:H1	1.73	0.70
1:C:7:GLN:HB2	1:C:412:ASN:ND2	2.06	0.70
1:B:4:PHE:CE1	1:B:392:ILE:HD12	2.27	0.70
1:G:346:GLU:OE2	1:G:355:HIS:NE2	2.21	0.70
1:A:395:ILE:CD1	1:A:402:ILE:CG2	2.49	0.69
1:B:21:ALA:HA	1:B:231:ASP:HB2	1.72	0.69
1:D:323:ILE:HB	1:D:352:VAL:HG13	1.73	0.69
1:E:370:LEU:H	1:E:370:LEU:HD23	1.58	0.69
1:A:176:ALA:O	1:A:217:GLY:HA3	1.91	0.69
1:G:333:MET:HG3	5:G:663:HOH:O	1.92	0.68
1:G:315:LEU:HD13	1:G:343:ALA:HB1	1.75	0.68
1:C:176:ALA:O	1:C:217:GLY:HA3	1.92	0.68
1:C:396:ASP:CG	1:C:415:ARG:HH22	1.95	0.68
1:B:418:GLY:O	1:B:419:GLU:CB	2.41	0.68
1:E:22:LYS:HZ1	3:E:502:ACT:H2	1.58	0.68
1:A:229:LEU:HB2	1:A:230:PRO:HD2	1.75	0.68
1:B:417:LYS:HG2	1:B:418:GLY:N	2.09	0.68
1:C:81:SER:HB3	1:C:108:GLN:HB2	1.75	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:29:LEU:HD23	1:A:41:ILE:HD12	1.74	0.68
1:B:417:LYS:HG2	1:B:418:GLY:H	1.57	0.68
1:E:103:ARG:NH1	1:E:104:PHE:HZ	1.91	0.67
1:E:369:ASP:HB3	1:E:372:ALA:HB3	1.76	0.67
1:E:108:GLN:HG2	1:E:144:LYS:HG2	1.75	0.67
1:F:176:ALA:O	1:F:217:GLY:HA3	1.95	0.67
1:B:4:PHE:CD1	1:B:392:ILE:CD1	2.78	0.67
1:G:243:ALA:HA	1:G:284:MET:CG	2.25	0.66
1:C:416:VAL:HG12	1:C:418:GLY:H	1.60	0.66
1:F:369:ASP:CB	1:F:372:ALA:HB3	2.25	0.66
1:D:149:GLY:O	1:D:150:ARG:HD3	1.96	0.66
1:D:42:GLN:HA	1:D:69:SER:HB3	1.78	0.66
1:E:36:GLU:HG2	1:E:103:ARG:NH2	2.11	0.66
1:H:370:LEU:CD1	1:H:397:ARG:CD	2.74	0.66
1:A:323:ILE:HB	1:A:352:VAL:CG1	2.26	0.66
1:E:105:GLY:HA2	1:E:147:VAL:HG12	1.78	0.66
1:A:229:LEU:HB2	1:A:230:PRO:CD	2.27	0.66
1:H:369:ASP:HB3	1:H:372:ALA:HB3	1.78	0.66
1:A:181:ILE:CG2	1:A:212:ARG:HD2	2.25	0.65
1:F:243:ALA:HA	1:F:284:MET:CG	2.26	0.65
1:A:317:ALA:O	1:A:356:GLY:HA3	1.96	0.65
1:B:176:ALA:O	1:B:217:GLY:HA3	1.95	0.65
1:A:370:LEU:O	1:A:371:ARG:HD2	1.96	0.65
1:B:401:ARG:HG2	5:B:616:HOH:O	1.96	0.65
1:G:126:ILE:HG23	1:G:136:ILE:HD13	1.77	0.65
1:D:137:LYS:HE3	1:D:139:GLU:OE1	1.97	0.65
1:E:243:ALA:HA	1:E:284:MET:HG2	1.78	0.65
1:F:81:SER:HB3	1:F:108:GLN:HB2	1.79	0.65
1:H:395:ILE:HG21	1:H:402:ILE:HG21	1.79	0.64
1:C:396:ASP:OD2	1:C:415:ARG:NH2	2.21	0.64
1:C:227:ARG:HD2	5:C:637:HOH:O	1.97	0.64
1:E:393:TYR:O	1:E:397:ARG:HG3	1.97	0.64
1:H:63:LYS:HB3	1:H:73:ASP:HB3	1.80	0.64
1:A:243:ALA:HA	1:A:284:MET:CG	2.26	0.64
1:E:128:GLY:HA3	1:E:169:ILE:HD11	1.79	0.64
1:B:118:GLY:CA	1:B:329:GLU:OE2	2.46	0.64
1:E:243:ALA:HA	1:E:284:MET:HG3	1.78	0.64
1:F:243:ALA:HA	1:F:284:MET:HG3	1.77	0.64
1:F:3:LYS:HA	1:F:392:ILE:HG23	1.80	0.64
1:A:111:LEU:HD12	1:A:112:PRO:HD2	1.80	0.64
1:D:112:PRO:HA	4:D:509:EDO:H22	1.80	0.64
1:D:82:ALA:HB3	1:D:109:VAL:HG13	1.80	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:29:LEU:HD23	1:B:41:ILE:HD12	1.79	0.63
1:D:243:ALA:HA	1:D:284:MET:CG	2.27	0.63
1:H:108:GLN:NE2	1:H:144:LYS:HE2	2.13	0.63
1:B:74:ALA:O	1:B:77:VAL:HG23	1.97	0.63
1:H:41:ILE:O	1:H:69:SER:HB2	1.98	0.63
1:D:38:PRO:HG3	1:D:73:ASP:OD2	1.97	0.63
1:A:243:ALA:HA	1:A:284:MET:HG3	1.80	0.63
1:G:41:ILE:O	1:G:69:SER:HB2	1.99	0.63
1:C:34:LEU:HD21	1:C:99:PRO:HA	1.81	0.63
1:G:29:LEU:HD23	1:G:41:ILE:HD12	1.81	0.63
1:G:196:ASN:HB3	4:G:505:EDO:H12	1.80	0.63
1:C:24:ALA:HB3	1:C:228:VAL:HG13	1.81	0.62
1:H:10:THR:HG21	1:H:410:GLY:O	1.99	0.62
1:B:418:GLY:C	1:B:419:GLU:HG3	2.11	0.62
1:B:34:LEU:HD22	1:B:175:LEU:HD11	1.82	0.62
1:E:282:LEU:HD23	1:E:282:LEU:C	2.20	0.62
1:A:306:MET:CE	1:A:309:GLN:NE2	2.61	0.62
1:B:152:LYS:HD2	1:B:177:GLU:O	1.99	0.62
1:G:369:ASP:HB3	1:G:372:ALA:HB3	1.82	0.62
1:F:204:LYS:HE3	1:F:218:VAL:HG12	1.82	0.62
1:D:108:GLN:HG3	5:D:646:HOH:O	1.98	0.61
1:A:320:THR:HG21	1:C:320:THR:HG21	1.81	0.61
1:E:46:LYS:HG2	1:E:66:ARG:NH1	2.15	0.61
1:G:48:LYS:HZ3	1:G:393:TYR:HB2	1.65	0.61
1:E:22:LYS:NZ	3:E:502:ACT:H2	2.16	0.61
1:G:335:VAL:HB	1:G:336:PRO:HD3	1.83	0.61
1:F:63:LYS:HB3	1:F:73:ASP:HB3	1.81	0.61
1:B:2:ASP:OD2	1:B:415:ARG:HD3	2.01	0.61
1:D:120:ARG:HH22	4:D:510:EDO:C1	2.07	0.61
1:F:323:ILE:HB	1:F:352:VAL:HG13	1.83	0.61
1:D:92:ALA:HA	4:D:504:EDO:H12	1.82	0.61
1:B:39:VAL:HG22	1:B:223:GLY:HA2	1.81	0.60
1:H:370:LEU:HD11	1:H:397:ARG:NE	2.16	0.60
1:H:313:LEU:C	1:H:313:LEU:HD23	2.22	0.60
1:B:334:HIS:HB3	1:B:372:ALA:HB1	1.83	0.60
1:B:3:LYS:HG3	1:B:3:LYS:O	2.02	0.60
1:B:367:ALA:HB1	1:B:373:SER:OG	2.01	0.60
1:D:124:LEU:HD11	1:D:160:LYS:HG2	1.84	0.60
1:B:4:PHE:CD2	1:B:413:ILE:HD11	2.36	0.60
1:F:3:LYS:HB2	1:F:389:VAL:O	2.00	0.60
1:B:373:SER:HB3	1:B:395:ILE:HG12	1.83	0.60
1:H:81:SER:HB3	1:H:108:GLN:HB2	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:369:ASP:C	1:A:371:ARG:H	2.05	0.59
1:H:176:ALA:O	1:H:217:GLY:HA3	2.02	0.59
1:E:41:ILE:O	1:E:69:SER:HB2	2.03	0.59
1:E:5:ARG:NH1	1:E:386:THR:HG21	2.17	0.59
1:A:150:ARG:HH12	1:A:219:GLU:HA	1.67	0.59
1:G:348:GLU:O	1:G:349:SER:HB3	2.03	0.59
1:G:340:ARG:HG2	1:G:340:ARG:HH11	1.66	0.59
1:H:366:MET:CE	1:H:391:ARG:HD2	2.32	0.59
1:E:150:ARG:HB2	1:E:177:GLU:CG	2.30	0.59
1:A:306:MET:HE1	1:A:309:GLN:HE21	1.65	0.59
1:A:204:LYS:HE2	1:A:218:VAL:HG12	1.84	0.59
1:D:63:LYS:HB3	1:D:73:ASP:HB3	1.84	0.59
1:A:40:GLU:HB3	1:A:225:VAL:HG22	1.84	0.59
1:B:48:LYS:HE3	1:B:397:ARG:HG2	1.85	0.59
1:A:116:ALA:O	1:A:330:ASN:ND2	2.35	0.59
1:E:323:ILE:HB	1:E:352:VAL:HG13	1.85	0.59
1:E:152:LYS:HD2	1:E:153:GLY:N	2.18	0.59
1:G:317:ALA:O	1:G:356:GLY:HA3	2.03	0.59
1:B:4:PHE:CE1	1:B:392:ILE:CD1	2.85	0.58
1:C:4:PHE:HE2	1:C:395:ILE:CD1	2.12	0.58
1:A:259:LEU:HD12	1:A:263:LEU:CG	2.31	0.58
1:C:233:ILE:HG23	1:C:306:MET:HE3	1.84	0.58
1:B:34:LEU:HD22	1:B:175:LEU:CD1	2.33	0.58
1:D:64:VAL:HG22	1:D:72:ILE:HD13	1.85	0.58
1:H:243:ALA:HA	1:H:284:MET:HG3	1.84	0.58
1:F:48:LYS:HZ1	1:F:393:TYR:HB2	1.68	0.58
1:C:36:GLU:OE1	1:C:220:ARG:NE	2.35	0.58
1:H:85:ASP:O	1:H:89:THR:HG23	2.03	0.58
1:A:370:LEU:HD12	1:A:370:LEU:O	2.03	0.58
1:H:152:LYS:HE3	5:H:627:HOH:O	2.03	0.58
1:G:1:MET:C	1:G:418:GLY:HA2	2.14	0.57
1:B:4:PHE:H	1:B:392:ILE:HG21	1.68	0.57
1:C:334:HIS:HB3	1:C:372:ALA:HB1	1.85	0.57
1:G:124:LEU:HD11	1:G:160:LYS:HG2	1.85	0.57
1:F:197:PHE:CZ	1:F:201:LEU:HD11	2.40	0.57
1:B:118:GLY:HA3	1:B:329:GLU:OE2	2.03	0.57
1:B:56:LEU:HB2	1:B:86:LEU:HD13	1.84	0.57
1:D:41:ILE:HG22	1:D:44:VAL:CG2	2.35	0.57
1:C:259:LEU:HD12	1:C:263:LEU:HG	1.86	0.57
1:D:66:ARG:HB3	1:D:70:VAL:HG22	1.86	0.57
1:F:391:ARG:HB3	1:F:393:TYR:CE2	2.40	0.57
1:E:152:LYS:HD2	1:E:153:GLY:H	1.70	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:333:MET:CE	1:A:333:MET:HA	2.35	0.57
1:E:373:SER:HB2	1:E:395:ILE:CD1	2.35	0.57
1:E:40:GLU:OE2	1:E:71:TRP:NE1	2.38	0.57
1:F:315:LEU:HD21	1:F:345:ALA:HB2	1.85	0.57
1:E:103:ARG:NH1	1:E:104:PHE:CZ	2.72	0.56
1:F:48:LYS:HZ3	1:F:393:TYR:HB2	1.70	0.56
1:A:15:GLU:HG2	1:A:250:VAL:HB	1.86	0.56
1:E:105:GLY:HA2	1:E:147:VAL:CG1	2.33	0.56
1:F:3:LYS:NZ	1:F:419:GLU:C	2.58	0.56
1:E:127:PHE:CE2	1:E:131:LYS:HE2	2.41	0.56
1:C:306:MET:HA	1:C:306:MET:HE2	1.88	0.56
1:A:395:ILE:HD11	1:A:402:ILE:HG21	0.75	0.56
1:D:243:ALA:HA	1:D:284:MET:HG3	1.88	0.56
1:A:395:ILE:HG23	1:A:396:ASP:N	2.21	0.56
1:E:248:LYS:HD2	1:E:283:ASP:OD2	2.05	0.56
1:B:314:ASN:HB3	1:B:354:CYS:HB2	1.87	0.56
1:D:64:VAL:HG22	1:D:72:ILE:CD1	2.36	0.55
1:B:17:THR:HA	1:B:252:ARG:HB2	1.87	0.55
1:A:94:ILE:HA	1:A:109:VAL:HG11	1.88	0.55
1:B:417:LYS:CG	1:B:418:GLY:H	2.19	0.55
1:G:81:SER:HB3	1:G:108:GLN:CB	2.36	0.55
1:B:29:LEU:HD23	1:B:41:ILE:CD1	2.37	0.55
1:H:127:PHE:CE2	1:H:131:LYS:HD2	2.41	0.55
1:E:330:ASN:OD1	1:H:330:ASN:HB2	2.06	0.55
1:B:372:ALA:O	1:B:375:SER:N	2.39	0.55
1:C:250:VAL:HG22	1:C:281:SER:HB2	1.88	0.55
1:C:182:ILE:HG22	1:C:185:ALA:HB2	1.89	0.55
1:A:81:SER:HB3	1:A:108:GLN:HB2	1.89	0.55
1:E:36:GLU:OE1	1:E:220:ARG:HB2	2.07	0.55
1:H:323:ILE:HB	1:H:352:VAL:CG1	2.37	0.55
1:D:56:LEU:HD23	1:D:56:LEU:C	2.26	0.55
1:B:40:GLU:HG3	1:B:71:TRP:NE1	2.22	0.55
1:C:370:LEU:HD11	1:C:399:TYR:CD1	2.42	0.54
1:D:94:ILE:HD12	1:D:122:VAL:HG11	1.89	0.54
3:H:503:ACT:H2	5:H:606:HOH:O	2.07	0.54
1:H:117:ILE:CG2	1:H:331:ARG:HG3	2.36	0.54
1:D:152:LYS:HD2	1:D:177:GLU:O	2.07	0.54
1:B:21:ALA:HB2	1:B:231:ASP:HA	1.90	0.54
1:G:64:VAL:HG22	1:G:72:ILE:HD13	1.89	0.54
1:D:313:LEU:C	1:D:313:LEU:HD23	2.27	0.54
1:A:56:LEU:C	1:A:56:LEU:HD23	2.27	0.54
1:E:103:ARG:HH11	1:E:104:PHE:HZ	1.55	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:48:LYS:NZ	1:B:393:TYR:HB2	2.22	0.54
1:E:373:SER:HB2	1:E:395:ILE:HD11	1.89	0.54
1:H:248:LYS:HB3	1:H:248:LYS:NZ	2.23	0.54
1:H:56:LEU:HD23	1:H:56:LEU:C	2.28	0.54
1:F:56:LEU:HD23	1:F:56:LEU:C	2.27	0.54
1:C:77:VAL:HB	1:C:104:PHE:CZ	2.43	0.54
1:E:56:LEU:HD23	1:E:56:LEU:O	2.07	0.54
1:F:323:ILE:HB	1:F:352:VAL:CG1	2.38	0.54
1:E:323:ILE:HB	1:E:352:VAL:CG1	2.37	0.54
1:B:9:PRO:HD3	1:B:384:GLU:HA	1.89	0.54
1:B:126:ILE:O	1:B:130:GLU:HG3	2.07	0.54
1:F:120:ARG:HB3	5:F:622:HOH:O	2.07	0.54
1:B:97:LEU:O	1:B:97:LEU:HD12	2.08	0.53
1:H:188:GLU:N	1:H:188:GLU:OE1	2.41	0.53
1:B:244:ILE:HA	1:B:289:PRO:HG2	1.89	0.53
1:D:299:HIS:ND1	1:D:300:PRO:HA	2.24	0.53
1:C:127:PHE:HB2	5:C:641:HOH:O	2.07	0.53
1:E:124:LEU:HD11	1:E:160:LYS:HG3	1.90	0.53
1:G:56:LEU:HD23	1:G:56:LEU:O	2.08	0.53
1:A:115:ASP:HB3	1:A:118:GLY:O	2.08	0.53
1:C:317:ALA:O	1:C:356:GLY:HA3	2.08	0.53
1:A:31:ALA:HB1	1:A:198:LEU:HD21	1.90	0.53
1:E:150:ARG:HH12	1:E:219:GLU:HA	1.73	0.53
1:G:111:LEU:HD12	1:G:112:PRO:HD2	1.91	0.53
1:B:395:ILE:HG21	1:B:402:ILE:HG21	1.91	0.53
1:H:62:THR:HG22	1:H:64:VAL:HG22	1.90	0.53
1:H:3:LYS:HB2	1:H:416:VAL:HB	1.91	0.53
1:C:299:HIS:CG	1:C:300:PRO:HA	2.43	0.53
1:F:416:VAL:HG12	1:F:417:LYS:N	2.23	0.53
1:H:317:ALA:O	1:H:356:GLY:HA3	2.09	0.53
1:B:317:ALA:O	1:B:356:GLY:HA3	2.09	0.53
1:B:45:PRO:O	1:B:50:ILE:HG13	2.09	0.53
1:E:74:ALA:O	1:E:77:VAL:HG23	2.09	0.53
1:D:46:LYS:HG2	1:D:66:ARG:CZ	2.39	0.53
1:B:46:LYS:N	1:B:400:GLU:OE1	2.35	0.53
1:E:5:ARG:HH12	1:E:386:THR:HG21	1.73	0.52
1:C:233:ILE:HG23	1:C:306:MET:CE	2.39	0.52
1:B:243:ALA:HA	1:B:284:MET:HG3	1.91	0.52
1:A:181:ILE:HG23	1:A:212:ARG:CG	2.40	0.52
1:C:111:LEU:HD12	1:C:112:PRO:HD2	1.90	0.52
1:A:306:MET:HA	1:A:306:MET:HE2	1.91	0.52
1:E:64:VAL:HG13	1:E:72:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:21:ALA:HA	1:H:231:ASP:HB2	1.91	0.52
1:D:118:GLY:O	1:D:119:ALA:HB3	2.09	0.52
1:A:152:LYS:HD2	1:A:177:GLU:O	2.09	0.52
1:C:316:VAL:HG23	1:C:316:VAL:O	2.08	0.52
1:E:150:ARG:HB2	1:E:177:GLU:HG3	1.91	0.52
1:B:97:LEU:HD11	1:B:145:ALA:HB3	1.92	0.52
1:A:416:VAL:HG12	1:A:418:GLY:H	1.74	0.52
1:C:40:GLU:HB3	1:C:225:VAL:HG22	1.92	0.52
1:C:243:ALA:HA	1:C:284:MET:HG3	1.92	0.52
1:B:213:ILE:HG22	1:B:215:ILE:HD11	1.91	0.52
1:B:108:GLN:NE2	1:B:144:LYS:HE2	2.24	0.52
1:B:249:ILE:HG12	1:B:250:VAL:N	2.24	0.52
1:E:299:HIS:CG	1:E:300:PRO:HA	2.45	0.52
1:C:41:ILE:HD11	1:C:197:PHE:CE1	2.45	0.52
1:F:33:LEU:HD21	1:F:57:LEU:CD2	2.38	0.52
1:E:330:ASN:CG	1:H:330:ASN:HB2	2.29	0.52
1:H:370:LEU:HD11	1:H:397:ARG:CZ	2.40	0.52
1:D:1:MET:N	1:D:418:GLY:O	2.43	0.52
1:H:37:GLU:HB2	1:H:223:GLY:N	2.25	0.52
1:B:87:VAL:HG21	1:B:110:SER:HB3	1.91	0.52
1:A:137:LYS:NZ	1:A:139:GLU:OE2	2.42	0.51
1:A:34:LEU:HD21	1:A:99:PRO:HA	1.91	0.51
1:C:126:ILE:HG23	1:C:136:ILE:HG21	1.92	0.51
1:B:119:ALA:N	1:B:329:GLU:OE2	2.44	0.51
1:C:233:ILE:CG2	1:C:306:MET:HE3	2.41	0.51
1:E:330:ASN:HB2	1:H:330:ASN:OD1	2.10	0.51
1:E:111:LEU:HD13	1:E:143:VAL:CG2	2.40	0.51
1:F:105:GLY:HA2	1:F:147:VAL:HG12	1.92	0.51
1:A:101:VAL:HG13	1:A:102:ALA:N	2.25	0.51
1:A:275:THR:HG22	1:A:280:ILE:HG12	1.92	0.51
1:E:278:ASP:OD1	1:E:278:ASP:N	2.42	0.51
1:B:220:ARG:O	1:B:221:LEU:HD23	2.11	0.51
1:E:123:ASP:HA	4:E:508:EDO:H21	1.93	0.51
1:D:4:PHE:HE1	1:D:415:ARG:HB2	1.75	0.51
1:A:124:LEU:HD11	1:A:160:LYS:HG2	1.93	0.51
1:D:204:LYS:HB2	1:D:216:GLU:HB3	1.92	0.51
1:E:57:LEU:O	1:E:62:THR:HB	2.11	0.51
1:E:369:ASP:CB	1:E:372:ALA:HB3	2.40	0.51
1:D:12:LEU:HD12	1:D:241:ALA:HB1	1.92	0.51
1:D:369:ASP:CB	1:D:372:ALA:HB3	2.35	0.51
1:G:299:HIS:ND1	1:G:300:PRO:HA	2.26	0.51
1:D:254:ALA:O	1:D:278:ASP:HA	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:276:GLY:HA3	1:C:279:TRP:NE1	2.26	0.50
1:A:259:LEU:CD1	1:A:263:LEU:CG	2.88	0.50
1:G:42:GLN:HA	1:G:69:SER:HB3	1.92	0.50
1:D:299:HIS:CG	1:D:300:PRO:HA	2.46	0.50
1:H:240:VAL:O	1:H:244:ILE:HG12	2.12	0.50
1:G:21:ALA:HA	1:G:231:ASP:HB2	1.92	0.50
1:E:115:ASP:OD2	1:E:117:ILE:HG12	2.12	0.50
1:H:282:LEU:C	1:H:282:LEU:HD23	2.32	0.50
1:A:115:ASP:OD2	1:A:116:ALA:N	2.45	0.50
1:G:131:LYS:HD3	1:G:156:ILE:HG23	1.94	0.50
1:D:13:GLN:HA	1:D:248:LYS:O	2.10	0.50
1:F:340:ARG:HG2	1:F:340:ARG:HH11	1.74	0.50
1:B:5:ARG:NE	1:B:416:VAL:HG21	2.26	0.50
1:E:124:LEU:HD11	1:E:160:LYS:CG	2.42	0.50
1:D:10:THR:HG21	1:D:411:ALA:HA	1.92	0.50
1:E:176:ALA:O	1:E:217:GLY:HA3	2.12	0.50
1:C:36:GLU:O	1:C:75:SER:HB3	2.12	0.50
1:H:62:THR:HG22	1:H:64:VAL:CG2	2.42	0.50
1:B:21:ALA:HA	1:B:231:ASP:CB	2.42	0.49
1:A:81:SER:CB	1:A:108:GLN:HB2	2.42	0.49
1:C:294:VAL:HB	1:C:323:ILE:HD13	1.93	0.49
1:B:37:GLU:HB2	1:B:223:GLY:N	2.23	0.49
1:B:180:THR:HB	1:B:215:ILE:HB	1.94	0.49
1:A:21:ALA:HA	1:A:231:ASP:HB2	1.94	0.49
1:F:50:ILE:O	1:F:54:MET:HG3	2.11	0.49
1:B:296:THR:HA	1:B:302:PHE:O	2.12	0.49
1:F:294:VAL:HB	1:F:323:ILE:HD13	1.94	0.49
1:B:48:LYS:HZ2	1:B:393:TYR:HB2	1.76	0.49
1:E:152:LYS:CE	5:E:632:HOH:O	2.60	0.49
1:E:152:LYS:HE3	5:E:632:HOH:O	2.11	0.49
1:H:329:GLU:HG2	1:H:330:ASN:H	1.76	0.49
1:B:35:ALA:O	1:B:74:ALA:HB3	2.13	0.49
1:C:94:ILE:HA	1:C:109:VAL:HG11	1.95	0.49
1:C:399:TYR:CD2	1:C:402:ILE:HD12	2.47	0.49
1:B:271:ALA:HB2	1:B:284:MET:SD	2.52	0.49
1:E:4:PHE:CD2	1:E:392:ILE:HG21	2.48	0.49
1:G:87:VAL:HG21	1:G:110:SER:HB3	1.95	0.49
1:H:366:MET:HE3	1:H:391:ARG:HD2	1.94	0.49
1:C:357:VAL:HG13	5:C:606:HOH:O	2.11	0.49
1:F:24:ALA:HB3	1:F:228:VAL:HG13	1.93	0.49
1:E:46:LYS:HG2	1:E:66:ARG:CZ	2.43	0.49
1:C:243:ALA:HA	1:C:284:MET:CG	2.43	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:367:ALA:HB1	1:H:373:SER:CB	2.43	0.49
1:F:330:ASN:HB2	1:G:330:ASN:HB2	1.95	0.48
1:C:87:VAL:HG21	1:C:110:SER:HB3	1.94	0.48
1:E:1:MET:H2	1:E:418:GLY:HA2	1.78	0.48
1:B:35:ALA:HB2	1:B:201:LEU:HD13	1.95	0.48
1:G:340:ARG:CG	1:G:340:ARG:HH11	2.26	0.48
1:B:360:LEU:O	1:B:384:GLU:N	2.44	0.48
1:A:282:LEU:HD23	1:A:282:LEU:C	2.34	0.48
1:B:299:HIS:CG	1:B:300:PRO:HA	2.48	0.48
1:D:276:GLY:HA3	1:D:279:TRP:NE1	2.28	0.48
1:E:294:VAL:HB	1:E:323:ILE:HD13	1.96	0.48
1:C:220:ARG:HG3	1:C:220:ARG:HH11	1.78	0.48
1:E:373:SER:CB	1:E:395:ILE:HD11	2.43	0.48
1:D:150:ARG:HG3	4:D:508:EDO:O1	2.14	0.48
1:H:21:ALA:HA	1:H:231:ASP:CB	2.44	0.48
1:D:22:LYS:HD3	1:D:371:ARG:NH1	2.28	0.48
1:B:234:GLU:HG3	1:B:238:PHE:CE2	2.49	0.48
1:F:45:PRO:HA	1:F:400:GLU:OE1	2.14	0.48
1:G:114:GLY:HA2	1:G:119:ALA:O	2.13	0.48
1:H:348:GLU:OE2	1:H:348:GLU:HA	2.13	0.48
1:F:331:ARG:H	3:F:503:ACT:CH3	2.22	0.48
1:G:160:LYS:HE3	5:G:655:HOH:O	2.13	0.48
1:A:83:PRO:HD2	1:A:86:LEU:HD12	1.96	0.48
1:B:117:ILE:HD11	1:B:120:ARG:NH1	2.28	0.48
1:F:330:ASN:CB	1:G:330:ASN:HB2	2.44	0.48
1:C:91:ARG:HG3	5:C:646:HOH:O	2.13	0.48
1:A:233:ILE:HG23	1:A:306:MET:CE	2.44	0.48
1:C:46:LYS:N	1:C:400:GLU:OE1	2.30	0.48
1:D:417:LYS:O	1:D:419:GLU:N	2.41	0.48
1:C:373:SER:O	1:C:377:VAL:HG23	2.13	0.47
1:B:220:ARG:HG3	1:B:220:ARG:HH11	1.79	0.47
1:B:234:GLU:OE2	1:B:238:PHE:HE2	1.97	0.47
1:B:407:ARG:HG3	1:B:411:ALA:O	2.13	0.47
1:E:308:ALA:HA	1:E:334:HIS:NE2	2.29	0.47
1:C:309:GLN:N	1:C:309:GLN:OE1	2.44	0.47
1:F:320:THR:HG21	1:H:320:THR:HG21	1.96	0.47
1:C:108:GLN:CG	1:C:144:LYS:HG2	2.43	0.47
1:F:3:LYS:HZ1	1:F:419:GLU:C	2.17	0.47
1:D:115:ASP:OD2	1:D:116:ALA:N	2.48	0.47
1:C:88:LYS:HE3	1:C:88:LYS:HB3	1.40	0.47
1:B:60:LEU:HD22	1:B:79:ASN:O	2.15	0.47
1:D:37:GLU:OE2	1:D:220:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:30:PHE:CE1	1:B:96:ALA:HB2	2.49	0.47
1:B:276:GLY:HA3	1:B:279:TRP:NE1	2.29	0.47
1:C:37:GLU:HB3	1:C:38:PRO:CD	2.44	0.47
1:E:56:LEU:C	1:E:56:LEU:HD23	2.34	0.47
1:E:64:VAL:HG13	1:E:72:ILE:CD1	2.45	0.47
1:B:273:ILE:O	1:B:274:GLU:HG2	2.15	0.47
1:D:37:GLU:O	1:D:39:VAL:HG23	2.14	0.47
1:H:369:ASP:CB	1:H:372:ALA:HB3	2.43	0.47
1:E:125:HIS:CE1	1:E:164:GLY:C	2.88	0.47
1:C:276:GLY:HA3	1:C:279:TRP:CE2	2.48	0.47
1:E:6:VAL:HG22	1:E:413:ILE:HG13	1.96	0.47
1:D:91:ARG:NH2	1:D:120:ARG:HB3	2.30	0.47
1:E:96:ALA:O	1:E:99:PRO:HD2	2.14	0.47
1:G:108:GLN:HG3	5:G:635:HOH:O	2.15	0.47
1:D:97:LEU:HB2	1:D:109:VAL:HG21	1.97	0.47
1:G:333:MET:O	1:G:336:PRO:HD2	2.15	0.47
1:E:128:GLY:HA3	1:E:169:ILE:CD1	2.45	0.47
1:E:42:GLN:HA	1:E:69:SER:CB	2.45	0.47
1:H:248:LYS:CB	1:H:248:LYS:NZ	2.78	0.47
1:B:282:LEU:HD21	1:B:284:MET:HG2	1.95	0.47
1:E:111:LEU:HD13	1:E:143:VAL:HG21	1.97	0.47
1:A:282:LEU:HD23	1:A:283:ASP:N	2.30	0.47
1:B:299:HIS:ND1	1:B:300:PRO:HA	2.30	0.47
1:B:13:GLN:HA	1:B:248:LYS:O	2.15	0.47
1:H:255:GLN:HG2	1:H:257:ASP:OD1	2.14	0.47
1:D:6:VAL:HG22	1:D:413:ILE:HG13	1.96	0.47
1:E:10:THR:HG21	1:E:410:GLY:O	2.15	0.47
1:H:81:SER:CB	1:H:108:GLN:HB2	2.44	0.47
1:A:20:GLY:HA3	1:A:43:ASN:O	2.15	0.47
1:D:22:LYS:HB2	1:D:47:LEU:CD1	2.44	0.47
1:H:29:LEU:HD23	1:H:41:ILE:CD1	2.45	0.47
1:A:323:ILE:HB	1:A:352:VAL:HG13	1.97	0.47
1:C:299:HIS:ND1	1:C:300:PRO:HA	2.30	0.47
1:C:115:ASP:CG	1:C:116:ALA:H	2.17	0.47
1:E:103:ARG:HB2	1:E:175:LEU:CD1	2.44	0.47
1:F:248:LYS:HA	1:F:282:LEU:O	2.15	0.47
1:F:85:ASP:O	1:F:89:THR:HG23	2.15	0.47
1:D:169:ILE:HG22	1:D:182:ILE:HD11	1.97	0.47
1:B:124:LEU:HD11	1:B:160:LYS:HG2	1.95	0.47
1:H:370:LEU:HD11	1:H:397:ARG:CD	2.43	0.46
1:B:236:GLY:O	1:B:240:VAL:HG23	2.15	0.46
1:H:251:CYS:O	1:H:279:TRP:HA	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:325:GLU:CG	1:D:329:GLU:H	2.28	0.46
1:G:74:ALA:HB3	5:G:637:HOH:O	2.15	0.46
1:H:233:ILE:HD12	1:H:305:ASP:HB2	1.95	0.46
1:C:277:GLU:HG3	3:C:502:ACT:O	2.15	0.46
1:C:3:LYS:CD	1:C:390:ASP:OD1	2.62	0.46
1:G:369:ASP:CB	1:G:372:ALA:HB3	2.45	0.46
1:B:273:ILE:HG22	1:B:274:GLU:N	2.30	0.46
1:D:325:GLU:HG3	1:D:329:GLU:H	1.80	0.46
1:F:233:ILE:HG21	1:F:371:ARG:CD	2.46	0.46
1:C:323:ILE:HB	1:C:352:VAL:HG12	1.97	0.46
1:A:315:LEU:HD23	1:A:354:CYS:HB3	1.96	0.46
1:F:249:ILE:HG12	1:F:250:VAL:N	2.30	0.46
1:D:243:ALA:HA	1:D:284:MET:HG2	1.96	0.46
1:E:59:GLN:C	1:E:61:GLY:H	2.18	0.46
1:F:157:VAL:O	4:F:509:EDO:H22	2.15	0.46
1:G:63:LYS:HB3	1:G:73:ASP:HB3	1.97	0.46
1:B:41:ILE:O	1:B:69:SER:HB2	2.16	0.46
1:F:41:ILE:HG23	1:F:228:VAL:HG23	1.97	0.46
1:D:116:ALA:O	1:D:330:ASN:ND2	2.38	0.46
1:D:60:LEU:O	1:D:77:VAL:HG13	2.16	0.46
1:C:266:LEU:O	1:C:269:ALA:HB3	2.16	0.46
1:B:282:LEU:HD23	1:B:282:LEU:C	2.35	0.46
1:F:288:ARG:NH2	1:F:317:ALA:O	2.48	0.46
1:H:160:LYS:HA	5:H:653:HOH:O	2.16	0.46
1:H:84:TYR:CE1	4:H:507:EDO:H12	2.50	0.46
1:H:108:GLN:CD	1:H:144:LYS:HE2	2.36	0.46
1:E:1:MET:H3	1:E:418:GLY:HA2	1.76	0.46
1:D:417:LYS:C	1:D:419:GLU:H	2.18	0.46
1:F:353:ILE:HD12	1:F:353:ILE:N	2.31	0.46
1:E:88:LYS:HG2	1:E:88:LYS:O	2.15	0.46
1:G:193:ASP:CG	1:G:229:LEU:HD22	2.36	0.46
1:D:21:ALA:HA	1:D:231:ASP:HB2	1.98	0.46
1:B:37:GLU:O	1:B:38:PRO:C	2.53	0.46
1:H:264:ALA:O	1:H:268:GLU:HG3	2.16	0.46
1:H:66:ARG:HB3	1:H:70:VAL:HG22	1.97	0.46
1:C:367:ALA:CB	1:C:373:SER:HB3	2.40	0.46
1:E:36:GLU:OE1	1:E:220:ARG:NE	2.49	0.46
1:G:331:ARG:NH2	1:G:371:ARG:HB2	2.30	0.46
1:H:320:THR:HA	1:H:354:CYS:O	2.16	0.46
1:G:315:LEU:HD23	1:G:354:CYS:HB3	1.98	0.46
1:B:213:ILE:HG22	1:B:215:ILE:CD1	2.45	0.46
1:H:249:ILE:HG12	1:H:250:VAL:N	2.31	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:147:VAL:HG13	1:A:147:VAL:O	2.16	0.46
1:B:14:GLY:O	1:B:249:ILE:HA	2.16	0.45
1:D:39:VAL:HG12	1:D:41:ILE:HD12	1.98	0.45
1:H:248:LYS:HZ3	1:H:248:LYS:HB3	1.80	0.45
1:D:213:ILE:HG22	1:D:215:ILE:HD11	1.97	0.45
1:F:299:HIS:CG	1:F:300:PRO:HA	2.51	0.45
1:C:20:GLY:HA3	1:C:43:ASN:O	2.16	0.45
1:C:47:LEU:HB3	1:C:397:ARG:O	2.16	0.45
1:D:51:ASP:HA	1:D:54:MET:CE	2.46	0.45
1:D:42:GLN:HA	1:D:69:SER:CB	2.46	0.45
1:G:48:LYS:HZ1	1:G:393:TYR:HB2	1.81	0.45
1:F:416:VAL:CG1	1:F:417:LYS:N	2.79	0.45
1:D:12:LEU:O	1:D:247:GLY:HA3	2.16	0.45
1:B:20:GLY:HA3	1:B:43:ASN:O	2.16	0.45
1:H:126:ILE:O	1:H:130:GLU:HG3	2.16	0.45
1:A:4:PHE:HE2	1:A:395:ILE:HD13	1.80	0.45
1:G:28:ILE:HD12	1:G:228:VAL:HG22	1.99	0.45
1:F:124:LEU:HD11	1:F:160:LYS:HG2	1.97	0.45
1:E:26:LEU:N	1:E:27:PRO:HD2	2.32	0.45
1:F:34:LEU:HD21	1:F:99:PRO:HA	1.97	0.45
1:B:85:ASP:HA	1:B:88:LYS:HE2	1.97	0.45
1:H:367:ALA:HB1	1:H:373:SER:HB2	1.97	0.45
1:B:335:VAL:HB	1:B:336:PRO:CD	2.47	0.45
1:F:116:ALA:HB1	1:F:333:MET:HE1	1.98	0.45
1:H:20:GLY:HA3	1:H:43:ASN:O	2.16	0.45
1:F:313:LEU:HD23	1:F:313:LEU:C	2.37	0.45
1:F:108:GLN:HG2	1:F:144:LYS:CG	2.34	0.45
1:D:59:GLN:OE1	1:D:79:ASN:ND2	2.49	0.45
1:B:376:LEU:O	1:B:379:ALA:HB3	2.17	0.45
1:G:299:HIS:CG	1:G:300:PRO:HA	2.51	0.45
1:G:115:ASP:OD2	1:G:117:ILE:HG12	2.17	0.45
1:A:105:GLY:HA2	1:A:147:VAL:CG1	2.47	0.45
1:B:316:VAL:HG23	1:B:316:VAL:O	2.17	0.45
1:B:111:LEU:HD12	1:B:112:PRO:HD2	1.98	0.45
1:C:22:LYS:HD2	1:C:398:GLY:HA2	1.97	0.45
1:F:309:GLN:OE1	1:F:309:GLN:N	2.39	0.45
1:G:108:GLN:CD	1:G:144:LYS:HE2	2.37	0.45
1:E:5:ARG:NH1	5:E:641:HOH:O	2.40	0.45
1:G:11:ARG:HD3	1:G:13:GLN:OE1	2.17	0.45
1:G:197:PHE:CZ	1:G:201:LEU:HD11	2.52	0.45
1:G:401:ARG:HA	5:G:642:HOH:O	2.17	0.45
1:H:59:GLN:NE2	1:H:86:LEU:HD11	2.32	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:299:HIS:ND1	1:F:300:PRO:HA	2.32	0.44
1:C:21:ALA:HA	1:C:231:ASP:HB2	1.98	0.44
1:D:31:ALA:HB1	1:D:198:LEU:HD21	1.98	0.44
1:C:395:ILE:HG23	1:C:396:ASP:N	2.32	0.44
1:C:220:ARG:HG3	1:C:220:ARG:NH1	2.33	0.44
1:E:265:LYS:HE3	1:E:293:THR:O	2.17	0.44
1:E:374:ALA:HB2	1:E:399:TYR:CE1	2.52	0.44
1:G:276:GLY:HA3	1:G:279:TRP:CE2	2.53	0.44
1:F:12:LEU:CD1	1:F:241:ALA:HB1	2.46	0.44
1:E:187:ARG:HD2	1:F:211:ASP:OD2	2.17	0.44
1:H:314:ASN:HD22	1:H:323:ILE:HD11	1.82	0.44
1:B:115:ASP:HB3	1:B:120:ARG:HD3	2.00	0.44
1:G:34:LEU:HD21	1:G:99:PRO:HA	2.00	0.44
1:F:64:VAL:HG13	1:F:72:ILE:HD13	2.00	0.44
1:G:331:ARG:HG2	1:G:331:ARG:O	2.18	0.44
1:A:181:ILE:HG23	1:A:212:ARG:HG3	1.99	0.44
1:G:131:LYS:HE3	1:G:156:ILE:HG12	2.00	0.44
1:B:5:ARG:HE	1:B:416:VAL:HG21	1.81	0.44
1:B:87:VAL:HG11	1:B:110:SER:O	2.17	0.44
1:B:218:VAL:HG21	1:B:221:LEU:HD21	2.00	0.44
1:E:37:GLU:HB3	1:E:38:PRO:CD	2.48	0.44
1:B:127:PHE:CZ	1:B:131:LYS:HE3	2.53	0.44
1:E:50:ILE:O	1:E:54:MET:HG3	2.17	0.44
1:H:167:VAL:HG12	4:H:508:EDO:H22	1.98	0.44
1:D:320:THR:HA	1:D:354:CYS:O	2.16	0.44
1:B:81:SER:CB	1:B:108:GLN:HG3	2.30	0.44
1:H:392:ILE:HD12	1:H:415:ARG:NH1	2.33	0.44
1:B:372:ALA:O	1:B:373:SER:C	2.56	0.44
1:D:124:LEU:HD11	1:D:160:LYS:CG	2.48	0.44
1:H:367:ALA:CB	1:H:373:SER:HB2	2.48	0.44
1:A:366:MET:CE	1:D:88:LYS:HD2	2.48	0.44
1:H:13:GLN:HA	1:H:248:LYS:O	2.18	0.44
1:E:109:VAL:HG12	1:E:110:SER:O	2.17	0.44
1:H:11:ARG:HD3	1:H:247:GLY:HA2	2.00	0.44
1:E:233:ILE:HG21	1:E:371:ARG:HD3	2.00	0.44
1:C:374:ALA:O	1:C:378:LEU:HG	2.18	0.44
1:G:193:ASP:CB	1:G:229:LEU:HD22	2.48	0.43
1:H:101:VAL:HG11	1:H:145:ALA:HB3	2.00	0.43
1:E:12:LEU:HD12	1:E:241:ALA:HB1	2.00	0.43
1:F:369:ASP:CG	1:F:372:ALA:HB3	2.38	0.43
1:H:67:IAS:CG	1:H:69:SER:N	2.81	0.43
1:B:308:ALA:HA	1:B:334:HIS:NE2	2.32	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:64:VAL:HG22	1:G:72:ILE:CD1	2.49	0.43
1:B:193:ASP:CG	1:B:229:LEU:HD22	2.38	0.43
1:F:39:VAL:HG12	1:F:40:GLU:N	2.32	0.43
1:A:374:ALA:HB2	1:A:399:TYR:CE1	2.53	0.43
1:D:3:LYS:HE2	1:D:390:ASP:OD1	2.18	0.43
1:B:24:ALA:HB3	1:B:228:VAL:HG13	1.99	0.43
1:A:395:ILE:CG2	1:A:396:ASP:N	2.81	0.43
1:B:108:GLN:HB3	1:B:144:LYS:HG2	1.99	0.43
1:D:41:ILE:HG22	1:D:44:VAL:HG23	1.99	0.43
1:A:323:ILE:HB	1:A:352:VAL:HG12	1.98	0.43
1:D:340:ARG:HG2	1:D:340:ARG:HH11	1.83	0.43
1:F:320:THR:HA	1:F:354:CYS:O	2.19	0.43
1:B:16:VAL:CG1	1:B:249:ILE:HD11	2.48	0.43
1:A:244:ILE:HD12	1:A:382:ILE:HD13	2.01	0.43
1:G:56:LEU:HD23	1:G:56:LEU:C	2.39	0.43
1:B:220:ARG:HG3	1:B:220:ARG:NH1	2.33	0.43
1:D:87:VAL:HG11	1:D:110:SER:O	2.18	0.43
1:E:396:ASP:CG	1:E:415:ARG:HH22	2.22	0.43
1:E:1:MET:C	1:E:418:GLY:HA2	2.39	0.43
1:D:335:VAL:HB	1:D:336:PRO:CD	2.48	0.43
1:H:289:PRO:HD3	5:H:601:HOH:O	2.18	0.43
1:B:416:VAL:HG12	1:B:417:LYS:N	2.33	0.43
1:E:256:PRO:HG3	1:E:280:ILE:HG13	2.00	0.43
1:A:22:LYS:HD3	1:A:398:GLY:HA2	2.01	0.43
1:A:35:ALA:HB1	1:A:222:GLY:O	2.19	0.43
1:G:371:ARG:HD3	1:G:371:ARG:HA	1.75	0.43
1:D:189:PRO:HD3	1:D:299:HIS:CD2	2.54	0.43
1:D:317:ALA:O	1:D:356:GLY:HA3	2.18	0.43
1:A:265:LYS:HA	1:A:265:LYS:HD3	1.78	0.43
1:D:151:LEU:O	1:D:176:ALA:HB1	2.19	0.43
1:A:308:ALA:HA	1:A:334:HIS:NE2	2.34	0.42
1:B:32:ALA:O	1:B:34:LEU:N	2.52	0.42
1:D:238:PHE:O	1:D:241:ALA:HB3	2.19	0.42
1:C:64:VAL:HG13	1:C:72:ILE:CD1	2.49	0.42
1:C:335:VAL:HB	1:C:336:PRO:CD	2.49	0.42
1:A:161:VAL:HG11	1:A:298:PRO:HB3	2.00	0.42
1:A:4:PHE:HE1	1:A:415:ARG:HB2	1.83	0.42
1:G:118:GLY:HA2	1:G:329:GLU:OE1	2.14	0.42
1:A:182:ILE:O	1:A:212:ARG:HA	2.19	0.42
1:E:63:LYS:O	1:E:72:ILE:HA	2.19	0.42
1:E:51:ASP:HA	1:E:54:MET:HE2	2.01	0.42
1:D:2:ASP:HB3	1:D:392:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:315:LEU:O	1:B:357:VAL:HG22	2.18	0.42
1:D:94:ILE:CD1	1:D:122:VAL:HG11	2.49	0.42
1:F:33:LEU:CD2	1:F:57:LEU:HD22	2.46	0.42
1:B:323:ILE:HB	1:B:352:VAL:HG13	2.01	0.42
1:E:85:ASP:O	1:E:89:THR:HG23	2.19	0.42
1:E:259:LEU:HD12	1:E:263:LEU:HG	2.01	0.42
1:C:254:ALA:O	1:C:278:ASP:HA	2.20	0.42
1:C:282:LEU:HD23	1:C:282:LEU:C	2.40	0.42
1:E:29:LEU:O	1:E:32:ALA:HB3	2.20	0.42
1:A:230:PRO:HG2	1:A:255:GLN:HB2	2.01	0.42
1:A:117:ILE:HG21	1:A:369:ASP:OD2	2.19	0.42
1:E:323:ILE:O	1:E:351:THR:HA	2.20	0.42
1:E:265:LYS:HA	1:E:265:LYS:HD3	1.84	0.42
1:H:235:THR:O	1:H:239:LEU:HG	2.19	0.42
1:D:308:ALA:HA	1:D:334:HIS:NE2	2.34	0.42
1:C:30:PHE:CZ	1:C:53:THR:HG23	2.54	0.42
1:H:402:ILE:HG23	1:H:403:GLU:N	2.35	0.42
1:B:315:LEU:HD21	1:B:345:ALA:HB2	2.01	0.42
1:E:232:ARG:HB2	1:E:259:LEU:HD23	2.01	0.42
1:B:313:LEU:C	1:B:313:LEU:HD23	2.40	0.42
1:C:370:LEU:HD11	1:C:399:TYR:CE1	2.54	0.42
1:H:42:GLN:HA	1:H:69:SER:CB	2.41	0.42
1:F:414:GLU:HG2	1:F:416:VAL:HG23	2.02	0.42
1:F:64:VAL:C	1:F:65:GLU:HG3	2.40	0.42
1:F:20:GLY:HA3	1:F:43:ASN:O	2.19	0.42
1:C:11:ARG:HD3	1:C:13:GLN:OE1	2.20	0.42
1:C:136:ILE:HA	1:C:144:LYS:O	2.20	0.42
1:A:21:ALA:HA	1:A:231:ASP:CB	2.49	0.42
1:D:34:LEU:HD21	1:D:99:PRO:HA	2.00	0.42
1:B:77:VAL:HB	1:B:104:PHE:CZ	2.55	0.42
1:A:333:MET:HE3	1:A:333:MET:HA	2.00	0.42
1:B:264:ALA:O	1:B:268:GLU:HG3	2.19	0.42
1:C:5:ARG:NH1	1:C:386:THR:HG21	2.35	0.42
1:H:370:LEU:HD12	1:H:397:ARG:CD	2.35	0.42
1:H:2:ASP:HB3	1:H:392:ILE:CD1	2.38	0.42
1:C:28:ILE:HG23	1:C:197:PHE:CD2	2.54	0.42
1:C:24:ALA:CB	1:C:228:VAL:HG13	2.48	0.42
1:E:111:LEU:HA	1:E:112:PRO:HD3	1.90	0.42
1:D:213:ILE:HG22	1:D:215:ILE:CD1	2.50	0.42
1:H:91:ARG:C	1:H:93:SER:H	2.23	0.42
1:G:182:ILE:HG22	1:G:185:ALA:HB2	2.00	0.42
1:E:132:LEU:HA	1:E:132:LEU:HD23	1.87	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:244:ILE:HD12	1:C:382:ILE:HD13	2.01	0.42
1:E:317:ALA:O	1:E:356:GLY:HA3	2.20	0.42
1:B:4:PHE:CE2	1:B:413:ILE:HD11	2.55	0.42
1:D:294:VAL:HB	1:D:323:ILE:HD13	2.00	0.42
1:B:83:PRO:CG	1:B:86:LEU:HD12	2.50	0.42
1:D:382:ILE:HD12	4:D:507:EDO:H22	2.01	0.42
1:A:189:PRO:HD3	1:A:299:HIS:CD2	2.55	0.42
1:H:55:LYS:HA	4:H:510:EDO:H22	2.02	0.42
1:C:392:ILE:HB	1:C:395:ILE:HG21	2.01	0.41
1:B:197:PHE:O	1:B:201:LEU:HG	2.20	0.41
1:C:64:VAL:O	1:C:65:GLU:HG3	2.20	0.41
1:E:103:ARG:HG2	1:E:104:PHE:CE1	2.54	0.41
1:E:81:SER:HB3	1:E:108:GLN:HB2	2.02	0.41
1:F:282:LEU:C	1:F:282:LEU:HD23	2.40	0.41
1:H:66:ARG:CB	1:H:70:VAL:HG22	2.50	0.41
2:A:501:UD1:H5'2	4:A:507:EDO:O2	2.20	0.41
1:H:256:PRO:HG3	1:H:280:ILE:CG1	2.50	0.41
1:B:369:ASP:C	1:B:371:ARG:H	2.23	0.41
1:H:117:ILE:HG22	1:H:331:ARG:HG3	2.01	0.41
1:H:56:LEU:HB2	1:H:86:LEU:HD13	2.02	0.41
1:B:189:PRO:HD3	1:B:299:HIS:CD2	2.55	0.41
1:B:30:PHE:HE1	1:B:96:ALA:HB2	1.85	0.41
1:B:273:ILE:CG2	1:B:274:GLU:N	2.84	0.41
1:G:245:SER:HB3	1:G:382:ILE:HG22	2.01	0.41
1:H:2:ASP:C	1:H:392:ILE:HG12	2.41	0.41
1:H:366:MET:HE2	1:H:391:ARG:HD2	2.01	0.41
1:A:81:SER:HA	1:A:108:GLN:O	2.20	0.41
1:A:298:PRO:HA	4:A:507:EDO:H11	2.03	0.41
1:E:203:ALA:HB2	1:E:221:LEU:HD21	2.03	0.41
1:G:22:LYS:HD3	1:G:371:ARG:NH2	2.35	0.41
1:H:236:GLY:O	1:H:240:VAL:HG23	2.20	0.41
1:C:37:GLU:HB3	1:C:38:PRO:HD2	2.02	0.41
1:E:195:ALA:HB3	1:E:208:GLN:HG3	2.02	0.41
1:G:50:ILE:O	1:G:54:MET:HG3	2.20	0.41
1:H:29:LEU:HD23	1:H:41:ILE:HD13	2.03	0.41
1:B:415:ARG:HG2	1:B:415:ARG:O	2.19	0.41
1:F:199:VAL:O	1:F:202:GLY:N	2.49	0.41
1:A:88:LYS:HG2	1:A:88:LYS:O	2.21	0.41
1:D:282:LEU:HD23	1:D:282:LEU:C	2.40	0.41
1:B:54:MET:HG2	1:B:64:VAL:HG11	2.02	0.41
1:C:161:VAL:O	3:C:503:ACT:H2	2.21	0.41
1:F:204:LYS:HG3	1:F:218:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:208:GLN:HA	1:A:213:ILE:HG12	2.03	0.41
1:D:252:ARG:O	1:D:253:ASN:HB2	2.21	0.41
1:H:370:LEU:HD12	1:H:397:ARG:HB2	2.03	0.41
1:D:12:LEU:CD1	1:D:241:ALA:HB1	2.51	0.41
1:C:196:ASN:HB2	1:C:226:TYR:OH	2.20	0.41
1:D:65:GLU:HG3	1:D:71:TRP:HB2	2.02	0.41
1:B:66:ARG:HD2	1:B:70:VAL:HG22	2.03	0.41
1:A:60:LEU:HA	1:A:79:ASN:HB3	2.03	0.41
1:C:392:ILE:C	1:C:395:ILE:HG22	2.15	0.41
1:C:39:VAL:HG12	1:C:41:ILE:CD1	2.50	0.41
1:B:373:SER:HB3	1:B:395:ILE:CG1	2.51	0.41
1:E:42:GLN:HA	1:E:69:SER:HB2	2.02	0.41
1:A:256:PRO:HG3	1:A:280:ILE:HG12	2.02	0.41
1:G:131:LYS:HB3	1:G:131:LYS:HE3	1.94	0.41
1:F:371:ARG:NH2	1:F:398:GLY:O	2.54	0.41
1:C:314:ASN:HB3	1:C:354:CYS:HB2	2.03	0.41
1:E:13:GLN:O	1:E:409:LEU:HA	2.21	0.41
1:B:16:VAL:HG11	1:B:249:ILE:HD11	2.03	0.41
1:H:370:LEU:CD1	1:H:397:ARG:CZ	2.99	0.41
1:G:340:ARG:NH1	1:G:340:ARG:CG	2.83	0.41
1:H:91:ARG:C	1:H:93:SER:N	2.73	0.41
1:F:263:LEU:HD22	1:F:273:ILE:HD13	2.02	0.41
1:D:283:ASP:OD2	1:D:285:HIS:CE1	2.74	0.41
1:C:67:IAS:CG	1:C:69:SER:N	2.84	0.41
1:C:2:ASP:HB3	1:C:392:ILE:HD11	2.03	0.40
1:C:4:PHE:CD1	1:C:392:ILE:HD13	2.56	0.40
1:D:91:ARG:NH2	1:D:120:ARG:CB	2.84	0.40
1:A:369:ASP:C	1:A:371:ARG:N	2.74	0.40
1:E:330:ASN:HB2	1:H:330:ASN:CG	2.42	0.40
1:H:117:ILE:HD12	1:H:328:PHE:CD2	2.56	0.40
1:H:56:LEU:HD23	1:H:56:LEU:O	2.20	0.40
1:E:57:LEU:O	1:E:62:THR:CB	2.69	0.40
1:B:57:LEU:HD23	1:B:57:LEU:HA	1.92	0.40
1:H:63:LYS:HG2	3:H:504:ACT:H3	2.03	0.40
1:F:315:LEU:HD22	1:F:343:ALA:HB1	2.01	0.40
1:A:196:ASN:OD1	1:A:208:GLN:NE2	2.55	0.40
1:E:33:LEU:HD13	1:E:100:LEU:HD21	2.03	0.40
1:G:147:VAL:HG13	1:G:147:VAL:O	2.20	0.40
1:C:367:ALA:HB1	1:C:373:SER:CB	2.44	0.40
1:A:314:ASN:ND2	1:A:323:ILE:HD11	2.36	0.40
1:B:190:GLU:N	1:B:190:GLU:OE1	2.50	0.40
1:A:4:PHE:HA	1:A:4:PHE:HD1	1.79	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:233:ILE:HG23	1:A:306:MET:HE3	2.03	0.40
1:F:1:MET:CE	1:F:391:ARG:HG2	2.50	0.40
1:B:401:ARG:HB3	1:B:404:ASP:OD2	2.21	0.40
1:B:395:ILE:HG21	1:B:402:ILE:CG2	2.52	0.40
1:D:24:ALA:HB3	1:D:228:VAL:HG13	2.03	0.40
1:C:4:PHE:CG	1:C:392:ILE:HG21	2.56	0.40
1:F:40:GLU:CD	1:F:71:TRP:HE1	2.25	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:419:GLU:O	1:H:139:GLU:OE2[2_456]	1.89	0.31

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	415/419 (99%)	398 (96%)	14 (3%)	3 (1%)	30	50
1	B	415/419 (99%)	386 (93%)	26 (6%)	3 (1%)	30	50
1	C	415/419 (99%)	404 (97%)	9 (2%)	2 (0%)	38	60
1	D	415/419 (99%)	398 (96%)	14 (3%)	3 (1%)	30	50
1	E	415/419 (99%)	389 (94%)	21 (5%)	5 (1%)	19	32
1	F	415/419 (99%)	399 (96%)	16 (4%)	0	100	100
1	G	415/419 (99%)	400 (96%)	15 (4%)	0	100	100
1	H	415/419 (99%)	397 (96%)	18 (4%)	0	100	100
All	All	3320/3352 (99%)	3171 (96%)	133 (4%)	16 (0%)	38	60

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	119	ALA

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Mol	Chain	Res	Type
1	E	60	LEU
1	E	77	VAL
1	B	33	LEU
1	A	417	LYS
1	B	92	ALA
1	B	370	LEU
1	C	92	ALA
1	D	118	GLY
1	E	140	GLU
1	A	148	ASN
1	A	370	LEU
1	D	418	GLY
1	E	222	GLY
1	C	77	VAL
1	E	392	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	329/329 (100%)	326 (99%)	3 (1%)	87	97
1	B	329/329 (100%)	324 (98%)	5 (2%)	76	93
1	C	329/329 (100%)	325 (99%)	4 (1%)	82	95
1	D	329/329 (100%)	327 (99%)	2 (1%)	92	98
1	E	329/329 (100%)	325 (99%)	4 (1%)	82	95
1	F	329/329 (100%)	325 (99%)	4 (1%)	82	95
1	G	329/329 (100%)	327 (99%)	2 (1%)	92	98
1	H	329/329 (100%)	326 (99%)	3 (1%)	87	97
All	All	2632/2632 (100%)	2605 (99%)	27 (1%)	85	97

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	ARG
1	A	193	ASP

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Mol	Chain	Res	Type
1	A	229	LEU
1	B	187	ARG
1	B	193	ASP
1	B	278	ASP
1	B	307	GLN
1	B	371	ARG
1	C	10	THR
1	C	187	ARG
1	C	259	LEU
1	C	371	ARG
1	D	59	GLN
1	D	187	ARG
1	E	22	LYS
1	E	66	ARG
1	E	187	ARG
1	E	391	ARG
1	F	135	GLU
1	F	187	ARG
1	F	229	LEU
1	F	371	ARG
1	G	187	ARG
1	G	229	LEU
1	H	135	GLU
1	H	187	ARG
1	H	371	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	79	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	IAS	A	67	1	7,7,8	6.97	1 (14%)	6,8,10	0.77	0
1	IAS	B	67	1	7,7,8	6.61	1 (14%)	6,8,10	0.91	0
1	IAS	C	67	1	7,7,8	6.79	1 (14%)	6,8,10	0.54	0
1	IAS	D	67	1	7,7,8	6.73	1 (14%)	6,8,10	1.52	1 (16%)
1	IAS	E	67	1	7,7,8	6.63	1 (14%)	6,8,10	1.36	1 (16%)
1	IAS	F	67	1	7,7,8	6.98	1 (14%)	6,8,10	0.62	0
1	IAS	G	67	1	7,7,8	7.03	2 (28%)	6,8,10	0.35	0
1	IAS	H	67	1	7,7,8	6.83	1 (14%)	6,8,10	1.33	1 (16%)

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
1	IAS	A	67	1	-	0/6/7/8	0/0/0/0
1	IAS	B	67	1	-	0/6/7/8	0/0/0/0
1	IAS	C	67	1	-	0/6/7/8	0/0/0/0
1	IAS	D	67	1	-	0/6/7/8	0/0/0/0
1	IAS	E	67	1	-	0/6/7/8	0/0/0/0
1	IAS	F	67	1	-	0/6/7/8	0/0/0/0
1	IAS	G	67	1	-	0/6/7/8	0/0/0/0
1	IAS	H	67	1	-	0/6/7/8	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	67	IAS	OD1-CG	18.32	1.24	1.11
1	A	67	IAS	OD1-CG	18.22	1.24	1.11
1	F	67	IAS	OD1-CG	18.22	1.24	1.11
1	H	67	IAS	OD1-CG	17.86	1.23	1.11
1	C	67	IAS	OD1-CG	17.76	1.23	1.11
1	D	67	IAS	OD1-CG	17.58	1.23	1.11
1	E	67	IAS	OD1-CG	17.32	1.23	1.11
1	B	67	IAS	OD1-CG	17.30	1.23	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	67	IAS	CB-CA	-2.16	1.52	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	67	IAS	C-CA-N	3.42	115.02	109.36
1	E	67	IAS	C-CA-N	3.29	114.81	109.36
1	H	67	IAS	C-CA-N	3.14	114.57	109.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates i

There are no carbohydrates in this entry.

5.6 Ligand geometry i

72 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	UD1	A	501	-	41,41,41	1.85	14 (34%)	58,62,62	1.35	7 (12%)
3	ACT	A	502	-	1,3,3	2.97	1 (100%)	0,3,3	0.00	-
3	ACT	A	503	-	1,3,3	1.82	0	0,3,3	0.00	-
3	ACT	A	504	-	1,3,3	2.24	1 (100%)	0,3,3	0.00	-
3	ACT	A	505	-	1,3,3	2.25	1 (100%)	0,3,3	0.00	-
4	EDO	A	506	-	3,3,3	0.62	0	2,2,2	0.38	0
4	EDO	A	507	-	3,3,3	0.55	0	2,2,2	0.41	0
4	EDO	A	508	-	3,3,3	0.59	0	2,2,2	0.34	0
4	EDO	A	509	-	3,3,3	0.63	0	2,2,2	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UD1	B	501	-	41,41,41	1.97	16 (39%)	58,62,62	1.35	7 (12%)
3	ACT	B	502	-	1,3,3	2.14	1 (100%)	0,3,3	0.00	-
4	EDO	B	503	-	3,3,3	0.44	0	2,2,2	0.49	0
4	EDO	B	504	-	3,3,3	0.53	0	2,2,2	0.39	0
4	EDO	B	505	-	3,3,3	0.50	0	2,2,2	0.40	0
2	UD1	C	501	-	41,41,41	1.88	14 (34%)	58,62,62	1.33	6 (10%)
3	ACT	C	502	-	1,3,3	1.93	0	0,3,3	0.00	-
3	ACT	C	503	-	1,3,3	2.54	1 (100%)	0,3,3	0.00	-
4	EDO	C	504	-	3,3,3	0.53	0	2,2,2	0.34	0
4	EDO	C	505	-	3,3,3	0.68	0	2,2,2	0.28	0
4	EDO	C	506	-	3,3,3	0.62	0	2,2,2	0.32	0
4	EDO	C	507	-	3,3,3	0.60	0	2,2,2	0.35	0
2	UD1	D	501	-	41,41,41	2.03	14 (34%)	58,62,62	1.44	8 (13%)
3	ACT	D	502	-	1,3,3	2.28	1 (100%)	0,3,3	0.00	-
3	ACT	D	503	-	1,3,3	1.88	0	0,3,3	0.00	-
4	EDO	D	504	-	3,3,3	0.49	0	2,2,2	0.46	0
4	EDO	D	505	-	3,3,3	0.44	0	2,2,2	0.43	0
4	EDO	D	506	-	3,3,3	0.72	0	2,2,2	0.24	0
4	EDO	D	507	-	3,3,3	0.53	0	2,2,2	0.36	0
4	EDO	D	508	-	3,3,3	0.66	0	2,2,2	0.26	0
4	EDO	D	509	-	3,3,3	0.54	0	2,2,2	0.36	0
4	EDO	D	510	-	3,3,3	0.62	0	2,2,2	0.39	0
2	UD1	E	501	-	41,41,41	2.05	14 (34%)	58,62,62	1.47	9 (15%)
3	ACT	E	502	-	1,3,3	1.50	0	0,3,3	0.00	-
3	ACT	E	503	-	1,3,3	1.89	0	0,3,3	0.00	-
3	ACT	E	504	-	1,3,3	1.91	0	0,3,3	0.00	-
4	EDO	E	505	-	3,3,3	0.59	0	2,2,2	0.35	0
4	EDO	E	506	-	3,3,3	0.64	0	2,2,2	0.29	0
4	EDO	E	507	-	3,3,3	0.70	0	2,2,2	0.28	0
4	EDO	E	508	-	3,3,3	0.63	0	2,2,2	0.28	0
4	EDO	E	509	-	3,3,3	0.44	0	2,2,2	0.39	0
4	EDO	E	510	-	3,3,3	0.68	0	2,2,2	0.24	0
4	EDO	E	511	-	3,3,3	0.62	0	2,2,2	0.32	0
2	UD1	F	501	-	41,41,41	1.86	10 (24%)	58,62,62	1.44	7 (12%)
3	ACT	F	502	-	1,3,3	2.19	1 (100%)	0,3,3	0.00	-
3	ACT	F	503	-	1,3,3	1.49	0	0,3,3	0.00	-
3	ACT	F	504	-	1,3,3	2.33	1 (100%)	0,3,3	0.00	-
4	EDO	F	505	-	3,3,3	0.54	0	2,2,2	0.38	0
4	EDO	F	506	-	3,3,3	0.57	0	2,2,2	0.38	0
4	EDO	F	507	-	3,3,3	0.58	0	2,2,2	0.32	0
4	EDO	F	508	-	3,3,3	0.57	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	F	509	-	3,3,3	0.64	0	2,2,2	0.37	0
2	UD1	G	501	-	41,41,41	1.89	11 (26%)	58,62,62	1.49	7 (12%)
4	EDO	G	502	-	3,3,3	0.52	0	2,2,2	0.35	0
4	EDO	G	503	-	3,3,3	0.56	0	2,2,2	0.38	0
4	EDO	G	504	-	3,3,3	0.67	0	2,2,2	0.28	0
4	EDO	G	505	-	3,3,3	0.57	0	2,2,2	0.36	0
4	EDO	G	506	-	3,3,3	0.63	0	2,2,2	0.32	0
4	EDO	G	507	-	3,3,3	0.66	0	2,2,2	0.27	0
4	EDO	G	508	-	3,3,3	0.94	0	2,2,2	0.34	0
2	UD1	H	501	-	41,41,41	2.15	14 (34%)	58,62,62	1.42	8 (13%)
3	ACT	H	502	-	1,3,3	1.90	0	0,3,3	0.00	-
3	ACT	H	503	-	1,3,3	0.51	0	0,3,3	0.00	-
3	ACT	H	504	-	1,3,3	1.18	0	0,3,3	0.00	-
3	ACT	H	505	-	1,3,3	2.21	1 (100%)	0,3,3	0.00	-
3	ACT	H	506	-	1,3,3	2.49	1 (100%)	0,3,3	0.00	-
4	EDO	H	507	-	3,3,3	0.56	0	2,2,2	0.32	0
4	EDO	H	508	-	3,3,3	0.67	0	2,2,2	0.30	0
4	EDO	H	509	-	3,3,3	0.60	0	2,2,2	0.33	0
4	EDO	H	510	-	3,3,3	0.60	0	2,2,2	0.34	0
4	EDO	H	511	-	3,3,3	0.60	0	2,2,2	0.37	0
4	EDO	H	512	-	3,3,3	0.61	0	2,2,2	0.37	0
4	EDO	H	513	-	3,3,3	0.62	0	2,2,2	0.33	0

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	UD1	A	501	-	-	0/25/63/63	0/3/3/3
3	ACT	A	502	-	-	0/0/0/0	0/0/0/0
3	ACT	A	503	-	-	0/0/0/0	0/0/0/0
3	ACT	A	504	-	-	0/0/0/0	0/0/0/0
3	ACT	A	505	-	-	0/0/0/0	0/0/0/0
4	EDO	A	506	-	-	0/1/1/1	0/0/0/0
4	EDO	A	507	-	-	0/1/1/1	0/0/0/0
4	EDO	A	508	-	-	0/1/1/1	0/0/0/0
4	EDO	A	509	-	-	0/1/1/1	0/0/0/0
2	UD1	B	501	-	-	0/25/63/63	0/3/3/3
3	ACT	B	502	-	-	0/0/0/0	0/0/0/0
4	EDO	B	503	-	-	0/1/1/1	0/0/0/0
4	EDO	B	504	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	505	-	-	0/1/1/1	0/0/0/0
2	UD1	C	501	-	-	0/25/63/63	0/3/3/3
3	ACT	C	502	-	-	0/0/0/0	0/0/0/0
3	ACT	C	503	-	-	0/0/0/0	0/0/0/0
4	EDO	C	504	-	-	0/1/1/1	0/0/0/0
4	EDO	C	505	-	-	0/1/1/1	0/0/0/0
4	EDO	C	506	-	-	0/1/1/1	0/0/0/0
4	EDO	C	507	-	-	0/1/1/1	0/0/0/0
2	UD1	D	501	-	-	0/25/63/63	0/3/3/3
3	ACT	D	502	-	-	0/0/0/0	0/0/0/0
3	ACT	D	503	-	-	0/0/0/0	0/0/0/0
4	EDO	D	504	-	-	0/1/1/1	0/0/0/0
4	EDO	D	505	-	-	0/1/1/1	0/0/0/0
4	EDO	D	506	-	-	0/1/1/1	0/0/0/0
4	EDO	D	507	-	-	0/1/1/1	0/0/0/0
4	EDO	D	508	-	-	0/1/1/1	0/0/0/0
4	EDO	D	509	-	-	0/1/1/1	0/0/0/0
4	EDO	D	510	-	-	0/1/1/1	0/0/0/0
2	UD1	E	501	-	-	0/25/63/63	0/3/3/3
3	ACT	E	502	-	-	0/0/0/0	0/0/0/0
3	ACT	E	503	-	-	0/0/0/0	0/0/0/0
3	ACT	E	504	-	-	0/0/0/0	0/0/0/0
4	EDO	E	505	-	-	0/1/1/1	0/0/0/0
4	EDO	E	506	-	-	0/1/1/1	0/0/0/0
4	EDO	E	507	-	-	0/1/1/1	0/0/0/0
4	EDO	E	508	-	-	0/1/1/1	0/0/0/0
4	EDO	E	509	-	-	0/1/1/1	0/0/0/0
4	EDO	E	510	-	-	0/1/1/1	0/0/0/0
4	EDO	E	511	-	-	0/1/1/1	0/0/0/0
2	UD1	F	501	-	-	0/25/63/63	0/3/3/3
3	ACT	F	502	-	-	0/0/0/0	0/0/0/0
3	ACT	F	503	-	-	0/0/0/0	0/0/0/0
3	ACT	F	504	-	-	0/0/0/0	0/0/0/0
4	EDO	F	505	-	-	0/1/1/1	0/0/0/0
4	EDO	F	506	-	-	0/1/1/1	0/0/0/0
4	EDO	F	507	-	-	0/1/1/1	0/0/0/0
4	EDO	F	508	-	-	0/1/1/1	0/0/0/0
4	EDO	F	509	-	-	0/1/1/1	0/0/0/0
2	UD1	G	501	-	-	0/25/63/63	0/3/3/3
4	EDO	G	502	-	-	0/1/1/1	0/0/0/0
4	EDO	G	503	-	-	0/1/1/1	0/0/0/0
4	EDO	G	504	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	G	505	-	-	0/1/1/1	0/0/0/0
4	EDO	G	506	-	-	0/1/1/1	0/0/0/0
4	EDO	G	507	-	-	0/1/1/1	0/0/0/0
4	EDO	G	508	-	-	0/1/1/1	0/0/0/0
2	UD1	H	501	-	-	0/25/63/63	0/3/3/3
3	ACT	H	502	-	-	0/0/0/0	0/0/0/0
3	ACT	H	503	-	-	0/0/0/0	0/0/0/0
3	ACT	H	504	-	-	0/0/0/0	0/0/0/0
3	ACT	H	505	-	-	0/0/0/0	0/0/0/0
3	ACT	H	506	-	-	0/0/0/0	0/0/0/0
4	EDO	H	507	-	-	0/1/1/1	0/0/0/0
4	EDO	H	508	-	-	0/1/1/1	0/0/0/0
4	EDO	H	509	-	-	0/1/1/1	0/0/0/0
4	EDO	H	510	-	-	0/1/1/1	0/0/0/0
4	EDO	H	511	-	-	0/1/1/1	0/0/0/0
4	EDO	H	512	-	-	0/1/1/1	0/0/0/0
4	EDO	H	513	-	-	0/1/1/1	0/0/0/0

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	UD1	PA-O3A	-5.71	1.49	1.59
2	H	501	UD1	PA-O3A	-5.62	1.49	1.59
2	F	501	UD1	PA-O3A	-5.36	1.50	1.59
2	E	501	UD1	PA-O3A	-5.19	1.50	1.59
2	G	501	UD1	PA-O3A	-5.14	1.50	1.59
2	B	501	UD1	PA-O3A	-4.95	1.50	1.59
2	H	501	UD1	C6-N1	4.63	1.43	1.35
2	A	501	UD1	PA-O3A	-4.60	1.51	1.59
2	C	501	UD1	C6-N1	4.57	1.43	1.35
2	D	501	UD1	C2-N1	4.31	1.43	1.38
2	E	501	UD1	C2-N1	4.20	1.43	1.38
2	E	501	UD1	C6-N1	4.16	1.42	1.35
2	D	501	UD1	C6-N1	4.04	1.42	1.35
2	B	501	UD1	C6-N1	4.01	1.42	1.35
2	H	501	UD1	C2-N1	4.00	1.42	1.38
2	G	501	UD1	C6-N1	3.96	1.42	1.35
2	F	501	UD1	C6-N1	3.89	1.42	1.35
2	B	501	UD1	C2B-C1B	-3.73	1.48	1.53
2	C	501	UD1	PA-O3A	-3.67	1.53	1.59
2	H	501	UD1	C2B-C1B	-3.63	1.48	1.53
2	G	501	UD1	C2-N1	3.60	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	UD1	C6-N1	3.56	1.41	1.35
2	H	501	UD1	O1'-C1'	3.50	1.48	1.42
2	E	501	UD1	O1'-C1'	3.34	1.48	1.42
2	A	501	UD1	O5'-C5'	3.29	1.52	1.44
2	D	501	UD1	O5'-C5'	3.29	1.52	1.44
2	C	501	UD1	C2-N1	2.97	1.41	1.38
3	A	502	ACT	CH3-C	2.97	1.53	1.48
2	E	501	UD1	O3B-C3B	2.96	1.50	1.43
2	E	501	UD1	C2B-C1B	-2.89	1.49	1.53
2	B	501	UD1	C2-N1	2.79	1.41	1.38
2	C	501	UD1	PB-O2B	-2.78	1.42	1.55
2	G	501	UD1	O5'-C5'	2.75	1.51	1.44
2	A	501	UD1	O2'-C2B	2.75	1.49	1.43
2	C	501	UD1	C2B-C1B	-2.74	1.49	1.53
2	H	501	UD1	O3'-C3'	2.73	1.49	1.43
2	F	501	UD1	O2'-C2B	2.73	1.49	1.43
2	H	501	UD1	PB-O1B	-2.70	1.41	1.51
2	E	501	UD1	O5'-C5'	2.70	1.51	1.44
2	D	501	UD1	O1'-C1'	2.68	1.47	1.42
2	G	501	UD1	O1'-C1'	2.65	1.47	1.42
2	B	501	UD1	O3B-C3B	2.63	1.49	1.43
2	G	501	UD1	PB-O2B	-2.63	1.43	1.55
2	B	501	UD1	C5-C4	2.62	1.47	1.40
2	A	501	UD1	C2-N1	2.60	1.41	1.38
2	B	501	UD1	O5'-C5'	2.60	1.50	1.44
2	A	501	UD1	C2B-C1B	-2.58	1.49	1.53
2	C	501	UD1	O1'-C1'	2.58	1.46	1.42
2	C	501	UD1	O3B-C3B	2.57	1.49	1.43
2	A	501	UD1	O4'-C4'	2.57	1.49	1.43
3	C	503	ACT	CH3-C	2.54	1.52	1.48
2	H	501	UD1	C5-C4	2.52	1.47	1.40
2	G	501	UD1	O2'-C2B	2.52	1.49	1.43
2	C	501	UD1	O2'-C2B	2.51	1.49	1.43
2	H	501	UD1	O5'-C5'	2.50	1.50	1.44
3	H	506	ACT	CH3-C	2.49	1.52	1.48
2	A	501	UD1	PB-O2B	-2.46	1.44	1.55
2	A	501	UD1	O3B-C3B	2.45	1.48	1.43
2	E	501	UD1	O2'-C2B	2.43	1.48	1.43
2	E	501	UD1	PB-O2B	-2.43	1.44	1.55
2	F	501	UD1	PB-O2B	-2.43	1.44	1.55
2	D	501	UD1	C8'-C7'	2.42	1.55	1.50
2	D	501	UD1	C5-C4	2.41	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	UD1	O2'-C2B	2.41	1.48	1.43
2	H	501	UD1	O2'-C2B	2.41	1.48	1.43
2	G	501	UD1	C8'-C7'	2.41	1.55	1.50
2	E	501	UD1	C5-C4	2.40	1.46	1.40
2	D	501	UD1	O3'-C3'	2.40	1.48	1.43
2	C	501	UD1	C8'-C7'	2.38	1.55	1.50
2	C	501	UD1	O5'-C5'	2.37	1.50	1.44
2	A	501	UD1	C8'-C7'	2.36	1.55	1.50
2	F	501	UD1	PB-O1B	-2.35	1.42	1.51
2	H	501	UD1	O3B-C3B	2.35	1.48	1.43
2	H	501	UD1	C1'-C2'	2.34	1.57	1.53
2	G	501	UD1	PB-O1B	-2.34	1.42	1.51
2	F	501	UD1	O3B-C3B	2.33	1.48	1.43
3	F	504	ACT	CH3-C	2.33	1.52	1.48
2	F	501	UD1	O5'-C5'	2.31	1.50	1.44
2	F	501	UD1	C2-N1	2.31	1.40	1.38
2	D	501	UD1	PB-O2B	-2.31	1.44	1.55
2	B	501	UD1	C4'-C5'	2.30	1.58	1.53
2	E	501	UD1	C8'-C7'	2.28	1.55	1.50
3	D	502	ACT	CH3-C	2.28	1.52	1.48
2	C	501	UD1	PB-O1B	-2.26	1.42	1.51
3	A	505	ACT	CH3-C	2.25	1.52	1.48
2	C	501	UD1	C5-C4	2.24	1.46	1.40
3	A	504	ACT	CH3-C	2.24	1.52	1.48
2	B	501	UD1	PB-O2B	-2.24	1.45	1.55
2	H	501	UD1	PB-O2B	-2.24	1.45	1.55
2	F	501	UD1	PA-O2A	-2.23	1.45	1.55
2	C	501	UD1	C4-N3	2.21	1.40	1.37
3	H	505	ACT	CH3-C	2.21	1.52	1.48
2	E	501	UD1	O3'-C3'	2.21	1.48	1.43
3	F	502	ACT	CH3-C	2.19	1.52	1.48
2	A	501	UD1	C5-C4	2.18	1.46	1.40
2	B	501	UD1	O2'-C2B	2.18	1.48	1.43
2	B	501	UD1	O4'-C4'	2.17	1.48	1.43
2	D	501	UD1	C4-N3	2.17	1.40	1.37
2	B	501	UD1	O3'-C3'	2.15	1.48	1.43
2	D	501	UD1	O5'-C1'	2.14	1.47	1.41
2	B	501	UD1	C8'-C7'	2.14	1.55	1.50
3	B	502	ACT	CH3-C	2.14	1.51	1.48
2	A	501	UD1	C2'-N2'	2.13	1.49	1.45
2	G	501	UD1	O3'-C3'	2.12	1.48	1.43
2	H	501	UD1	C8'-C7'	2.12	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	UD1	PB-O1B	-2.12	1.43	1.51
2	E	501	UD1	O5'-C1'	2.12	1.47	1.41
2	E	501	UD1	PB-O1B	-2.11	1.43	1.51
2	A	501	UD1	O2-C2	2.09	1.27	1.23
2	D	501	UD1	C3B-C4B	2.06	1.58	1.53
2	B	501	UD1	O1'-C1'	2.05	1.45	1.42
2	F	501	UD1	O3'-C3'	2.04	1.47	1.43
2	B	501	UD1	C3B-C4B	2.03	1.58	1.53
2	B	501	UD1	C1'-C2'	2.02	1.56	1.53
2	A	501	UD1	PA-O2A	-2.02	1.46	1.55
2	C	501	UD1	O3'-C3'	2.01	1.47	1.43
2	G	501	UD1	C5-C4	2.01	1.45	1.40

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501	UD1	C2-N1-C1B	5.86	121.88	118.21
2	F	501	UD1	C2-N1-C1B	5.58	121.70	118.21
2	E	501	UD1	C2-N1-C1B	5.35	121.56	118.21
2	D	501	UD1	C2-N1-C1B	4.80	121.22	118.21
2	H	501	UD1	C2-N1-C1B	4.73	121.17	118.21
2	A	501	UD1	C2-N1-C1B	3.93	120.67	118.21
2	C	501	UD1	C2-N1-C1B	3.81	120.60	118.21
2	G	501	UD1	O2'-C2B-C1B	3.60	122.11	111.23
2	D	501	UD1	O2'-C2B-C1B	3.50	121.82	111.23
2	B	501	UD1	N3-C2-N1	3.41	118.82	115.97
2	H	501	UD1	O3B-C3B-C4B	3.39	121.06	111.08
2	B	501	UD1	O3B-C3B-C4B	3.37	121.00	111.08
2	E	501	UD1	O2'-C2B-C1B	3.35	121.36	111.23
2	B	501	UD1	C2-N1-C1B	3.28	120.27	118.21
2	H	501	UD1	O2'-C2B-C1B	3.10	120.60	111.23
2	G	501	UD1	O3B-C3B-C4B	3.09	120.17	111.08
2	C	501	UD1	O2'-C2B-C1B	3.06	120.48	111.23
2	D	501	UD1	O3B-C3B-C4B	3.04	120.05	111.08
2	F	501	UD1	O2'-C2B-C1B	3.04	120.43	111.23
2	A	501	UD1	O2'-C2B-C1B	2.99	120.28	111.23
2	E	501	UD1	O3B-C3B-C4B	2.98	119.87	111.08
2	C	501	UD1	O3B-C3B-C4B	2.98	119.86	111.08
2	A	501	UD1	O3B-C3B-C4B	2.95	119.77	111.08
2	A	501	UD1	O2'-C2B-C3B	2.95	121.42	111.83
2	F	501	UD1	O2'-C2B-C3B	2.91	121.30	111.83
2	B	501	UD1	O2'-C2B-C3B	2.91	121.29	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	UD1	O2'-C2B-C3B	2.84	121.08	111.83
2	H	501	UD1	O2'-C2B-C3B	2.79	120.93	111.83
2	C	501	UD1	O2'-C2B-C3B	2.79	120.92	111.83
2	E	501	UD1	N3-C2-N1	2.79	118.30	115.97
2	F	501	UD1	O3B-C3B-C4B	2.77	119.25	111.08
2	D	501	UD1	O2'-C2B-C3B	2.74	120.74	111.83
2	G	501	UD1	N3-C2-N1	2.64	118.18	115.97
2	B	501	UD1	O2'-C2B-C1B	2.64	119.20	111.23
2	G	501	UD1	O2'-C2B-C3B	2.62	120.37	111.83
2	C	501	UD1	N3-C2-N1	2.55	118.10	115.97
2	H	501	UD1	N3-C2-N1	2.48	118.04	115.97
2	H	501	UD1	O3A-PA-O5B	2.47	114.47	103.41
2	A	501	UD1	N3-C2-N1	2.47	118.04	115.97
2	D	501	UD1	N3-C2-N1	2.37	117.95	115.97
2	G	501	UD1	O2A-PA-O3A	2.36	116.35	105.14
2	B	501	UD1	O2A-PA-O3A	2.36	116.34	105.14
2	F	501	UD1	N3-C2-N1	2.35	117.93	115.97
2	E	501	UD1	O2A-PA-O3A	2.30	116.05	105.14
2	H	501	UD1	C4'-C3'-C2'	-2.28	107.20	110.44
2	A	501	UD1	O2A-PA-O3A	2.24	115.78	105.14
2	C	501	UD1	O2B-PB-O3A	2.22	115.67	105.14
2	D	501	UD1	O2A-PA-O3A	2.20	115.56	105.14
2	F	501	UD1	O2A-PA-O3A	2.15	115.32	105.14
2	A	501	UD1	O2B-PB-O3A	2.13	115.26	105.14
2	B	501	UD1	C2B-C3B-C4B	-2.13	98.41	102.65
2	H	501	UD1	O2A-PA-O3A	2.10	115.08	105.14
2	E	501	UD1	O3A-PA-O5B	2.08	112.71	103.41
2	F	501	UD1	O3A-PA-O5B	2.05	112.58	103.41
2	G	501	UD1	O2B-PB-O3A	2.05	114.87	105.14
2	E	501	UD1	O2B-PB-O3A	2.04	114.80	105.14
2	E	501	UD1	O3A-PB-O1'	2.03	108.61	103.48
2	D	501	UD1	O5'-C5'-C6'	2.02	111.31	106.34
2	D	501	UD1	O2B-PB-O3A	2.01	114.68	105.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	419/419 (100%)	-0.16	3 (0%) 84 86	22, 36, 52, 87	0
1	B	419/419 (100%)	0.49	38 (9%) 9 8	30, 53, 75, 94	0
1	C	419/419 (100%)	-0.02	6 (1%) 72 74	24, 42, 58, 81	0
1	D	419/419 (100%)	-0.03	10 (2%) 56 58	22, 39, 58, 83	0
1	E	419/419 (100%)	0.10	15 (3%) 41 42	19, 42, 71, 92	0
1	F	419/419 (100%)	-0.06	11 (2%) 53 55	24, 40, 59, 84	0
1	G	419/419 (100%)	-0.05	8 (1%) 64 66	22, 39, 56, 93	0
1	H	419/419 (100%)	-0.09	8 (1%) 64 66	19, 36, 52, 89	0
All	All	3352/3352 (100%)	0.02	99 (2%) 49 50	19, 40, 64, 94	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	419	GLU	9.6
1	B	418	GLY	9.0
1	H	419	GLU	7.5
1	B	419	GLU	6.5
1	G	419	GLU	6.3
1	B	417	LYS	6.3
1	H	418	GLY	6.2
1	H	417	LYS	6.1
1	F	419	GLU	5.2
1	E	418	GLY	5.1
1	E	419	GLU	4.7
1	A	419	GLU	4.6
1	G	418	GLY	4.5
1	E	63	LYS	4.3
1	E	277	GLU	3.9
1	F	418	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.8
1	B	277	GLU	3.7
1	D	419	GLU	3.6
1	D	418	GLY	3.6
1	B	287	LYS	3.6
1	B	63	LYS	3.5
1	E	329	GLU	3.4
1	E	417	LYS	3.4
1	G	417	LYS	3.4
1	E	65	GLU	3.4
1	D	148	ASN	3.3
1	B	359	LYS	3.2
1	C	287	LYS	3.2
1	D	76	ASN	3.1
1	B	248	LYS	3.0
1	C	1	MET	3.0
1	E	38	PRO	3.0
1	F	1	MET	3.0
1	B	38	PRO	3.0
1	B	401	ARG	3.0
1	F	277	GLU	2.9
1	D	1	MET	2.9
1	B	127	PHE	2.9
1	F	127	PHE	2.9
1	C	63	LYS	2.8
1	B	61	GLY	2.8
1	H	1	MET	2.8
1	B	2	ASP	2.8
1	E	401	ARG	2.8
1	E	71	TRP	2.7
1	E	85	ASP	2.7
1	G	1	MET	2.7
1	F	177	GLU	2.7
1	B	76	ASN	2.7
1	B	285	HIS	2.7
1	B	78	ASN	2.7
1	B	71	TRP	2.7
1	B	67	IAS	2.7
1	D	149	GLY	2.6
1	E	76	ASN	2.6
1	C	418	GLY	2.6
1	E	78	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	252	ARG	2.5
1	B	15	GLU	2.5
1	B	358	GLU	2.5
1	E	1	MET	2.5
1	F	219	GLU	2.5
1	B	80	PHE	2.5
1	G	76	ASN	2.5
1	H	391	ARG	2.4
1	D	78	ASN	2.4
1	F	359	LYS	2.4
1	B	42	GLN	2.4
1	B	83	PRO	2.4
1	B	416	VAL	2.3
1	F	358	GLU	2.3
1	A	212	ARG	2.3
1	B	79	ASN	2.3
1	D	127	PHE	2.3
1	B	9	PRO	2.3
1	B	46	LYS	2.2
1	F	68	GLY	2.2
1	B	384	GLU	2.2
1	D	150	ARG	2.2
1	B	7	GLN	2.2
1	G	277	GLU	2.2
1	H	416	VAL	2.2
1	H	127	PHE	2.2
1	D	417	LYS	2.1
1	B	318	GLU	2.1
1	B	219	GLU	2.1
1	G	116	ALA	2.1
1	B	370	LEU	2.1
1	B	241	ALA	2.1
1	B	220	ARG	2.1
1	H	148	ASN	2.1
1	E	177	GLU	2.1
1	G	287	LYS	2.1
1	B	86	LEU	2.1
1	B	217	GLY	2.0
1	B	3	LYS	2.0
1	F	252	ARG	2.0
1	C	384	GLU	2.0

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

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	IAS	B	67	8/9	0.35	1.53	73,74,76,76	0
1	IAS	D	67	8/9	0.25	0.58	56,57,61,62	0
1	IAS	F	67	8/9	0.24	0.50	59,60,62,64	0
1	IAS	G	67	8/9	0.19	0.21	36,38,41,42	0
1	IAS	E	67	8/9	0.27	0.01	68,70,71,72	0
1	IAS	C	67	8/9	0.17	-0.18	49,52,52,53	0
1	IAS	A	67	8/9	0.10	-0.48	34,36,37,37	0
1	IAS	H	67	8/9	0.10	-0.98	34,35,37,38	0

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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	EDO	A	507	4/4	0.40	19.16	35,35,37,40	0
3	ACT	B	502	4/4	0.24	10.22	69,71,71,71	0
4	EDO	D	506	4/4	0.26	10.22	48,50,52,53	0
4	EDO	E	510	4/4	0.42	9.88	59,62,63,63	0
3	ACT	H	505	4/4	0.31	9.70	57,58,59,60	0
3	ACT	C	503	4/4	0.30	9.56	52,53,55,56	0
3	ACT	A	505	4/4	0.37	8.13	72,72,73,73	0
3	ACT	F	503	4/4	0.34	7.90	49,52,52,52	0
4	EDO	A	509	4/4	0.30	7.32	55,56,56,56	0
3	ACT	H	502	4/4	0.32	7.29	55,57,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	EDO	F	508	4/4	0.22	6.09	59,62,62,63	0
4	EDO	C	506	4/4	0.23	5.56	55,57,57,58	0
4	EDO	G	505	4/4	0.29	5.51	62,63,64,64	0
4	EDO	H	513	4/4	0.33	5.48	56,56,56,57	0
4	EDO	G	504	4/4	0.18	5.04	45,45,46,47	0
4	EDO	F	509	4/4	0.26	5.01	44,45,47,49	0
3	ACT	E	503	4/4	0.30	4.53	74,75,75,75	0
3	ACT	F	502	4/4	0.47	4.23	69,69,70,70	0
4	EDO	E	507	4/4	0.21	4.14	45,46,47,47	0
4	EDO	B	505	4/4	0.32	3.56	59,59,59,60	0
3	ACT	H	503	4/4	0.17	3.23	42,45,46,47	0
3	ACT	C	502	4/4	0.36	3.10	74,75,75,76	0
4	EDO	G	507	4/4	0.20	2.91	48,49,50,51	0
3	ACT	A	503	4/4	0.33	2.75	67,68,68,69	0
4	EDO	H	510	4/4	0.25	2.54	56,58,59,60	0
4	EDO	E	506	4/4	0.24	2.27	48,48,50,52	0
3	ACT	A	502	4/4	0.22	2.24	47,51,51,51	0
4	EDO	H	509	4/4	0.21	2.22	58,58,59,61	0
4	EDO	C	507	4/4	0.32	2.09	54,54,54,54	0
4	EDO	F	506	4/4	0.15	1.94	59,59,61,61	0
4	EDO	G	506	4/4	0.29	1.72	57,58,58,58	0
3	ACT	H	506	4/4	0.18	1.65	57,57,58,58	0
3	ACT	A	504	4/4	0.23	1.56	52,54,54,56	0
4	EDO	B	503	4/4	0.18	1.45	44,44,44,48	0
4	EDO	C	505	4/4	0.24	1.43	51,54,55,56	0
3	ACT	D	502	4/4	0.20	1.40	52,54,55,56	0
4	EDO	E	508	4/4	0.23	1.25	54,54,55,55	0
3	ACT	F	504	4/4	0.34	1.21	68,70,70,70	0
4	EDO	D	510	4/4	0.17	1.14	44,47,48,51	0
4	EDO	D	504	4/4	0.16	1.07	39,40,41,43	0
4	EDO	D	507	4/4	0.24	1.03	58,59,59,61	0
3	ACT	D	503	4/4	0.23	1.01	68,68,69,69	0
3	ACT	H	504	4/4	0.22	0.98	58,58,58,59	0
4	EDO	G	508	4/4	0.24	0.86	46,47,48,49	0
3	ACT	E	504	4/4	0.44	0.72	81,81,82,82	0
3	ACT	E	502	4/4	0.16	0.63	63,64,64,65	0
4	EDO	G	503	4/4	0.15	0.61	51,51,51,53	0
4	EDO	E	509	4/4	0.14	0.60	45,46,47,49	0
4	EDO	F	507	4/4	0.17	0.58	60,63,63,64	0
4	EDO	D	509	4/4	0.15	0.50	61,62,62,62	0
4	EDO	A	506	4/4	0.13	0.20	32,34,35,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	EDO	D	505	4/4	0.14	0.03	48,49,49,51	0
4	EDO	H	512	4/4	0.14	-0.09	34,36,36,39	0
4	EDO	H	511	4/4	0.16	-0.14	54,56,57,58	0
4	EDO	D	508	4/4	0.22	-0.20	58,59,60,60	0
4	EDO	G	502	4/4	0.11	-0.28	35,36,37,39	0
4	EDO	H	507	4/4	0.11	-0.42	42,42,43,44	0
2	UD1	D	501	39/39	0.11	-0.43	18,28,37,37	0
4	EDO	E	505	4/4	0.13	-0.48	51,55,55,57	0
2	UD1	G	501	39/39	0.10	-0.55	25,30,42,44	0
2	UD1	E	501	39/39	0.10	-0.55	23,30,35,35	0
2	UD1	A	501	39/39	0.10	-0.57	18,29,37,41	0
2	UD1	H	501	39/39	0.10	-0.57	27,32,39,40	0
4	EDO	H	508	4/4	0.12	-0.59	50,52,52,52	0
2	UD1	F	501	39/39	0.11	-0.60	24,32,37,40	0
4	EDO	C	504	4/4	0.11	-0.62	37,37,37,37	0
4	EDO	A	508	4/4	0.11	-0.64	53,53,54,54	0
4	EDO	B	504	4/4	0.14	-0.71	59,60,61,61	0
4	EDO	F	505	4/4	0.11	-0.72	43,44,44,45	0
2	UD1	C	501	39/39	0.10	-0.89	24,29,37,40	0
2	UD1	B	501	39/39	0.12	-0.92	31,38,42,44	0
4	EDO	E	511	4/4	0.18	-0.99	62,64,65,65	0

6.5 Other polymers ⓘ

There are no such residues in this entry.