



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 06:35 PM BST

PDB ID : 6NN8
Title : The structure of human liver pyruvate kinase, hLPYK-S531E
Authors : McFarlane, J.S.; Ronnebaum, T.A.; Meneely, K.M.; Fenton, A.W.; Lamb, A.L.
Deposited on : 2019-01-14
Resolution : 2.42 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

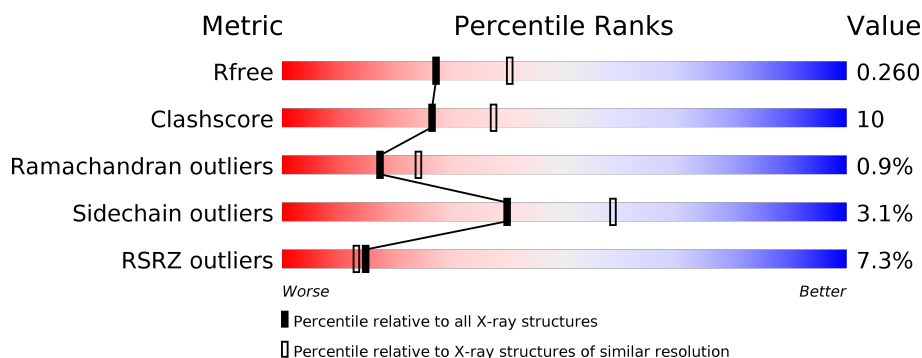
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	543	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>• 7%</div> </div> </div>
1	B	543	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• 5%</div> </div> </div>
1	C	543	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>8%</div> </div> </div>
1	D	543	<div> <div>6%</div> <div> <div></div> <div>59%</div> <div>17%</div> <div>• 22%</div> </div> </div>
1	E	543	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• 6%</div> </div> </div>
1	F	543	<div> <div>7%</div> <div> <div></div> <div>54%</div> <div>22%</div> <div>• 23%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	543	
1	H	543	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	604	-	-	X	-
2	EDO	G	601	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 57131 atoms, of which 28756 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 Pyruvate kinase PKLR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	505	Total	C	H	N	O	S	0	0	0
			7738	2410	3909	690	711	18			
1	B	518	Total	C	H	N	O	S	0	0	0
			7937	2473	4006	710	730	18			
1	C	499	Total	C	H	N	O	S	0	0	0
			7675	2390	3880	683	704	18			
1	D	421	Total	C	H	N	O	S	0	1	0
			6468	2018	3259	580	592	19			
1	E	509	Total	C	H	N	O	S	0	0	0
			7828	2438	3957	701	714	18			
1	F	417	Total	C	H	N	O	S	0	0	0
			6429	2006	3239	577	589	18			
1	G	395	Total	C	H	N	O	S	0	0	0
			6086	1895	3076	542	555	18			
1	H	407	Total	C	H	N	O	S	0	0	0
			6310	1965	3184	568	575	18			

There are 24 discrepancies between the modelled and reference sequences:

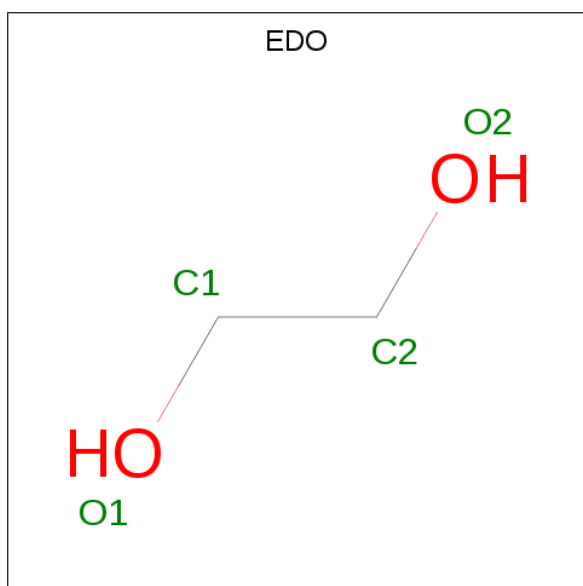
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P30613
A	2	GLU	-	expression tag	UNP P30613
A	531	GLU	SER	engineered mutation	UNP P30613
B	1	MET	-	expression tag	UNP P30613
B	2	GLU	-	expression tag	UNP P30613
B	531	GLU	SER	engineered mutation	UNP P30613
C	1	MET	-	expression tag	UNP P30613
C	2	GLU	-	expression tag	UNP P30613
C	531	GLU	SER	engineered mutation	UNP P30613
D	1	MET	-	expression tag	UNP P30613
D	2	GLU	-	expression tag	UNP P30613
D	531	GLU	SER	engineered mutation	UNP P30613
E	1	MET	-	expression tag	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2	GLU	-	expression tag	UNP P30613
E	531	GLU	SER	engineered mutation	UNP P30613
F	1	MET	-	expression tag	UNP P30613
F	2	GLU	-	expression tag	UNP P30613
F	531	GLU	SER	engineered mutation	UNP P30613
G	1	MET	-	expression tag	UNP P30613
G	2	GLU	-	expression tag	UNP P30613
G	531	GLU	SER	engineered mutation	UNP P30613
H	1	MET	-	expression tag	UNP P30613
H	2	GLU	-	expression tag	UNP P30613
H	531	GLU	SER	engineered mutation	UNP P30613

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	H	O	0	0
			10	2	6	2		
2	E	1	Total	C	H	O	0	0
			10	2	6	2		
2	E	1	Total	C	H	O	0	0
			10	2	6	2		
2	E	1	Total	C	H	O	0	0
			10	2	6	2		
2	E	1	Total	C	H	O	0	0
			10	2	6	2		
2	E	1	Total	C	H	O	0	0
			10	2	6	2		
2	F	1	Total	C	H	O	0	0
			10	2	6	2		
2	F	1	Total	C	H	O	0	0
			10	2	6	2		
2	G	1	Total	C	H	O	0	0
			10	2	6	2		
2	G	1	Total	C	H	O	0	0
			10	2	6	2		
2	H	1	Total	C	H	O	0	0
			10	2	6	2		
2	H	1	Total	C	H	O	0	0
			10	2	6	2		
2	H	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	71	Total	O	0	0
			71	71		
3	B	58	Total	O	0	0
			58	58		
3	C	54	Total	O	0	0
			54	54		
3	D	16	Total	O	0	0
			16	16		
3	E	34	Total	O	0	0
			34	34		

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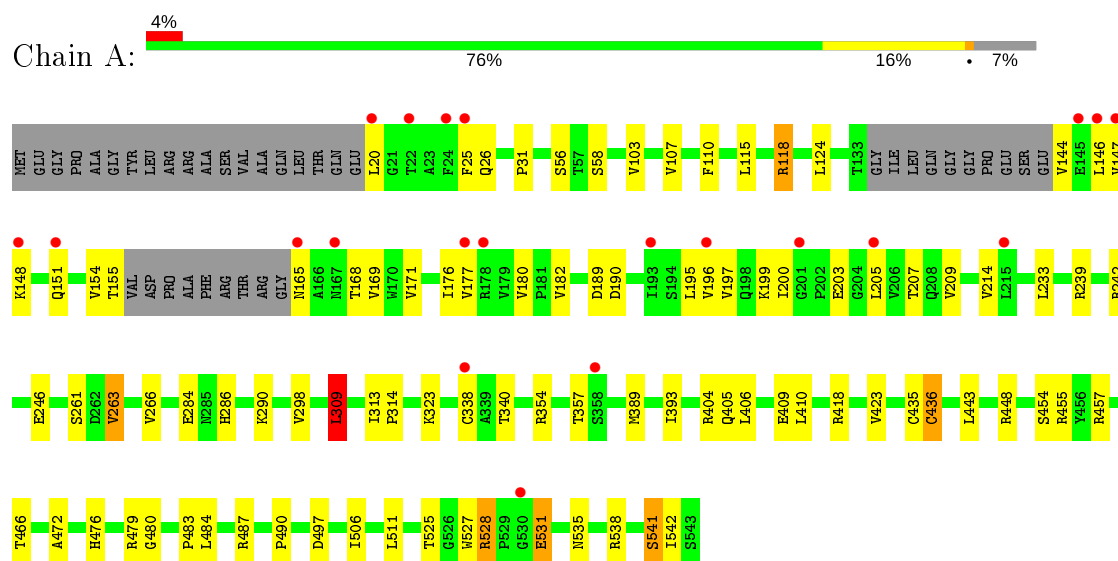
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	6	Total 6	O 6	0	0
3	G	10	Total 10	O 10	0	0
3	H	1	Total 1	O 1	0	0

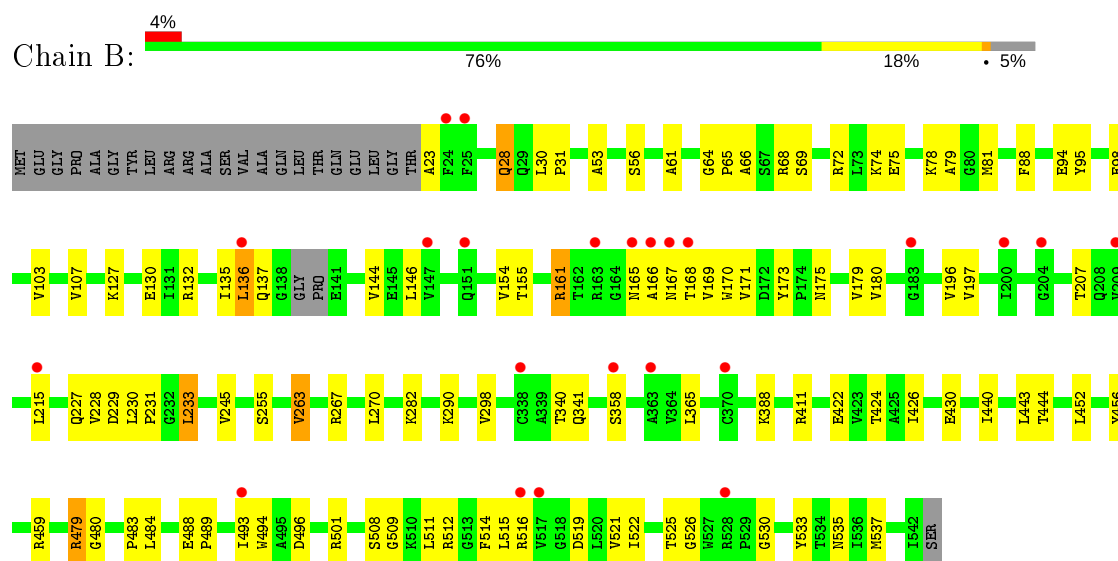
3 Residue-property plots

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

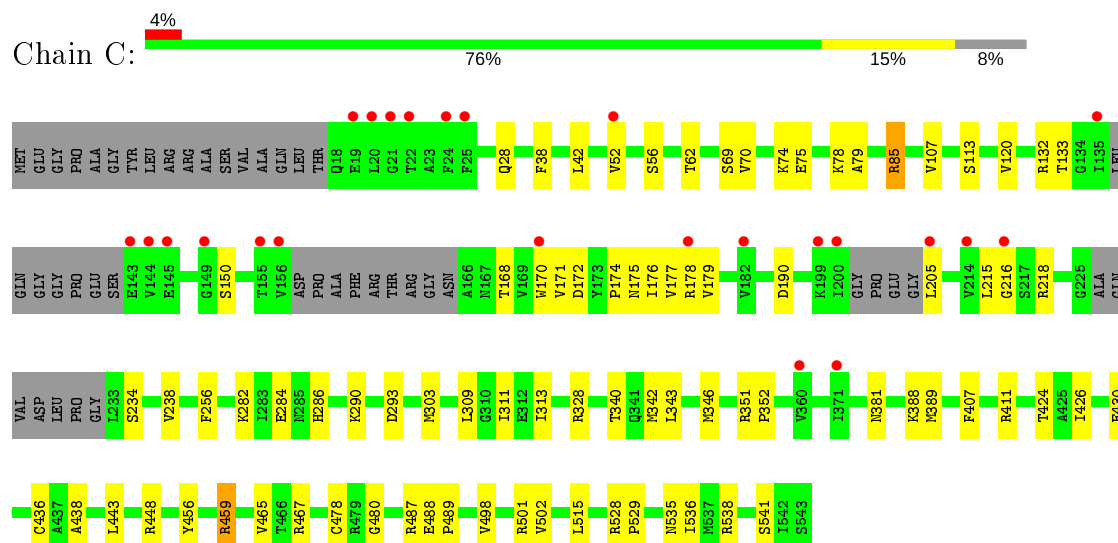
• Molecule 1: Pyruvate kinase PKLR



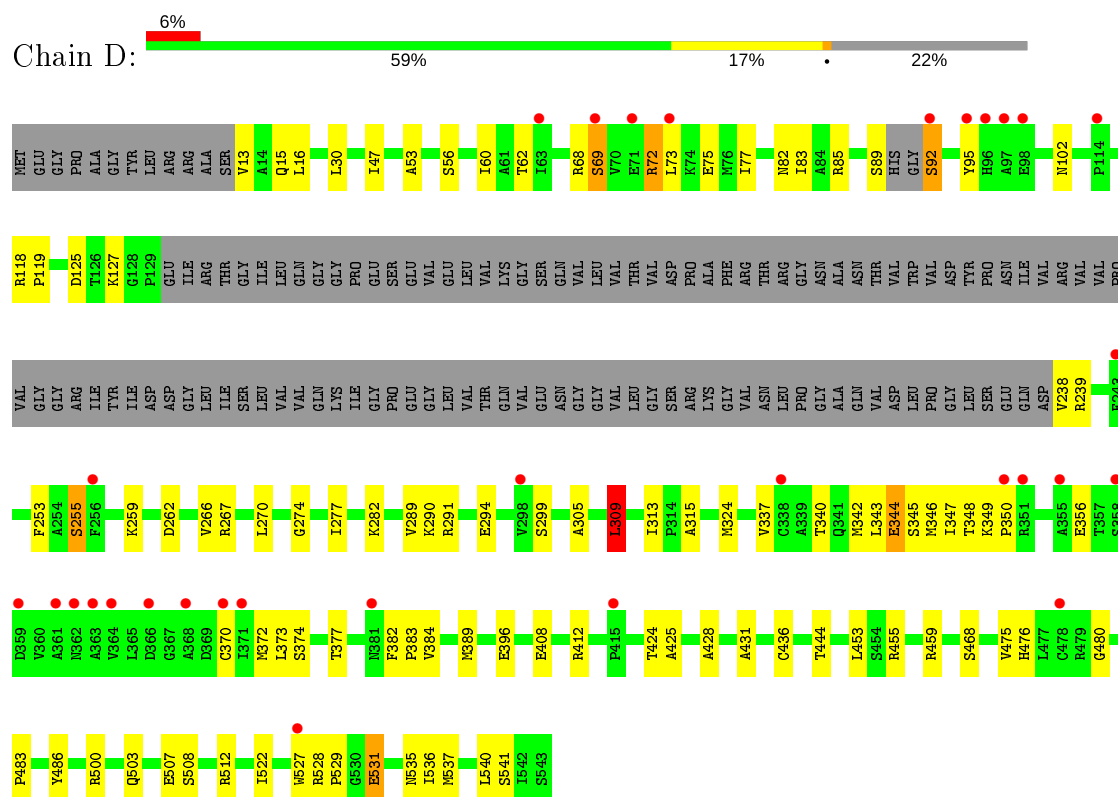
• Molecule 1: Pyruvate kinase PKLR



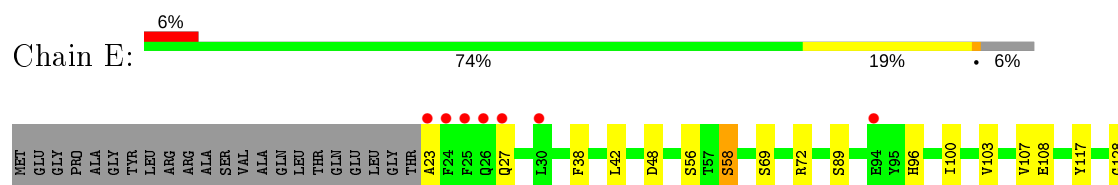
• Molecule 1: Pyruvate kinase PKLR

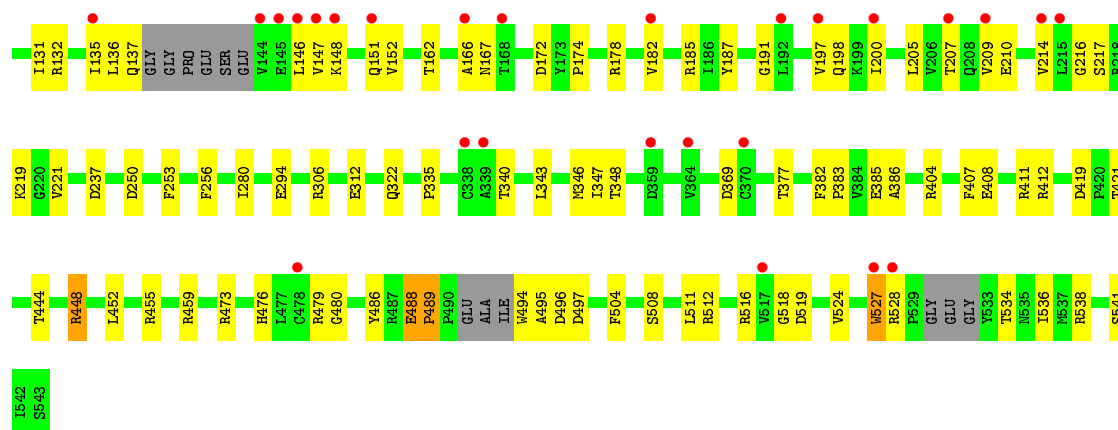


- Molecule 1: Pyruvate kinase PKLR

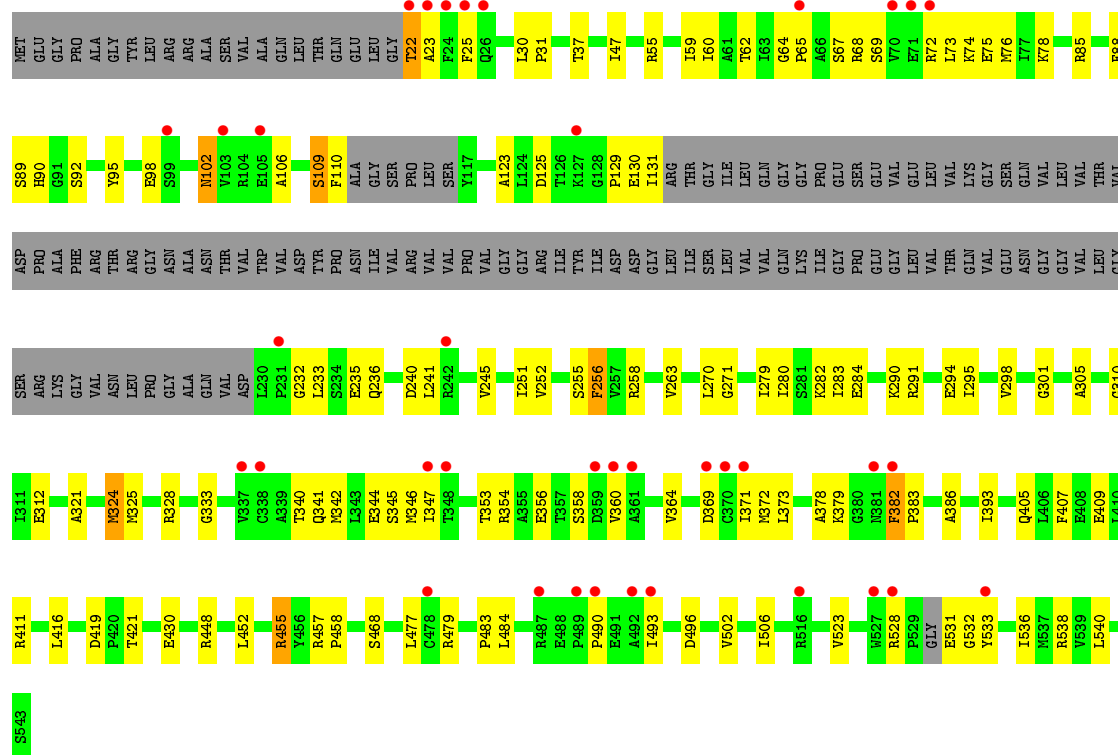


- Molecule 1: Pyruvate kinase PKLR

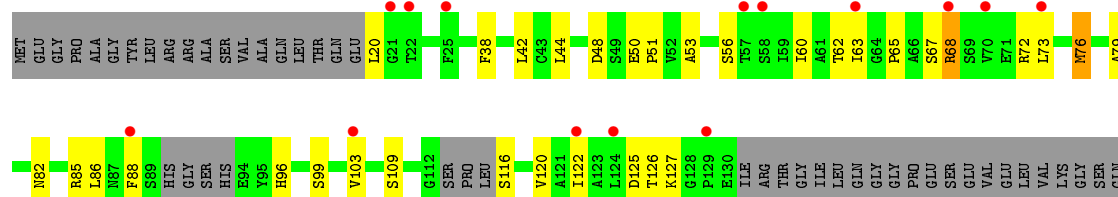


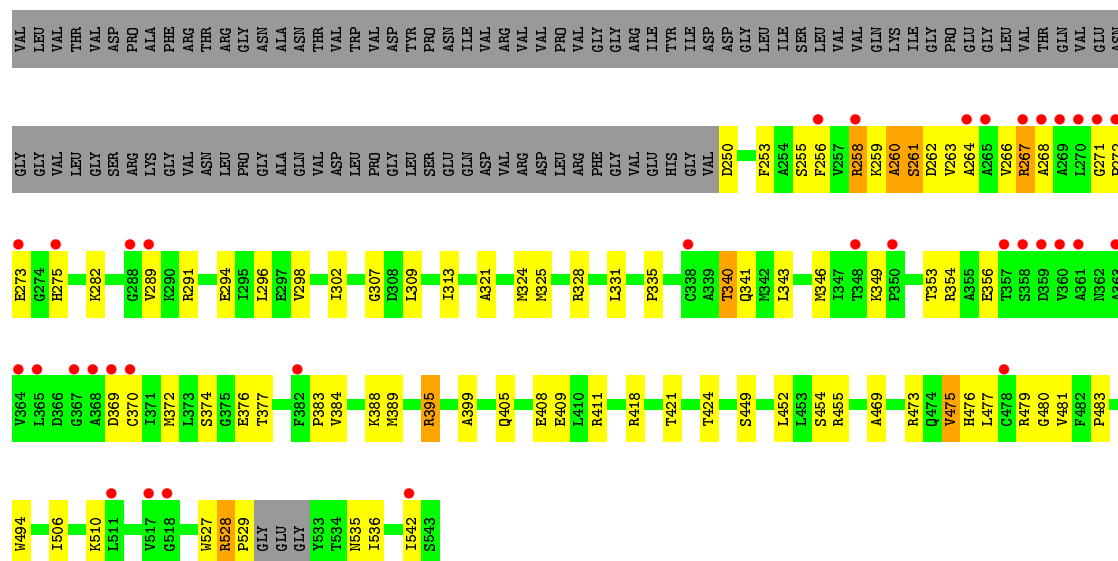


• Molecule 1: Pyruvate kinase PKLR

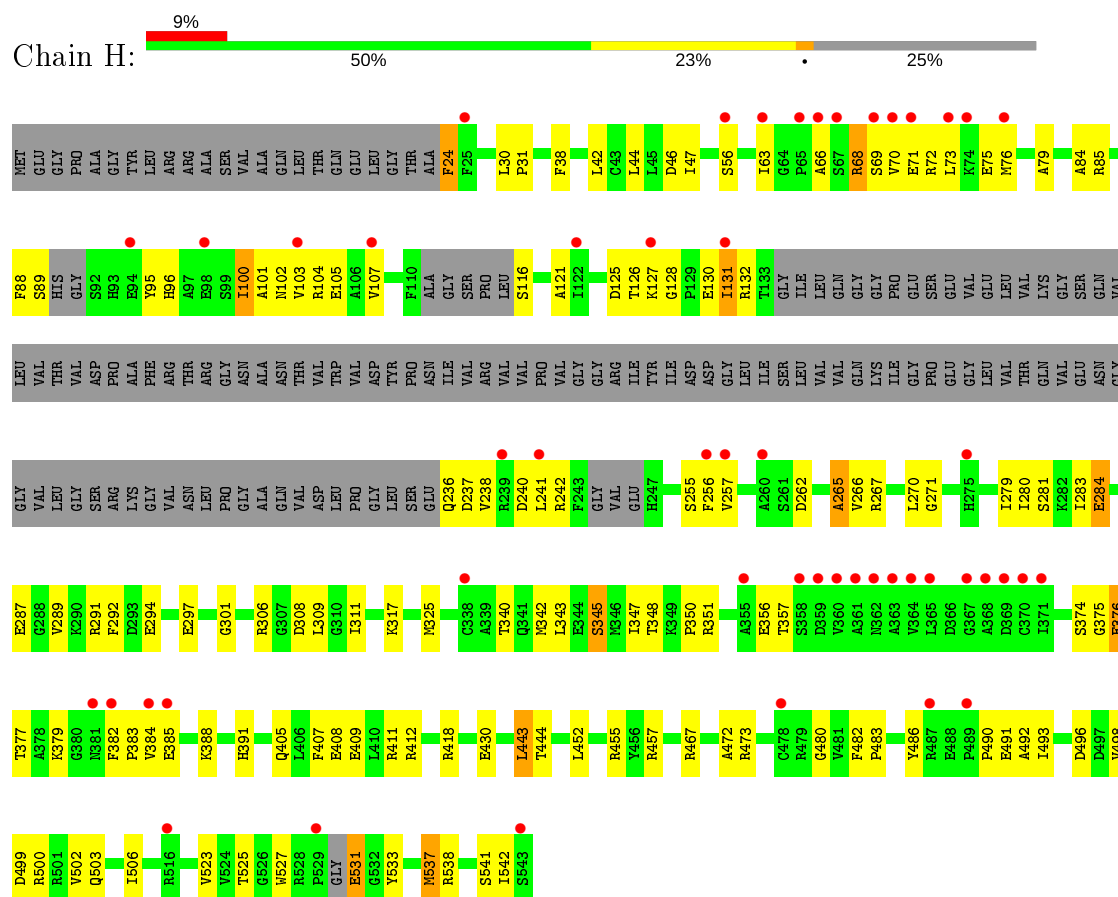


• Molecule 1: Pyruvate kinase PKLR





● Molecule 1: Pyruvate kinase PKLR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.91Å 139.41Å 181.29Å 90.00° 103.35° 90.00°	Depositor
Resolution (Å)	39.54 – 2.42 39.54 – 2.42	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.54-2.42) 98.7 (39.54-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.208 , 0.260 0.208 , 0.260	Depositor DCC
R_{free} test set	2006 reflections (1.16%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	57131	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.74	2/3890 (0.1%)	0.85	5/5269 (0.1%)
1	B	0.67	0/3995	0.81	2/5413 (0.0%)
1	C	0.66	2/3852 (0.1%)	0.80	5/5212 (0.1%)
1	D	0.63	0/3263	0.75	2/4412 (0.0%)
1	E	0.64	0/3933	0.82	4/5326 (0.1%)
1	F	0.57	0/3241	0.74	0/4380
1	G	0.58	0/3055	0.73	1/4127 (0.0%)
1	H	0.59	0/3173	0.75	2/4283 (0.0%)
All	All	0.64	4/28402 (0.0%)	0.79	21/38422 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	VAL	CB-CG2	-5.78	1.40	1.52
1	C	436	CYS	CB-SG	-5.43	1.73	1.81
1	C	478	CYS	CB-SG	-5.38	1.73	1.81
1	A	338	CYS	CB-SG	5.03	1.90	1.82

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	479	ARG	NE-CZ-NH1	-9.02	115.79	120.30
1	B	459	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	D	459	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	448	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	C	459	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	C	85	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	E	538	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	309	LEU	CB-CG-CD2	-5.67	101.36	111.00
1	C	448	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	487	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	E	448	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	418	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	487	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	H	412	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	C	467	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	E	72	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	118	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	D	309	LEU	CA-CB-CG	5.07	126.97	115.30
1	H	418	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	G	44	LEU	CB-CG-CD2	5.05	119.58	111.00
1	B	479	ARG	NE-CZ-NH2	5.03	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	531	GLU	Peptide
1	B	533	TYR	Peptide

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	3829	3909	3907	77	0
1	B	3931	4006	4005	66	0
1	C	3795	3880	3876	54	0
1	D	3209	3259	3270	74	0
1	E	3871	3957	3954	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3190	3239	3239	90	0
1	G	3010	3076	3072	96	0
1	H	3126	3184	3179	93	0
2	A	40	60	60	12	0
2	B	28	42	42	5	0
2	C	24	36	36	3	0
2	D	16	24	24	2	0
2	E	28	42	42	6	0
2	F	8	12	12	0	0
2	G	8	12	12	9	0
2	H	12	18	18	3	0
3	A	71	0	0	0	0
3	B	58	0	0	1	0
3	C	54	0	0	1	0
3	D	16	0	0	1	0
3	E	34	0	0	1	0
3	F	6	0	0	0	0
3	G	10	0	0	2	0
3	H	1	0	0	0	0
All	All	28375	28756	28748	588	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 10.

All (588) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:HD21	1:A:214:VAL:HG22	1.26	1.13
1:E:185:ARG:NH1	1:E:210:GLU:OE2	2.03	0.92
1:F:483:PRO:O	1:F:484:LEU:HD23	1.70	0.91
1:G:53:ALA:HB3	2:G:601:EDO:H12	1.50	0.91
1:D:266:VAL:O	1:D:270:LEU:HD12	1.70	0.91
1:H:444:THR:OG1	1:H:531:GLU:OE2	1.88	0.90
1:E:346:MET:HE3	1:E:386:ALA:HA	1.52	0.90
1:G:260:ALA:O	1:G:263:VAL:HG22	1.70	0.90
1:E:343:LEU:HD13	1:E:346:MET:HE1	1.51	0.90
1:G:263:VAL:HG21	1:G:298:VAL:HG21	1.52	0.89
1:D:444:THR:OG1	1:D:531:GLU:OE2	1.94	0.85
1:A:263:VAL:HG21	1:A:298:VAL:HG23	1.61	0.82
1:E:294:GLU:OE1	3:E:701:HOH:O	1.98	0.82
1:A:118:ARG:H	2:A:604:EDO:H12	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:ILE:HD12	1:E:217:SER:HB2	1.60	0.82
1:B:53:ALA:HB3	2:B:604:EDO:H21	1.63	0.80
1:G:76:MET:O	1:G:79:ALA:N	2.15	0.80
1:G:85:ARG:NH2	1:G:125:ASP:OD2	2.14	0.79
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.65	0.79
1:H:408:GLU:OE2	1:H:411:ARG:NH2	2.16	0.79
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.66	0.78
1:F:263:VAL:HG21	1:F:298:VAL:HG23	1.66	0.78
1:H:493:ILE:HD12	1:H:496:ASP:OD2	1.83	0.77
1:B:493:ILE:HD12	1:B:496:ASP:OD2	1.85	0.77
1:C:28:GLN:O	1:C:459:ARG:NH2	2.17	0.77
1:F:62:THR:HG21	1:F:85:ARG:HH11	1.51	0.76
1:D:408:GLU:OE2	1:D:412:ARG:NH2	2.19	0.76
1:E:527:TRP:CD1	1:E:536:ILE:HD11	2.23	0.74
1:D:337:VAL:HG22	1:D:370:CYS:HB2	1.68	0.73
1:A:146:LEU:CD2	1:A:214:VAL:HG22	2.13	0.73
1:E:135:ILE:HD12	1:E:217:SER:CB	2.18	0.73
1:G:340:THR:HG22	1:G:341:GLN:HG3	1.71	0.73
1:A:146:LEU:HD23	1:A:214:VAL:HA	1.72	0.72
1:F:89:SER:O	1:F:90:HIS:ND1	2.22	0.71
1:E:312:GLU:OE2	2:E:602:EDO:H12	1.90	0.71
1:A:118:ARG:N	2:A:604:EDO:H12	2.05	0.71
1:H:68:ARG:NH2	1:H:95:TYR:O	2.22	0.71
1:C:411:ARG:HG2	1:C:426:ILE:HD11	1.71	0.71
1:E:516:ARG:N	1:E:519:ASP:OD2	2.22	0.71
1:A:146:LEU:O	1:A:148:LYS:HG3	1.91	0.71
1:F:353:THR:HG23	1:F:356:GLU:OE1	1.90	0.70
1:F:67:SER:O	1:F:73:LEU:HD21	1.90	0.70
1:G:263:VAL:HG21	1:G:298:VAL:CG2	2.21	0.70
1:E:494:TRP:O	1:E:496:ASP:N	2.23	0.70
1:E:346:MET:CE	1:E:386:ALA:HA	2.21	0.70
1:H:284:GLU:HA	1:H:309:LEU:HG	1.73	0.70
1:A:182:VAL:HG13	1:A:200:ILE:HD12	1.73	0.69
1:F:354:ARG:NH2	1:G:307:GLY:O	2.24	0.69
1:F:62:THR:HG22	1:F:85:ARG:HB3	1.74	0.69
1:B:171:VAL:HG12	1:B:173:TYR:H	1.58	0.69
1:C:75:GLU:OE2	1:C:78:LYS:NZ	2.22	0.69
1:E:518:GLY:O	1:G:418:ARG:NH2	2.26	0.68
1:A:147:VAL:CG1	1:A:209:VAL:HG21	2.23	0.68
1:A:110:PHE:HB2	2:A:604:EDO:H11	1.74	0.68
1:F:290:LYS:HE2	1:G:48:ASP:OD2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:498:VAL:O	1:H:502:VAL:HG23	1.95	0.67
1:H:68:ARG:O	1:H:102:ASN:ND2	2.27	0.67
1:D:527:TRP:CE3	1:D:528:ARG:HG2	2.29	0.67
2:G:601:EDO:H11	3:G:704:HOH:O	1.95	0.67
1:E:421:THR:HG22	1:E:452:LEU:HD12	1.78	0.66
1:G:67:SER:HA	1:G:72:ARG:HG3	1.77	0.66
1:A:58:SER:HB3	2:A:601:EDO:O2	1.96	0.66
1:G:353:THR:HG23	1:G:356:GLU:OE1	1.95	0.66
1:E:343:LEU:HD13	1:E:346:MET:CE	2.25	0.65
1:A:182:VAL:HG13	1:A:200:ILE:CD1	2.26	0.65
1:B:180:VAL:HG23	1:B:197:VAL:HG21	1.79	0.65
1:E:476:HIS:ND1	2:E:603:EDO:H21	2.12	0.64
1:A:147:VAL:HG12	1:A:209:VAL:HG21	1.80	0.64
1:E:136:LEU:HD12	1:E:217:SER:HB3	1.79	0.64
1:G:260:ALA:O	1:G:263:VAL:N	2.30	0.64
1:A:56:SER:HB2	1:A:480:GLY:HA2	1.80	0.63
1:B:290:LYS:HA	1:B:290:LYS:HE2	1.79	0.63
1:F:346:MET:HE1	1:F:386:ALA:HA	1.80	0.63
1:E:527:TRP:O	1:E:528:ARG:HG2	1.99	0.63
1:D:347:ILE:HG22	1:D:348:THR:HG23	1.79	0.62
1:D:69:SER:HB2	1:D:72:ARG:H	1.64	0.62
1:A:455:ARG:HA	2:A:608:EDO:H11	1.82	0.62
1:G:399:ALA:HB2	2:G:601:EDO:H22	1.82	0.62
1:D:503:GLN:O	1:D:507:GLU:HG2	2.00	0.62
1:C:177:VAL:HG12	1:C:205:LEU:HD13	1.82	0.62
1:E:419:ASP:OD2	1:E:448:ARG:NH2	2.26	0.62
1:A:457:ARG:HH12	2:A:608:EDO:H12	1.65	0.62
1:D:267:ARG:HA	1:D:270:LEU:HD13	1.82	0.62
1:G:60:ILE:HG21	1:G:372:MET:HE2	1.81	0.61
1:A:144:VAL:O	1:A:144:VAL:HG12	1.99	0.61
1:A:118:ARG:H	2:A:604:EDO:C1	2.12	0.61
1:G:264:ALA:HA	1:G:267:ARG:HB3	1.82	0.61
1:D:486:TYR:OH	1:D:500:ARG:HG2	2.00	0.61
1:F:333:GLY:HA2	1:F:455:ARG:HG2	1.82	0.61
1:A:404:ARG:CZ	1:D:412:ARG:HD2	2.30	0.61
1:C:426:ILE:HD12	1:C:456:TYR:CE1	2.35	0.61
1:G:528:ARG:HG3	1:G:529:PRO:N	2.16	0.61
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.82	0.60
1:F:324:MET:HE1	1:F:325:MET:HG2	1.83	0.60
1:G:475:VAL:HG22	1:G:481:VAL:HG11	1.83	0.60
1:D:238:VAL:HB	1:D:239:ARG:NH1	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:THR:HG22	1:F:85:ARG:HD3	1.84	0.60
1:E:136:LEU:HD11	1:E:216:GLY:O	2.02	0.60
1:F:346:MET:CE	1:F:386:ALA:HA	2.31	0.59
1:G:73:LEU:HD13	1:G:103:VAL:HA	1.84	0.59
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.84	0.59
1:B:263:VAL:HG21	1:B:298:VAL:HG23	1.84	0.58
1:C:538:ARG:HG3	1:F:536:ILE:HG12	1.83	0.58
1:D:290:LYS:NZ	1:H:46:ASP:OD1	2.35	0.58
1:A:242:ARG:O	1:A:246:GLU:HG3	2.02	0.58
1:F:256:PHE:N	1:F:284:GLU:OE1	2.36	0.58
1:F:241:LEU:O	1:F:245:VAL:HG23	2.03	0.58
1:F:62:THR:HG23	1:F:373:LEU:O	2.03	0.58
1:C:70:VAL:O	1:C:74:LYS:HG3	2.03	0.58
1:G:272:PRO:O	1:G:275:HIS:ND1	2.37	0.58
1:G:82:ASN:HB3	1:G:476:HIS:CD2	2.39	0.58
1:E:108:GLU:OE2	1:E:117:TYR:OH	2.21	0.57
1:G:268:ALA:O	1:G:271:GLY:N	2.38	0.57
1:G:262:ASP:O	1:G:266:VAL:HG23	2.04	0.57
1:A:454:SER:OG	1:A:479:ARG:O	2.20	0.57
1:G:418:ARG:HG3	1:G:418:ARG:HH11	1.69	0.57
1:H:457:ARG:HH12	2:H:602:EDO:H12	1.70	0.56
1:B:146:LEU:HG	1:B:215:LEU:HD22	1.87	0.56
1:A:118:ARG:HB2	2:A:604:EDO:H21	1.87	0.56
1:F:47:ILE:HD13	1:G:289:VAL:HG11	1.88	0.56
1:H:100:ILE:HG22	1:H:104:ARG:HD2	1.87	0.56
1:B:53:ALA:HB3	2:B:604:EDO:C2	2.36	0.56
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.86	0.56
1:D:62:THR:HA	1:D:85:ARG:HB3	1.87	0.56
1:H:267:ARG:CZ	1:H:279:ILE:HD12	2.36	0.56
1:A:405:GLN:O	1:A:409:GLU:HG3	2.06	0.55
1:B:267:ARG:HH11	1:B:267:ARG:HG2	1.70	0.55
1:C:38:PHE:CE2	1:C:42:LEU:HD11	2.42	0.55
1:G:506:ILE:O	1:G:510:LYS:HG3	2.05	0.55
1:D:266:VAL:HG12	1:D:270:LEU:HD11	1.87	0.55
1:C:407:PHE:CZ	1:C:411:ARG:HD3	2.42	0.55
1:D:475:VAL:CG2	1:D:483:PRO:HB3	2.37	0.55
1:F:62:THR:HG21	1:F:85:ARG:NH1	2.19	0.55
1:G:51:PRO:HB2	2:G:601:EDO:H21	1.88	0.55
1:G:395:ARG:O	2:G:601:EDO:H22	2.07	0.55
1:B:231:PRO:HB2	1:B:233:LEU:O	2.06	0.55
1:B:28:GLN:HB3	2:B:604:EDO:H11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:407:PHE:O	1:E:411:ARG:HG2	2.06	0.54
1:F:263:VAL:CG2	1:F:298:VAL:HG23	2.36	0.54
1:G:63:ILE:O	1:G:63:ILE:HD12	2.07	0.54
1:H:375:GLY:O	1:H:377:THR:N	2.40	0.54
1:C:175:ASN:O	1:C:179:VAL:HG23	2.08	0.54
1:D:305:ALA:O	1:D:309:LEU:HB2	2.07	0.54
1:E:135:ILE:CD1	1:E:217:SER:HB2	2.36	0.54
1:A:239:ARG:NH1	1:A:242:ARG:HH12	2.04	0.54
1:C:430:GLU:OE2	1:F:430:GLU:OE2	2.25	0.54
1:F:85:ARG:NE	1:F:125:ASP:OD2	2.40	0.54
1:D:68:ARG:O	1:D:102:ASN:ND2	2.40	0.54
1:E:335:PRO:HA	1:E:369:ASP:OD2	2.07	0.54
1:H:257:VAL:HG21	1:H:281:SER:HB3	1.89	0.54
1:H:256:PHE:N	1:H:284:GLU:OE1	2.38	0.54
1:B:426:ILE:HD13	1:B:456:TYR:CE1	2.42	0.54
1:H:347:ILE:HG22	1:H:348:THR:HG23	1.89	0.54
1:B:68:ARG:NH2	1:B:98:GLU:HB3	2.23	0.54
1:H:238:VAL:HG12	1:H:242:ARG:HE	1.73	0.54
1:E:96:HIS:O	1:E:100:ILE:HG13	2.08	0.54
1:G:259:LYS:HB3	1:G:291:ARG:HE	1.73	0.54
1:H:347:ILE:HG22	1:H:348:THR:CG2	2.38	0.54
1:H:287:GLU:O	1:H:291:ARG:HG3	2.08	0.53
1:A:538:ARG:HG2	1:D:536:ILE:HG12	1.90	0.53
1:E:56:SER:HB2	1:E:480:GLY:CA	2.37	0.53
1:H:128:GLY:HA2	1:H:237:ASP:OD2	2.08	0.53
1:H:24:PHE:N	1:H:24:PHE:CD2	2.75	0.53
1:C:498:VAL:O	1:C:502:VAL:HG23	2.09	0.53
1:F:47:ILE:CD1	1:G:289:VAL:HG11	2.38	0.53
1:D:125:ASP:HA	1:D:253:PHE:HB2	1.90	0.53
1:D:72:ARG:O	1:D:75:GLU:N	2.42	0.53
1:B:165:ASN:HB3	1:B:167:ASN:H	1.74	0.53
1:C:293:ASP:OD1	1:C:328:ARG:NH1	2.42	0.53
1:H:384:VAL:O	1:H:388:LYS:HG3	2.09	0.53
1:G:331:LEU:O	1:G:455:ARG:NH2	2.41	0.53
1:A:144:VAL:HG13	1:A:214:VAL:HG12	1.92	0.53
1:C:538:ARG:CG	1:F:536:ILE:HG12	2.39	0.53
1:F:502:VAL:O	1:F:506:ILE:HG13	2.10	0.52
1:G:122:ILE:O	1:G:250:ASP:HB2	2.09	0.52
1:G:343:LEU:HD23	1:G:356:GLU:HB3	1.91	0.52
1:E:136:LEU:HD11	1:E:216:GLY:C	2.30	0.52
1:G:353:THR:OG1	1:G:356:GLU:N	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:GLN:HB3	1:C:52:VAL:HG22	1.90	0.52
1:F:523:VAL:HG21	1:F:540:LEU:HD12	1.92	0.52
1:G:263:VAL:HG23	1:G:264:ALA:N	2.23	0.52
1:H:292:PHE:HE2	1:H:325:MET:HE2	1.74	0.52
1:C:56:SER:HB2	1:C:480:GLY:CA	2.38	0.52
1:F:291:ARG:O	1:F:294:GLU:HG2	2.09	0.52
1:G:296:LEU:HD13	1:G:302:ILE:HG13	1.92	0.52
1:B:422:GLU:HG2	1:B:452:LEU:HD13	1.91	0.52
1:D:289:VAL:HG11	1:H:47:ILE:CD1	2.40	0.52
1:G:255:SER:HA	1:G:282:LYS:HD3	1.91	0.52
1:A:233:LEU:HD13	1:A:266:VAL:HG22	1.91	0.52
1:A:527:TRP:HD1	1:A:535:ASN:OD1	1.93	0.52
1:G:421:THR:HG22	1:G:452:LEU:HD12	1.91	0.52
1:F:421:THR:HG22	1:F:452:LEU:CD1	2.39	0.52
1:D:527:TRP:O	1:D:528:ARG:HD3	2.09	0.52
1:D:82:ASN:HB3	1:D:476:HIS:ND1	2.25	0.52
1:E:103:VAL:O	1:E:107:VAL:HG23	2.10	0.52
1:D:47:ILE:CD1	1:H:289:VAL:HG11	2.40	0.52
1:H:383:PRO:HG2	1:H:384:VAL:HG23	1.92	0.52
1:H:405:GLN:O	1:H:409:GLU:HG3	2.10	0.52
1:D:262:ASP:O	1:D:266:VAL:HG23	2.10	0.51
1:D:428:ALA:HB2	1:D:537:MET:HG3	1.91	0.51
1:F:364:VAL:O	1:F:479:ARG:NH1	2.43	0.51
1:F:88:PHE:CD2	1:F:240:ASP:HB3	2.45	0.51
1:G:405:GLN:O	1:G:409:GLU:HG3	2.11	0.51
1:H:38:PHE:CE2	1:H:42:LEU:HD11	2.46	0.51
1:C:28:GLN:HA	3:C:736:HOH:O	2.10	0.51
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.92	0.51
1:E:135:ILE:HG23	1:E:162:THR:HA	1.91	0.51
1:G:85:ARG:NE	1:G:125:ASP:OD2	2.44	0.51
1:A:290:LYS:HA	1:A:290:LYS:HE2	1.91	0.51
1:D:527:TRP:CD2	1:D:528:ARG:HG2	2.46	0.51
1:F:342:MET:CE	1:F:371:ILE:HG22	2.40	0.51
1:D:60:ILE:HG12	1:D:83:ILE:HB	1.91	0.51
1:H:266:VAL:O	1:H:270:LEU:HG	2.11	0.51
1:A:195:LEU:CD2	1:A:209:VAL:HG22	2.41	0.51
1:F:345:SER:HB3	1:F:356:GLU:OE1	2.11	0.51
1:G:353:THR:HG23	1:G:356:GLU:CD	2.30	0.51
1:H:56:SER:CB	1:H:480:GLY:HA2	2.40	0.51
1:C:215:LEU:HD12	1:C:216:GLY:N	2.26	0.51
1:D:15:GLN:HG2	3:D:712:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:528:ARG:HG3	1:G:529:PRO:CD	2.41	0.51
1:H:283:ILE:HG13	1:H:325:MET:HE3	1.92	0.51
1:B:179:VAL:HG21	1:B:227:GLN:O	2.11	0.51
1:A:203:GLU:HG2	1:A:203:GLU:O	2.11	0.50
1:B:64:GLY:O	1:B:68:ARG:HG3	2.10	0.50
1:C:133:THR:HA	1:C:170:TRP:O	2.10	0.50
1:F:75:GLU:HA	1:F:78:LYS:HD3	1.92	0.50
1:H:284:GLU:OE2	1:H:308:ASP:OD2	2.29	0.50
1:H:79:ALA:HB2	1:H:384:VAL:HG13	1.92	0.50
1:B:444:THR:O	2:B:605:EDO:H22	2.11	0.50
1:B:483:PRO:O	1:B:484:LEU:HD23	2.11	0.50
1:C:132:ARG:O	1:C:171:VAL:HA	2.11	0.50
1:G:469:ALA:O	1:G:473:ARG:HG3	2.11	0.50
1:H:455:ARG:HA	2:H:602:EDO:H11	1.92	0.50
1:A:233:LEU:CD1	1:A:266:VAL:HG22	2.41	0.50
1:B:135:ILE:HG22	1:B:136:LEU:O	2.12	0.50
1:G:335:PRO:HB3	1:G:477:LEU:O	2.12	0.50
1:B:255:SER:HA	1:B:282:LYS:HD3	1.93	0.50
1:H:280:ILE:HD12	1:H:301:GLY:HA3	1.92	0.50
1:H:443:LEU:HD22	1:H:525:THR:HG22	1.94	0.50
1:F:493:ILE:HB	1:F:496:ASP:OD2	2.12	0.50
1:B:68:ARG:HD2	1:B:95:TYR:OH	2.11	0.50
1:C:438:ALA:HB3	1:C:515:LEU:HD23	1.94	0.50
1:D:396:GLU:OE2	1:H:317:LYS:HE2	2.11	0.50
1:D:47:ILE:O	1:H:317:LYS:NZ	2.34	0.50
1:F:345:SER:HB2	1:F:353:THR:HG23	1.94	0.50
1:G:67:SER:HA	1:G:72:ARG:CG	2.40	0.50
1:E:459:ARG:HE	2:E:607:EDO:H21	1.77	0.50
1:A:144:VAL:HG13	1:A:214:VAL:CG1	2.42	0.50
1:F:321:ALA:O	1:F:325:MET:HG3	2.11	0.50
1:B:144:VAL:HG22	1:B:166:ALA:HB2	1.93	0.49
1:E:494:TRP:O	1:E:497:ASP:N	2.43	0.49
1:D:350:PRO:HB3	1:D:382:PHE:CE1	2.47	0.49
1:F:340:THR:HG22	1:F:341:GLN:HG3	1.94	0.49
1:F:55:ARG:CZ	1:F:59:ILE:HD12	2.41	0.49
1:F:72:ARG:O	1:F:76:MET:HG2	2.12	0.49
1:G:494:TRP:CE3	1:G:529:PRO:HG3	2.47	0.49
1:E:146:LEU:HD23	1:E:214:VAL:HA	1.93	0.49
1:G:67:SER:OG	1:G:377:THR:O	2.17	0.49
1:G:475:VAL:CG2	1:G:481:VAL:HG11	2.41	0.49
1:C:215:LEU:HD12	1:C:216:GLY:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:ASP:OD1	1:E:473:ARG:NE	2.39	0.49
1:G:260:ALA:O	1:G:261:SER:C	2.51	0.49
1:G:506:ILE:HG23	1:G:542:ILE:HD12	1.95	0.49
1:B:180:VAL:O	1:B:180:VAL:HG23	2.12	0.49
1:E:58:SER:HB2	2:E:603:EDO:H22	1.95	0.49
1:H:103:VAL:O	1:H:107:VAL:HG23	2.12	0.49
1:B:165:ASN:HB3	1:B:168:THR:H	1.78	0.49
1:G:421:THR:CG2	1:G:452:LEU:HD12	2.43	0.49
1:H:71:GLU:OE2	1:H:72:ARG:HG3	2.12	0.49
1:D:377:THR:HA	1:D:383:PRO:HB3	1.95	0.49
1:A:423:VAL:HG12	1:D:431:ALA:HB1	1.94	0.49
1:E:38:PHE:CE2	1:E:42:LEU:HD11	2.47	0.49
1:G:38:PHE:CE2	1:G:42:LEU:HD11	2.47	0.48
1:H:343:LEU:HD23	1:H:356:GLU:HB3	1.94	0.48
1:F:455:ARG:HH21	1:F:455:ARG:CB	2.26	0.48
1:B:30:LEU:N	1:B:31:PRO:CD	2.76	0.48
1:D:343:LEU:HD23	1:D:356:GLU:HB3	1.95	0.48
1:F:60:ILE:HB	1:F:372:MET:HG3	1.96	0.48
1:G:126:THR:HG22	1:G:127:LYS:N	2.29	0.48
1:G:384:VAL:HG12	1:G:388:LYS:HE3	1.95	0.48
1:F:421:THR:HG22	1:F:452:LEU:HD12	1.95	0.48
1:H:88:PHE:O	1:H:127:LYS:HD2	2.13	0.48
1:H:88:PHE:CE2	1:H:240:ASP:HB3	2.49	0.48
1:F:369:ASP:HB3	1:F:477:LEU:O	2.14	0.48
1:G:309:LEU:O	1:G:313:ILE:HG12	2.14	0.48
1:G:418:ARG:HG3	1:G:418:ARG:NH1	2.29	0.48
1:H:262:ASP:O	1:H:265:ALA:HB3	2.13	0.48
1:A:200:ILE:HA	1:A:205:LEU:HD23	1.95	0.48
1:F:310:GLY:HA3	1:G:354:ARG:HE	1.79	0.48
1:F:324:MET:HE2	1:F:328:ARG:HG3	1.95	0.48
1:H:73:LEU:HD13	1:H:103:VAL:HA	1.95	0.48
1:B:424:THR:OG1	1:B:535:ASN:HA	2.14	0.48
1:C:411:ARG:NH2	1:F:411:ARG:HH22	2.12	0.48
1:B:175:ASN:ND2	1:B:229:ASP:OD2	2.42	0.48
1:E:172:ASP:O	1:E:174:PRO:HD3	2.14	0.48
1:F:256:PHE:HZ	1:F:312:GLU:OE1	1.97	0.48
1:E:197:VAL:HA	1:E:207:THR:HG22	1.96	0.47
1:G:56:SER:HB2	1:G:480:GLY:CA	2.43	0.47
1:A:286:HIS:CE1	1:A:290:LYS:HG3	2.49	0.47
1:B:245:VAL:HG21	1:B:270:LEU:O	2.15	0.47
1:B:515:LEU:HD22	1:B:521:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:488:GLU:HB3	1:E:489:PRO:CD	2.45	0.47
1:F:531:GLU:O	1:F:533:TYR:N	2.47	0.47
1:H:283:ILE:HG13	1:H:325:MET:CE	2.44	0.47
1:H:486:TYR:OH	1:H:500:ARG:HG2	2.14	0.47
1:H:499:ASP:O	1:H:503:GLN:HG2	2.15	0.47
1:F:342:MET:HE1	1:F:371:ILE:HG22	1.95	0.47
1:B:511:LEU:HD22	1:B:511:LEU:O	2.14	0.47
1:D:309:LEU:O	1:D:313:ILE:HG12	2.14	0.47
1:D:424:THR:OG1	1:D:535:ASN:HA	2.14	0.47
1:F:353:THR:HB	1:G:341:GLN:OE1	2.15	0.47
1:G:50:GLU:OE1	1:G:50:GLU:HA	2.14	0.47
1:F:74:LYS:HE2	1:F:109:SER:OG	2.13	0.47
1:F:65:PRO:HD2	1:F:379:LYS:HG2	1.97	0.47
1:H:66:ALA:O	1:H:72:ARG:HD2	2.14	0.47
1:C:133:THR:O	1:C:218:ARG:HA	2.14	0.47
1:C:79:ALA:HB1	1:C:388:LYS:HG3	1.97	0.47
1:F:98:GLU:O	1:F:102:ASN:OD1	2.32	0.47
1:F:344:GLU:HG2	1:F:347:ILE:HD12	1.97	0.47
1:F:129:PRO:HG2	1:F:232:GLY:O	2.15	0.47
1:C:411:ARG:HH21	1:F:411:ARG:HH22	1.61	0.47
1:A:476:HIS:ND1	2:A:601:EDO:C2	2.78	0.47
1:C:176:ILE:HG23	1:C:177:VAL:N	2.29	0.47
1:F:256:PHE:HD2	1:F:258:ARG:HE	1.61	0.47
1:B:196:VAL:O	1:B:207:THR:HA	2.15	0.47
1:D:540:LEU:HA	2:D:602:EDO:H21	1.97	0.47
1:E:382:PHE:HB3	1:E:385:GLU:HB2	1.96	0.47
1:H:63:ILE:HD11	1:H:84:ALA:HB1	1.97	0.47
1:A:180:VAL:HG12	1:A:197:VAL:HG21	1.97	0.46
1:A:410:LEU:HD13	1:A:455:ARG:O	2.15	0.46
1:H:72:ARG:O	1:H:76:MET:N	2.44	0.46
1:C:443:LEU:HD23	1:C:465:VAL:HB	1.96	0.46
1:F:233:LEU:HD23	1:F:233:LEU:H	1.79	0.46
2:G:601:EDO:C1	3:G:704:HOH:O	2.59	0.46
1:G:65:PRO:HA	1:G:68:ARG:HD3	1.97	0.46
1:A:176:ILE:HG23	1:A:177:VAL:N	2.30	0.46
1:C:286:HIS:CE1	1:C:290:LYS:HG3	2.50	0.46
1:E:23:ALA:O	1:E:27:GLN:HG3	2.16	0.46
1:G:454:SER:HB2	1:G:479:ARG:O	2.15	0.46
1:H:482:PHE:CD1	1:H:482:PHE:N	2.83	0.46
1:B:144:VAL:CG2	1:B:166:ALA:HB2	2.45	0.46
1:D:92:SER:O	1:D:95:TYR:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:92:SER:H	1:F:95:TYR:HB3	1.81	0.46
1:G:85:ARG:CZ	1:G:125:ASP:OD2	2.63	0.46
1:A:483:PRO:O	1:A:484:LEU:HD23	2.15	0.46
1:C:107:VAL:HG21	1:C:120:VAL:HB	1.98	0.46
1:D:289:VAL:HG11	1:H:47:ILE:HD13	1.97	0.46
1:E:412:ARG:NH1	1:G:408:GLU:OE2	2.48	0.46
1:F:102:ASN:OD1	1:F:102:ASN:N	2.48	0.46
1:D:372:MET:HG2	1:D:373:LEU:N	2.31	0.46
1:G:335:PRO:HA	1:G:369:ASP:OD1	2.16	0.46
1:A:25:PHE:O	1:A:31:PRO:HD3	2.15	0.46
1:B:488:GLU:OE1	1:B:489:PRO:HD3	2.16	0.46
1:E:147:VAL:CG1	1:E:209:VAL:HG21	2.46	0.46
1:G:260:ALA:C	1:G:263:VAL:HG22	2.34	0.46
1:H:486:TYR:OH	1:H:500:ARG:CG	2.64	0.46
1:B:443:LEU:HD22	1:B:525:THR:HG22	1.97	0.46
1:F:64:GLY:HA3	1:F:378:ALA:HB1	1.97	0.46
1:G:73:LEU:HA	1:G:76:MET:HG3	1.98	0.46
1:A:146:LEU:HD23	1:A:214:VAL:CA	2.44	0.45
1:A:26:GLN:O	1:A:26:GLN:HG3	2.15	0.45
1:E:486:TYR:HD1	1:E:504:PHE:CD2	2.34	0.45
1:F:284:GLU:HG2	1:F:305:ALA:HB3	1.97	0.45
1:F:280:ILE:HD12	1:F:301:GLY:HA3	1.97	0.45
1:G:116:SER:OG	1:G:116:SER:O	2.28	0.45
1:B:23:ALA:N	3:B:709:HOH:O	2.49	0.45
1:E:256:PHE:HZ	2:E:602:EDO:H22	1.79	0.45
1:H:101:ALA:O	1:H:105:GLU:HG3	2.16	0.45
1:A:165:ASN:O	1:A:168:THR:O	2.34	0.45
1:A:506:ILE:HG23	1:A:542:ILE:HD12	1.98	0.45
1:D:346:MET:HA	1:D:349:LYS:O	2.17	0.45
1:G:324:MET:O	1:G:328:ARG:HG3	2.15	0.45
1:D:13:VAL:HA	1:D:16:LEU:HD12	1.97	0.45
1:D:69:SER:HB2	1:D:72:ARG:HB2	1.99	0.45
1:E:135:ILE:CG2	1:E:162:THR:HG22	2.47	0.45
1:A:20:LEU:HD12	1:A:20:LEU:N	2.32	0.45
1:D:73:LEU:O	1:D:77:ILE:HG13	2.16	0.45
1:G:424:THR:OG1	1:G:535:ASN:HA	2.16	0.45
1:G:63:ILE:HD11	1:G:86:LEU:HD22	1.97	0.45
1:H:96:HIS:O	1:H:100:ILE:HG13	2.17	0.45
1:E:182:VAL:O	1:E:197:VAL:O	2.35	0.45
1:E:132:ARG:HA	1:E:219:LYS:O	2.16	0.45
1:H:343:LEU:O	1:H:376:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD12	1:A:511:LEU:HD13	1.99	0.45
1:C:190:ASP:HA	1:C:311:ILE:HD11	1.97	0.45
1:D:425:ALA:HB1	1:D:453:LEU:HD23	1.99	0.45
1:F:382:PHE:N	1:F:383:PRO:CD	2.79	0.45
1:F:455:ARG:HH21	1:F:455:ARG:HB3	1.80	0.45
1:B:430:GLU:OE1	1:H:411:ARG:HD2	2.17	0.45
1:H:491:GLU:HG3	1:H:492:ALA:H	1.82	0.45
1:C:256:PHE:N	1:C:284:GLU:OE1	2.45	0.45
1:F:92:SER:O	1:F:95:TYR:N	2.50	0.45
1:A:176:ILE:CG2	1:A:177:VAL:N	2.79	0.45
1:D:455:ARG:O	1:D:455:ARG:CG	2.62	0.45
1:F:30:LEU:N	1:F:31:PRO:CD	2.80	0.45
1:F:455:ARG:CG	1:F:455:ARG:HH21	2.30	0.45
1:H:350:PRO:HG2	1:H:351:ARG:HG3	1.97	0.45
1:H:379:LYS:HG3	1:H:379:LYS:O	2.17	0.45
1:H:79:ALA:HB2	1:H:384:VAL:CG1	2.47	0.45
1:A:58:SER:CB	2:A:601:EDO:O2	2.62	0.44
1:D:267:ARG:HA	1:D:270:LEU:CD1	2.48	0.44
1:D:53:ALA:HB2	2:D:603:EDO:H22	1.98	0.44
1:F:252:VAL:HG21	1:F:270:LEU:HD11	1.99	0.44
1:G:60:ILE:CG2	1:G:372:MET:HE2	2.45	0.44
1:F:37:THR:HB	1:G:409:GLU:CD	2.37	0.44
1:B:175:ASN:O	1:B:179:VAL:HG12	2.18	0.44
1:E:524:VAL:HG12	1:E:534:THR:CG2	2.46	0.44
1:B:508:SER:O	1:B:512:ARG:HG3	2.18	0.44
1:D:373:LEU:HD23	1:D:373:LEU:HA	1.79	0.44
1:F:419:ASP:OD2	1:F:448:ARG:NH2	2.38	0.44
1:H:452:LEU:O	1:H:455:ARG:HG2	2.17	0.44
1:B:72:ARG:O	1:B:75:GLU:N	2.50	0.44
1:D:118:ARG:O	1:D:119:PRO:C	2.56	0.44
1:F:25:PHE:CG	1:F:25:PHE:O	2.69	0.44
1:B:180:VAL:CG2	1:B:197:VAL:HG21	2.48	0.44
1:G:346:MET:HA	1:G:349:LYS:O	2.17	0.44
1:G:88:PHE:CE1	1:G:96:HIS:ND1	2.86	0.44
1:H:382:PHE:HB3	1:H:385:GLU:HB2	2.00	0.44
1:A:457:ARG:NH1	2:A:608:EDO:H12	2.29	0.44
1:A:466:THR:CG2	1:A:472:ALA:HB2	2.47	0.44
1:C:172:ASP:O	1:C:174:PRO:HD3	2.17	0.44
1:G:395:ARG:O	2:G:601:EDO:C2	2.66	0.44
1:H:237:ASP:O	1:H:241:LEU:HG	2.17	0.44
1:B:501:ARG:NH1	2:B:605:EDO:O2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:VAL:CG2	1:E:198:GLN:O	2.66	0.44
1:B:263:VAL:CG2	1:B:298:VAL:HG23	2.46	0.43
1:E:152:VAL:N	1:E:207:THR:O	2.38	0.43
1:C:234:SER:O	1:C:238:VAL:HG23	2.18	0.43
1:C:309:LEU:O	1:C:313:ILE:HG12	2.18	0.43
1:C:443:LEU:HB3	2:C:601:EDO:H12	2.00	0.43
1:D:75:GLU:HB3	1:D:384:VAL:HG21	2.00	0.43
1:B:228:VAL:HG12	1:B:230:LEU:H	1.82	0.43
1:D:255:SER:HA	1:D:282:LYS:HD3	1.98	0.43
1:D:315:ALA:O	1:H:357:THR:HG21	2.18	0.43
1:D:389:MET:HE2	1:D:389:MET:HA	2.00	0.43
1:E:147:VAL:HG13	1:E:209:VAL:HG21	2.00	0.43
1:G:263:VAL:CG2	1:G:264:ALA:N	2.81	0.43
1:H:523:VAL:O	1:H:537:MET:HA	2.18	0.43
1:B:180:VAL:O	1:B:180:VAL:CG2	2.66	0.43
1:C:342:MET:O	1:C:343:LEU:HD23	2.18	0.43
1:C:528:ARG:HB2	1:C:529:PRO:HD2	2.01	0.43
1:D:270:LEU:H	1:D:270:LEU:HD12	1.83	0.43
1:D:528:ARG:HB3	1:D:529:PRO:CD	2.48	0.43
1:A:144:VAL:CG1	1:A:214:VAL:CG1	2.96	0.43
1:B:79:ALA:HB1	1:B:388:LYS:HG3	2.00	0.43
1:F:62:THR:CG2	1:F:85:ARG:HD3	2.48	0.43
1:E:408:GLU:OE1	1:G:408:GLU:OE2	2.35	0.43
1:H:506:ILE:HG23	1:H:542:ILE:HD12	2.00	0.43
1:A:263:VAL:CG2	1:A:298:VAL:HG23	2.38	0.43
1:B:154:VAL:HA	1:B:169:VAL:O	2.17	0.43
1:A:354:ARG:HG2	1:B:341:GLN:OE1	2.19	0.43
1:E:347:ILE:HG22	1:E:348:THR:HG23	2.01	0.43
1:F:457:ARG:N	1:F:458:PRO:CD	2.82	0.43
1:A:490:PRO:HA	1:A:497:ASP:OD1	2.18	0.43
1:A:56:SER:HB2	1:A:480:GLY:CA	2.48	0.43
1:B:494:TRP:HH2	1:B:526:GLY:O	2.01	0.43
1:C:352:PRO:HG3	1:C:389:MET:HG2	2.01	0.43
1:E:128:GLY:HA2	1:E:237:ASP:OD2	2.18	0.43
1:H:472:ALA:O	1:H:483:PRO:HG3	2.18	0.43
1:C:424:THR:OG1	1:C:535:ASN:HA	2.19	0.43
1:E:411:ARG:HD3	1:G:411:ARG:NH2	2.33	0.43
1:E:508:SER:O	1:E:512:ARG:HG3	2.19	0.43
1:F:123:ALA:HA	1:F:251:ILE:O	2.17	0.43
1:G:527:TRP:HB3	1:G:536:ILE:HD11	2.01	0.43
1:H:72:ARG:O	1:H:75:GLU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:THR:HA	1:C:85:ARG:HB3	2.01	0.43
1:E:187:TYR:CD1	1:E:191:GLY:HA2	2.54	0.43
1:H:267:ARG:NH1	1:H:279:ILE:HD12	2.33	0.43
1:B:130:GLU:OE1	1:B:132:ARG:NH2	2.51	0.43
1:E:136:LEU:O	1:E:137:GLN:CB	2.67	0.43
1:E:527:TRP:HD1	1:E:536:ILE:HD11	1.75	0.43
1:H:292:PHE:CE2	1:H:325:MET:HE2	2.53	0.43
1:H:374:SER:N	1:H:376:GLU:OE1	2.50	0.43
1:H:467:ARG:NH2	1:H:490:PRO:HA	2.34	0.43
1:B:61:ALA:HB3	1:B:81:MET:SD	2.59	0.42
1:D:274:GLY:HA2	1:D:277:ILE:CG1	2.49	0.42
1:E:306:ARG:HD3	1:E:322:GLN:OE1	2.18	0.42
1:G:56:SER:CB	1:G:480:GLY:HA2	2.47	0.42
1:B:146:LEU:HG	1:B:215:LEU:CD2	2.49	0.42
1:A:541:SER:N	2:A:609:EDO:H22	2.34	0.42
1:B:103:VAL:O	1:B:107:VAL:HG23	2.19	0.42
1:D:125:ASP:OD2	1:D:282:LYS:HE3	2.19	0.42
1:A:323:LYS:HE3	1:B:365:LEU:CD1	2.49	0.42
1:A:406:LEU:HD21	1:A:457:ARG:HG3	2.01	0.42
1:D:508:SER:O	1:D:512:ARG:HG3	2.19	0.42
1:E:421:THR:CG2	1:E:452:LEU:HD12	2.49	0.42
1:F:68:ARG:HD2	1:F:95:TYR:OH	2.20	0.42
1:H:257:VAL:HG21	1:H:281:SER:HA	2.00	0.42
1:H:257:VAL:HG21	1:H:281:SER:CB	2.49	0.42
1:C:282:LYS:HG2	1:C:303:MET:HB3	2.02	0.42
1:E:377:THR:HA	1:E:383:PRO:HB3	2.02	0.42
1:C:536:ILE:HG12	1:F:538:ARG:HG2	2.02	0.42
1:H:85:ARG:NE	1:H:125:ASP:OD2	2.48	0.42
1:H:44:LEU:HA	1:H:44:LEU:HD23	1.86	0.42
1:H:121:ALA:HB2	1:H:473:ARG:HB3	2.00	0.42
1:B:440:ILE:HA	1:B:522:ILE:O	2.20	0.42
1:G:56:SER:HB2	1:G:480:GLY:N	2.35	0.42
1:C:178:ARG:HB2	1:C:178:ARG:NH1	2.34	0.42
1:H:79:ALA:CB	1:H:384:VAL:HG13	2.50	0.42
1:A:357:THR:HG22	1:A:393:ILE:HD11	2.01	0.42
1:A:443:LEU:HG	1:A:525:THR:HG22	2.01	0.42
1:F:360:VAL:HB	1:F:393:ILE:HG21	2.02	0.42
1:B:88:PHE:O	1:B:127:LYS:HB2	2.20	0.41
1:C:175:ASN:OD1	1:C:178:ARG:NH1	2.53	0.41
1:C:381:ASN:O	2:C:606:EDO:H21	2.19	0.41
1:D:89:SER:OG	1:D:127:LYS:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:333:GLY:HA2	1:F:455:ARG:CG	2.48	0.41
1:G:528:ARG:HG3	1:G:529:PRO:HD2	2.01	0.41
1:D:384:VAL:O	1:D:384:VAL:HG12	2.20	0.41
1:D:428:ALA:HB1	1:D:522:ILE:HG21	2.01	0.41
1:E:197:VAL:HG22	1:E:207:THR:HG22	2.02	0.41
1:E:452:LEU:O	1:E:455:ARG:HG2	2.21	0.41
1:F:279:ILE:C	1:F:280:ILE:HD13	2.41	0.41
1:H:294:GLU:O	1:H:297:GLU:HB3	2.20	0.41
1:A:155:THR:CG2	1:A:203:GLU:O	2.67	0.41
1:B:535:ASN:O	1:H:538:ARG:HA	2.20	0.41
1:C:426:ILE:HD12	1:C:456:TYR:CZ	2.54	0.41
1:A:423:VAL:CG1	1:D:431:ALA:HB1	2.50	0.41
1:H:30:LEU:N	1:H:31:PRO:CD	2.83	0.41
1:B:514:PHE:N	1:B:514:PHE:CD1	2.86	0.41
1:C:351:ARG:NH2	1:E:191:GLY:O	2.53	0.41
1:E:200:ILE:HG12	1:E:205:LEU:CD2	2.50	0.41
1:H:430:GLU:HA	1:H:430:GLU:OE2	2.20	0.41
1:C:290:LYS:HE3	1:E:48:ASP:OD2	2.19	0.41
1:D:527:TRP:CE3	1:D:528:ARG:CG	2.99	0.41
1:E:58:SER:CB	2:E:603:EDO:H22	2.50	0.41
1:B:509:GLY:HA3	1:B:515:LEU:HD12	2.02	0.41
1:B:74:LYS:O	1:B:78:LYS:HG3	2.19	0.41
1:G:296:LEU:HD13	1:G:302:ILE:CG1	2.51	0.41
1:G:321:ALA:O	1:G:325:MET:HG3	2.21	0.41
1:H:325:MET:HB3	1:H:325:MET:HE2	1.93	0.41
1:A:154:VAL:HA	1:A:169:VAL:O	2.20	0.41
1:A:171:VAL:HG21	1:A:176:ILE:HD13	2.02	0.41
1:F:22:THR:OG1	1:F:23:ALA:N	2.52	0.41
1:F:283:ILE:HD11	1:F:295:ILE:HG21	2.03	0.41
1:F:405:GLN:O	1:F:409:GLU:HG3	2.21	0.41
1:G:475:VAL:HG11	1:G:483:PRO:HB3	2.01	0.41
1:A:124:LEU:HD23	1:A:124:LEU:C	2.41	0.41
1:C:488:GLU:HB3	1:C:489:PRO:HD2	2.03	0.41
1:F:64:GLY:C	1:F:378:ALA:O	2.59	0.41
1:H:306:ARG:NH2	1:H:342:MET:HG2	2.35	0.41
1:A:196:VAL:O	1:A:207:THR:HA	2.21	0.41
1:A:389:MET:SD	1:A:393:ILE:HD11	2.61	0.41
1:C:172:ASP:O	1:C:174:PRO:CD	2.69	0.41
1:A:404:ARG:NE	1:D:412:ARG:HD2	2.35	0.41
1:G:51:PRO:HB2	2:G:601:EDO:C2	2.51	0.41
1:H:291:ARG:NE	1:H:294:GLU:OE1	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LYS:O	1:A:205:LEU:HA	2.21	0.41
1:A:527:TRP:CE3	1:A:528:ARG:HB3	2.56	0.41
1:D:30:LEU:HA	1:D:30:LEU:HD23	1.95	0.41
1:E:131:ILE:HG22	1:E:221:VAL:HB	2.03	0.41
1:E:152:VAL:HG22	1:E:167:ASN:HA	2.03	0.41
1:F:342:MET:O	1:F:356:GLU:HB3	2.21	0.41
1:A:103:VAL:O	1:A:107:VAL:HG23	2.20	0.41
1:A:435:CYS:O	1:A:436:CYS:C	2.59	0.41
1:C:343:LEU:HD13	1:C:346:MET:CE	2.50	0.41
1:D:324:MET:SD	1:D:324:MET:C	2.99	0.41
1:D:540:LEU:HD12	1:D:541:SER:H	1.86	0.41
1:F:130:GLU:HG2	1:F:131:ILE:N	2.36	0.41
1:H:375:GLY:C	1:H:377:THR:N	2.75	0.41
1:A:313:ILE:HB	1:A:314:PRO:HD2	2.03	0.40
1:C:501:ARG:HH12	2:C:601:EDO:C1	2.34	0.40
1:F:236:GLN:O	1:F:240:ASP:OD2	2.40	0.40
1:G:376:GLU:O	1:G:383:PRO:HA	2.21	0.40
1:H:308:ASP:O	1:H:311:ILE:HG12	2.21	0.40
1:A:182:VAL:HA	1:A:197:VAL:HG12	2.03	0.40
1:B:64:GLY:O	1:B:66:ALA:N	2.54	0.40
1:E:494:TRP:C	1:E:496:ASP:N	2.75	0.40
1:G:253:PHE:HB3	1:G:282:LYS:HD2	2.02	0.40
1:B:516:ARG:O	1:B:519:ASP:HB2	2.21	0.40
1:B:64:GLY:O	1:B:65:PRO:C	2.59	0.40
1:D:291:ARG:O	1:D:294:GLU:HG2	2.22	0.40
1:D:344:GLU:HG3	1:D:347:ILE:HD12	2.02	0.40
1:G:291:ARG:O	1:G:294:GLU:HG2	2.20	0.40
1:G:120:VAL:O	1:G:473:ARG:HD2	2.22	0.40
1:G:62:THR:HA	1:G:85:ARG:HB3	2.02	0.40
1:H:308:ASP:OD2	2:H:601:EDO:H22	2.21	0.40
1:H:70:VAL:HG23	1:H:102:ASN:ND2	2.37	0.40
1:A:284:GLU:C	1:A:309:LEU:HD13	2.41	0.40
1:B:155:THR:O	1:B:170:TRP:HA	2.20	0.40
1:B:537:MET:HB3	1:H:537:MET:HG3	2.03	0.40
1:F:106:ALA:O	1:F:110:PHE:CE1	2.75	0.40
1:F:255:SER:HA	1:F:282:LYS:HD3	2.03	0.40
1:G:256:PHE:O	1:G:258:ARG:HD3	2.22	0.40
1:D:455:ARG:HG3	1:D:455:ARG:O	2.22	0.40
1:E:253:PHE:HD1	1:E:280:ILE:HB	1.86	0.40
1:G:399:ALA:HB2	2:G:601:EDO:C2	2.50	0.40
1:H:527:TRP:NE1	1:H:533:TYR:HB3	2.36	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	499/543 (92%)	484 (97%)	12 (2%)	3 (1%)	25	35
1	B	514/543 (95%)	495 (96%)	14 (3%)	5 (1%)	15	22
1	C	489/543 (90%)	471 (96%)	17 (4%)	1 (0%)	47	61
1	D	416/543 (77%)	405 (97%)	10 (2%)	1 (0%)	47	61
1	E	501/543 (92%)	481 (96%)	13 (3%)	7 (1%)	11	14
1	F	409/543 (75%)	378 (92%)	26 (6%)	5 (1%)	13	17
1	G	385/543 (71%)	355 (92%)	27 (7%)	3 (1%)	19	27
1	H	395/543 (73%)	366 (93%)	22 (6%)	7 (2%)	8	10
All	All	3608/4344 (83%)	3435 (95%)	141 (4%)	32 (1%)	17	24

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	151	GLN
1	E	495	ALA
1	B	137	GLN
1	E	166	ALA
1	F	532	GLY
1	H	376	GLU
1	A	151	GLN
1	A	189	ASP
1	C	340	THR
1	E	148	LYS
1	E	489	PRO
1	G	261	SER
1	H	100	ILE
1	H	340	THR

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Mol	Chain	Res	Type
1	H	345	SER
1	A	340	THR
1	B	161	ARG
1	B	340	THR
1	E	488	GLU
1	F	416	LEU
1	H	265	ALA
1	H	271	GLY
1	B	530	GLY
1	D	340	THR
1	G	340	THR
1	B	28	GLN
1	E	340	THR
1	F	271	GLY
1	F	490	PRO
1	G	260	ALA
1	F	382	PHE
1	H	131	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	405/433 (94%)	398 (98%)	7 (2%)	60	77
1	B	415/433 (96%)	406 (98%)	9 (2%)	52	69
1	C	402/433 (93%)	397 (99%)	5 (1%)	71	84
1	D	336/433 (78%)	321 (96%)	15 (4%)	27	42
1	E	410/433 (95%)	401 (98%)	9 (2%)	52	69
1	F	334/433 (77%)	322 (96%)	12 (4%)	35	52
1	G	314/433 (72%)	299 (95%)	15 (5%)	25	40
1	H	328/433 (76%)	309 (94%)	19 (6%)	20	31
All	All	2944/3464 (85%)	2853 (97%)	91 (3%)	40	58

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	ASP
1	A	261	SER
1	A	309	LEU
1	A	436	CYS
1	A	528	ARG
1	A	531	GLU
1	A	541	SER
1	B	69	SER
1	B	94	GLU
1	B	136	LEU
1	B	161	ARG
1	B	233	LEU
1	B	263	VAL
1	B	358	SER
1	B	411	ARG
1	B	479	ARG
1	C	69	SER
1	C	113	SER
1	C	150	SER
1	C	168	THR
1	C	541	SER
1	D	69	SER
1	D	72	ARG
1	D	92	SER
1	D	255	SER
1	D	259	LYS
1	D	299	SER
1	D	309	LEU
1	D	342	MET
1	D	344	GLU
1	D	345	SER
1	D	374	SER
1	D	436[A]	CYS
1	D	436[B]	CYS
1	D	468	SER
1	D	531	GLU
1	E	58	SER
1	E	69	SER
1	E	89	SER
1	E	178	ARG
1	E	404	ARG
1	E	444	THR
1	E	511	LEU

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Mol	Chain	Res	Type
1	E	527	TRP
1	E	541	SER
1	F	22	THR
1	F	69	SER
1	F	102	ASN
1	F	109	SER
1	F	235	GLU
1	F	256	PHE
1	F	324	MET
1	F	358	SER
1	F	407	PHE
1	F	455	ARG
1	F	468	SER
1	F	528	ARG
1	G	20	LEU
1	G	68	ARG
1	G	76	MET
1	G	99	SER
1	G	109	SER
1	G	258	ARG
1	G	267	ARG
1	G	273	GLU
1	G	370	CYS
1	G	374	SER
1	G	389	MET
1	G	395	ARG
1	G	449	SER
1	G	475	VAL
1	G	528	ARG
1	H	24	PHE
1	H	68	ARG
1	H	69	SER
1	H	89	SER
1	H	116	SER
1	H	126	THR
1	H	130	GLU
1	H	131	ILE
1	H	132	ARG
1	H	236	GLN
1	H	255	SER
1	H	284	GLU
1	H	345	SER

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Mol	Chain	Res	Type
1	H	391	HIS
1	H	407	PHE
1	H	443	LEU
1	H	531	GLU
1	H	537	MET
1	H	541	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	403	HIS
1	H	403	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

41 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	EDO	A	608	-	3,3,3	0.95	0	2,2,2	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	E	607	-	3,3,3	0.57	0	2,2,2	0.69	0
2	EDO	H	603	-	3,3,3	0.45	0	2,2,2	0.51	0
2	EDO	H	602	-	3,3,3	0.47	0	2,2,2	0.58	0
2	EDO	C	605	-	3,3,3	0.44	0	2,2,2	0.40	0
2	EDO	B	606	-	3,3,3	0.41	0	2,2,2	0.39	0
2	EDO	H	601	-	3,3,3	0.68	0	2,2,2	0.55	0
2	EDO	G	602	-	3,3,3	0.52	0	2,2,2	0.12	0
2	EDO	A	610	-	3,3,3	0.49	0	2,2,2	0.42	0
2	EDO	A	603	-	3,3,3	0.55	0	2,2,2	0.12	0
2	EDO	D	601	-	3,3,3	0.52	0	2,2,2	0.05	0
2	EDO	E	603	-	3,3,3	0.61	0	2,2,2	0.36	0
2	EDO	C	604	-	3,3,3	0.44	0	2,2,2	0.75	0
2	EDO	B	602	-	3,3,3	0.43	0	2,2,2	0.51	0
2	EDO	E	606	-	3,3,3	0.43	0	2,2,2	0.70	0
2	EDO	E	602	-	3,3,3	0.68	0	2,2,2	0.36	0
2	EDO	C	603	-	3,3,3	0.36	0	2,2,2	1.01	0
2	EDO	C	606	-	3,3,3	0.57	0	2,2,2	0.14	0
2	EDO	D	602	-	3,3,3	0.59	0	2,2,2	0.50	0
2	EDO	B	601	-	3,3,3	0.57	0	2,2,2	0.45	0
2	EDO	F	601	-	3,3,3	0.53	0	2,2,2	0.20	0
2	EDO	D	604	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	A	607	-	3,3,3	0.57	0	2,2,2	0.14	0
2	EDO	E	604	-	3,3,3	0.62	0	2,2,2	0.84	0
2	EDO	E	605	-	3,3,3	0.46	0	2,2,2	0.03	0
2	EDO	E	601	-	3,3,3	0.60	0	2,2,2	1.06	0
2	EDO	B	603	-	3,3,3	1.05	0	2,2,2	1.13	0
2	EDO	B	607	-	3,3,3	0.44	0	2,2,2	0.63	0
2	EDO	A	602	-	3,3,3	0.45	0	2,2,2	0.39	0
2	EDO	A	606	-	3,3,3	0.52	0	2,2,2	0.15	0
2	EDO	B	605	-	3,3,3	0.52	0	2,2,2	0.21	0
2	EDO	A	609	-	3,3,3	0.46	0	2,2,2	0.55	0
2	EDO	A	601	-	3,3,3	0.59	0	2,2,2	1.57	1 (50%)
2	EDO	A	604	-	3,3,3	0.48	0	2,2,2	0.31	0
2	EDO	B	604	-	3,3,3	0.64	0	2,2,2	1.30	0
2	EDO	A	605	-	3,3,3	0.81	0	2,2,2	0.49	0
2	EDO	C	601	-	3,3,3	0.79	0	2,2,2	0.54	0
2	EDO	D	603	-	3,3,3	0.46	0	2,2,2	0.48	0
2	EDO	G	601	-	3,3,3	0.43	0	2,2,2	0.63	0
2	EDO	F	602	-	3,3,3	0.49	0	2,2,2	0.20	0
2	EDO	C	602	-	3,3,3	0.73	0	2,2,2	0.32	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	EDO	A	608	-	-	1/1/1/1	-
2	EDO	E	607	-	-	0/1/1/1	-
2	EDO	H	603	-	-	1/1/1/1	-
2	EDO	H	602	-	-	1/1/1/1	-
2	EDO	C	605	-	-	0/1/1/1	-
2	EDO	B	606	-	-	1/1/1/1	-
2	EDO	H	601	-	-	0/1/1/1	-
2	EDO	G	602	-	-	0/1/1/1	-
2	EDO	A	610	-	-	0/1/1/1	-
2	EDO	A	603	-	-	0/1/1/1	-
2	EDO	D	601	-	-	1/1/1/1	-
2	EDO	E	603	-	-	1/1/1/1	-
2	EDO	C	604	-	-	1/1/1/1	-
2	EDO	B	602	-	-	1/1/1/1	-
2	EDO	E	606	-	-	0/1/1/1	-
2	EDO	E	602	-	-	1/1/1/1	-
2	EDO	C	603	-	-	1/1/1/1	-
2	EDO	C	606	-	-	1/1/1/1	-
2	EDO	D	602	-	-	0/1/1/1	-
2	EDO	B	601	-	-	0/1/1/1	-
2	EDO	F	601	-	-	1/1/1/1	-
2	EDO	D	604	-	-	1/1/1/1	-
2	EDO	A	607	-	-	1/1/1/1	-
2	EDO	E	604	-	-	0/1/1/1	-
2	EDO	E	605	-	-	1/1/1/1	-
2	EDO	E	601	-	-	0/1/1/1	-
2	EDO	B	603	-	-	0/1/1/1	-
2	EDO	B	607	-	-	1/1/1/1	-
2	EDO	A	602	-	-	1/1/1/1	-
2	EDO	A	606	-	-	1/1/1/1	-
2	EDO	B	605	-	-	0/1/1/1	-
2	EDO	A	609	-	-	1/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
2	EDO	A	604	-	-	1/1/1/1	-
2	EDO	B	604	-	-	0/1/1/1	-
2	EDO	A	605	-	-	1/1/1/1	-
2	EDO	C	601	-	-	0/1/1/1	-
2	EDO	D	603	-	-	1/1/1/1	-
2	EDO	G	601	-	-	0/1/1/1	-
2	EDO	F	602	-	-	1/1/1/1	-
2	EDO	C	602	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	EDO	O1-C1-C2	-2.22	95.90	111.91

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	EDO	O1-C1-C2-O2
2	H	603	EDO	O1-C1-C2-O2
2	B	606	EDO	O1-C1-C2-O2
2	E	602	EDO	O1-C1-C2-O2
2	A	605	EDO	O1-C1-C2-O2
2	F	602	EDO	O1-C1-C2-O2
2	D	604	EDO	O1-C1-C2-O2
2	H	602	EDO	O1-C1-C2-O2
2	A	604	EDO	O1-C1-C2-O2
2	D	603	EDO	O1-C1-C2-O2
2	A	608	EDO	O1-C1-C2-O2
2	A	609	EDO	O1-C1-C2-O2
2	C	604	EDO	O1-C1-C2-O2
2	E	603	EDO	O1-C1-C2-O2
2	C	606	EDO	O1-C1-C2-O2
2	A	607	EDO	O1-C1-C2-O2
2	E	605	EDO	O1-C1-C2-O2
2	C	602	EDO	O1-C1-C2-O2
2	B	602	EDO	O1-C1-C2-O2
2	F	601	EDO	O1-C1-C2-O2
2	B	607	EDO	O1-C1-C2-O2
2	A	602	EDO	O1-C1-C2-O2
2	C	603	EDO	O1-C1-C2-O2
2	A	606	EDO	O1-C1-C2-O2

There are no ring outliers.

16 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	608	EDO	3	0
2	E	607	EDO	1	0
2	H	602	EDO	2	0
2	H	601	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	603	EDO	3	0
2	E	602	EDO	2	0
2	C	606	EDO	1	0
2	D	602	EDO	1	0
2	B	605	EDO	2	0
2	A	609	EDO	1	0
2	A	601	EDO	3	0
2	A	604	EDO	5	0
2	B	604	EDO	3	0
2	C	601	EDO	2	0
2	D	603	EDO	1	0
2	G	601	EDO	9	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	505/543 (93%)	0.14	21 (4%) 36 34	26, 41, 73, 88	0
1	B	518/543 (95%)	0.27	23 (4%) 34 32	26, 45, 75, 88	0
1	C	499/543 (91%)	0.26	24 (4%) 30 28	30, 45, 72, 92	0
1	D	421/543 (77%)	0.48	31 (7%) 14 13	30, 58, 82, 91	0
1	E	509/543 (93%)	0.30	33 (6%) 18 17	28, 48, 77, 92	0
1	F	417/543 (76%)	0.54	37 (8%) 9 8	39, 63, 85, 94	0
1	G	395/543 (72%)	0.66	49 (12%) 4 3	38, 62, 85, 95	0
1	H	407/543 (74%)	0.69	50 (12%) 4 3	41, 64, 85, 93	0
All	All	3671/4344 (84%)	0.40	268 (7%) 15 13	26, 53, 82, 95	0

All (268) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	272	PRO	7.5
1	E	25	PHE	6.6
1	E	146	LEU	6.6
1	G	270	LEU	5.5
1	A	215	LEU	5.3
1	H	63	ILE	5.0
1	H	381	ASN	4.9
1	B	25	PHE	4.8
1	F	25	PHE	4.7
1	C	144	VAL	4.6
1	C	135	ILE	4.6
1	A	147	VAL	4.5
1	H	107	VAL	4.4
1	H	370	CYS	4.3
1	G	511	LEU	4.3
1	E	147	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	363	ALA	4.2
1	G	370	CYS	4.2
1	F	348	THR	4.2
1	A	24	PHE	4.1
1	G	25	PHE	4.1
1	G	265	ALA	4.0
1	G	122	ILE	4.0
1	F	99	SER	4.0
1	H	239	ARG	3.9
1	A	178	ARG	3.9
1	F	493	ILE	3.8
1	A	146	LEU	3.8
1	F	72	ARG	3.7
1	B	147	VAL	3.7
1	H	359	ASP	3.7
1	F	381	ASN	3.7
1	E	24	PHE	3.7
1	F	242	ARG	3.6
1	F	516	ARG	3.6
1	H	338	CYS	3.6
1	C	22	THR	3.6
1	H	529	PRO	3.6
1	D	381	ASN	3.6
1	D	351	ARG	3.5
1	G	382	PHE	3.4
1	H	363	ALA	3.4
1	D	73	LEU	3.4
1	G	542	ILE	3.4
1	F	370	CYS	3.4
1	G	124	LEU	3.4
1	A	530	GLY	3.3
1	F	23	ALA	3.3
1	G	129	PRO	3.3
1	B	517	VAL	3.3
1	D	63	ILE	3.3
1	G	350	PRO	3.3
1	G	517	VAL	3.3
1	G	338	CYS	3.3
1	D	97	ALA	3.3
1	H	67	SER	3.3
1	H	103	VAL	3.2
1	E	527	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	516	ARG	3.2
1	D	361	ALA	3.2
1	G	288	GLY	3.2
1	C	155	THR	3.2
1	G	258	ARG	3.2
1	H	362	ASN	3.2
1	H	260	ALA	3.2
1	D	96	HIS	3.2
1	A	20	LEU	3.2
1	A	151	GLN	3.1
1	C	216	GLY	3.1
1	D	368	ALA	3.1
1	E	168	THR	3.1
1	F	487	ARG	3.1
1	F	71	GLU	3.1
1	E	23	ALA	3.1
1	D	415	PRO	3.0
1	H	69	SER	3.0
1	A	145	GLU	3.0
1	B	370	CYS	3.0
1	F	527	TRP	3.0
1	G	22	THR	3.0
1	G	70	VAL	2.9
1	B	338	CYS	2.9
1	H	371	ILE	2.9
1	H	131	ILE	2.9
1	C	214	VAL	2.9
1	A	25	PHE	2.9
1	H	489	PRO	2.9
1	E	30	LEU	2.9
1	H	355	ALA	2.9
1	D	243	PHE	2.9
1	A	165	ASN	2.8
1	C	360	VAL	2.8
1	G	264	ALA	2.8
1	G	348	THR	2.8
1	H	487	ARG	2.8
1	C	205	LEU	2.8
1	C	52	VAL	2.8
1	H	70	VAL	2.8
1	G	63	ILE	2.8
1	A	148	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	338	CYS	2.8
1	H	74	LYS	2.8
1	G	271	GLY	2.8
1	B	528	ARG	2.8
1	G	268	ALA	2.8
1	B	166	ALA	2.8
1	B	493	ILE	2.8
1	C	200	ILE	2.8
1	E	26	GLN	2.7
1	B	168	THR	2.7
1	H	25	PHE	2.7
1	H	65	PRO	2.7
1	C	156	VAL	2.7
1	D	98	GLU	2.7
1	H	122	ILE	2.7
1	D	114	PRO	2.7
1	G	273	GLU	2.7
1	G	478	CYS	2.7
1	E	214	VAL	2.7
1	G	58	SER	2.7
1	C	24	PHE	2.7
1	D	95	TYR	2.7
1	H	94	GLU	2.7
1	D	370	CYS	2.7
1	B	215	LEU	2.7
1	E	144	VAL	2.6
1	D	256	PHE	2.6
1	F	490	PRO	2.6
1	E	215	LEU	2.6
1	H	256	PHE	2.6
1	F	103	VAL	2.6
1	H	73	LEU	2.6
1	D	69	SER	2.6
1	D	366	ASP	2.6
1	F	528	ARG	2.6
1	E	182	VAL	2.6
1	F	533	TYR	2.6
1	C	20	LEU	2.5
1	F	22	THR	2.5
1	D	362	ASN	2.5
1	D	358	SER	2.5
1	B	163	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	71	GLU	2.5
1	B	136	LEU	2.5
1	H	367	GLY	2.5
1	G	267	ARG	2.5
1	G	359	ASP	2.5
1	H	361	ALA	2.5
1	B	183	GLY	2.5
1	E	192	LEU	2.5
1	G	360	VAL	2.5
1	H	56	SER	2.5
1	D	355	ALA	2.5
1	C	371	ILE	2.4
1	G	289	VAL	2.4
1	A	201	GLY	2.4
1	D	350	PRO	2.4
1	A	22	THR	2.4
1	E	166	ALA	2.4
1	C	170	TRP	2.4
1	C	149	GLY	2.4
1	F	347	ILE	2.4
1	F	24	PHE	2.4
1	G	21	GLY	2.4
1	F	478	CYS	2.4
1	G	369	ASP	2.4
1	F	360	VAL	2.4
1	D	478	CYS	2.4
1	G	361	ALA	2.4
1	H	66	ALA	2.4
1	C	19	GLU	2.4
1	F	337	VAL	2.4
1	G	368	ALA	2.4
1	G	358	SER	2.4
1	F	338	CYS	2.4
1	E	339	ALA	2.3
1	G	269	ALA	2.3
1	B	167	ASN	2.3
1	D	364	VAL	2.3
1	C	178	ARG	2.3
1	B	200	ILE	2.3
1	B	24	PHE	2.3
1	G	88	PHE	2.3
1	F	359	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	478	CYS	2.3
1	G	357	THR	2.3
1	E	135	ILE	2.3
1	E	200	ILE	2.3
1	C	25	PHE	2.3
1	G	365	LEU	2.3
1	F	65	PRO	2.3
1	C	145	GLU	2.3
1	E	145	GLU	2.3
1	E	364	VAL	2.3
1	G	68	ARG	2.3
1	H	543	SER	2.3
1	B	363	ALA	2.3
1	D	359	ASP	2.3
1	G	364	VAL	2.2
1	G	367	GLY	2.2
1	A	358	SER	2.2
1	B	151	GLN	2.2
1	E	94	GLU	2.2
1	F	105	GLU	2.2
1	A	177	VAL	2.2
1	E	148	LYS	2.2
1	E	370	CYS	2.2
1	E	478	CYS	2.2
1	A	205	LEU	2.2
1	H	241	LEU	2.2
1	D	527	TRP	2.2
1	E	209	VAL	2.2
1	A	338	CYS	2.2
1	F	492	ALA	2.2
1	H	358	SER	2.2
1	A	196	VAL	2.2
1	E	27	GLN	2.2
1	H	385	GLU	2.2
1	F	26	GLN	2.2
1	H	275	HIS	2.2
1	C	199	LYS	2.2
1	H	98	GLU	2.2
1	H	384	VAL	2.1
1	A	167	ASN	2.1
1	G	363	ALA	2.1
1	C	143	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	92	SER	2.1
1	E	528	ARG	2.1
1	G	73	LEU	2.1
1	E	338	CYS	2.1
1	F	127	LYS	2.1
1	H	364	VAL	2.1
1	H	368	ALA	2.1
1	E	207	THR	2.1
1	D	71	GLU	2.1
1	C	21	GLY	2.1
1	C	182	VAL	2.1
1	G	103	VAL	2.1
1	F	489	PRO	2.1
1	D	371	ILE	2.1
1	H	365	LEU	2.1
1	H	127	LYS	2.1
1	H	382	PHE	2.1
1	B	165	ASN	2.1
1	H	257	VAL	2.1
1	H	360	VAL	2.1
1	H	369	ASP	2.1
1	F	371	ILE	2.1
1	B	358	SER	2.1
1	G	256	PHE	2.1
1	G	518	GLY	2.1
1	H	76	MET	2.0
1	F	231	PRO	2.0
1	F	361	ALA	2.0
1	B	204	GLY	2.0
1	F	382	PHE	2.0
1	E	359	ASP	2.0
1	F	369	ASP	2.0
1	D	298	VAL	2.0
1	E	517	VAL	2.0
1	F	70	VAL	2.0
1	G	275	HIS	2.0
1	A	193	ILE	2.0
1	H	516	ARG	2.0
1	G	57	THR	2.0
1	B	209	VAL	2.0
1	E	197	VAL	2.0
1	E	151	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	H	601	4/4	0.72	0.39	61,73,86,86	0
2	EDO	H	603	4/4	0.73	0.21	65,78,84,87	0
2	EDO	E	607	4/4	0.76	0.24	46,68,82,93	0
2	EDO	F	601	4/4	0.76	0.20	58,74,88,89	0
2	EDO	C	606	4/4	0.77	0.21	51,62,64,69	0
2	EDO	A	603	4/4	0.77	0.26	62,74,82,82	0
2	EDO	G	602	4/4	0.80	0.22	56,72,86,86	0
2	EDO	E	604	4/4	0.80	0.55	54,65,73,77	0
2	EDO	B	603	4/4	0.81	0.40	43,56,73,73	0
2	EDO	B	604	4/4	0.82	0.29	45,63,72,76	0
2	EDO	A	602	4/4	0.83	0.16	65,78,89,89	0
2	EDO	D	602	4/4	0.85	0.17	54,65,74,78	0
2	EDO	A	608	4/4	0.85	0.28	36,45,54,54	0
2	EDO	A	610	4/4	0.85	0.15	56,68,83,83	0
2	EDO	A	604	4/4	0.86	0.28	44,55,65,79	0
2	EDO	F	602	4/4	0.86	0.25	67,80,89,91	0
2	EDO	C	602	4/4	0.86	0.42	41,57,70,81	0
2	EDO	D	603	4/4	0.87	0.20	49,59,70,71	0
2	EDO	B	607	4/4	0.87	0.19	62,74,90,90	0
2	EDO	D	601	4/4	0.87	0.35	57,73,87,87	0
2	EDO	A	601	4/4	0.88	0.27	46,56,58,58	0
2	EDO	A	609	4/4	0.88	0.24	49,59,70,72	0
2	EDO	A	605	4/4	0.89	0.39	35,56,65,71	0
2	EDO	A	607	4/4	0.89	0.28	41,56,59,71	0
2	EDO	H	602	4/4	0.90	0.31	45,59,71,72	0
2	EDO	D	604	4/4	0.90	0.28	61,74,76,85	0
2	EDO	C	603	4/4	0.90	0.26	45,55,66,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	B	601	4/4	0.91	0.23	43,54,58,65	0
2	EDO	B	605	4/4	0.91	0.24	49,59,60,63	0
2	EDO	B	602	4/4	0.92	0.13	50,60,69,82	0
2	EDO	C	601	4/4	0.93	0.19	41,49,53,58	0
2	EDO	C	604	4/4	0.94	0.11	52,63,73,73	0
2	EDO	E	606	4/4	0.94	0.13	54,65,74,89	0
2	EDO	G	601	4/4	0.94	0.17	49,59,74,74	0
2	EDO	E	605	4/4	0.94	0.22	50,64,68,82	0
2	EDO	E	602	4/4	0.94	0.24	40,55,66,66	0
2	EDO	A	606	4/4	0.95	0.13	42,50,60,60	0
2	EDO	E	601	4/4	0.95	0.22	44,53,65,69	0
2	EDO	E	603	4/4	0.96	0.17	42,51,67,80	0
2	EDO	B	606	4/4	0.96	0.27	47,58,64,70	0
2	EDO	C	605	4/4	0.96	0.20	43,58,69,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.