



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:12 AM UTC

PDB ID : 6NN7 / pdb_00006nn7
Title : The structure of human liver pyruvate kinase, hLPYK-GGG
Authors : McFarlane, J.S.; Ronnebaum, T.A.; Meneely, K.M.; Fenton, A.W.; Lamb, A.L.
Deposited on : 2019-01-14
Resolution : 2.32 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

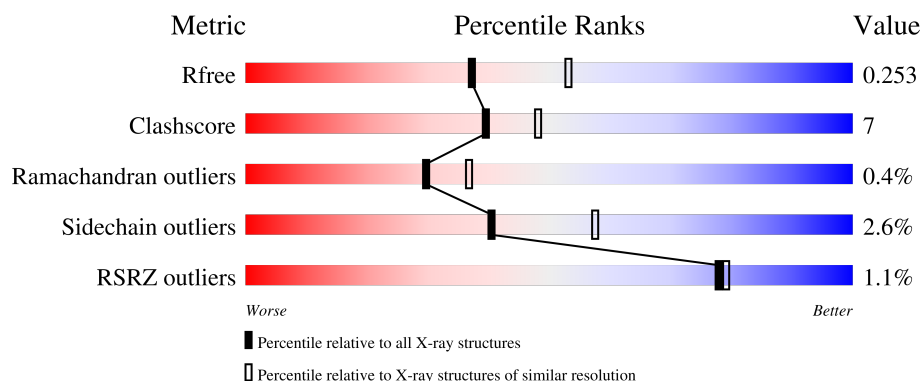
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	542	83% 11% 5%
1	B	542	68% 8% 24%
1	C	542	83% 11% 5%
1	D	542	73% 15% 12%
1	E	542	83% 12% 5%

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Mol	Chain	Length	Quality of chain
1	F	542	
1	G	542	
1	H	542	

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	C	603	-	-	X	-
2	EDO	C	605	-	-	X	-
4	FLC	C	601	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 58243 atoms, of which 29236 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	516	Total	C	H	N	O	S	0	0	0
			7927	2469	4006	706	728	18			
1	B	414	Total	C	H	N	O	S	0	0	0
			6369	1980	3212	574	585	18			
1	C	514	Total	C	H	N	O	S	0	0	0
			7851	2440	3964	705	724	18			
1	E	518	Total	C	H	N	O	S	0	0	0
			7919	2463	3998	710	730	18			
1	D	479	Total	C	H	N	O	S	0	0	0
			7361	2295	3715	658	675	18			
1	F	406	Total	C	H	N	O	S	0	0	0
			6256	1943	3158	562	575	18			
1	G	496	Total	C	H	N	O	S	0	0	0
			7660	2388	3869	685	700	18			
1	H	398	Total	C	H	N	O	S	0	0	0
			6118	1895	3092	552	561	18			

There are 32 discrepancies between the modelled and reference sequences:

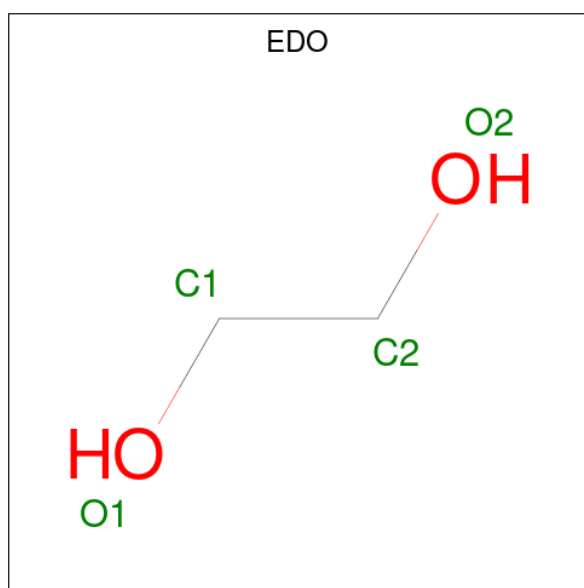
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P30613
A	2	GLU	-	expression tag	UNP P30613
A	?	-	PRO	deletion	UNP P30613
A	531	GLY	SER	engineered mutation	UNP P30613
B	1	MET	-	expression tag	UNP P30613
B	2	GLU	-	expression tag	UNP P30613
B	?	-	PRO	deletion	UNP P30613
B	531	GLY	SER	engineered mutation	UNP P30613
C	1	MET	-	expression tag	UNP P30613
C	2	GLU	-	expression tag	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	531	GLY	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	?	-	PRO	deletion	UNP P30613
E	531	GLY	SER	engineered mutation	UNP P30613
D	1	MET	-	expression tag	UNP P30613
D	2	GLU	-	expression tag	UNP P30613
D	?	-	PRO	deletion	UNP P30613
D	531	GLY	SER	engineered mutation	UNP P30613
F	1	MET	-	expression tag	UNP P30613
F	2	GLU	-	expression tag	UNP P30613
F	?	-	PRO	deletion	UNP P30613
F	531	GLY	SER	engineered mutation	UNP P30613
G	1	MET	-	expression tag	UNP P30613
G	2	GLU	-	expression tag	UNP P30613
G	?	-	PRO	deletion	UNP P30613
G	531	GLY	SER	engineered mutation	UNP P30613
H	1	MET	-	expression tag	UNP P30613
H	2	GLU	-	expression tag	UNP P30613
H	?	-	PRO	deletion	UNP P30613
H	531	GLY	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		

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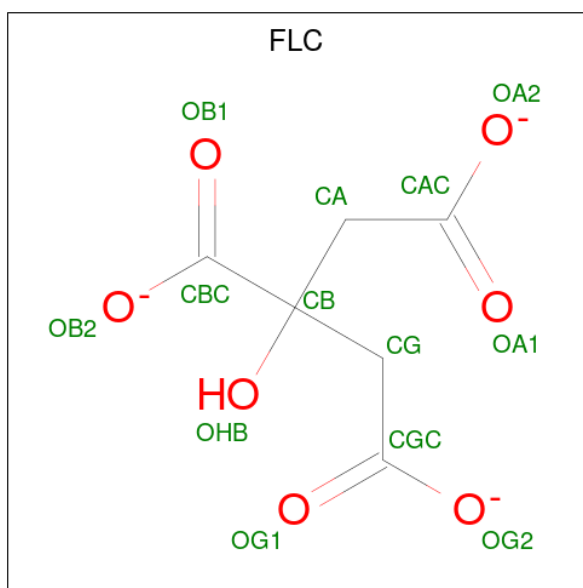
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			13	3	7	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			13	3	7	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	F	1	Total	C	H	O	0	0
			14	3	8	3		
3	F	1	Total	C	H	O	0	0
			14	3	8	3		
3	G	1	Total	C	H	O	0	0
			14	3	8	3		
3	H	1	Total	C	H	O	0	0
			14	3	8	3		
3	H	1	Total	C	H	O	0	0
			14	3	8	3		

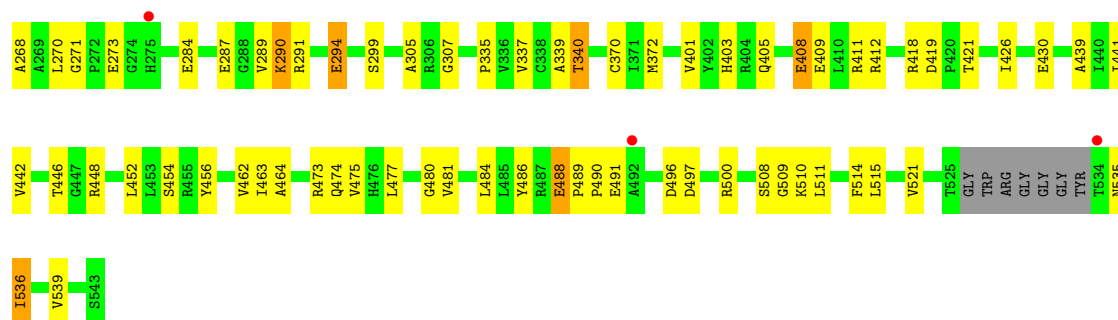
- Molecule 4 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



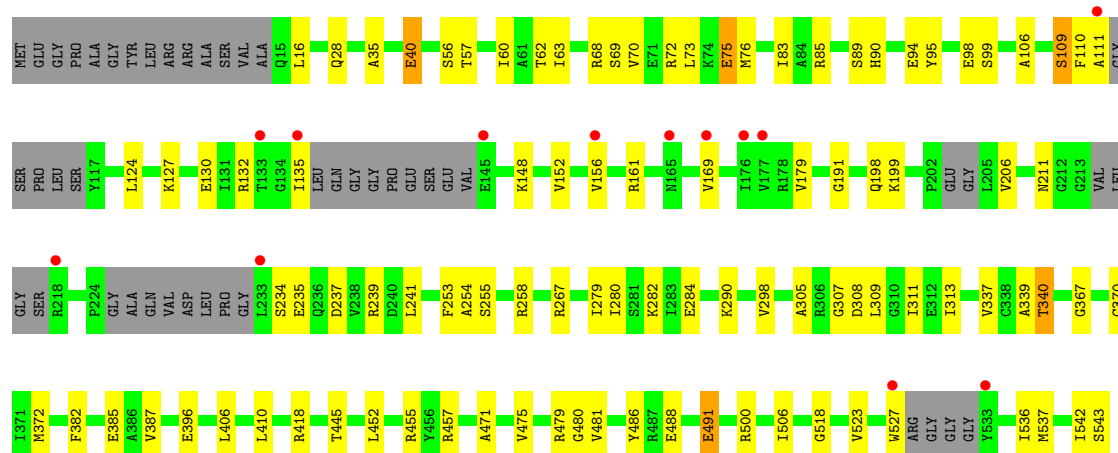
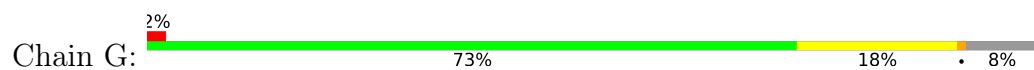
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			18	6	5	7		
4	D	1	Total	C	H	O	0	0
			18	6	5	7		

- Molecule 5 is water.

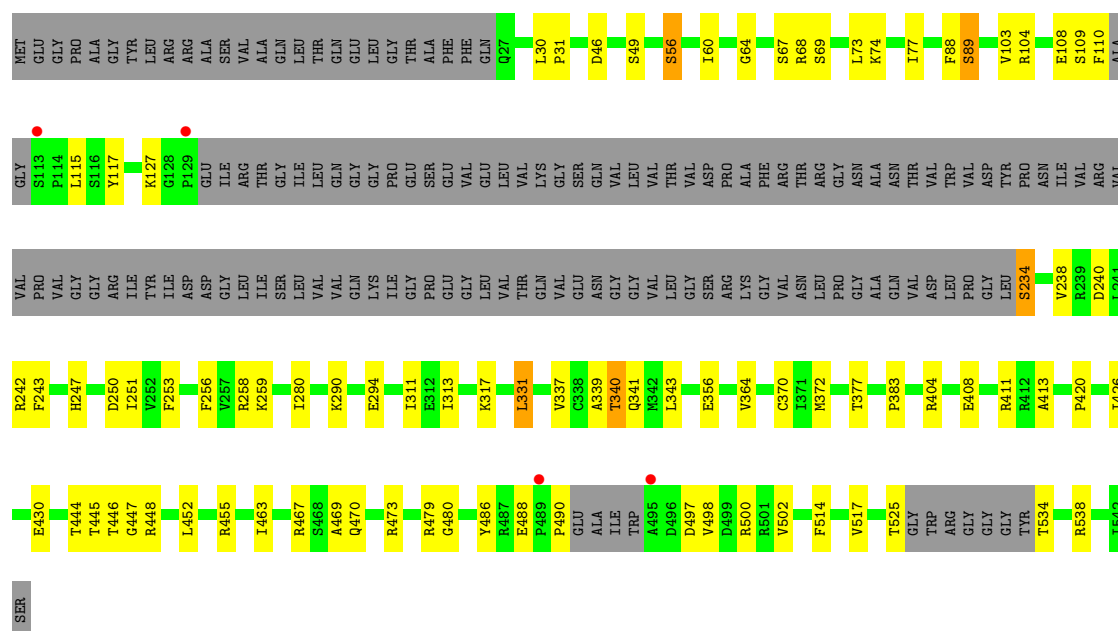
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	87	Total	O	0	0
			87	87		
5	B	63	Total	O	0	0
			63	63		
5	C	67	Total	O	0	0
			67	67		
5	E	64	Total	O	0	0
			64	64		
5	D	73	Total	O	0	0
			73	73		
5	F	15	Total	O	0	0
			15	15		
5	G	11	Total	O	0	0
			11	11		
5	H	2	Total	O	0	0
			2	2		



• Molecule 1: Pyruvate kinase PKLR



• Molecule 1: Pyruvate kinase PKLR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.36Å 106.20Å 151.71Å 76.44° 80.06° 71.37°	Depositor
Resolution (Å)	39.06 – 2.32 39.06 – 2.32	Depositor EDS
% Data completeness (in resolution range)	89.4 (39.06-2.32) 89.4 (39.06-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.31Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.191 , 0.251 0.194 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (1.02%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	58243	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: FLC, EDO, GOL

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	0.64	0/3981	0.74	0/5392
1	B	0.62	0/3206	0.79	0/4333
1	C	0.61	0/3949	0.75	0/5349
1	D	0.58	0/3699	0.73	0/4998
1	E	0.59	0/3985	0.73	0/5399
1	F	0.53	0/3143	0.72	0/4245
1	G	0.50	0/3847	0.69	0/5203
1	H	0.46	0/3068	0.65	0/4143
All	All	0.57	0/28878	0.73	0/39062

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	C	0	1
1	G	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	112	GLY	Peptide
1	G	254	ALA	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	3921	4006	4004	40	0
1	B	3157	3212	3212	33	0
1	C	3887	3964	3963	55	0
1	D	3646	3715	3708	51	0
1	E	3921	3998	3997	39	0
1	F	3098	3158	3156	71	0
1	G	3791	3869	3868	68	0
1	H	3026	3092	3091	52	0
2	A	8	12	12	2	0
2	B	8	12	12	0	0
2	C	28	42	42	11	0
2	D	4	6	6	3	0
2	E	8	12	12	2	0
2	F	4	6	6	2	0
2	G	8	12	12	0	0
3	A	12	16	16	0	0
3	B	12	15	16	1	0
3	C	6	8	8	0	0
3	D	6	8	8	0	0
3	E	18	23	24	0	0
3	F	12	16	16	1	0
3	G	6	8	8	1	0
3	H	12	16	16	1	0
4	C	13	5	5	1	0
4	D	13	5	5	2	0
5	A	87	0	0	1	0
5	B	63	0	0	2	0
5	C	67	0	0	4	0
5	D	73	0	0	1	0
5	E	64	0	0	1	0
5	F	15	0	0	0	0
5	G	11	0	0	0	0
5	H	2	0	0	0	0
All	All	29007	29236	29223	385	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 7.

All (385) 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:B:236:GLN:OE1	1:B:239:ARG:NH2	1.98	0.96
1:F:337:VAL:HG22	1:F:370:CYS:HB2	1.52	0.90
1:G:527:TRP:HB2	1:G:536:ILE:HD11	1.57	0.87
1:H:446:THR:HG22	3:H:602:GOL:H31	1.55	0.86
1:F:419:ASP:OD2	1:F:448:ARG:NH2	2.14	0.81
1:D:144:VAL:HG21	1:D:166:ALA:HB2	1.63	0.79
1:D:156:VAL:HG12	1:D:171:VAL:HG22	1.65	0.77
1:G:475:VAL:HG11	1:G:481:VAL:HG11	1.66	0.77
1:G:475:VAL:CG1	1:G:481:VAL:HG11	2.14	0.76
1:H:444:THR:HG22	1:H:447:GLY:H	1.50	0.75
1:G:471:ALA:O	1:G:475:VAL:HG23	1.86	0.75
1:D:263:VAL:HG21	1:D:298:VAL:HG23	1.68	0.75
1:C:512:ARG:HH11	1:C:512:ARG:HB3	1.52	0.74
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.69	0.73
1:E:233:LEU:HD21	1:E:266:VAL:HG22	1.70	0.72
1:C:122:ILE:HD12	2:C:603:EDO:H11	1.69	0.72
1:G:255:SER:O	1:G:284:GLU:OE1	2.08	0.72
1:F:339:ALA:HB1	1:F:372:MET:HE2	1.71	0.72
1:D:260:ALA:O	1:D:263:VAL:HG22	1.91	0.71
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.72	0.71
1:A:419:ASP:OD2	1:A:448:ARG:NH2	2.23	0.71
1:G:339:ALA:HB1	1:G:372:MET:HE2	1.73	0.70
1:C:538:ARG:NH1	1:C:540:LEU:HD21	2.05	0.70
1:B:527:TRP:HB3	1:B:536:ILE:HD11	1.73	0.70
1:E:527:TRP:HE3	1:E:536:ILE:HD11	1.55	0.70
1:H:444:THR:CG2	1:H:447:GLY:H	2.07	0.67
1:E:165:ASN:HB3	2:E:601:EDO:H11	1.77	0.67
1:D:263:VAL:HG21	1:D:298:VAL:CG2	2.24	0.66
1:B:419:ASP:OD2	1:B:448:ARG:NH2	2.21	0.65
1:F:475:VAL:CG2	1:F:481:VAL:HG11	2.27	0.65
1:G:76:MET:HE2	1:G:387:VAL:HG21	1.79	0.65
1:F:475:VAL:HG22	1:F:481:VAL:HG11	1.79	0.65
1:H:73:LEU:HD13	1:H:103:VAL:HA	1.79	0.63
1:H:337:VAL:HG22	1:H:370:CYS:HB2	1.80	0.62
1:E:162:THR:HG22	1:E:162:THR:O	1.99	0.62
1:A:56:SER:HB2	1:A:480:GLY:HA2	1.82	0.62
1:D:527:TRP:HB2	1:D:536:ILE:HD11	1.80	0.62
1:H:331:LEU:HD21	1:H:413:ALA:HB1	1.80	0.62
1:E:165:ASN:CB	2:E:601:EDO:H11	2.30	0.62
1:C:510:LYS:NZ	1:C:543:SER:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:411:ARG:HD3	1:H:426:ILE:HD11	1.82	0.61
1:C:155:THR:HG22	1:C:157:ASP:H	1.64	0.61
1:B:521:VAL:CG1	1:B:542:ILE:HD11	2.30	0.61
1:C:418:ARG:NH2	5:C:706:HOH:O	2.33	0.61
1:E:115:LEU:HD23	1:E:508:SER:OG	2.01	0.61
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.82	0.61
1:H:343:LEU:HD23	1:H:356:GLU:HB3	1.82	0.61
1:A:418:ARG:NH1	1:C:435:CYS:O	2.35	0.60
1:D:28:GLN:HG3	1:D:52:VAL:HG22	1.84	0.60
1:C:473:ARG:NE	2:C:603:EDO:H21	2.17	0.59
1:E:339:ALA:HB1	1:E:372:MET:HE2	1.83	0.59
1:D:130:GLU:OE1	1:D:132:ARG:NH2	2.35	0.59
1:F:463:ILE:CG2	1:F:484:LEU:HD12	2.32	0.59
1:G:63:ILE:HD12	1:G:73:LEU:HD21	1.85	0.59
1:C:28:GLN:HG2	1:C:52:VAL:HG22	1.83	0.58
1:A:188:ILE:HB	1:A:193:ILE:HB	1.84	0.58
1:E:47:ILE:CD1	1:F:289:VAL:HG11	2.33	0.58
4:D:601:FLC:CAC	4:D:601:FLC:OG1	2.52	0.58
1:C:512:ARG:HB3	1:C:512:ARG:NH1	2.17	0.58
1:E:337:VAL:HG22	1:E:370:CYS:HB2	1.85	0.58
1:G:62:THR:OG1	1:G:85:ARG:NH1	2.36	0.58
1:H:490:PRO:HB3	1:H:497:ASP:OD1	2.04	0.58
1:G:396:GLU:OE2	1:H:317:LYS:NZ	2.33	0.57
1:C:28:GLN:CG	1:C:52:VAL:HG22	2.34	0.57
1:D:68:ARG:NH2	5:D:705:HOH:O	2.38	0.57
1:H:104:ARG:O	1:H:108:GLU:HG2	2.04	0.56
1:B:411:ARG:HG2	1:B:426:ILE:HD11	1.87	0.56
1:C:318:VAL:HG12	2:C:605:EDO:H21	1.86	0.56
1:C:114:PRO:HG2	1:C:117:TYR:N	2.19	0.56
1:G:35:ALA:HB1	1:G:40:GLU:HB3	1.87	0.56
1:E:177:VAL:HA	1:E:205:LEU:HD21	1.87	0.56
1:C:239:ARG:HD3	1:G:518:GLY:HA3	1.87	0.56
1:F:243:PHE:CE1	1:F:247:HIS:CE1	2.94	0.56
1:C:471:ALA:O	1:C:475:VAL:HG13	2.05	0.56
1:F:486:TYR:CZ	1:F:488:GLU:HG3	2.41	0.56
1:C:104:ARG:HH21	2:C:603:EDO:H22	1.71	0.56
1:F:268:ALA:O	1:F:271:GLY:N	2.33	0.55
1:F:426:ILE:HD12	1:F:456:TYR:CZ	2.40	0.55
1:G:239:ARG:HB3	1:G:239:ARG:CZ	2.35	0.55
1:G:106:ALA:O	1:G:109:SER:HB3	2.05	0.55
1:H:411:ARG:HD2	1:H:411:ARG:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:475:VAL:HG12	1:G:481:VAL:HG11	1.89	0.55
1:A:451:GLN:OE1	2:A:602:EDO:H21	2.05	0.55
1:G:72:ARG:O	1:G:75:GLU:N	2.39	0.55
1:G:406:LEU:HD11	1:G:410:LEU:HD11	1.88	0.55
1:H:64:GLY:O	1:H:68:ARG:HG3	2.06	0.55
1:G:491:GLU:OE2	1:G:500:ARG:NH2	2.39	0.55
1:B:26:GLN:N	1:B:30:LEU:HD23	2.21	0.55
1:A:148:LYS:HG3	1:A:149:GLY:N	2.20	0.55
1:D:72:ARG:O	1:D:76:MET:HG2	2.07	0.54
4:D:601:FLC:OA1	4:D:601:FLC:OHB	2.11	0.54
1:C:339:ALA:O	1:C:340:THR:HB	2.08	0.53
1:D:35:ALA:HB2	1:D:44:LEU:HD12	1.89	0.53
1:D:69:SER:OG	2:D:602:EDO:C2	2.56	0.53
1:F:442:VAL:HG13	1:F:464:ALA:HA	1.90	0.53
1:G:110:PHE:O	1:G:111:ALA:CB	2.56	0.53
1:F:446:THR:HG22	3:F:603:GOL:O1	2.08	0.53
1:H:339:ALA:HB1	1:H:372:MET:HE2	1.89	0.53
1:D:443:LEU:HG	1:D:525:THR:HG22	1.89	0.53
1:D:69:SER:OG	2:D:602:EDO:H22	2.09	0.53
1:G:367:GLY:O	1:G:457:ARG:NH2	2.41	0.52
1:C:256:PHE:CZ	2:C:606:EDO:H12	2.43	0.52
1:A:455:ARG:HG3	1:A:455:ARG:HH11	1.74	0.52
1:F:70:VAL:O	1:F:74:LYS:HG3	2.08	0.52
1:A:449:SER:OG	1:A:534:THR:HG21	2.10	0.52
1:E:527:TRP:CE3	1:E:536:ILE:HD11	2.41	0.52
1:E:155:THR:HG21	1:E:160:PHE:CD2	2.44	0.52
1:D:55:ARG:HB2	1:D:395:ARG:HG3	1.91	0.52
1:F:251:ILE:HG22	1:F:252:VAL:N	2.25	0.51
1:C:319:PHE:HA	2:C:605:EDO:C2	2.40	0.51
1:C:512:ARG:NH1	1:C:514:PHE:CZ	2.78	0.51
1:F:93:HIS:O	1:F:97:ALA:N	2.39	0.51
1:G:253:PHE:HB3	1:G:282:LYS:HD2	1.92	0.51
1:D:27:GLN:NE2	1:D:50:GLU:OE1	2.44	0.51
1:A:337:VAL:HG22	1:A:370:CYS:HB2	1.93	0.51
1:H:467:ARG:NH2	1:H:488:GLU:O	2.44	0.51
1:G:152:VAL:CG1	1:G:169:VAL:HG23	2.40	0.51
1:D:156:VAL:HG12	1:D:171:VAL:CG2	2.36	0.51
1:A:517:VAL:HG12	1:A:543:SER:OG	2.10	0.51
1:D:173:TYR:CD2	1:D:176:ILE:HG23	2.46	0.51
1:F:405:GLN:O	1:F:409:GLU:HG3	2.11	0.51
1:H:525:THR:C	1:H:534:THR:HG23	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ALA:HB3	1:B:515:LEU:HD23	1.91	0.50
1:G:110:PHE:O	1:G:111:ALA:HB2	2.11	0.50
1:B:521:VAL:HG11	1:B:542:ILE:HD11	1.93	0.50
1:F:511:LEU:HD13	1:F:511:LEU:C	2.37	0.50
1:C:47:ILE:HD13	1:D:289:VAL:HG11	1.93	0.50
1:C:118:ARG:CZ	1:C:512:ARG:NH2	2.75	0.50
1:G:445:THR:H	3:G:603:GOL:H12	1.77	0.50
1:G:199:LYS:HB2	1:G:206:VAL:HG11	1.94	0.50
1:E:416:LEU:HB2	1:G:16:LEU:HD11	1.93	0.50
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.94	0.50
1:H:89:SER:HA	1:H:127:LYS:HG3	1.94	0.50
1:A:527:TRP:HA	1:A:536:ILE:HD11	1.94	0.49
1:F:462:VAL:HG11	1:F:481:VAL:HG22	1.93	0.49
1:C:114:PRO:HD2	1:C:117:TYR:N	2.26	0.49
1:G:234:SER:OG	1:G:237:ASP:N	2.36	0.49
1:A:197:VAL:HA	1:A:207:THR:HG22	1.94	0.49
1:C:75:GLU:HG3	1:C:384:VAL:HG11	1.94	0.49
1:B:488:GLU:OE1	1:B:488:GLU:N	2.46	0.49
1:H:411:ARG:HD2	1:H:411:ARG:C	2.37	0.49
1:B:56:SER:HB2	1:B:480:GLY:CA	2.42	0.49
1:F:251:ILE:HD13	1:F:477:LEU:HD21	1.95	0.49
1:F:462:VAL:HG13	1:F:462:VAL:O	2.12	0.49
1:C:331:LEU:HD11	1:C:413:ALA:HB1	1.95	0.49
1:G:199:LYS:HB2	1:G:206:VAL:CG1	2.43	0.49
1:G:94:GLU:O	1:G:98:GLU:HG3	2.12	0.48
1:D:133:THR:HA	1:D:170:TRP:O	2.13	0.48
1:F:411:ARG:NH2	1:H:408:GLU:OE2	2.46	0.48
1:B:521:VAL:HG13	1:B:542:ILE:HD11	1.93	0.48
1:C:339:ALA:HB1	1:C:372:MET:HE2	1.95	0.48
1:B:408:GLU:HG2	1:B:411:ARG:HH21	1.77	0.48
1:F:462:VAL:CG1	1:F:481:VAL:HG22	2.44	0.48
1:A:414:ALA:HB2	1:A:455:ARG:HH21	1.79	0.48
1:B:494:TRP:CH2	1:B:526:GLY:O	2.66	0.48
1:D:93:HIS:NE2	1:D:240:ASP:OD1	2.36	0.48
1:C:118:ARG:CZ	1:C:512:ARG:HH21	2.26	0.48
1:D:114:PRO:HB3	1:D:487:ARG:NH1	2.29	0.48
1:C:515:LEU:HD22	1:C:521:VAL:HG11	1.96	0.48
1:F:63:ILE:HD12	1:F:73:LEU:HD21	1.96	0.48
1:G:124:LEU:C	1:G:124:LEU:HD23	2.39	0.48
1:C:104:ARG:HH21	2:C:603:EDO:C2	2.27	0.47
1:C:107:VAL:HG21	1:C:120:VAL:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:VAL:O	5:E:701:HOH:O	2.20	0.47
1:D:124:LEU:C	1:D:124:LEU:HD23	2.39	0.47
1:F:474:GLN:O	1:F:477:LEU:HD12	2.13	0.47
1:H:446:THR:HG23	1:H:448:ARG:H	1.78	0.47
1:H:498:VAL:O	1:H:502:VAL:HG23	2.15	0.47
1:G:284:GLU:OE2	1:G:308:ASP:HB2	2.14	0.47
1:E:335:PRO:HB3	1:E:477:LEU:O	2.13	0.47
1:F:446:THR:HG23	1:F:448:ARG:H	1.80	0.47
1:H:452:LEU:O	1:H:455:ARG:HG2	2.14	0.47
1:C:55:ARG:HB2	1:C:395:ARG:HG2	1.96	0.47
1:G:89:SER:O	1:G:90:HIS:ND1	2.47	0.47
1:G:130:GLU:OE1	1:G:132:ARG:NH1	2.47	0.47
1:A:408:GLU:OE1	1:C:412:ARG:NH2	2.48	0.47
1:B:463:ILE:HD11	1:B:514:PHE:HE1	1.80	0.47
1:A:137:GLN:HG3	1:A:164:GLY:O	2.15	0.47
1:H:331:LEU:HD21	1:H:413:ALA:CB	2.44	0.47
1:C:470:GLN:NE2	5:C:707:HOH:O	2.39	0.47
1:F:484:LEU:HD21	1:F:508:SER:OG	2.15	0.47
1:A:421:THR:HG1	1:A:533:TYR:HD1	1.62	0.46
1:F:307:GLY:CA	1:F:340:THR:HG21	2.44	0.46
1:F:454:SER:OG	2:F:601:EDO:C1	2.64	0.46
1:C:47:ILE:CD1	1:D:289:VAL:HG11	2.45	0.46
1:E:527:TRP:HE3	1:E:536:ILE:CD1	2.27	0.46
1:G:198:GLN:O	1:G:199:LYS:HG3	2.15	0.46
1:G:267:ARG:NH2	1:G:279:ILE:HD12	2.31	0.46
1:H:67:SER:O	1:H:73:LEU:HD21	2.15	0.46
1:F:539:VAL:HG11	1:H:420:PRO:HB3	1.98	0.46
1:G:307:GLY:CA	1:G:340:THR:HG21	2.44	0.46
1:F:242:ARG:HA	1:F:245:VAL:HG12	1.97	0.46
1:F:441:ILE:HG13	1:F:521:VAL:HG21	1.97	0.46
1:F:454:SER:OG	2:F:601:EDO:H12	2.16	0.46
1:H:411:ARG:HD3	1:H:426:ILE:CD1	2.44	0.46
1:A:23:ALA:O	1:A:27:GLN:HG3	2.15	0.46
1:G:284:GLU:HG2	1:G:305:ALA:HB3	1.97	0.46
1:B:493:ILE:HG23	1:B:496:ASP:CG	2.41	0.46
1:E:486:TYR:CE2	1:E:488:GLU:HB2	2.51	0.46
1:F:510:LYS:HA	1:F:515:LEU:O	2.16	0.46
1:D:469:ALA:HA	1:D:485:LEU:HD13	1.98	0.46
1:G:68:ARG:NH1	1:G:95:TYR:CZ	2.84	0.46
1:F:430:GLU:HG2	1:H:430:GLU:HG3	1.98	0.45
1:A:255:SER:HA	1:A:282:LYS:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:407:PHE:O	1:E:411:ARG:HG2	2.16	0.45
1:D:339:ALA:O	1:D:340:THR:HB	2.16	0.45
1:F:439:ALA:O	1:F:521:VAL:HG23	2.15	0.45
1:H:256:PHE:O	1:H:258:ARG:HG3	2.16	0.45
1:C:493:ILE:CG2	1:C:496:ASP:OD2	2.65	0.45
1:D:339:ALA:HB1	1:D:372:MET:HE2	1.99	0.45
1:F:535:ASN:OD1	1:F:536:ILE:HD12	2.17	0.45
1:G:235:GLU:O	1:G:239:ARG:HG3	2.17	0.45
1:E:331:LEU:HD12	1:E:331:LEU:O	2.16	0.45
1:F:419:ASP:OD1	1:F:419:ASP:C	2.60	0.45
1:F:535:ASN:O	1:H:538:ARG:HA	2.16	0.45
1:G:75:GLU:HA	1:G:75:GLU:OE1	2.16	0.45
1:D:73:LEU:HD13	1:D:103:VAL:HA	1.98	0.45
1:D:284:GLU:OE2	1:D:308:ASP:OD2	2.35	0.45
1:F:462:VAL:HG12	1:F:480:GLY:O	2.15	0.45
1:G:148:LYS:HZ2	1:G:211:ASN:HA	1.81	0.45
1:G:523:VAL:O	1:G:537:MET:HA	2.17	0.45
1:C:403:HIS:O	1:C:404:ARG:C	2.59	0.45
1:E:292:PHE:CE1	1:E:325:MET:HG2	2.52	0.45
1:D:69:SER:CB	2:D:602:EDO:H21	2.46	0.45
1:H:74:LYS:HE3	1:H:109:SER:OG	2.17	0.45
1:A:155:THR:O	1:A:170:TRP:HA	2.17	0.45
1:B:522:ILE:HG23	1:B:537:MET:HE3	1.98	0.45
1:C:290:LYS:HD2	1:D:48:ASP:OD2	2.17	0.45
1:F:56:SER:HB3	1:F:480:GLY:HA2	1.99	0.45
1:G:135:ILE:N	1:G:135:ILE:HD12	2.32	0.45
1:G:506:ILE:HG23	1:G:542:ILE:HD12	1.99	0.45
1:E:30:LEU:O	1:E:34:MET:HG2	2.16	0.45
1:E:402:TYR:CE2	1:E:405:GLN:HB2	2.52	0.45
1:D:144:VAL:CG2	1:D:166:ALA:HB2	2.40	0.45
1:H:234:SER:O	1:H:238:VAL:HG23	2.17	0.45
1:B:434:LYS:NZ	1:D:415:PRO:O	2.47	0.44
1:F:287:GLU:OE2	1:F:291:ARG:NH1	2.50	0.44
1:E:162:THR:O	1:E:162:THR:CG2	2.65	0.44
1:D:165:ASN:OD1	1:D:168:THR:N	2.48	0.44
1:F:462:VAL:CG1	1:F:481:VAL:HA	2.48	0.44
1:H:340:THR:O	1:H:341:GLN:HB2	2.17	0.44
1:D:165:ASN:OD1	1:D:165:ASN:C	2.60	0.44
1:C:403:HIS:CE1	1:C:459:ARG:HG2	2.52	0.44
1:E:343:LEU:HD23	1:E:356:GLU:HB3	2.00	0.44
1:D:424:THR:OG1	1:D:535:ASN:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:VAL:O	1:E:179:VAL:CG1	2.64	0.44
1:F:426:ILE:HD12	1:F:456:TYR:CE1	2.52	0.44
1:G:337:VAL:HG22	1:G:370:CYS:HB2	1.99	0.44
1:H:30:LEU:N	1:H:31:PRO:CD	2.81	0.44
1:H:469:ALA:HB1	1:H:473:ARG:HH22	1.83	0.44
1:A:19:GLU:OE1	1:C:418:ARG:NH1	2.51	0.44
1:F:124:LEU:C	1:F:124:LEU:HD23	2.42	0.44
1:A:419:ASP:O	1:A:423:VAL:HG23	2.17	0.44
1:B:30:LEU:N	1:B:31:PRO:CD	2.80	0.44
1:H:60:ILE:HB	1:H:372:MET:HG3	2.00	0.44
1:H:250:ASP:C	1:H:251:ILE:HG13	2.43	0.44
1:H:486:TYR:OH	1:H:500:ARG:NH1	2.51	0.44
1:A:416:LEU:N	1:A:416:LEU:HD23	2.32	0.44
1:E:236:GLN:NE2	1:E:240:ASP:OD1	2.51	0.44
1:G:60:ILE:HG12	1:G:83:ILE:HB	2.00	0.44
1:E:128:GLY:HA2	1:E:237:ASP:OD2	2.18	0.43
1:H:46:ASP:HB3	1:H:49:SER:HB2	2.00	0.43
1:A:469:ALA:HA	1:A:485:LEU:HD13	1.98	0.43
1:D:194:SER:OG	1:D:211:ASN:HB2	2.18	0.43
1:F:284:GLU:HG2	1:F:305:ALA:HB3	1.99	0.43
1:A:486:TYR:CZ	1:A:488:GLU:HB2	2.54	0.43
1:B:243:PHE:CD1	1:B:243:PHE:C	2.95	0.43
1:B:515:LEU:HD22	1:B:542:ILE:CD1	2.49	0.43
1:E:87:ASN:OD1	1:E:89:SER:HB2	2.19	0.43
1:G:406:LEU:HD21	1:G:457:ARG:HG2	1.99	0.43
1:F:421:THR:HG22	1:F:452:LEU:HD12	2.01	0.43
1:G:152:VAL:HG11	1:G:169:VAL:HG23	2.00	0.43
1:B:412:ARG:NH1	1:D:404:ARG:HD3	2.32	0.43
1:C:319:PHE:HB3	2:C:605:EDO:H22	2.00	0.43
1:D:309:LEU:O	1:D:313:ILE:HG12	2.18	0.43
1:H:243:PHE:CE2	1:H:247:HIS:CE1	3.07	0.43
1:H:445:THR:O	1:H:445:THR:HG22	2.19	0.43
1:A:451:GLN:OE1	2:A:602:EDO:C2	2.66	0.43
1:C:259:LYS:CE	5:C:709:HOH:O	2.67	0.43
1:D:51:PRO:HG3	1:D:396:GLU:CD	2.43	0.43
1:G:68:ARG:NH1	1:G:99:SER:OG	2.51	0.43
1:G:253:PHE:HD1	1:G:280:ILE:HB	1.83	0.43
1:G:309:LEU:O	1:G:313:ILE:HG12	2.19	0.43
1:H:88:PHE:CD2	1:H:240:ASP:HB3	2.53	0.43
1:F:235:GLU:O	1:F:239:ARG:HG3	2.19	0.43
1:G:339:ALA:HB1	1:G:372:MET:CE	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:VAL:HG22	1:B:543:SER:OXT	2.19	0.43
1:C:246:GLU:OE2	1:E:528:ARG:NH1	2.41	0.43
1:E:518:GLY:O	1:G:418:ARG:NH2	2.51	0.43
1:H:56:SER:HB3	1:H:480:GLY:HA2	2.00	0.43
1:H:377:THR:HA	1:H:383:PRO:HB3	2.00	0.43
1:A:133:THR:HA	1:A:170:TRP:O	2.19	0.43
1:F:412:ARG:NH2	1:H:404:ARG:HG2	2.34	0.43
1:C:155:THR:HG22	1:C:157:ASP:N	2.32	0.42
1:C:259:LYS:HE2	5:C:709:HOH:O	2.19	0.42
1:G:237:ASP:O	1:G:241:LEU:HG	2.19	0.42
1:G:406:LEU:CD1	1:G:410:LEU:HD11	2.49	0.42
1:A:284:GLU:C	1:A:309:LEU:HD13	2.44	0.42
1:A:423:VAL:HG12	1:C:431:ALA:HB1	2.00	0.42
1:E:27:GLN:HB3	1:E:50:GLU:O	2.19	0.42
1:F:462:VAL:HG13	1:F:481:VAL:HA	2.01	0.42
1:F:509:GLY:O	1:F:514:PHE:N	2.52	0.42
1:D:482:PHE:CD1	1:D:482:PHE:N	2.87	0.42
1:F:273:GLU:H	1:F:273:GLU:CD	2.25	0.42
1:F:335:PRO:HB3	1:F:477:LEU:O	2.19	0.42
1:A:72:ARG:HA	1:A:72:ARG:HD3	1.86	0.42
1:B:26:GLN:O	1:B:27:GLN:NE2	2.44	0.42
1:B:438:ALA:HB1	1:B:514:PHE:O	2.19	0.42
1:E:118:ARG:HH21	1:E:118:ARG:HG3	1.84	0.42
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.55	0.42
1:A:152:VAL:HG13	1:A:209:VAL:HG23	2.02	0.42
1:B:494:TRP:CZ3	1:B:526:GLY:O	2.72	0.42
1:H:463:ILE:HD11	1:H:514:PHE:HD2	1.83	0.42
1:B:527:TRP:HB3	1:B:536:ILE:CD1	2.47	0.42
1:F:496:ASP:O	1:F:500:ARG:HG3	2.19	0.42
1:F:539:VAL:CG1	1:H:420:PRO:HB3	2.49	0.42
1:B:493:ILE:HG23	1:B:496:ASP:HB2	2.00	0.42
1:E:181:PRO:O	1:E:182:VAL:C	2.63	0.42
1:E:408:GLU:HG3	1:E:411:ARG:HH12	1.84	0.42
1:F:408:GLU:OE1	1:H:408:GLU:OE1	2.38	0.42
1:C:243:PHE:CD1	1:C:243:PHE:C	2.97	0.42
1:F:260:ALA:HB2	1:F:294:GLU:HG3	2.02	0.42
1:G:57:THR:OG1	1:G:479:ARG:HD2	2.20	0.42
1:B:449:SER:OG	3:B:603:GOL:H31	2.20	0.42
1:C:421:THR:HG23	1:C:534:THR:HB	2.01	0.42
1:C:538:ARG:CZ	1:C:540:LEU:HD21	2.50	0.42
1:E:419:ASP:OD1	1:E:419:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:412:ARG:HD3	1:H:404:ARG:CZ	2.50	0.42
1:A:330:ASN:O	1:A:455:ARG:NH1	2.53	0.42
1:A:28:GLN:HA	5:A:763:HOH:O	2.19	0.41
1:D:24:PHE:CD1	1:D:24:PHE:C	2.98	0.41
1:G:382:PHE:HB3	1:G:385:GLU:OE1	2.20	0.41
1:C:137:GLN:HE22	2:C:607:EDO:H12	1.85	0.41
1:D:253:PHE:HD1	1:D:280:ILE:HB	1.86	0.41
1:F:243:PHE:CE1	1:F:247:HIS:ND1	2.88	0.41
1:A:154:VAL:HG22	1:A:169:VAL:CG2	2.50	0.41
1:B:290:LYS:NZ	5:B:707:HOH:O	2.49	0.41
1:C:403:HIS:ND1	1:C:459:ARG:NH1	2.68	0.41
1:E:154:VAL:HA	1:E:169:VAL:O	2.21	0.41
1:E:346:MET:HA	1:E:349:LYS:O	2.20	0.41
1:D:154:VAL:O	1:D:200:ILE:C	2.63	0.41
1:D:258:ARG:HB3	1:D:287:GLU:HG2	2.02	0.41
1:G:68:ARG:NH2	1:G:98:GLU:HB2	2.35	0.41
1:A:415:PRO:O	1:A:416:LEU:C	2.62	0.41
1:F:401:VAL:CG2	1:F:403:HIS:NE2	2.83	0.41
1:G:191:GLY:HA3	1:G:311:ILE:HG23	2.02	0.41
1:G:382:PHE:HB3	1:G:385:GLU:HB2	2.01	0.41
1:A:37:THR:HB	1:B:409:GLU:CD	2.45	0.41
1:C:515:LEU:HD12	1:C:515:LEU:C	2.45	0.41
1:D:421:THR:HG23	1:D:534:THR:HB	2.03	0.41
1:F:339:ALA:O	1:F:340:THR:HB	2.20	0.41
1:F:489:PRO:O	1:F:490:PRO:C	2.63	0.41
1:C:412:ARG:HG3	1:C:412:ARG:HH11	1.86	0.41
2:C:605:EDO:H11	1:D:358:SER:HB2	2.01	0.41
1:D:57:THR:OG1	1:D:479:ARG:HD2	2.20	0.41
1:F:475:VAL:HG21	1:F:481:VAL:HG11	1.99	0.41
1:F:491:GLU:HB2	1:F:497:ASP:HB2	2.01	0.41
1:G:68:ARG:O	1:G:68:ARG:HG2	2.21	0.41
1:G:298:VAL:HG12	1:G:298:VAL:O	2.21	0.41
1:C:319:PHE:CA	2:C:605:EDO:H22	2.51	0.41
4:C:601:FLC:OG1	4:C:601:FLC:CA	2.69	0.41
1:E:323:LYS:HB3	1:F:42:LEU:HD22	2.01	0.41
1:F:250:ASP:CG	1:F:473:ARG:HE	2.29	0.41
1:H:364:VAL:O	1:H:479:ARG:NH1	2.44	0.41
1:C:193:ILE:HD11	1:C:213:GLY:CA	2.51	0.41
1:A:414:ALA:CB	1:A:455:ARG:HH21	2.34	0.40
1:A:435:CYS:HB2	1:A:520:LEU:HD12	2.03	0.40
1:A:253:PHE:HD1	1:A:280:ILE:HB	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:SER:HG	1:D:237:ASP:CG	2.29	0.40
1:F:236:GLN:OE1	1:F:239:ARG:NH1	2.55	0.40
1:F:290:LYS:HE2	1:F:290:LYS:HA	2.03	0.40
1:G:452:LEU:O	1:G:455:ARG:HG2	2.22	0.40
1:A:414:ALA:HB2	1:A:455:ARG:NH2	2.35	0.40
1:H:253:PHE:HD1	1:H:280:ILE:HB	1.86	0.40
1:H:444:THR:HG21	1:H:447:GLY:CA	2.51	0.40
1:F:94:GLU:OE1	1:F:94:GLU:O	2.40	0.40
1:F:287:GLU:OE2	1:F:291:ARG:CZ	2.69	0.40
1:G:135:ILE:HD12	1:G:161:ARG:O	2.21	0.40
1:H:108:GLU:C	1:H:110:PHE:H	2.30	0.40
1:A:258:ARG:C	1:A:295:ILE:HD11	2.47	0.40
1:B:258:ARG:HD3	5:B:733:HOH:O	2.21	0.40
1:B:411:ARG:NH2	1:D:411:ARG:NH1	2.70	0.40
1:C:93:HIS:HB2	1:G:543:SER:HB3	2.03	0.40
1:F:68:ARG:NH2	1:F:98:GLU:HB3	2.37	0.40
1:G:68:ARG:NH2	1:G:95:TYR:O	2.46	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	508/542 (94%)	495 (97%)	12 (2%)	1 (0%)	43	53
1	B	408/542 (75%)	392 (96%)	15 (4%)	1 (0%)	43	53
1	C	510/542 (94%)	497 (98%)	12 (2%)	1 (0%)	43	53
1	D	461/542 (85%)	447 (97%)	12 (3%)	2 (0%)	30	37
1	E	516/542 (95%)	498 (96%)	16 (3%)	2 (0%)	30	37
1	F	398/542 (73%)	378 (95%)	19 (5%)	1 (0%)	36	45
1	G	482/542 (89%)	466 (97%)	12 (2%)	4 (1%)	16	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	388/542 (72%)	375 (97%)	11 (3%)	2 (0%)	24	30
All	All	3671/4336 (85%)	3548 (97%)	109 (3%)	14 (0%)	30	37

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	117	TYR
1	C	340	THR
1	E	416	LEU
1	D	340	THR
1	G	109	SER
1	H	340	THR
1	A	340	THR
1	B	340	THR
1	E	340	THR
1	F	340	THR
1	G	28	GLN
1	G	340	THR
1	G	491	GLU
1	D	490	PRO

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	416/431 (96%)	409 (98%)	7 (2%)	53	70
1	B	331/431 (77%)	322 (97%)	9 (3%)	39	56
1	C	410/431 (95%)	404 (98%)	6 (2%)	57	73
1	D	385/431 (89%)	375 (97%)	10 (3%)	40	57
1	E	414/431 (96%)	403 (97%)	11 (3%)	39	56
1	F	326/431 (76%)	315 (97%)	11 (3%)	32	47
1	G	401/431 (93%)	392 (98%)	9 (2%)	45	63
1	H	320/431 (74%)	305 (95%)	15 (5%)	23	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3003/3448 (87%)	2925 (97%)	78 (3%)	40 57

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	THR
1	A	188	ILE
1	A	227	GLN
1	A	228	VAL
1	A	263	VAL
1	A	534	THR
1	A	541	SER
1	B	52	VAL
1	B	256	PHE
1	B	416	LEU
1	B	488	GLU
1	B	493	ILE
1	B	508	SER
1	B	520	LEU
1	B	534	THR
1	B	537	MET
1	C	71	GLU
1	C	86	LEU
1	C	113	SER
1	C	190	ASP
1	C	294	GLU
1	C	429	VAL
1	E	89	SER
1	E	140	PRO
1	E	179	VAL
1	E	198	GLN
1	E	263	VAL
1	E	358	SER
1	E	412	ARG
1	E	426	ILE
1	E	491	GLU
1	E	506	ILE
1	E	541	SER
1	D	50	GLU
1	D	179	VAL
1	D	214	VAL
1	D	261	SER

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Mol	Chain	Res	Type
1	D	412	ARG
1	D	487	ARG
1	D	488	GLU
1	D	491	GLU
1	D	536	ILE
1	D	540	LEU
1	F	76	MET
1	F	94	GLU
1	F	255	SER
1	F	270	LEU
1	F	290	LYS
1	F	294	GLU
1	F	299	SER
1	F	408	GLU
1	F	418	ARG
1	F	488	GLU
1	F	536	ILE
1	G	40	GLU
1	G	69	SER
1	G	70	VAL
1	G	75	GLU
1	G	127	LYS
1	G	156	VAL
1	G	179	VAL
1	G	258	ARG
1	G	290	LYS
1	H	56	SER
1	H	69	SER
1	H	77	ILE
1	H	89	SER
1	H	115	LEU
1	H	234	SER
1	H	242	ARG
1	H	259	LYS
1	H	290	LYS
1	H	294	GLU
1	H	311	ILE
1	H	313	ILE
1	H	331	LEU
1	H	470	GLN
1	H	517	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	211	ASN
1	B	247	HIS
1	B	275	HIS
1	B	286	HIS
1	C	165	ASN
1	C	330	ASN
1	E	211	ASN
1	E	470	GLN
1	D	90	HIS
1	D	470	GLN
1	D	503	GLN
1	F	90	HIS
1	G	151	GLN
1	G	275	HIS
1	G	286	HIS
1	G	405	GLN
1	H	405	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

33 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	C	602	-	3,3,3	0.45	0	2,2,2	0.34	0
3	GOL	E	604	-	5,5,5	0.93	0	5,5,5	1.52	1 (20%)
3	GOL	B	603	-	5,5,5	0.72	0	5,5,5	0.79	0
3	GOL	H	602	-	5,5,5	0.53	0	5,5,5	0.57	0
3	GOL	A	603	-	5,5,5	0.67	0	5,5,5	1.08	0
3	GOL	A	604	-	5,5,5	0.52	0	5,5,5	1.47	1 (20%)
2	EDO	C	608	-	3,3,3	0.39	0	2,2,2	0.43	0
3	GOL	E	603	-	5,5,5	0.46	0	5,5,5	0.56	0
2	EDO	G	601	-	3,3,3	0.43	0	2,2,2	0.41	0
3	GOL	C	609	-	5,5,5	0.95	0	5,5,5	1.28	1 (20%)
2	EDO	C	604	-	3,3,3	0.46	0	2,2,2	0.26	0
2	EDO	A	601	-	3,3,3	0.40	0	2,2,2	0.68	0
2	EDO	G	602	-	3,3,3	0.49	0	2,2,2	0.59	0
2	EDO	C	603	-	3,3,3	0.48	0	2,2,2	0.34	0
3	GOL	D	603	-	5,5,5	0.50	0	5,5,5	1.10	0
4	FLC	D	601	-	12,12,12	1.49	1 (8%)	17,17,17	1.51	2 (11%)
2	EDO	F	601	-	3,3,3	0.46	0	2,2,2	0.87	0
2	EDO	C	606	-	3,3,3	0.61	0	2,2,2	0.35	0
2	EDO	A	602	-	3,3,3	0.42	0	2,2,2	0.71	0
4	FLC	C	601	-	12,12,12	2.12	2 (16%)	17,17,17	3.06	9 (52%)
2	EDO	C	607	-	3,3,3	0.46	0	2,2,2	0.37	0
2	EDO	B	602	-	3,3,3	0.56	0	2,2,2	0.15	0
3	GOL	G	603	-	5,5,5	0.68	0	5,5,5	1.50	1 (20%)
2	EDO	E	601	-	3,3,3	0.46	0	2,2,2	0.41	0
3	GOL	H	601	-	5,5,5	0.40	0	5,5,5	0.35	0
3	GOL	F	602	-	5,5,5	0.53	0	5,5,5	0.69	0
2	EDO	B	601	-	3,3,3	0.51	0	2,2,2	0.74	0
2	EDO	D	602	-	3,3,3	0.55	0	2,2,2	0.59	0
3	GOL	F	603	-	5,5,5	0.68	0	5,5,5	0.84	0
2	EDO	C	605	-	3,3,3	0.54	0	2,2,2	0.33	0
2	EDO	E	602	-	3,3,3	0.41	0	2,2,2	0.60	0
3	GOL	E	605	-	5,5,5	0.61	0	5,5,5	1.11	0
3	GOL	B	604	-	5,5,5	0.63	0	5,5,5	0.82	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	C	602	-	-	1/1/1/1	-
3	GOL	E	604	-	-	2/4/4/4	-
3	GOL	B	603	-	-	2/4/4/4	-
3	GOL	H	602	-	-	4/4/4/4	-
3	GOL	A	603	-	-	0/4/4/4	-
3	GOL	A	604	-	-	4/4/4/4	-
2	EDO	C	608	-	-	0/1/1/1	-
3	GOL	E	603	-	-	4/4/4/4	-
2	EDO	G	601	-	-	1/1/1/1	-
3	GOL	C	609	-	-	2/4/4/4	-
2	EDO	C	604	-	-	0/1/1/1	-
2	EDO	A	601	-	-	1/1/1/1	-
2	EDO	G	602	-	-	1/1/1/1	-
2	EDO	C	603	-	-	0/1/1/1	-
3	GOL	D	603	-	-	3/4/4/4	-
4	FLC	D	601	-	-	9/16/16/16	-
2	EDO	F	601	-	-	1/1/1/1	-
2	EDO	C	606	-	-	0/1/1/1	-
2	EDO	A	602	-	-	1/1/1/1	-
4	FLC	C	601	-	-	8/16/16/16	-
2	EDO	C	607	-	-	0/1/1/1	-
2	EDO	B	602	-	-	0/1/1/1	-
3	GOL	G	603	-	-	3/4/4/4	-
2	EDO	E	601	-	-	1/1/1/1	-
3	GOL	H	601	-	-	2/4/4/4	-
3	GOL	F	602	-	-	2/4/4/4	-
2	EDO	B	601	-	-	1/1/1/1	-
2	EDO	D	602	-	-	1/1/1/1	-
3	GOL	F	603	-	-	2/4/4/4	-
2	EDO	C	605	-	-	1/1/1/1	-
2	EDO	E	602	-	-	0/1/1/1	-
3	GOL	E	605	-	-	2/4/4/4	-
3	GOL	B	604	-	-	3/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	FLC	CB-CBC	5.85	1.59	1.53
4	D	601	FLC	CB-CBC	2.62	1.56	1.53
4	C	601	FLC	CA-CB	-2.10	1.51	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	FLC	OB2-CBC-CB	5.37	123.44	113.14
4	C	601	FLC	CA-CB-CBC	5.30	121.76	110.03
4	C	601	FLC	OB2-CBC-OB1	-5.15	107.38	123.86
4	C	601	FLC	OA2-CAC-OA1	-4.05	112.91	123.33
4	C	601	FLC	OA2-CAC-CA	3.93	126.78	114.35
4	D	601	FLC	OB2-CBC-CB	3.81	120.46	113.14
4	C	601	FLC	OB1-CBC-CB	3.57	129.02	122.09
4	C	601	FLC	OHB-CB-CG	-3.21	102.06	109.38
3	G	603	GOL	O2-C2-C3	2.67	120.24	109.18
3	E	604	GOL	O1-C1-C2	2.49	121.59	110.38
4	C	601	FLC	OHB-CB-CA	-2.36	103.99	109.38
3	A	604	GOL	O2-C2-C1	-2.22	99.98	109.18
4	D	601	FLC	OB2-CBC-OB1	-2.17	116.92	123.86
4	C	601	FLC	OHB-CB-CBC	2.08	111.91	108.96
3	C	609	GOL	C3-C2-C1	2.03	119.24	111.80

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	GOL	O1-C1-C2-C3
3	A	604	GOL	C1-C2-C3-O3
3	B	603	GOL	O1-C1-C2-C3
3	C	609	GOL	C1-C2-C3-O3
3	C	609	GOL	O2-C2-C3-O3
3	E	603	GOL	O1-C1-C2-C3
3	E	603	GOL	C1-C2-C3-O3
3	E	604	GOL	O1-C1-C2-C3
3	E	605	GOL	O1-C1-C2-C3
3	F	602	GOL	O1-C1-C2-C3
3	F	603	GOL	C1-C2-C3-O3
3	G	603	GOL	C1-C2-C3-O3
4	C	601	FLC	CG-CB-CBC-OB1
4	C	601	FLC	CG-CB-CBC-OB2
4	C	601	FLC	OHB-CB-CBC-OB1
4	C	601	FLC	OHB-CB-CBC-OB2
4	D	601	FLC	CAC-CA-CB-CBC
4	D	601	FLC	CAC-CA-CB-CG
4	D	601	FLC	CAC-CA-CB-OHB
4	D	601	FLC	CG-CB-CBC-OB1
4	D	601	FLC	CG-CB-CBC-OB2

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Mol	Chain	Res	Type	Atoms
4	D	601	FLC	OHB-CB-CBC-OB1
4	D	601	FLC	OHB-CB-CBC-OB2
4	C	601	FLC	CAC-CA-CB-CBC
4	C	601	FLC	CAC-CA-CB-CG
3	E	605	GOL	O1-C1-C2-O2
3	D	603	GOL	O2-C2-C3-O3
3	F	602	GOL	O1-C1-C2-O2
3	H	601	GOL	O1-C1-C2-O2
3	H	602	GOL	O2-C2-C3-O3
3	B	604	GOL	C1-C2-C3-O3
3	D	603	GOL	O1-C1-C2-C3
3	D	603	GOL	C1-C2-C3-O3
3	H	601	GOL	O1-C1-C2-C3
3	H	602	GOL	O1-C1-C2-C3
3	H	602	GOL	C1-C2-C3-O3
3	A	604	GOL	O1-C1-C2-O2
3	A	604	GOL	O2-C2-C3-O3
3	E	603	GOL	O1-C1-C2-O2
3	E	604	GOL	O1-C1-C2-O2
3	F	603	GOL	O2-C2-C3-O3
3	G	603	GOL	O2-C2-C3-O3
4	C	601	FLC	CAC-CA-CB-OHB
2	B	601	EDO	O1-C1-C2-O2
3	B	603	GOL	O1-C1-C2-O2
3	E	603	GOL	O2-C2-C3-O3
2	E	601	EDO	O1-C1-C2-O2
2	D	602	EDO	O1-C1-C2-O2
3	H	602	GOL	O1-C1-C2-O2
2	G	602	EDO	O1-C1-C2-O2
2	C	605	EDO	O1-C1-C2-O2
3	B	604	GOL	O2-C2-C3-O3
4	D	601	FLC	CA-CB-CBC-OB2
3	B	604	GOL	O1-C1-C2-O2
3	G	603	GOL	O1-C1-C2-O2
4	D	601	FLC	CA-CB-CBC-OB1
2	G	601	EDO	O1-C1-C2-O2
4	C	601	FLC	OHB-CB-CG-CGC
2	A	601	EDO	O1-C1-C2-O2
2	A	602	EDO	O1-C1-C2-O2
2	C	602	EDO	O1-C1-C2-O2
2	F	601	EDO	O1-C1-C2-O2

There are no ring outliers.

14 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	603	GOL	1	0
3	H	602	GOL	1	0
2	C	603	EDO	4	0
4	D	601	FLC	2	0
2	F	601	EDO	2	0
2	C	606	EDO	1	0
2	A	602	EDO	2	0
4	C	601	FLC	1	0
2	C	607	EDO	1	0
3	G	603	GOL	1	0
2	E	601	EDO	2	0
2	D	602	EDO	3	0
3	F	603	GOL	1	0
2	C	605	EDO	5	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	516/542 (95%)	-0.32	3 (0%) 85 86	21, 39, 70, 97	0
1	B	414/542 (76%)	-0.30	3 (0%) 84 85	25, 39, 65, 93	0
1	C	514/542 (94%)	-0.38	1 (0%) 91 91	25, 39, 59, 83	0
1	D	479/542 (88%)	-0.13	9 (1%) 66 68	25, 42, 78, 95	0
1	E	518/542 (95%)	-0.30	1 (0%) 91 91	26, 41, 65, 86	0
1	F	406/542 (74%)	0.22	6 (1%) 72 73	34, 52, 81, 96	0
1	G	496/542 (91%)	0.20	13 (2%) 57 60	35, 56, 78, 94	0
1	H	398/542 (73%)	0.18	4 (1%) 79 81	39, 59, 81, 96	0
All	All	3741/4336 (86%)	-0.12	40 (1%) 78 79	21, 46, 75, 97	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	527	TRP	4.5
1	E	25	PHE	4.4
1	G	111	ALA	4.2
1	G	169	VAL	3.8
1	D	23	ALA	3.7
1	D	179	VAL	3.6
1	D	170	TRP	3.4
1	F	111	ALA	3.4
1	D	176	ILE	3.3
1	A	527	TRP	3.2
1	F	275	HIS	3.2
1	H	129	PRO	3.2
1	C	114	PRO	3.1
1	G	135	ILE	2.9
1	F	116	SER	2.8
1	G	165	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	25	PHE	2.8
1	G	527	TRP	2.7
1	D	158	PRO	2.6
1	D	415	PRO	2.6
1	B	131	ILE	2.6
1	F	492	ALA	2.5
1	G	533	TYR	2.5
1	A	182	VAL	2.5
1	H	113	SER	2.5
1	G	233	LEU	2.4
1	B	130	GLU	2.4
1	D	531	GLY	2.4
1	H	495	ALA	2.2
1	G	145	GLU	2.2
1	G	133	THR	2.2
1	G	176	ILE	2.1
1	G	156	VAL	2.1
1	A	166	ALA	2.1
1	G	218	ARG	2.1
1	G	177	VAL	2.1
1	D	218	ARG	2.1
1	D	154	VAL	2.1
1	F	534	THR	2.1
1	H	489	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
3	GOL	A	603	6/6	0.62	0.23	49,64,74,79	0
2	EDO	G	601	4/4	0.72	0.21	52,64,77,77	0
3	GOL	H	602	6/6	0.77	0.16	52,64,75,77	0
3	GOL	F	603	6/6	0.79	0.16	52,66,81,81	0
3	GOL	D	603	6/6	0.79	0.16	47,58,70,70	0
3	GOL	E	605	6/6	0.82	0.14	32,49,59,71	0
3	GOL	E	604	6/6	0.83	0.19	36,50,60,63	0
3	GOL	G	603	6/6	0.84	0.15	44,56,78,82	0
3	GOL	B	603	6/6	0.85	0.12	35,51,67,67	0
3	GOL	B	604	6/6	0.85	0.12	36,50,70,70	0
2	EDO	C	608	4/4	0.85	0.12	48,57,66,68	0
2	EDO	E	602	4/4	0.85	0.11	36,45,55,66	0
3	GOL	A	604	6/6	0.86	0.15	27,44,61,64	0
3	GOL	C	609	6/6	0.86	0.14	28,43,55,55	0
4	FLC	D	601	13/13	0.86	0.10	44,59,72,72	0
2	EDO	F	601	4/4	0.87	0.12	48,58,65,72	0
3	GOL	F	602	6/6	0.87	0.14	43,63,75,80	0
2	EDO	C	602	4/4	0.88	0.18	50,60,69,71	0
3	GOL	E	603	6/6	0.88	0.15	50,64,75,77	0
3	GOL	H	601	6/6	0.89	0.14	51,64,76,76	0
2	EDO	E	601	4/4	0.90	0.14	27,44,53,59	0
2	EDO	A	602	4/4	0.90	0.14	43,55,66,66	0
2	EDO	G	602	4/4	0.90	0.12	42,50,55,56	0
4	FLC	C	601	13/13	0.91	0.11	31,44,54,63	0
2	EDO	C	606	4/4	0.91	0.12	39,47,54,55	0
2	EDO	C	604	4/4	0.92	0.10	41,49,55,57	0
2	EDO	C	603	4/4	0.92	0.15	38,46,56,58	0
2	EDO	B	602	4/4	0.93	0.10	40,48,53,53	0
2	EDO	D	602	4/4	0.94	0.12	37,50,54,65	0
2	EDO	C	605	4/4	0.94	0.13	29,45,54,58	0
2	EDO	B	601	4/4	0.94	0.11	38,45,48,55	0
2	EDO	C	607	4/4	0.94	0.07	43,54,59,68	0
2	EDO	A	601	4/4	0.95	0.07	29,38,49,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.