



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:58 PM UTC

PDB ID : 6NN8 / pdb_00006nn8
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

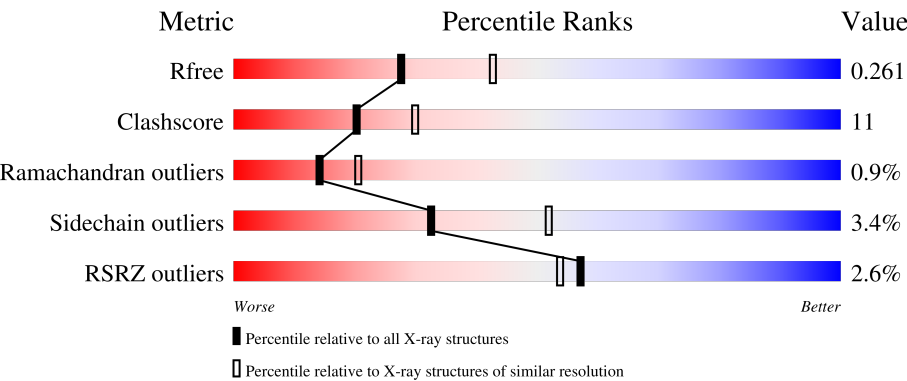
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	543	3% 76% 16% 7%
1	B	543	% 75% 20% 5%
1	C	543	% 76% 16% 8%
1	D	543	2% 58% 18% 22%
1	E	543	2% 74% 19% 6%

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Mol	Chain	Length	Quality of chain
1	F	543	
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:

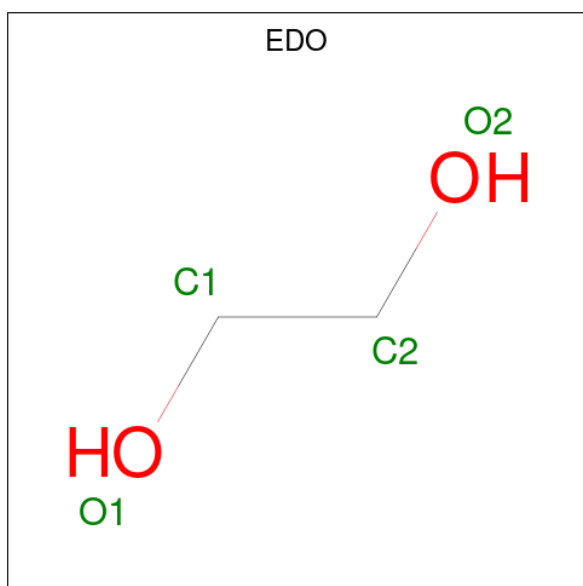
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P30613
A	2	GLU	-	expression tag	UNP P30613
A	531	GLU	SER	engineered mutation	UNP P30613
B	1	MET	-	expression tag	UNP P30613
B	2	GLU	-	expression tag	UNP P30613
B	531	GLU	SER	engineered mutation	UNP P30613
C	1	MET	-	expression 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 (CCD ID: 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	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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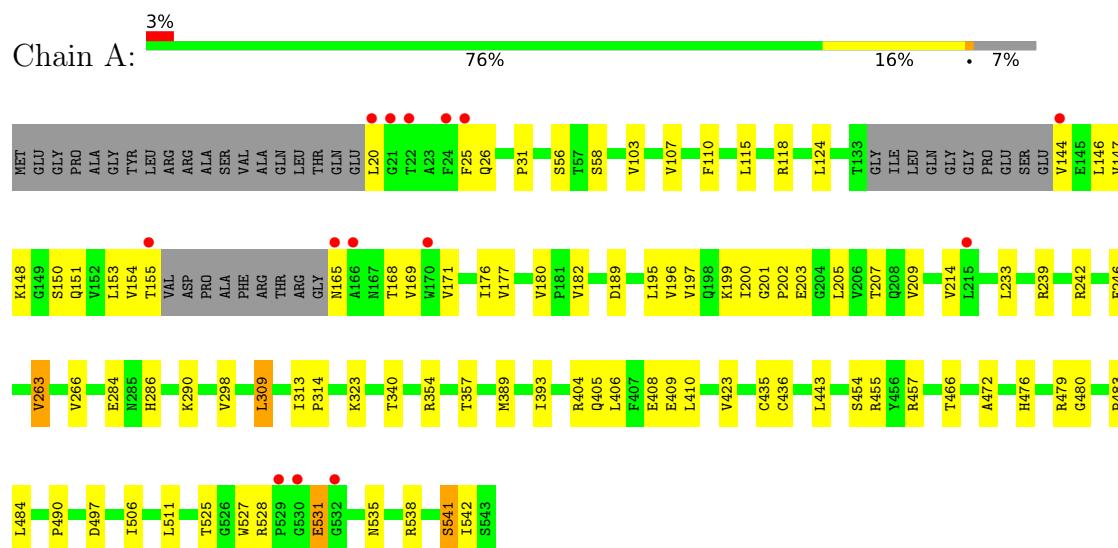
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	6	Total 6	O 6	0	0
3	G	10	Total 10	O 10	0	0
3	H	1	Total 1	O 1	0	0

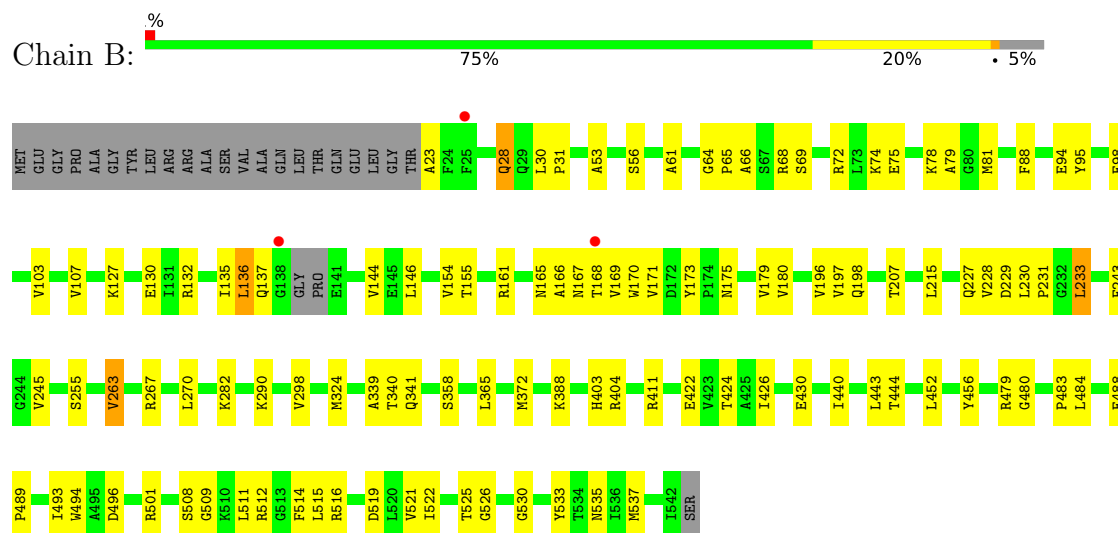
3 Residue-property plots [i](#)

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

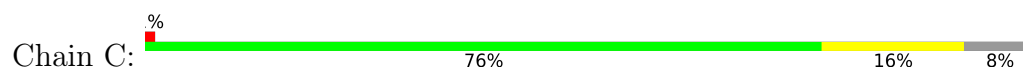
• Molecule 1: Pyruvate kinase PKLR

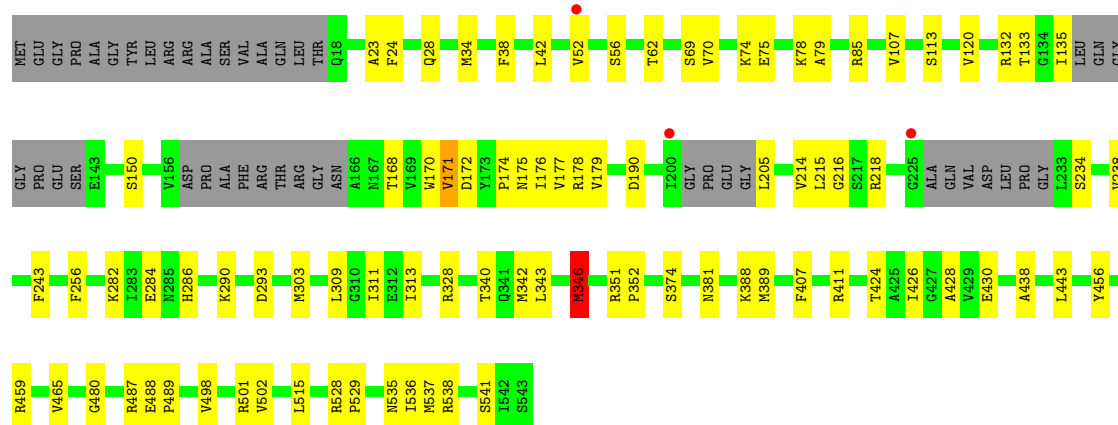


• Molecule 1: Pyruvate kinase PKLR

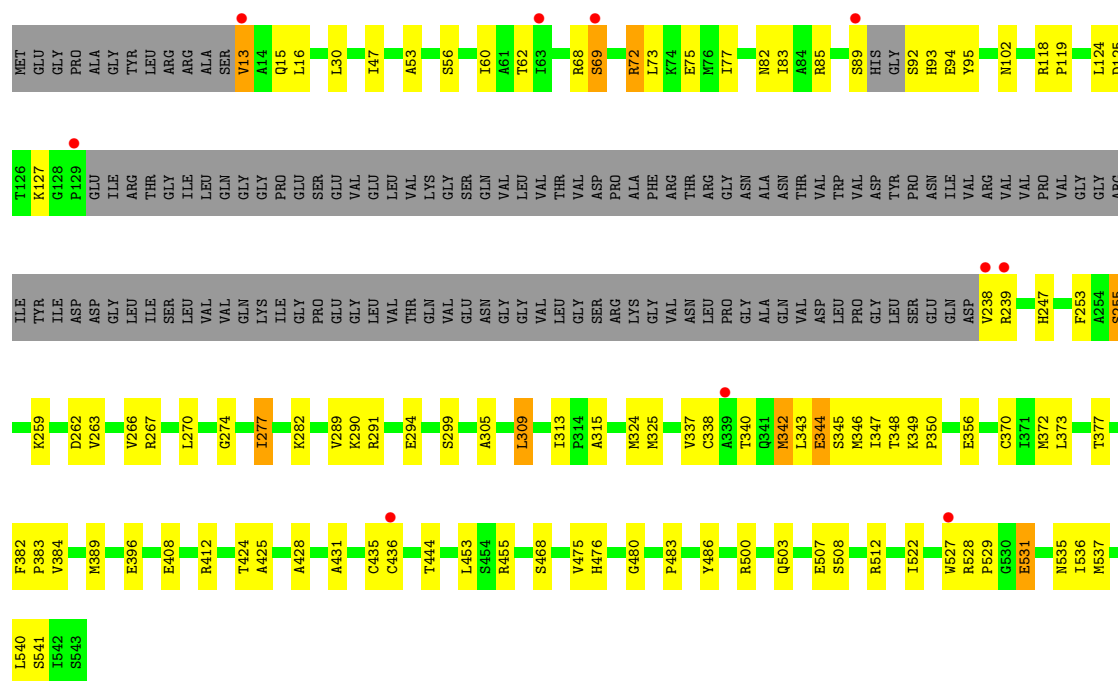


• Molecule 1: Pyruvate kinase PKLR

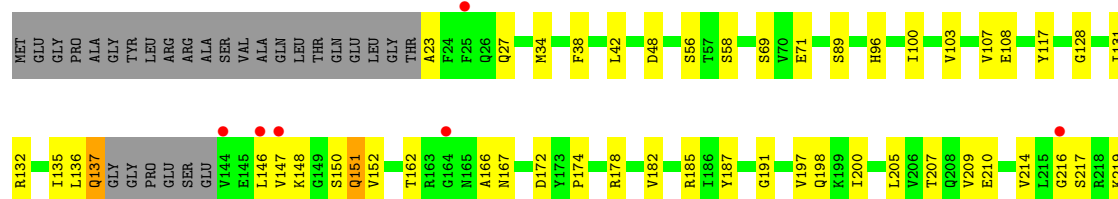
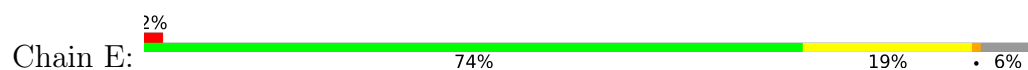


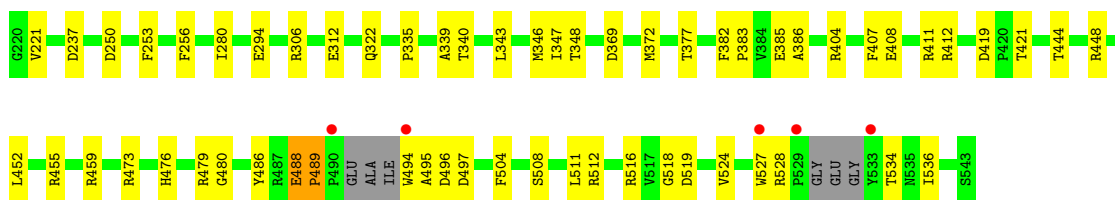


• Molecule 1: Pyruvate kinase PKLR

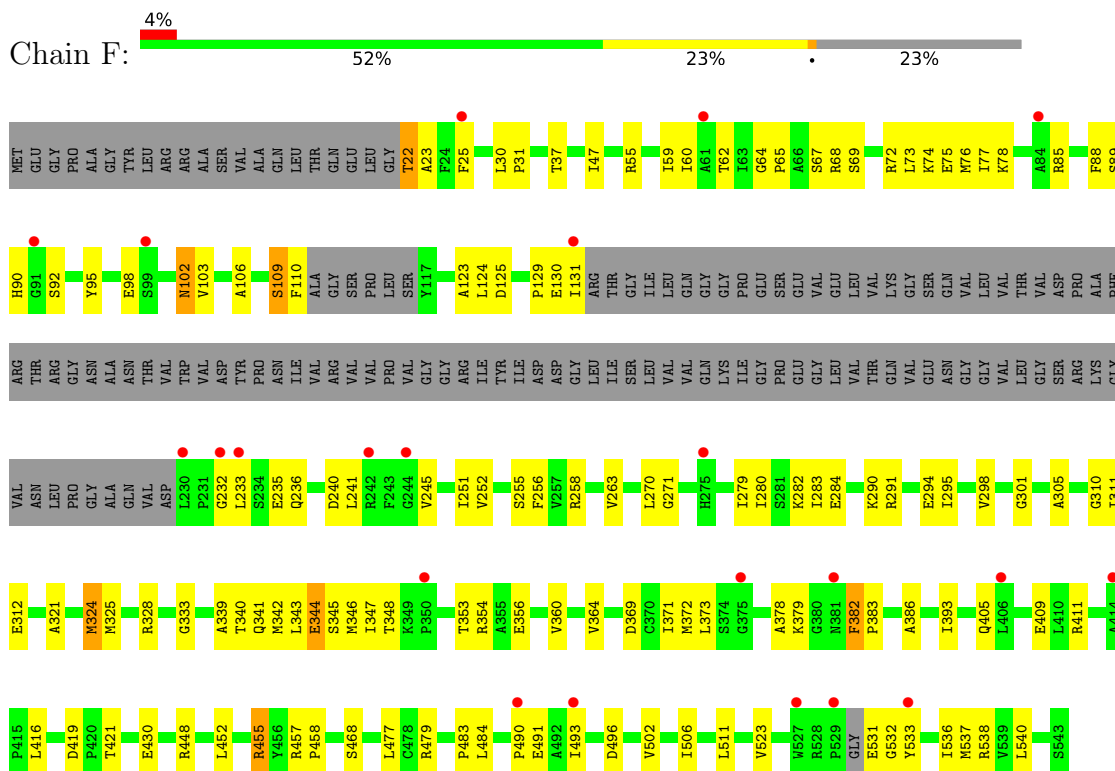


• Molecule 1: Pyruvate kinase PKLR

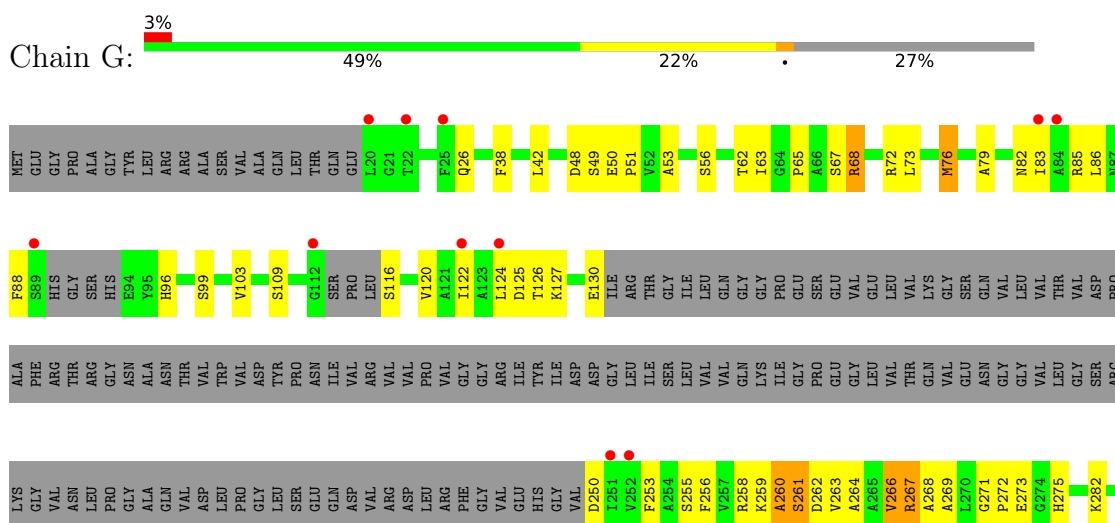


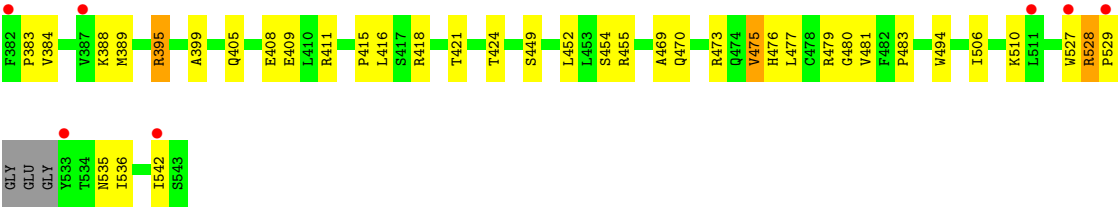


- Molecule 1: Pyruvate kinase PKLR

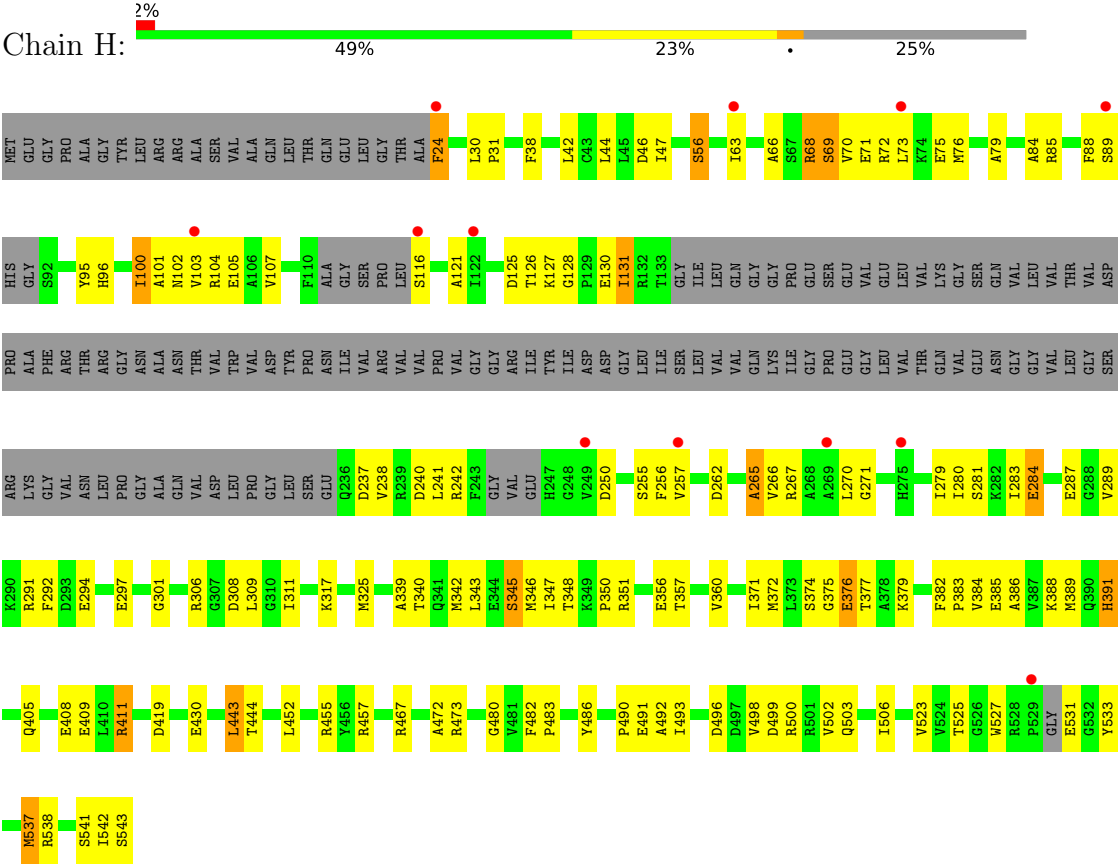


- Molecule 1: Pyruvate kinase PKLR





● 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 0.209 , 0.261	Depositor DCC
R_{free} test set	2008 reflections (1.14%)	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)	0.37 , 38.9	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	0.70	0/3890	0.83	2/5269 (0.0%)
1	B	0.64	0/3995	0.78	0/5413
1	C	0.64	2/3852 (0.1%)	0.79	0/5212
1	D	0.60	0/3263	0.74	0/4412
1	E	0.62	0/3933	0.82	4/5326 (0.1%)
1	F	0.54	0/3241	0.71	0/4380
1	G	0.54	0/3055	0.72	0/4127
1	H	0.55	0/3173	0.73	0/4283
All	All	0.61	2/28402 (0.0%)	0.77	6/38422 (0.0%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	346	MET	SD-CE	-5.82	1.65	1.79
1	C	374	SER	C-O	5.39	1.30	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	150	SER	CA-C-N	6.27	133.51	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	150	SER	C-N-CA	6.27	133.51	121.54
1	A	150	SER	CA-C-N	6.21	133.40	121.54
1	A	150	SER	C-N-CA	6.21	133.40	121.54
1	E	151	GLN	N-CA-C	5.75	123.05	110.80
1	E	479	ARG	NE-CZ-NH1	-5.71	115.79	121.50

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

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	78	0
1	B	3931	4006	4005	71	0
1	C	3795	3880	3876	60	0
1	D	3209	3259	3270	80	0
1	E	3871	3957	3954	79	0
1	F	3190	3239	3239	97	0
1	G	3010	3076	3072	104	0
1	H	3126	3184	3179	107	0
2	A	40	60	60	12	0
2	B	28	42	42	7	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	641	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 11.

All (641) 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:343:LEU:HD13	1:E:346:MET:HE2	1.44	1.00
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:F:346:MET:HE1	1:F:386:ALA:HA	1.53	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:G:260:ALA:O	1:G:263:VAL:HG22	1.70	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
1:E:135:ILE:HD12	1:E:217:SER:HB2	1.60	0.82
1:C:537:MET:HE3	1:F:537:MET:HE3	1.61	0.81
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:F:342:MET:HE1	1:F:371:ILE:HG22	1.63	0.78
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:346:MET:CE	1:E:386:ALA:HA	2.21	0.71
1:F:67:SER:O	1:F:73:LEU:HD21	1.90	0.70
1:F:353:THR:HG23	1:F:356:GLU:OE1	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: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
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: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:343:LEU:HD13	1:E:346:MET:CE	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:527:TRP:O	1:E:528:ARG:HG2	1.99	0.63
1:D:69:SER:HB2	1:D:72:ARG:H	1.64	0.62
1:D:347:ILE:HG22	1:D:348:THR:HG23	1.79	0.62
1:E:346:MET:HE3	1:E:386:ALA:HA	1.80	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:G:67:SER:OG	1:G:377:THR:O	2.17	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:B:324:MET:HE2	2:B:606:EDO:C1	2.30	0.62
1:A:118:ARG:H	2:A:604:EDO:C1	2.12	0.61
1:A:144:VAL:HG12	1:A:144:VAL:O	1.99	0.61
1:B:324:MET:HE2	2:B:606:EDO:H12	1.81	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:D:389:MET:HA	1:D:389:MET:HE2	1.83	0.61
1:C:426:ILE:HD12	1:C:456:TYR:CE1	2.35	0.61
1:H:342:MET:HE1	1:H:371:ILE:CG2	2.31	0.61
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.82	0.60
1:G:475:VAL:HG22	1:G:481:VAL:HG11	1.83	0.60
1:G:528:ARG:HG3	1:G:529:PRO:N	2.16	0.60
1:D:238:VAL:HB	1:D:239:ARG:NH1	2.17	0.60
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:346:MET:CE	1:F:386:ALA:HA	2.31	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:339:ALA:HB1	1:E:372:MET:HE2	1.86	0.57
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:E:136:LEU:HD11	1:E:216:GLY:C	2.30	0.57
1:H:339:ALA:HB1	1:H:372:MET:HE2	1.87	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:HG2	1:B:267:ARG:HH11	1.70	0.55
1:G:353:THR:HG23	1:G:356:GLU:CD	2.30	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:H:283:ILE:HB	1:H:325:MET:HE1	1.87	0.55
1:H:346:MET:HE1	1:H:385:GLU:C	2.31	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:28:GLN:HB3	2:B:604:EDO:H11	1.88	0.55
1:B:231:PRO:HB2	1:B:233:LEU:O	2.06	0.55
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:H:342:MET:HE2	1:H:360:VAL:HG22	1.89	0.54
1:G:63:ILE:HD12	1:G:63:ILE:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:283:ILE:HG13	1:H:325:MET:HE1	1.90	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:256:PHE:N	1:H:284:GLU:OE1	2.38	0.54
1:H:257:VAL:HG21	1:H:281:SER:HB3	1.89	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:F:339:ALA:HB1	1:F:372:MET:HE2	1.90	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:24:PHE:N	1:H:24:PHE:CD2	2.75	0.53
1:H:128:GLY:HA2	1:H:237:ASP:OD2	2.08	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:72:ARG:O	1:D:75:GLU:N	2.42	0.53
1:D:125:ASP:HA	1:D:253:PHE:HB2	1.90	0.53
1:H:292:PHE:CE2	1:H:325:MET:HE3	2.43	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:260:ALA:O	1:G:261:SER:C	2.51	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: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:E:346:MET:HE1	1:E:386:ALA:HA	1.91	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: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:47:ILE:CD1	1:H:289:VAL:HG11	2.40	0.52
1:D:82:ASN:HB3	1:D:476:HIS:ND1	2.25	0.52
1:D:527:TRP:O	1:D:528:ARG:HD3	2.09	0.52
1:E:103:VAL:O	1:E:107:VAL:HG23	2.10	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:88:PHE:CD2	1:F:240:ASP:HB3	2.45	0.51
1:F:364:VAL:O	1:F:479:ARG:NH1	2.43	0.51
1:H:292:PHE:CD2	1:H:325:MET:HE3	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:HE2	1:A:290:LYS:HA	1.91	0.51
1:D:527:TRP:CD2	1:D:528:ARG:HG2	2.46	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: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
1:G:528:ARG:HG3	1:G:529:PRO:CD	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:VAL:HG21	1:B:227:GLN:O	2.11	0.51
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:79:ALA:HB2	1:H:384:VAL:HG13	1.92	0.50
1:H:284:GLU:OE2	1:H:308:ASP:OD2	2.29	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:G:260:ALA:C	1:G:263:VAL:HG22	2.34	0.50
1:C:132:ARG:O	1:C:171:VAL:HA	2.11	0.50
1:D:47:ILE:O	1:H:317:LYS:NZ	2.34	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: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:37:THR:HB	1:G:409:GLU:CD	2.37	0.50
1:F:321:ALA:O	1:F:325:MET:HG3	2.11	0.50
1:A:203:GLU:O	1:A:203:GLU:HG2	2.11	0.49
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:G:303:MET:HE3	1:G:372:MET:HE1	1.92	0.49
1:H:346:MET:HE1	1:H:386:ALA:N	2.27	0.49
1:D:350:PRO:HB3	1:D:382:PHE:CE1	2.47	0.49
1:F:55:ARG:CZ	1:F:59:ILE:HD12	2.41	0.49
1:F:340:THR:HG22	1:F:341:GLN:HG3	1.94	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:475:VAL:CG2	1:G:481:VAL:HG11	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:LEU:HD12	1:C:216:GLY:H	1.77	0.49
1:E:250:ASP:OD1	1:E:473:ARG:NE	2.39	0.49
1:G:506:ILE:HG23	1:G:542:ILE:HD12	1.95	0.49
1:B:180:VAL:HG23	1:B:180:VAL:O	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:D:118:ARG:O	1:D:119:PRO:C	2.56	0.49
1:E:34:MET:HA	1:E:34:MET:HE3	1.95	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:A:423:VAL:HG12	1:D:431:ALA:HB1	1.94	0.49
1:D:377:THR:HA	1:D:383:PRO:HB3	1.95	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:CB	1:F:455:ARG:HH21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:LEU:HD22	1:B:521:VAL:HG11	1.96	0.47
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: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:G:304:VAL:HG22	1:G:325:MET:HE3	1.96	0.47
1:F:65:PRO:HD2	1:F:379:LYS:HG2	1.97	0.47
1:F:74:LYS:HE2	1:F:109:SER:OG	2.13	0.47
1:H:66:ALA:O	1:H:72:ARG:HD2	2.14	0.47
1:C:79:ALA:HB1	1:C:388:LYS:HG3	1.97	0.47
1:C:133:THR:O	1:C:218:ARG:HA	2.14	0.47
1:F:98:GLU:O	1:F:102:ASN:OD1	2.32	0.47
1:C:411:ARG:HH21	1:F:411:ARG:HH22	1.61	0.47
1:F:129:PRO:HG2	1:F:232:GLY:O	2.15	0.47
1:F:344:GLU:HG2	1:F:347:ILE:HD12	1.97	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:G:26:GLN:O	1:G:49:SER:OG	2.31	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
1:G:65:PRO:HA	1:G:68:ARG:HD3	1.97	0.46
2:G:601:EDO:C1	3:G:704:HOH:O	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:92:SER:H	1:F:95:TYR:HB3	1.81	0.46
1:F:279:ILE:C	1:F:280:ILE:HD13	2.41	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:A:124:LEU:C	1:A:124:LEU:HD23	2.41	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: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:26:GLN:HG3	1:A:26:GLN:O	2.15	0.45
1:A:146:LEU:HD23	1:A:214:VAL:CA	2.44	0.45
1:E:486:TYR:HD1	1:E:504:PHE:CD2	2.34	0.45
1:F:64:GLY:C	1:F:378:ALA:O	2.59	0.45
1:F:280:ILE:HD12	1:F:301:GLY:HA3	1.97	0.45
1:F:284:GLU:HG2	1:F:305:ALA:HB3	1.97	0.45
1:G:116:SER:O	1:G:116:SER:OG	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:435:CYS:O	1:A:436:CYS:C	2.59	0.45
1:A:506:ILE:HG23	1:A:542:ILE:HD12	1.98	0.45
1:D:324:MET:SD	1:D:324:MET:C	2.99	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:H:283:ILE:CB	1:H:325:MET:HE1	2.47	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:E:494:TRP:C	1:E:496:ASP:N	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:HD12	1:A:20:LEU:N	2.32	0.45
1:B:64:GLY:O	1:B:65:PRO:C	2.59	0.45
1:D:73:LEU:O	1:D:77:ILE:HG13	2.16	0.45
1:E:185:ARG:NH1	1:E:210:GLU:CD	2.74	0.45
1:G:63:ILE:HD11	1:G:86:LEU:HD22	1.97	0.45
1:G:424:THR:OG1	1:G:535:ASN:HA	2.16	0.45
1:H:96:HIS:O	1:H:100:ILE:HG13	2.17	0.45
1:A:284:GLU:C	1:A:309:LEU:HD13	2.41	0.45
1:E:132:ARG:HA	1:E:219:LYS:O	2.16	0.45
1:E:182:VAL:O	1:E:197:VAL:O	2.35	0.45
1:H:343:LEU:O	1:H:376:GLU:HG2	2.16	0.45
1:A:115:LEU:HD12	1:A:511:LEU:HD13	1.99	0.45
1:B:430:GLU:OE1	1:H:411:ARG:HD2	2.17	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:H:346:MET:HE2	1:H:346:MET:HB3	1.91	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:HH21	1:F:455:ARG:CG	2.30	0.45
1:G:347:ILE:CD1	1:G:375:GLY:C	2.90	0.45
1:H:79:ALA:HB2	1:H:384:VAL:CG1	2.47	0.45
1:H:350:PRO:HG2	1:H:351:ARG:HG3	1.97	0.45
1:A:58:SER:CB	2:A:601:EDO:O2	2.62	0.44
1:C:428:ALA:HA	1:C:537:MET:HE2	1.99	0.44
1:D:53:ALA:HB2	2:D:603:EDO:H22	1.98	0.44
1:D:267:ARG:HA	1:D:270:LEU:CD1	2.48	0.44
1:F:252:VAL:HG21	1:F:270:LEU:HD11	1.99	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:F:324:MET:HE3	1:F:328:ARG:HG3	1.98	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:G:527:TRP:H	1:G:527:TRP:CD1	2.34	0.44
1:H:379:LYS:O	1:H:379:LYS:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:452:LEU:O	1:H:455:ARG:HG2	2.17	0.44
1:D:338:CYS:O	1:D:342:MET:HE2	2.17	0.44
1:B:72:ARG:O	1:B:75:GLU:N	2.50	0.44
1:F:25:PHE:O	1:F:25:PHE:CG	2.69	0.44
1:B:180:VAL:CG2	1:B:197:VAL:HG21	2.48	0.44
1:F:324:MET:HE2	1:F:325:MET:HA	2.00	0.44
1:G:88:PHE:CE1	1:G:96:HIS:ND1	2.86	0.44
1:G:346:MET:HA	1:G:349:LYS:O	2.17	0.44
1:D:349:LYS:C	1:D:382:PHE:CE2	2.95	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:243:PHE:CD1	1:B:243:PHE:C	2.96	0.44
1:B:501:ARG:NH1	2:B:605:EDO:O2	2.49	0.44
1:C:343:LEU:HD13	1:C:346:MET:HE3	1.99	0.44
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:G:303:MET:HE2	1:G:339:ALA:HB2	1.99	0.43
1:H:375:GLY:C	1:H:377:THR:N	2.75	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:F:124:LEU:C	1:F:124:LEU:HD23	2.42	0.43
1:F:324:MET:HE3	1:F:328:ARG:NE	2.33	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: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:G:268:ALA:O	1:G:269:ALA:C	2.61	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:HD12	1:D:270:LEU:H	1.83	0.43
1:D:528:ARG:HB3	1:D:529:PRO:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:408:GLU:OE1	1:G:408:GLU:OE2	2.35	0.43
1:F:62:THR:CG2	1:F:85:ARG:HD3	2.48	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:A:354:ARG:HG2	1:B:341:GLN:OE1	2.19	0.43
1:B:154:VAL:HA	1:B:169:VAL:O	2.17	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:56:SER:HB2	1:A:480:GLY:CA	2.48	0.43
1:A:490:PRO:HA	1:A:497:ASP:OD1	2.18	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:D:93:HIS:O	1:D:94:GLU:C	2.60	0.43
1:E:128:GLY:HA2	1:E:237:ASP:OD2	2.18	0.43
1:F:342:MET:CE	1:F:371:ILE:HG22	2.40	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:346:MET:HE3	1:G:350:PRO:O	2.19	0.43
1:G:527:TRP:HB3	1:G:536:ILE:HD11	2.01	0.43
1:H:68:ARG:HH21	1:H:95:TYR:C	2.26	0.43
1:H:72:ARG:O	1:H:75:GLU:N	2.52	0.43
1:A:201:GLY:O	1:A:202:PRO:C	2.60	0.43
1:B:339:ALA:HB1	1:B:372:MET:HE2	2.01	0.43
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:F:343:LEU:HD13	1:F:346:MET:HE2	2.01	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:F:77:ILE:O	1:F:78:LYS:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:403:HIS:O	1:B:404:ARG:C	2.62	0.42
1:D:125:ASP:OD2	1:D:282:LYS:HE3	2.19	0.42
1:E:343:LEU:CD1	1:E:346:MET:HE2	2.31	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:G:124:LEU:C	1:G:124:LEU:HD23	2.45	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:H:342:MET:HE1	1:H:371:ILE:HG22	2.00	0.42
1:C:243:PHE:CD1	1:C:243:PHE:C	2.97	0.42
1:C:282:LYS:HG2	1:C:303:MET:HB3	2.02	0.42
1:C:536:ILE:HG12	1:F:538:ARG:HG2	2.02	0.42
1:E:377:THR:HA	1:E:383:PRO:HB3	2.02	0.42
1:H:44:LEU:HD23	1:H:44:LEU:HA	1.86	0.42
1:H:85:ARG:NE	1:H:125:ASP:OD2	2.48	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
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:185:ARG:HH12	1:E:210:GLU:CD	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:423:VAL:CG1	1:D:431:ALA:HB1	2.50	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:H:30:LEU:N	1:H:31:PRO:CD	2.83	0.41
1:B:514:PHE:CD1	1:B:514:PHE:N	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:419:ASP:OD1	1:H:419:ASP:C	2.63	0.41
1:H:430:GLU:OE2	1:H:430:GLU:HA	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:74:LYS:O	1:B:78:LYS:HG3	2.19	0.41
1:B:509:GLY:HA3	1:B:515:LEU:HD12	2.02	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:391:HIS:ND1	1:H:391:HIS:C	2.77	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:E:494:TRP:C	1:E:496:ASP:H	2.29	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:C:488:GLU:HB3	1:C:489:PRO:HD2	2.03	0.41
1:D:289:VAL:HG22	1:D:325:MET:HE2	2.02	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:199:LYS:O	1:A:205:LEU:HA	2.21	0.41
1:A:389:MET:SD	1:A:393:ILE:HD11	2.61	0.41
1:A:404:ARG:NE	1:D:412:ARG:HD2	2.35	0.41
1:A:527:TRP:CE3	1:A:528:ARG:HB3	2.56	0.41
1:C:172:ASP:O	1:C:174:PRO:CD	2.69	0.41
1:D:30:LEU:HD23	1:D:30:LEU:HA	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:G:51:PRO:HB2	2:G:601:EDO:C2	2.51	0.41
1:G:415:PRO:O	1:G:416:LEU:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:70:VAL:CG2	1:H:102:ASN:CG	2.94	0.41
1:H:250:ASP:CG	1:H:473:ARG:HE	2.27	0.41
1:H:291:ARG:NE	1:H:294:GLU:OE1	2.41	0.41
1:A:103:VAL:O	1:A:107:VAL:HG23	2.20	0.41
1:C:34:MET:HE2	1:C:34:MET:HB2	1.89	0.41
1:C:343:LEU:HD13	1:C:346:MET:CE	2.50	0.41
1:D:85:ARG:HH21	1:D:125:ASP:CG	2.29	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:69:SER:C	1:H:71:GLU:N	2.78	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:F:324:MET:HE3	1:F:328:ARG:CD	2.52	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: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: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:62:THR:HA	1:G:85:ARG:HB3	2.02	0.40
1:G:120:VAL:O	1:G:473:ARG:HD2	2.22	0.40
1:G:291:ARG:O	1:G:294:GLU:HG2	2.20	0.40
1:H:70:VAL:HG23	1:H:102:ASN:ND2	2.37	0.40
1:H:308:ASP:OD2	2:H:601:EDO:H22	2.21	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:C:23:ALA:O	1:C:24:PHE:C	2.65	0.40
1:D:455:ARG:O	1:D:455:ARG:HG3	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%)	21	30
1	B	514/543 (95%)	495 (96%)	14 (3%)	5 (1%)	12	18
1	C	489/543 (90%)	471 (96%)	17 (4%)	1 (0%)	43	57
1	D	416/543 (77%)	405 (97%)	10 (2%)	1 (0%)	43	57
1	E	501/543 (92%)	481 (96%)	13 (3%)	7 (1%)	9	12
1	F	409/543 (75%)	378 (92%)	26 (6%)	5 (1%)	10	15
1	G	385/543 (71%)	355 (92%)	27 (7%)	3 (1%)	16	23
1	H	395/543 (73%)	366 (93%)	22 (6%)	7 (2%)	6	8
All	All	3608/4344 (83%)	3435 (95%)	141 (4%)	32 (1%)	14	20

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
1	H	345	SER
1	A	340	THR
1	B	161	ARG

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Mol	Chain	Res	Type
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%)	399 (98%)	6 (2%)	57	75
1	B	415/433 (96%)	406 (98%)	9 (2%)	45	66
1	C	402/433 (93%)	392 (98%)	10 (2%)	42	62
1	D	336/433 (78%)	318 (95%)	18 (5%)	20	33
1	E	410/433 (95%)	402 (98%)	8 (2%)	48	68
1	F	334/433 (77%)	320 (96%)	14 (4%)	26	43
1	G	314/433 (72%)	296 (94%)	18 (6%)	18	31
1	H	328/433 (76%)	309 (94%)	19 (6%)	18	30
All	All	2944/3464 (85%)	2842 (96%)	102 (4%)	32	51

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	LEU
1	A	263	VAL
1	A	309	LEU
1	A	408	GLU
1	A	531	GLU
1	A	541	SER
1	B	69	SER
1	B	94	GLU
1	B	136	LEU
1	B	198	GLN
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	135	ILE
1	C	150	SER
1	C	168	THR
1	C	171	VAL
1	C	214	VAL
1	C	346	MET
1	C	487	ARG
1	C	541	SER
1	D	13	VAL
1	D	69	SER
1	D	72	ARG
1	D	124	LEU
1	D	247	HIS
1	D	255	SER
1	D	259	LYS
1	D	263	VAL
1	D	277	ILE
1	D	299	SER
1	D	309	LEU
1	D	342	MET
1	D	344	GLU
1	D	345	SER
1	D	436[A]	CYS
1	D	436[B]	CYS
1	D	468	SER
1	D	531	GLU

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Mol	Chain	Res	Type
1	E	69	SER
1	E	71	GLU
1	E	89	SER
1	E	137	GLN
1	E	178	ARG
1	E	404	ARG
1	E	444	THR
1	E	511	LEU
1	F	22	THR
1	F	69	SER
1	F	102	ASN
1	F	103	VAL
1	F	109	SER
1	F	235	GLU
1	F	311	ILE
1	F	324	MET
1	F	344	GLU
1	F	348	THR
1	F	455	ARG
1	F	468	SER
1	F	491	GLU
1	F	511	LEU
1	G	68	ARG
1	G	76	MET
1	G	83	ILE
1	G	99	SER
1	G	109	SER
1	G	130	GLU
1	G	266	VAL
1	G	267	ARG
1	G	273	GLU
1	G	316	GLU
1	G	370	CYS
1	G	374	SER
1	G	389	MET
1	G	395	ARG
1	G	449	SER
1	G	470	GLN
1	G	475	VAL
1	G	528	ARG
1	H	24	PHE
1	H	56	SER

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Mol	Chain	Res	Type
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	255	SER
1	H	284	GLU
1	H	345	SER
1	H	389	MET
1	H	391	HIS
1	H	411	ARG
1	H	443	LEU
1	H	537	MET
1	H	541	SER
1	H	543	SER

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

Mol	Chain	Res	Type
1	A	90	HIS
1	A	405	GLN
1	B	28	GLN
1	B	208	GLN
1	B	222	ASN
1	B	403	HIS
1	B	405	GLN
1	C	405	GLN
1	C	470	GLN
1	D	28	GLN
1	D	405	GLN
1	E	28	GLN
1	E	247	HIS
1	E	403	HIS
1	E	405	GLN
1	F	27	GLN
1	F	28	GLN
1	F	405	GLN
1	G	405	GLN
1	G	451	GLN
1	H	93	HIS

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Mol	Chain	Res	Type
1	H	403	HIS
1	H	405	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	F	601	-	3,3,3	0.48	0	2,2,2	0.19	0
2	EDO	A	608	-	3,3,3	0.90	0	2,2,2	0.55	0
2	EDO	A	605	-	3,3,3	0.75	0	2,2,2	0.46	0
2	EDO	C	601	-	3,3,3	0.75	0	2,2,2	0.45	0
2	EDO	E	601	-	3,3,3	0.59	0	2,2,2	1.06	0
2	EDO	E	602	-	3,3,3	0.62	0	2,2,2	0.38	0
2	EDO	D	601	-	3,3,3	0.46	0	2,2,2	0.04	0
2	EDO	A	607	-	3,3,3	0.52	0	2,2,2	0.08	0
2	EDO	F	602	-	3,3,3	0.44	0	2,2,2	0.24	0
2	EDO	A	604	-	3,3,3	0.43	0	2,2,2	0.24	0
2	EDO	A	601	-	3,3,3	0.57	0	2,2,2	1.53	1 (50%)
2	EDO	C	603	-	3,3,3	0.32	0	2,2,2	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	606	-	3,3,3	0.38	0	2,2,2	0.43	0
2	EDO	B	605	-	3,3,3	0.47	0	2,2,2	0.26	0
2	EDO	E	606	-	3,3,3	0.41	0	2,2,2	0.72	0
2	EDO	G	601	-	3,3,3	0.41	0	2,2,2	0.62	0
2	EDO	E	603	-	3,3,3	0.55	0	2,2,2	0.40	0
2	EDO	H	601	-	3,3,3	0.62	0	2,2,2	0.48	0
2	EDO	H	602	-	3,3,3	0.43	0	2,2,2	0.57	0
2	EDO	D	603	-	3,3,3	0.41	0	2,2,2	0.40	0
2	EDO	C	604	-	3,3,3	0.40	0	2,2,2	0.77	0
2	EDO	B	602	-	3,3,3	0.39	0	2,2,2	0.52	0
2	EDO	E	604	-	3,3,3	0.56	0	2,2,2	0.80	0
2	EDO	B	601	-	3,3,3	0.53	0	2,2,2	0.37	0
2	EDO	C	606	-	3,3,3	0.51	0	2,2,2	0.09	0
2	EDO	E	607	-	3,3,3	0.51	0	2,2,2	0.66	0
2	EDO	D	602	-	3,3,3	0.53	0	2,2,2	0.50	0
2	EDO	D	604	-	3,3,3	0.40	0	2,2,2	0.38	0
2	EDO	C	602	-	3,3,3	0.67	0	2,2,2	0.26	0
2	EDO	A	606	-	3,3,3	0.47	0	2,2,2	0.12	0
2	EDO	C	605	-	3,3,3	0.41	0	2,2,2	0.43	0
2	EDO	A	602	-	3,3,3	0.41	0	2,2,2	0.42	0
2	EDO	H	603	-	3,3,3	0.41	0	2,2,2	0.54	0
2	EDO	B	603	-	3,3,3	0.99	0	2,2,2	1.00	0
2	EDO	A	609	-	3,3,3	0.43	0	2,2,2	0.56	0
2	EDO	E	605	-	3,3,3	0.41	0	2,2,2	0.09	0
2	EDO	A	610	-	3,3,3	0.44	0	2,2,2	0.40	0
2	EDO	G	602	-	3,3,3	0.47	0	2,2,2	0.17	0
2	EDO	B	607	-	3,3,3	0.41	0	2,2,2	0.66	0
2	EDO	A	603	-	3,3,3	0.49	0	2,2,2	0.07	0
2	EDO	B	604	-	3,3,3	0.58	0	2,2,2	1.16	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	F	601	-	-	1/1/1/1	-
2	EDO	A	608	-	-	1/1/1/1	-
2	EDO	A	605	-	-	1/1/1/1	-
2	EDO	C	601	-	-	0/1/1/1	-
2	EDO	E	601	-	-	1/1/1/1	-
2	EDO	E	602	-	-	1/1/1/1	-
2	EDO	D	601	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	607	-	-	1/1/1/1	-
2	EDO	F	602	-	-	1/1/1/1	-
2	EDO	A	604	-	-	1/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
2	EDO	C	603	-	-	1/1/1/1	-
2	EDO	B	606	-	-	1/1/1/1	-
2	EDO	B	605	-	-	0/1/1/1	-
2	EDO	E	606	-	-	0/1/1/1	-
2	EDO	G	601	-	-	0/1/1/1	-
2	EDO	E	603	-	-	1/1/1/1	-
2	EDO	H	601	-	-	0/1/1/1	-
2	EDO	H	602	-	-	1/1/1/1	-
2	EDO	D	603	-	-	1/1/1/1	-
2	EDO	C	604	-	-	1/1/1/1	-
2	EDO	B	602	-	-	1/1/1/1	-
2	EDO	E	604	-	-	1/1/1/1	-
2	EDO	B	601	-	-	0/1/1/1	-
2	EDO	C	606	-	-	1/1/1/1	-
2	EDO	E	607	-	-	1/1/1/1	-
2	EDO	D	602	-	-	0/1/1/1	-
2	EDO	D	604	-	-	1/1/1/1	-
2	EDO	C	602	-	-	1/1/1/1	-
2	EDO	A	606	-	-	1/1/1/1	-
2	EDO	C	605	-	-	0/1/1/1	-
2	EDO	A	602	-	-	1/1/1/1	-
2	EDO	H	603	-	-	1/1/1/1	-
2	EDO	B	603	-	-	0/1/1/1	-
2	EDO	A	609	-	-	1/1/1/1	-
2	EDO	E	605	-	-	1/1/1/1	-
2	EDO	A	610	-	-	0/1/1/1	-
2	EDO	G	602	-	-	0/1/1/1	-
2	EDO	B	607	-	-	1/1/1/1	-
2	EDO	A	603	-	-	0/1/1/1	-
2	EDO	B	604	-	-	0/1/1/1	-

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	-2.16	95.90	112.39

There are no chirality outliers.

All (27) torsion outliers are listed below:

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

There are no ring outliers.

17 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	608	EDO	3	0
2	C	601	EDO	2	0
2	E	602	EDO	2	0
2	A	604	EDO	5	0
2	A	601	EDO	3	0
2	B	606	EDO	2	0
2	B	605	EDO	2	0
2	G	601	EDO	9	0
2	E	603	EDO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	601	EDO	1	0
2	H	602	EDO	2	0
2	D	603	EDO	1	0
2	C	606	EDO	1	0
2	E	607	EDO	1	0
2	D	602	EDO	1	0
2	A	609	EDO	1	0
2	B	604	EDO	3	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%)	-0.25	14 (2%) 55 51	29, 44, 81, 97	0
1	B	518/543 (95%)	-0.17	3 (0%) 85 84	28, 50, 82, 98	0
1	C	499/543 (91%)	-0.19	3 (0%) 85 84	31, 49, 79, 99	0
1	D	421/543 (77%)	0.27	10 (2%) 59 56	31, 64, 90, 101	1 (0%)
1	E	509/543 (93%)	-0.07	11 (2%) 62 59	28, 53, 84, 102	0
1	F	417/543 (76%)	0.44	22 (5%) 32 28	42, 69, 93, 103	0
1	G	395/543 (72%)	0.45	19 (4%) 35 32	42, 69, 94, 106	0
1	H	407/543 (74%)	0.51	12 (2%) 53 50	45, 71, 94, 106	0
All	All	3671/4344 (84%)	0.09	94 (2%) 57 54	28, 58, 90, 106	1 (0%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	225	GLY	5.2
1	H	24	PHE	5.0
1	E	146	LEU	4.5
1	D	13	VAL	4.2
1	H	63	ILE	4.0
1	H	529	PRO	3.8
1	A	155	THR	3.7
1	G	112	GLY	3.3
1	F	131	ILE	3.3
1	E	533	TYR	3.2
1	A	530	GLY	3.2
1	G	20	LEU	3.2
1	F	533	TYR	3.2
1	F	99	SER	3.1
1	F	61	ALA	3.1
1	F	527	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	527	TRP	3.1
1	E	25	PHE	3.0
1	D	238	VAL	3.0
1	E	527	TRP	3.0
1	A	144	VAL	2.9
1	B	25	PHE	2.9
1	A	529	PRO	2.9
1	F	230	LEU	2.8
1	C	200	ILE	2.8
1	F	25	PHE	2.8
1	G	122	ILE	2.8
1	E	529	PRO	2.7
1	A	166	ALA	2.7
1	G	533	TYR	2.7
1	B	138	GLY	2.7
1	F	244	GLY	2.6
1	D	239	ARG	2.5
1	F	529	PRO	2.5
1	G	382	PHE	2.5
1	G	387	VAL	2.5
1	D	69	SER	2.5
1	G	542	ILE	2.5
1	G	251	ILE	2.5
1	A	20	LEU	2.5
1	F	242	ARG	2.5
1	D	436[A]	CYS	2.5
1	A	532	GLY	2.5
1	G	511	LEU	2.5
1	E	144	VAL	2.5
1	A	21	GLY	2.4
1	G	529	PRO	2.4
1	E	164	GLY	2.4
1	G	124	LEU	2.4
1	H	103	VAL	2.4
1	E	494	TRP	2.4
1	F	91	GLY	2.4
1	F	406	LEU	2.4
1	H	116	SER	2.3
1	F	493	ILE	2.3
1	H	122	ILE	2.3
1	A	24	PHE	2.3
1	A	25	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	84	ALA	2.3
1	A	22	THR	2.3
1	D	339	ALA	2.3
1	H	249	VAL	2.3
1	H	275	HIS	2.2
1	G	89	SER	2.2
1	H	73	LEU	2.2
1	G	25	PHE	2.2
1	E	490	PRO	2.2
1	G	252	VAL	2.2
1	F	233	LEU	2.2
1	F	414	ALA	2.2
1	A	215	LEU	2.2
1	H	89	SER	2.2
1	D	63	ILE	2.2
1	D	527	TRP	2.2
1	F	232	GLY	2.1
1	F	375	GLY	2.1
1	D	129	PRO	2.1
1	F	275	HIS	2.1
1	F	381	ASN	2.1
1	C	52	VAL	2.1
1	A	170	TRP	2.1
1	H	269	ALA	2.1
1	B	168	THR	2.1
1	D	89	SER	2.1
1	E	147	VAL	2.1
1	F	490	PRO	2.1
1	E	216	GLY	2.0
1	G	83	ILE	2.0
1	F	350	PRO	2.0
1	H	257	VAL	2.0
1	F	84	ALA	2.0
1	A	165	ASN	2.0
1	G	22	THR	2.0
1	G	350	PRO	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	E	604	4/4	0.55	0.36	54,65,73,77	0
2	EDO	H	601	4/4	0.56	0.32	61,73,86,86	0
2	EDO	F	602	4/4	0.61	0.28	67,80,89,91	0
2	EDO	D	601	4/4	0.64	0.29	57,73,87,87	0
2	EDO	A	602	4/4	0.64	0.24	65,78,89,89	0
2	EDO	H	603	4/4	0.66	0.21	65,78,84,87	0
2	EDO	E	607	4/4	0.68	0.21	46,68,82,93	0
2	EDO	B	603	4/4	0.69	0.30	43,56,73,73	0
2	EDO	F	601	4/4	0.71	0.24	58,74,88,89	0
2	EDO	A	605	4/4	0.76	0.27	35,56,65,71	0
2	EDO	C	602	4/4	0.78	0.28	41,57,70,81	0
2	EDO	A	603	4/4	0.79	0.15	62,74,82,82	0
2	EDO	G	602	4/4	0.79	0.25	56,72,86,86	0
2	EDO	C	601	4/4	0.83	0.15	41,49,53,58	0
2	EDO	D	602	4/4	0.85	0.14	54,65,74,78	0
2	EDO	C	606	4/4	0.85	0.13	51,62,64,69	0
2	EDO	A	610	4/4	0.86	0.13	56,68,83,83	0
2	EDO	B	607	4/4	0.86	0.14	62,74,90,90	0
2	EDO	B	606	4/4	0.87	0.15	47,58,64,70	0
2	EDO	D	604	4/4	0.87	0.14	61,74,76,85	0
2	EDO	E	603	4/4	0.87	0.15	42,51,67,80	0
2	EDO	A	604	4/4	0.87	0.13	44,55,65,79	0
2	EDO	A	601	4/4	0.87	0.15	46,56,58,58	0
2	EDO	A	608	4/4	0.88	0.15	36,45,54,54	0
2	EDO	B	604	4/4	0.89	0.18	45,63,72,76	0
2	EDO	E	606	4/4	0.89	0.10	54,65,74,89	0
2	EDO	E	605	4/4	0.90	0.13	50,64,68,82	0
2	EDO	B	601	4/4	0.90	0.12	43,54,58,65	0
2	EDO	B	602	4/4	0.90	0.12	50,60,69,82	0
2	EDO	H	602	4/4	0.90	0.15	45,59,71,72	0
2	EDO	C	603	4/4	0.90	0.12	45,55,66,70	0
2	EDO	A	609	4/4	0.91	0.10	49,59,70,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	B	605	4/4	0.91	0.17	49,59,60,63	0
2	EDO	C	604	4/4	0.92	0.09	52,63,73,73	0
2	EDO	D	603	4/4	0.92	0.14	49,59,70,71	0
2	EDO	G	601	4/4	0.94	0.10	49,59,74,74	0
2	EDO	A	607	4/4	0.95	0.13	41,56,59,71	0
2	EDO	A	606	4/4	0.95	0.10	42,50,60,60	0
2	EDO	E	601	4/4	0.95	0.10	44,53,65,69	0
2	EDO	E	602	4/4	0.95	0.12	40,55,66,66	0
2	EDO	C	605	4/4	0.97	0.08	43,58,69,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.