



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2020 – 06:21 PM EST

PDB ID : 6V3O
Title : Crystal structure of the T-state of maize C4-phosphoenolpyruvate carboxylase in complex with citrate
Authors : Carrizosa-Carbajal, E.I.; Munoz-Clares, R.A.; Gonzalez-Segura, L.
Deposited on : 2019-11-26
Resolution : 2.91 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

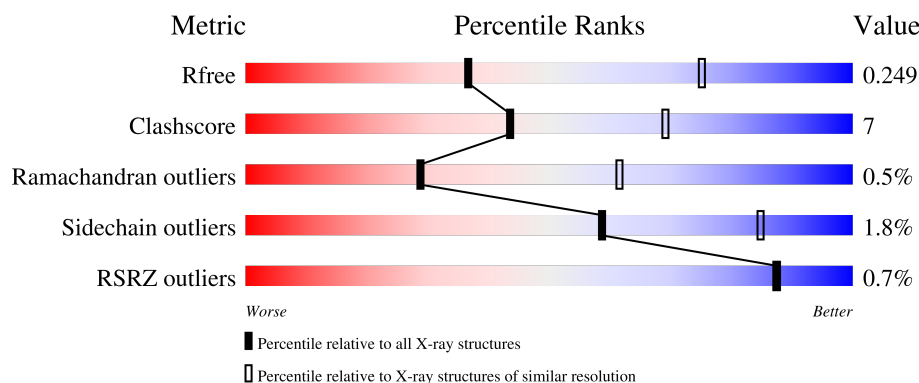
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 Å.

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






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	970	<div> <div>80%</div> <div>16%</div> <div>..</div> </div>
1	B	970	<div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	C	970	<div> <div>%</div> <div>81%</div> <div>15%</div> <div>.</div> </div>
1	D	970	<div> <div>%</div> <div>78%</div> <div>17%</div> <div>.</div> </div>
1	E	970	<div> <div>82%</div> <div>14%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	970	 81% 15% • •
1	G	970	 % 74% 20% • 5%
1	H	970	 % 78% 17% • •

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	SO4	A	1002	-	-	X	-
2	SO4	H	1002	-	-	X	-
3	FLC	C	1003	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 59688 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phosphoenolpyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	940	Total	C	N	O	S	0	0	0
			7488	4748	1307	1403	30			
1	B	942	Total	C	N	O	S	0	0	0
			7479	4737	1309	1403	30			
1	C	930	Total	C	N	O	S	0	0	0
			7390	4680	1294	1386	30			
1	D	927	Total	C	N	O	S	0	0	0
			7366	4665	1290	1381	30			
1	E	942	Total	C	N	O	S	0	0	0
			7502	4755	1310	1407	30			
1	F	944	Total	C	N	O	S	0	0	0
			7496	4748	1312	1406	30			
1	G	925	Total	C	N	O	S	0	0	0
			7359	4661	1289	1379	30			
1	H	930	Total	C	N	O	S	0	0	0
			7394	4684	1294	1386	30			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



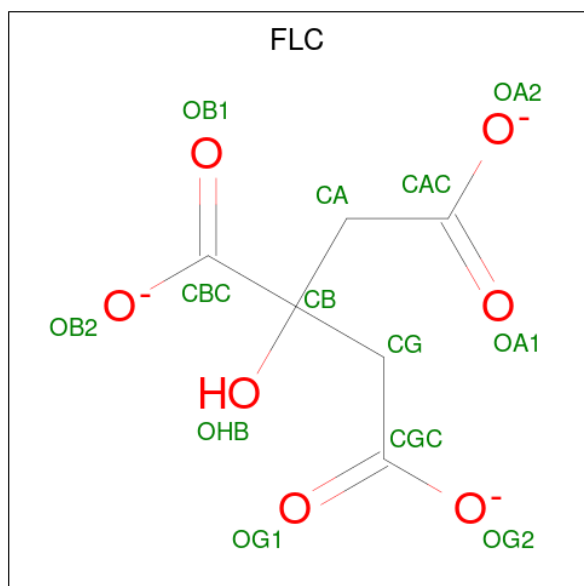
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



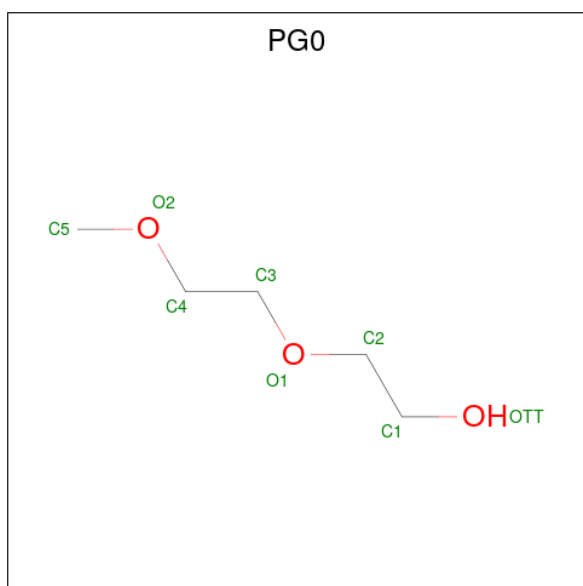
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			13	6	7		
3	E	1	Total	C	O	0	0
			13	6	7		
3	F	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			8	5	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		

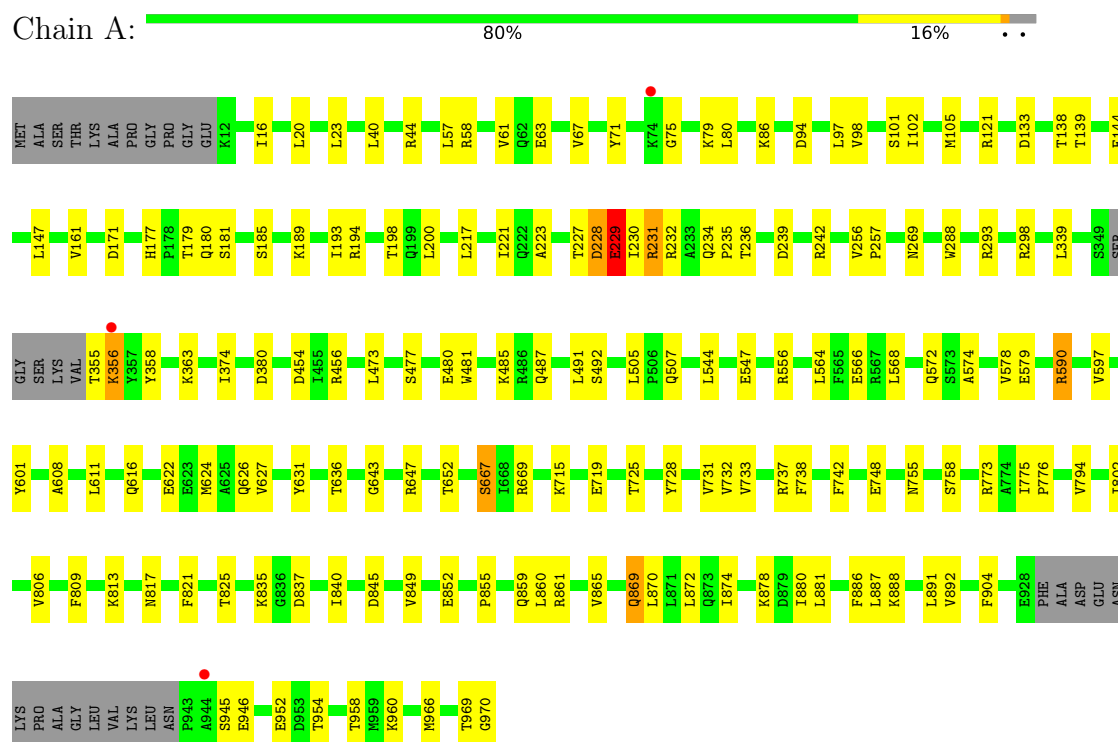
- Molecule 6 is water.

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

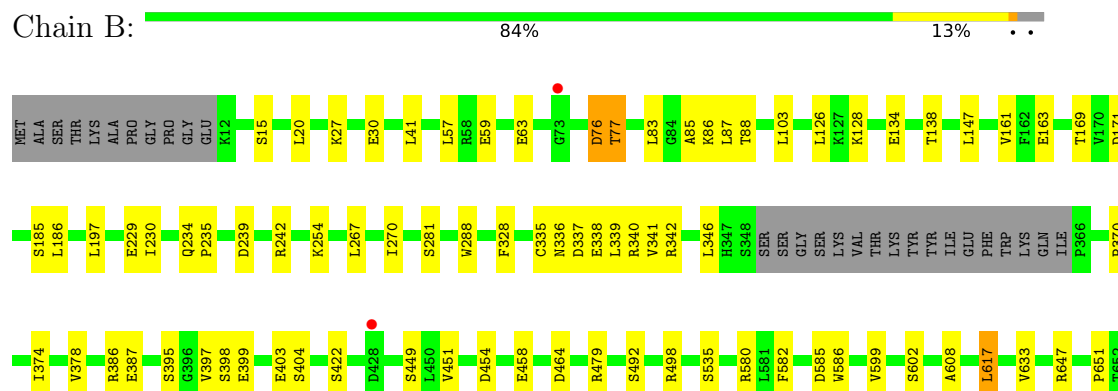
3 Residue-property plots

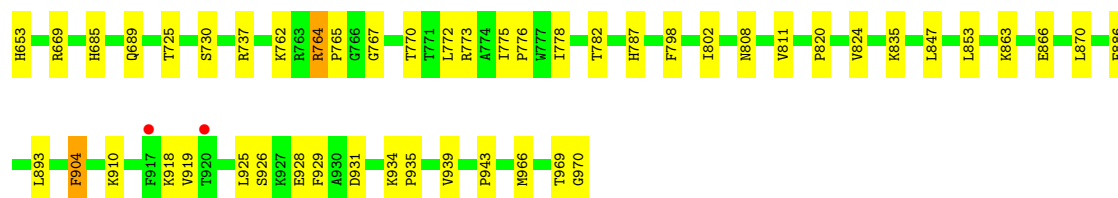
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Phosphoenolpyruvate carboxylase

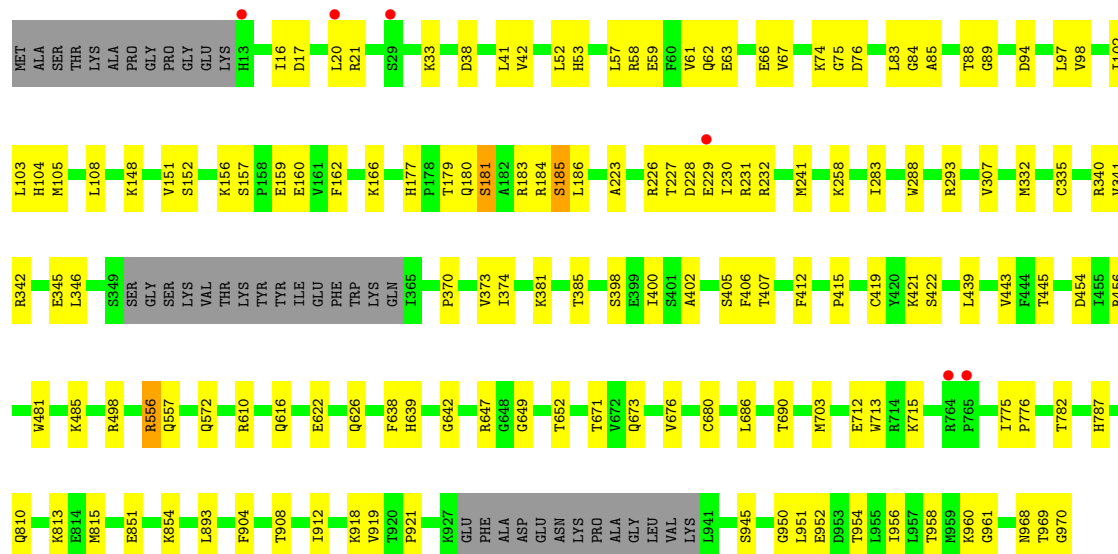
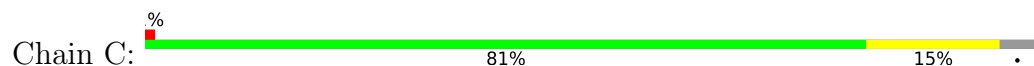


• Molecule 1: Phosphoenolpyruvate carboxylase

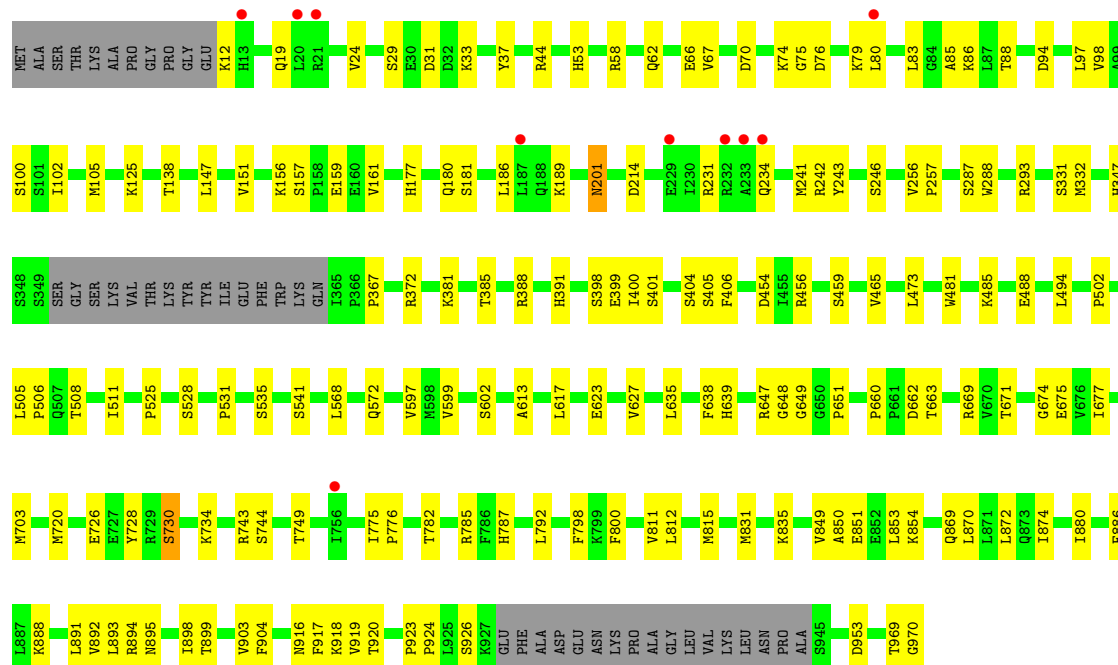
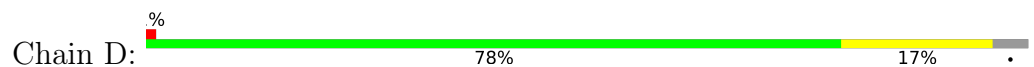





● Molecule 1: Phosphoenolpyruvate carboxylase

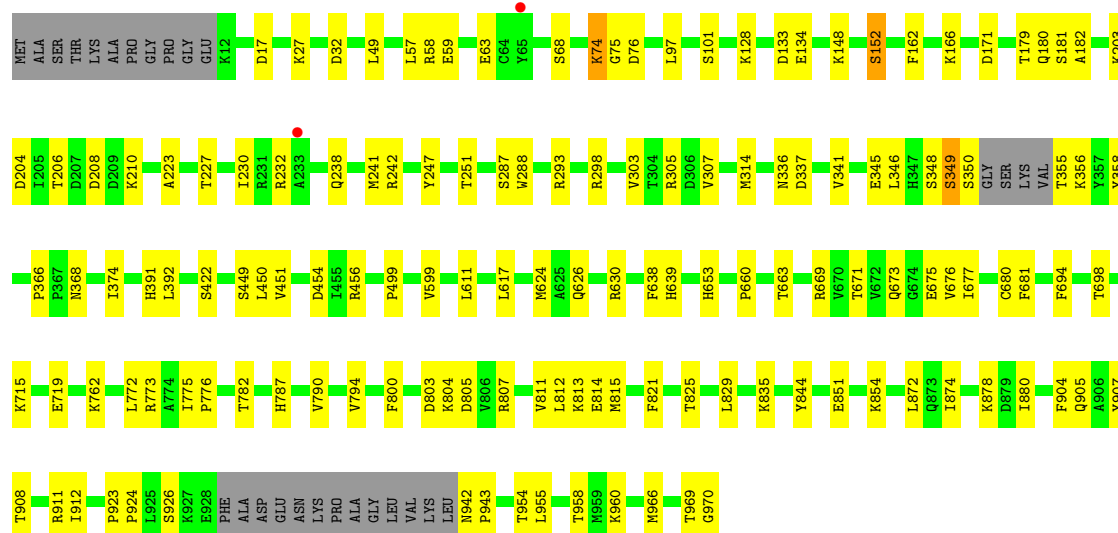


● Molecule 1: Phosphoenolpyruvate carboxylase




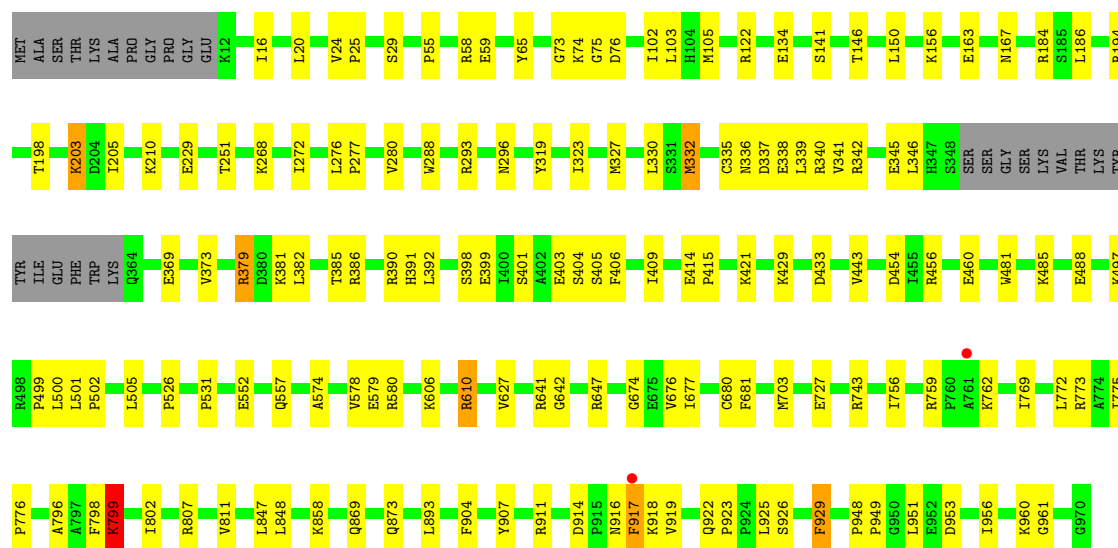
- Molecule 1: Phosphoenolpyruvate carboxylase

Chain E:  82% 14% .




- Molecule 1: Phosphoenolpyruvate carboxylase

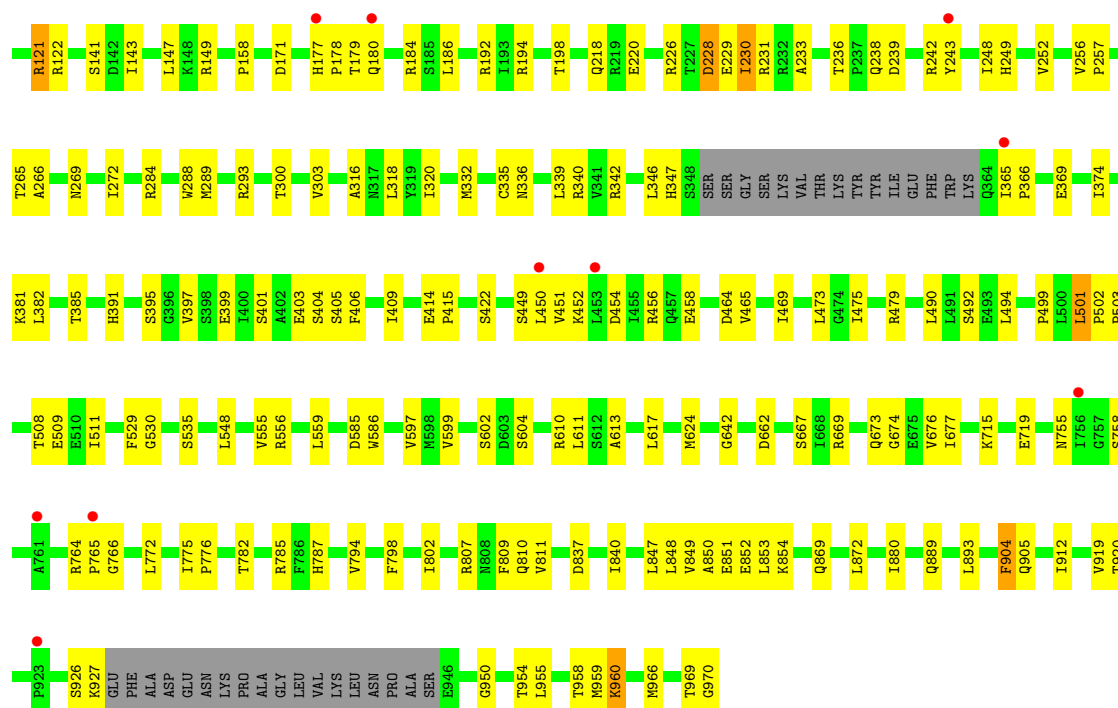
Chain F:  81% 15% . .



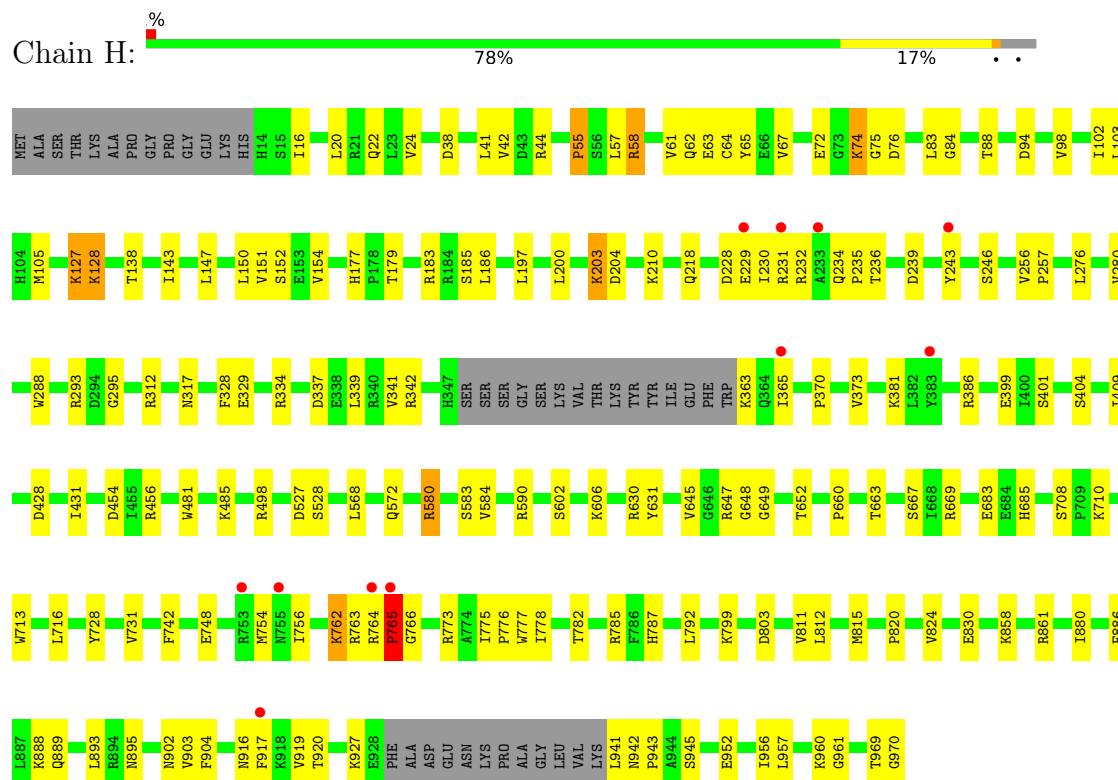
- Molecule 1: Phosphoenolpyruvate carboxylase

Chain G:  74% 20% 5%





● Molecule 1: Phosphoenolpyruvate carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	140.69Å 217.98Å 173.57Å 90.00° 91.05° 90.00°	Depositor
Resolution (Å)	49.20 – 2.91 49.20 – 2.91	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.20-2.91) 93.7 (49.20-2.91)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.218 , 0.249 0.218 , 0.249	Depositor DCC
R_{free} test set	11281 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.198 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	59688	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 2.12% 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: GOL, FLC, SO4, PG0

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	0.30	0/7646	0.47	0/10351
1	B	0.30	0/7635	0.47	0/10339
1	C	0.30	0/7543	0.47	0/10213
1	D	0.31	0/7518	0.48	0/10179
1	E	0.29	0/7660	0.47	0/10371
1	F	0.33	2/7652 (0.0%)	0.48	1/10363 (0.0%)
1	G	0.29	0/7511	0.48	0/10168
1	H	0.54	2/7546 (0.0%)	0.49	3/10217 (0.0%)
All	All	0.34	4/60711 (0.0%)	0.48	4/82201 (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	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	765	PRO	N-CD	-37.80	0.94	1.47
1	F	799	LYS	CE-NZ	11.88	1.78	1.49
1	H	765	PRO	CG-CD	7.87	1.76	1.50
1	F	799	LYS	CD-CE	-5.20	1.38	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	799	LYS	CA-CB-CG	-7.81	96.21	113.40
1	H	765	PRO	CA-CB-CG	-6.63	91.40	104.00
1	H	765	PRO	CB-CG-CD	-6.14	82.55	106.50
1	H	765	PRO	N-CD-CG	-5.06	95.62	103.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	229	GLU	Peptide
1	B	928	GLU	Peptide
1	B	931	ASP	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	7488	0	7474	107	0
1	B	7479	0	7472	77	0
1	C	7390	0	7387	102	0
1	D	7366	0	7360	99	0
1	E	7502	0	7484	84	0
1	F	7496	0	7490	99	1
1	G	7359	0	7356	133	1
1	H	7394	0	7397	118	0
2	A	15	0	0	3	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	15	0	0	0	0
2	E	15	0	0	0	0
2	F	15	0	0	1	0
2	G	15	0	0	0	0
2	H	15	0	0	2	0
3	A	13	0	5	1	0
3	B	26	0	10	4	0
3	C	13	0	5	4	0
3	E	13	0	5	2	0
3	F	13	0	5	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	8	0	12	1	0
5	G	6	0	8	0	0
5	H	6	0	8	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
6	G	2	0	0	0	0
6	H	1	0	0	0	0
All	All	59688	0	59478	801	1

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 (801) 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:H:765:PRO:CD	1:H:765:PRO:CG	1.76	1.57
1:F:799:LYS:CE	1:F:799:LYS:NZ	1.78	1.43
1:A:355:THR:O	1:A:356:LYS:HE2	1.48	1.09
1:F:911:ARG:HH21	1:F:919:VAL:HG11	1.21	1.06
1:H:762:LYS:HD3	1:H:765:PRO:HA	1.38	1.04
1:A:355:THR:O	1:A:356:LYS:CE	2.11	0.97
1:G:177:HIS:HD2	1:G:178:PRO:HD2	1.30	0.96
1:E:782:THR:HG22	1:E:787:HIS:HD2	1.35	0.91
1:G:184:ARG:HH12	1:G:243:TYR:HD1	1.22	0.87
1:D:785:ARG:HH12	1:D:899:THR:HG22	1.39	0.87
1:B:918:LYS:HG2	1:B:919:VAL:O	1.74	0.87
1:G:186:LEU:HD23	1:G:186:LEU:O	1.73	0.87
1:A:355:THR:O	1:A:356:LYS:CD	2.22	0.87
1:A:597:VAL:HG11	1:A:624:MET:HE1	1.57	0.86
1:B:342:ARG:O	1:B:346:LEU:HD12	1.73	0.86
1:B:342:ARG:O	1:B:346:LEU:CD1	2.24	0.85
1:H:762:LYS:CD	1:H:765:PRO:HA	2.05	0.85
1:G:248:ILE:HA	1:G:252:VAL:HG22	1.58	0.85
1:A:491:LEU:HD11	1:A:544:LEU:HD13	1.59	0.84
1:A:568:LEU:HD11	1:A:608:ALA:HB3	1.59	0.83
1:F:799:LYS:CD	1:F:799:LYS:NZ	2.44	0.80
1:H:16:ILE:HD11	1:H:42:VAL:HG21	1.62	0.80
1:C:57:LEU:HD21	1:C:97:LEU:HD22	1.64	0.79
1:D:83:LEU:HA	1:D:86:LYS:HE2	1.65	0.79
1:G:177:HIS:CD2	1:G:178:PRO:HD2	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:335:CYS:HB2	1:F:339:LEU:HD23	1.64	0.79
1:G:764:ARG:HG2	1:G:765:PRO:HD2	1.65	0.78
1:F:102:ILE:HA	1:F:105:MET:HE3	1.65	0.78
1:F:911:ARG:NH2	1:F:919:VAL:HG11	1.97	0.77
1:H:16:ILE:CD1	1:H:42:VAL:HG21	2.14	0.77
1:F:497:LYS:HB2	1:G:473:LEU:HD23	1.67	0.76
1:D:851:GLU:HA	1:D:854:LYS:HG3	1.68	0.76
1:G:339:LEU:HD11	1:G:374:ILE:HG13	1.68	0.76
1:F:911:ARG:HE	1:F:919:VAL:CG2	1.99	0.76
1:B:762:LYS:HB3	1:B:772:LEU:HA	1.68	0.75
1:G:336:ASN:OD1	1:G:422:SER:HA	1.86	0.75
1:A:339:LEU:HD11	1:A:374:ILE:HG13	1.67	0.74
1:G:469:ILE:HD11	1:G:501:LEU:HD12	1.69	0.73
1:G:88:THR:HB	1:G:919:VAL:HG11	1.69	0.73
1:B:599:VAL:HB	1:B:617:LEU:HD11	1.70	0.72
1:F:203:LYS:H	1:F:203:LYS:HD2	1.55	0.72
1:E:782:THR:HG22	1:E:787:HIS:CD2	2.23	0.72
1:H:203:LYS:HD2	1:H:204:ASP:HB2	1.70	0.72
1:G:764:ARG:HH21	1:G:766:GLY:HA3	1.55	0.71
1:F:296:ASN:HB2	1:F:759:ARG:HG3	1.73	0.71
1:A:355:THR:O	1:A:356:LYS:HD3	1.89	0.71
1:C:16:ILE:CD1	1:C:42:VAL:HG21	2.21	0.70
1:D:256:VAL:HG23	1:D:257:PRO:HD3	1.72	0.70
1:H:24:VAL:HG21	1:H:889:GLN:HG3	1.72	0.70
1:F:399:GLU:HG3	1:G:399:GLU:HG3	1.74	0.70
1:C:556:ARG:NH1	1:C:557:GLN:HE22	1.90	0.70
1:C:102:ILE:HA	1:C:105:MET:HE3	1.74	0.69
1:C:16:ILE:HD11	1:C:42:VAL:HG21	1.74	0.69
1:B:582:PHE:CE2	1:B:633:VAL:HG21	2.27	0.69
1:F:337:ASP:OD1	1:F:338:GLU:N	2.26	0.69
1:B:772:LEU:HD13	1:B:773:ARG:N	2.07	0.69
1:C:20:LEU:HD22	1:C:893:LEU:HD22	1.76	0.68
1:B:782:THR:HG22	1:B:787:HIS:HD2	1.56	0.68
1:E:835:LYS:HB3	1:E:966:MET:HE1	1.74	0.68
1:D:37:TYR:HE1	1:D:201:ASN:OD1	1.76	0.68
1:F:251:THR:HG21	1:F:681:PHE:O	1.94	0.68
1:H:762:LYS:HD2	1:H:765:PRO:HB3	1.75	0.68
1:H:295:GLY:HA3	1:H:773:ARG:NH2	2.08	0.67
1:A:945:SER:OG	1:A:952:GLU:OE1	2.09	0.67
1:G:490:LEU:O	1:G:494:LEU:HD12	1.94	0.67
1:H:941:LEU:HD13	1:H:942:ASN:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:LEU:C	1:G:186:LEU:HD23	2.15	0.67
1:G:602:SER:OG	1:G:970:GLY:OXT	2.11	0.67
1:A:234:GLN:HE21	1:A:755:ASN:HD22	1.43	0.66
1:F:526:PRO:HG3	1:F:557:GLN:HG3	1.77	0.66
1:H:916:ASN:O	1:H:917:PHE:HB3	1.95	0.66
1:D:505:LEU:HD12	1:D:506:PRO:HD2	1.77	0.66
1:B:772:LEU:HD13	1:B:773:ARG:O	1.96	0.66
1:D:385:THR:HG22	1:D:406:PHE:H	1.61	0.65
1:F:917:PHE:O	1:F:919:VAL:HG23	1.96	0.65
1:F:385:THR:HG22	1:F:406:PHE:H	1.62	0.65
1:H:63:GLU:O	1:H:67:VAL:HG23	1.97	0.65
1:A:888:LYS:O	1:A:892:VAL:HG23	1.96	0.64
1:D:186:LEU:HD12	1:D:189:LYS:HD2	1.79	0.64
1:C:680:CYS:HB3	1:C:690:THR:HG21	1.79	0.64
1:G:785:ARG:HD2	1:G:966:MET:HE2	1.79	0.64
1:H:83:LEU:HD23	1:H:903:VAL:HG21	1.80	0.64
1:B:835:LYS:HB3	1:B:966:MET:HE1	1.80	0.64
1:C:374:ILE:HD11	1:C:419:CYS:SG	2.37	0.64
1:H:428:ASP:HB3	1:H:431:ILE:HD12	1.79	0.63
1:C:223:ALA:O	1:C:227:THR:HG23	1.97	0.63
1:D:85:ALA:O	1:D:88:THR:OG1	2.15	0.63
1:E:251:THR:HG21	1:E:681:PHE:O	1.98	0.63
1:B:847:LEU:O	1:B:910:LYS:HE2	1.99	0.63
1:B:186:LEU:HD13	1:B:229:GLU:HG3	1.80	0.63
1:B:782:THR:HG22	1:B:787:HIS:CD2	2.33	0.63
1:G:905:GLN:HB2	1:G:958:THR:HG21	1.81	0.63
1:A:230:ILE:HG22	1:A:232:ARG:N	2.14	0.63
1:C:228:ASP:OD2	1:C:230:ILE:HG13	1.98	0.63
1:H:38:ASP:O	1:H:42:VAL:HG22	1.99	0.63
1:F:911:ARG:HE	1:F:919:VAL:HG21	1.63	0.63
1:H:41:LEU:HD21	1:H:197:LEU:HD13	1.80	0.62
1:C:157:SER:HB3	1:C:160:GLU:HG3	1.81	0.62
1:E:232:ARG:HE	1:E:943:PRO:HD2	1.63	0.62
1:B:242:ARG:NH2	3:B:1003:FLC:HG1	2.14	0.62
1:E:59:GLU:O	1:E:63:GLU:HG3	1.99	0.62
1:A:647:ARG:NE	3:A:1004:FLC:OA1	2.31	0.62
1:B:939:VAL:CG1	1:B:943:PRO:HA	2.29	0.62
1:G:121:ARG:HH12	1:H:204:ASP:HB3	1.65	0.62
1:A:236:THR:HG23	1:A:239:ASP:H	1.65	0.62
1:G:385:THR:HG22	1:G:405:SER:HB3	1.82	0.62
1:H:229:GLU:HG3	1:H:957:LEU:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:674:GLY:O	1:D:677:ILE:HG22	2.00	0.62
1:E:49:LEU:HD11	1:E:57:LEU:HD22	1.82	0.62
1:A:102:ILE:HA	1:A:105:MET:HE2	1.81	0.62
1:F:385:THR:CG2	1:F:406:PHE:H	2.13	0.61
1:H:127:LYS:O	1:H:128:LYS:HB2	1.98	0.61
1:C:556:ARG:HG3	1:C:557:GLN:OE1	1.99	0.61
1:E:969:THR:OG1	1:E:970:GLY:N	2.33	0.61
1:H:16:ILE:HB	1:H:65:TYR:HE2	1.63	0.61
1:B:20:LEU:HD22	1:B:893:LEU:HD22	1.83	0.61
1:D:177:HIS:HD2	1:D:180:GLN:H	1.46	0.61
1:H:317:ASN:HD21	1:H:386:ARG:HH11	1.48	0.61
1:C:227:THR:HG21	1:D:331:SER:OG	2.01	0.61
1:E:499:PRO:O	1:H:498:ARG:NH1	2.33	0.61
1:C:341:VAL:O	1:C:345:GLU:HG3	2.00	0.61
1:G:50:GLN:HE21	1:G:58:ARG:HH11	1.49	0.61
1:E:872:LEU:HD21	1:E:880:ILE:HD12	1.81	0.61
1:D:102:ILE:HA	1:D:105:MET:HE3	1.81	0.60
1:G:385:THR:CG2	1:G:406:PHE:H	2.14	0.60
1:A:57:LEU:HD21	1:A:97:LEU:HD22	1.83	0.60
1:C:639:HIS:O	1:C:671:THR:HG23	2.01	0.60
1:H:317:ASN:HD21	1:H:386:ARG:NH1	1.99	0.60
1:C:180:GLN:OE1	1:C:960:LYS:HD3	2.02	0.60
1:G:597:VAL:HG21	1:G:624:MET:HE1	1.83	0.60
1:C:104:HIS:NE2	1:C:229:GLU:OE1	2.34	0.60
1:D:870:LEU:O	1:D:874:ILE:HD12	2.01	0.60
1:A:230:ILE:HG22	1:A:232:ARG:H	1.67	0.60
1:E:391:HIS:ND1	1:H:399:GLU:OE2	2.35	0.60
1:E:639:HIS:O	1:E:671:THR:HG23	2.01	0.60
1:A:177:HIS:CE1	1:A:180:GLN:HB2	2.37	0.60
1:B:342:ARG:O	1:B:346:LEU:HD13	2.01	0.60
1:C:38:ASP:O	1:C:42:VAL:HG22	2.01	0.60
1:E:954:THR:O	1:E:958:THR:HG23	2.01	0.60
1:A:234:GLN:NE2	1:A:755:ASN:HD22	2.00	0.60
1:A:802:ILE:HG23	1:A:809:PHE:HB2	1.83	0.59
1:C:385:THR:CG2	1:C:406:PHE:H	2.15	0.59
1:H:370:PRO:O	1:H:373:VAL:HG12	2.01	0.59
1:F:399:GLU:OE2	1:G:391:HIS:ND1	2.34	0.59
1:D:24:VAL:HG12	1:D:892:VAL:HG21	1.85	0.59
1:G:464:ASP:OD1	1:G:479:ARG:NH2	2.31	0.59
1:F:847:LEU:HB2	1:F:848:LEU:HD22	1.85	0.59
1:F:580:ARG:HG3	1:F:580:ARG:HH11	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:347:HIS:CE1	1:G:365:ILE:HD11	2.38	0.59
1:G:494:LEU:HD11	1:G:548:LEU:HB2	1.83	0.59
1:H:55:PRO:O	1:H:58:ARG:N	2.35	0.59
1:B:647:ARG:NH2	3:B:1004:FLC:OA1	2.36	0.59
1:B:764:ARG:HG2	1:B:765:PRO:HD2	1.85	0.59
1:C:968:ASN:HD21	3:C:1003:FLC:HA2	1.68	0.59
1:D:62:GLN:O	1:D:66:GLU:HG3	2.02	0.59
1:D:639:HIS:O	1:D:671:THR:HG23	2.02	0.59
1:G:465:VAL:HG22	1:G:511:ILE:HG23	1.84	0.59
1:C:231:ARG:HH12	1:C:960:LYS:NZ	2.01	0.58
1:H:20:LEU:HD22	1:H:893:LEU:HD22	1.84	0.58
1:D:37:TYR:CE1	1:D:201:ASN:OD1	2.57	0.58
1:H:61:VAL:HG12	1:H:98:VAL:HG13	1.85	0.58
1:B:339:LEU:HD21	1:B:370:PRO:HB2	1.85	0.58
1:E:345:GLU:O	1:E:348:SER:OG	2.19	0.58
1:F:501:LEU:HD13	1:F:502:PRO:O	2.04	0.58
1:G:851:GLU:HA	1:G:854:LYS:HG3	1.85	0.58
1:H:74:LYS:O	1:H:76:ASP:N	2.34	0.58
1:A:636:THR:HG1	1:A:667:SER:HG	1.25	0.58
1:G:385:THR:HG22	1:G:406:PHE:H	1.68	0.58
1:D:177:HIS:CD2	1:D:180:GLN:HB3	2.39	0.58
1:E:179:THR:HG23	1:E:180:GLN:HG2	1.85	0.58
1:G:177:HIS:ND1	1:G:180:GLN:HB3	2.18	0.58
1:A:715:LYS:O	1:A:719:GLU:HG3	2.04	0.58
1:E:676:VAL:HG12	1:E:680:CYS:SG	2.44	0.58
1:B:498:ARG:HB2	1:D:473:LEU:HD13	1.85	0.58
1:D:19:GLN:OE1	1:D:66:GLU:HA	2.04	0.58
1:F:342:ARG:NH1	1:F:346:LEU:HD21	2.19	0.58
1:F:429:LYS:HE3	1:F:433:ASP:OD2	2.03	0.58
1:G:336:ASN:OD1	1:G:422:SER:CA	2.51	0.58
1:G:236:THR:HG23	1:G:239:ASP:H	1.68	0.57
1:E:206:THR:HG22	1:E:208:ASP:H	1.69	0.57
1:F:956:ILE:HG22	1:F:960:LYS:HD2	1.86	0.57
1:C:918:LYS:HG2	1:C:919:VAL:N	2.20	0.57
1:E:821:PHE:O	1:E:825:THR:HG23	2.05	0.57
1:D:388:ARG:NH1	1:D:400:ILE:O	2.37	0.57
1:F:20:LEU:HD22	1:F:893:LEU:HD22	1.87	0.56
1:H:710:LYS:HE2	1:H:713:TRP:CZ2	2.40	0.56
1:A:568:LEU:HD11	1:A:608:ALA:CB	2.32	0.56
1:A:636:THR:OG1	1:A:667:SER:OG	2.06	0.56
1:G:798:PHE:O	1:G:802:ILE:HG12	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:626:GLN:O	1:E:630:ARG:HG3	2.04	0.56
1:H:337:ASP:O	1:H:341:VAL:HG13	2.05	0.56
1:H:762:LYS:HD2	1:H:765:PRO:CB	2.35	0.56
1:D:181:SER:HB2	1:D:243:TYR:CE2	2.41	0.56
1:F:156:LYS:HE3	1:F:703:MET:HB3	1.87	0.56
1:B:336:ASN:HB3	1:B:339:LEU:H	1.70	0.56
1:D:568:LEU:O	1:D:572:GLN:HG3	2.06	0.56
1:C:62:GLN:O	1:C:66:GLU:HG3	2.05	0.56
1:F:727:GLU:OE2	1:F:796:ALA:HB2	2.04	0.56
1:C:556:ARG:HG3	1:C:557:GLN:NE2	2.21	0.56
1:D:157:SER:OG	1:D:159:GLU:HG3	2.04	0.56
1:C:969:THR:OG1	1:C:970:GLY:N	2.38	0.56
1:D:508:THR:HG23	1:D:511:ILE:H	1.71	0.56
1:E:206:THR:HG22	1:E:208:ASP:N	2.21	0.56
1:F:869:GLN:O	1:F:873:GLN:HG2	2.06	0.56
1:G:905:GLN:HB2	1:G:958:THR:CG2	2.36	0.56
1:B:41:LEU:HD21	1:B:197:LEU:HD13	1.88	0.56
1:C:374:ILE:CD1	1:C:419:CYS:SG	2.93	0.56
1:C:556:ARG:HH11	1:C:557:GLN:HE22	1.51	0.56
1:D:812:LEU:HA	1:D:815:MET:HE2	1.87	0.56
1:E:241:MET:HG3	1:E:307:VAL:HG13	1.88	0.56
1:H:72:GLU:OE2	1:H:895:ASN:ND2	2.32	0.56
1:C:67:VAL:HG21	1:C:83:LEU:HD13	1.88	0.56
1:F:409:ILE:HD12	1:F:409:ILE:H	1.71	0.56
1:G:837:ASP:OD2	1:G:840:ILE:HG13	2.06	0.56
1:A:742:PHE:CZ	1:A:748:GLU:HG3	2.42	0.55
1:D:74:LYS:O	1:D:76:ASP:N	2.38	0.55
1:E:790:VAL:HG12	1:E:829:LEU:HD23	1.88	0.55
1:C:385:THR:HG22	1:C:405:SER:HB3	1.87	0.55
1:C:810:GLN:HG2	1:C:813:LYS:HE3	1.88	0.55
1:A:71:TYR:CD1	1:A:80:LEU:HD11	2.41	0.55
1:B:335:CYS:HB2	1:B:339:LEU:HD22	1.88	0.55
1:C:556:ARG:HG3	1:C:557:GLN:CD	2.26	0.55
1:H:812:LEU:HA	1:H:815:MET:HE2	1.89	0.55
1:G:17:ASP:OD1	1:G:18:ALA:N	2.40	0.55
1:B:969:THR:OG1	1:B:970:GLY:N	2.38	0.55
1:C:810:GLN:HE21	1:C:813:LYS:NZ	2.04	0.55
1:G:382:LEU:O	1:G:385:THR:OG1	2.24	0.55
1:H:94:ASP:O	1:H:98:VAL:HG23	2.07	0.55
1:C:918:LYS:HG2	1:C:919:VAL:H	1.71	0.55
1:G:192:ARG:NH2	1:H:329:GLU:HG2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:ARG:HG2	1:D:456:ARG:O	2.07	0.55
1:G:950:GLY:O	1:G:954:THR:HG22	2.07	0.55
1:C:951:LEU:HA	1:C:954:THR:HG22	1.89	0.55
1:H:102:ILE:HA	1:H:105:MET:HE3	1.89	0.54
1:B:235:PRO:HB2	1:B:239:ASP:HB2	1.90	0.54
1:B:27:LYS:HE2	1:B:30:GLU:HA	1.90	0.54
1:G:179:THR:O	1:G:960:LYS:HE2	2.07	0.54
1:H:830:GLU:HG3	1:H:880:ILE:HG13	1.88	0.54
1:F:163:GLU:O	1:F:167:ASN:ND2	2.38	0.54
1:F:922:GLN:HG2	1:F:923:PRO:HD2	1.88	0.54
1:G:342:ARG:O	1:G:346:LEU:HD22	2.08	0.54
1:C:908:THR:O	1:C:912:ILE:HG13	2.07	0.54
1:H:228:ASP:OD1	1:H:230:ILE:HG12	2.07	0.54
1:H:230:ILE:HG13	1:H:232:ARG:HG2	1.90	0.54
1:A:872:LEU:HD21	1:A:880:ILE:HD12	1.89	0.54
1:C:945:SER:OG	1:C:952:GLU:OE1	2.24	0.54
1:F:336:ASN:O	1:F:340:ARG:HB2	2.07	0.54
1:E:238:GLN:O	1:E:242:ARG:HG3	2.07	0.54
1:E:803:ASP:HB2	1:E:804:LYS:NZ	2.22	0.54
1:E:811:VAL:O	1:E:815:MET:HG3	2.07	0.54
1:B:685:HIS:O	1:B:689:GLN:HG2	2.08	0.54
1:B:85:ALA:O	1:B:88:THR:OG1	2.26	0.53
1:C:686:LEU:O	1:C:690:THR:HG23	2.08	0.53
1:F:727:GLU:OE2	1:F:796:ALA:CB	2.56	0.53
1:A:235:PRO:O	1:A:298:ARG:NH1	2.41	0.53
1:D:385:THR:CG2	1:D:406:PHE:H	2.21	0.53
1:G:50:GLN:NE2	1:G:58:ARG:HH11	2.05	0.53
1:H:236:THR:HG23	1:H:239:ASP:H	1.73	0.53
1:D:744:SER:HB2	1:D:849:VAL:HG12	1.90	0.53
1:E:805:ASP:OD2	1:E:807:ARG:NH1	2.42	0.53
1:D:775:ILE:HB	1:D:776:PRO:HD3	1.90	0.53
1:E:908:THR:O	1:E:912:ILE:HG13	2.08	0.53
1:C:400:ILE:HD12	1:C:400:ILE:H	1.73	0.53
1:E:305:ARG:NH2	1:E:392:LEU:O	2.40	0.53
1:G:919:VAL:HG22	1:G:920:THR:H	1.74	0.53
1:D:80:LEU:HB3	1:D:903:VAL:HG11	1.90	0.53
1:G:288:TRP:CD1	1:G:454:ASP:HB2	2.44	0.53
1:A:194:ARG:O	1:A:198:THR:HG23	2.09	0.53
1:A:20:LEU:HA	1:A:23:LEU:HD12	1.90	0.53
1:A:887:LEU:O	1:A:891:LEU:HG	2.09	0.53
1:D:782:THR:HG23	1:D:787:HIS:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:366:PRO:HB2	1:G:369:GLU:HG3	1.91	0.53
1:G:772:LEU:HD11	1:G:776:PRO:HB2	1.90	0.53
1:D:177:HIS:HD2	1:D:180:GLN:N	2.07	0.53
1:D:831:MET:SD	1:D:835:LYS:HE2	2.48	0.53
1:D:969:THR:OG1	1:D:970:GLY:N	2.41	0.53
1:G:238:GLN:O	1:G:242:ARG:HG3	2.09	0.53
1:G:905:GLN:CB	1:G:958:THR:HG21	2.39	0.53
1:H:401:SER:O	1:H:404:SER:OG	2.24	0.53
1:F:341:VAL:O	1:F:345:GLU:HG3	2.09	0.52
1:F:342:ARG:O	1:F:346:LEU:HG	2.09	0.52
1:H:183:ARG:HB2	2:H:1002:SO4:O3	2.09	0.52
1:H:234:GLN:HG3	1:H:235:PRO:HD2	1.91	0.52
1:C:381:LYS:O	1:C:385:THR:HG23	2.08	0.52
1:D:647:ARG:O	1:D:649:GLY:N	2.37	0.52
1:A:57:LEU:O	1:A:61:VAL:HG23	2.09	0.52
1:D:347:HIS:NE2	1:D:367:PRO:HB3	2.25	0.52
1:F:392:LEU:HD22	1:F:398:SER:HB2	1.91	0.52
1:G:228:ASP:O	1:G:229:GLU:HB3	2.09	0.52
1:B:939:VAL:HG12	1:B:943:PRO:HA	1.90	0.52
1:C:782:THR:HG23	1:C:787:HIS:HE1	1.73	0.52
1:F:381:LYS:O	1:F:385:THR:HG23	2.10	0.52
1:A:180:GLN:HG3	1:A:960:LYS:HG3	1.91	0.52
1:C:647:ARG:HB3	3:C:1003:FLC:OA1	2.09	0.52
1:F:323:ILE:HG22	1:F:327:MET:HE2	1.91	0.52
1:A:647:ARG:O	1:A:652:THR:OG1	2.23	0.52
1:G:20:LEU:HA	1:G:23:LEU:HD12	1.92	0.52
1:G:785:ARG:HD2	1:G:966:MET:CE	2.39	0.52
1:A:293:ARG:HG2	1:A:456:ARG:O	2.10	0.52
1:C:908:THR:HG23	1:C:951:LEU:HD22	1.92	0.52
1:D:916:ASN:O	1:D:917:PHE:HB3	2.10	0.52
1:E:337:ASP:O	1:E:341:VAL:HG13	2.10	0.52
1:G:192:ARG:HH22	1:H:329:GLU:HG2	1.74	0.52
1:E:203:LYS:HG3	1:E:204:ASP:N	2.25	0.51
1:A:16:ILE:HD12	1:A:20:LEU:HD21	1.92	0.51
1:C:610:ARG:NH2	1:C:642:GLY:O	2.39	0.51
1:G:807:ARG:O	1:G:811:VAL:HG23	2.10	0.51
1:A:229:GLU:OE2	1:A:230:ILE:HG13	2.10	0.51
1:E:775:ILE:HB	1:E:776:PRO:HD3	1.92	0.51
1:H:568:LEU:HD21	1:H:572:GLN:OE1	2.11	0.51
1:E:812:LEU:HA	1:E:815:MET:HE2	1.93	0.51
1:G:872:LEU:HD21	1:G:880:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:527:ASP:OD1	1:H:527:ASP:N	2.43	0.51
1:D:459:SER:OG	1:D:535:SER:O	2.25	0.51
1:H:811:VAL:O	1:H:815:MET:HG3	2.10	0.51
1:C:181:SER:H	1:C:231:ARG:NH2	2.09	0.51
1:G:265:THR:O	1:G:269:ASN:ND2	2.39	0.51
1:E:762:LYS:HG2	1:E:772:LEU:HA	1.92	0.51
1:E:358:TYR:O	1:F:386:ARG:NH2	2.44	0.51
1:G:184:ARG:HH11	1:G:184:ARG:HG3	1.74	0.51
1:C:572:GLN:HE21	1:C:616:GLN:NE2	2.09	0.51
1:D:623:GLU:O	1:D:627:VAL:HG23	2.10	0.51
1:D:147:LEU:HD22	1:D:161:VAL:HG11	1.92	0.51
1:G:230:ILE:HD12	1:G:231:ARG:HE	1.76	0.51
1:H:150:LEU:HA	1:H:154:VAL:HG22	1.93	0.51
1:H:312:ARG:NH1	1:H:528:SER:OG	2.44	0.51
1:A:732:VAL:HG23	1:A:738:PHE:CE2	2.46	0.51
1:E:912:ILE:HD12	1:E:955:LEU:HD22	1.93	0.51
1:B:820:PRO:O	1:B:824:VAL:HG13	2.12	0.50
1:C:103:LEU:HD13	1:C:961:GLY:HA2	1.93	0.50
1:E:223:ALA:O	1:E:227:THR:HG23	2.11	0.50
1:F:647:ARG:HH21	3:F:1004:FLC:CGC	2.24	0.50
1:B:798:PHE:O	1:B:802:ILE:HG12	2.11	0.50
1:E:336:ASN:HB2	1:E:422:SER:HB2	1.92	0.50
1:G:473:LEU:HB2	1:G:475:ILE:HD12	1.92	0.50
1:H:276:LEU:HG	1:H:280:VAL:HG21	1.91	0.50
1:A:568:LEU:CD1	1:A:608:ALA:HB3	2.38	0.50
1:A:861:ARG:O	1:A:865:VAL:HG13	2.10	0.50
1:C:227:THR:CG2	1:D:331:SER:OG	2.59	0.50
1:D:892:VAL:HG23	1:D:893:LEU:HG	1.93	0.50
1:H:293:ARG:HG2	1:H:456:ARG:O	2.11	0.50
1:A:622:GLU:O	1:A:626:GLN:HG2	2.11	0.50
1:C:88:THR:HB	1:C:919:VAL:HG21	1.93	0.50
1:D:917:PHE:C	1:D:918:LYS:HD2	2.32	0.50
1:H:762:LYS:CD	1:H:765:PRO:CA	2.84	0.50
1:G:184:ARG:NH1	1:G:243:TYR:HD1	2.02	0.50
1:C:88:THR:HB	1:C:919:VAL:HG11	1.94	0.50
1:G:802:ILE:HD12	1:G:809:PHE:HD1	1.76	0.50
1:H:454:ASP:OD2	1:H:669:ARG:NH2	2.39	0.50
1:B:83:LEU:O	1:B:86:LYS:HG2	2.12	0.50
1:C:63:GLU:O	1:C:67:VAL:HG13	2.11	0.50
1:C:88:THR:OG1	1:C:89:GLY:N	2.45	0.50
1:D:381:LYS:O	1:D:385:THR:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:847:LEU:HB2	1:G:848:LEU:HD22	1.93	0.50
1:G:85:ALA:O	1:G:88:THR:OG1	2.30	0.50
1:H:481:TRP:HB3	1:H:485:LYS:HB3	1.94	0.50
1:A:564:LEU:HG	1:A:566:GLU:HG3	1.93	0.50
1:G:782:THR:HG22	1:G:787:HIS:ND1	2.25	0.50
1:B:57:LEU:HD12	1:B:925:LEU:HD23	1.92	0.49
1:D:156:LYS:HE3	1:D:703:MET:HB3	1.92	0.49
1:D:894:ARG:O	1:D:898:ILE:HG13	2.12	0.49
1:E:293:ARG:HG2	1:E:456:ARG:O	2.12	0.49
1:G:102:ILE:O	1:G:106:LEU:HD12	2.12	0.49
1:E:715:LYS:O	1:E:719:GLU:HG3	2.12	0.49
1:A:732:VAL:HG13	1:A:733:VAL:HG23	1.94	0.49
1:B:464:ASP:OD1	1:B:479:ARG:NH1	2.39	0.49
1:C:231:ARG:CZ	1:C:231:ARG:HB2	2.42	0.49
1:E:773:ARG:O	1:E:776:PRO:HD2	2.13	0.49
1:G:256:VAL:HG23	1:G:257:PRO:HD3	1.93	0.49
1:H:580:ARG:O	1:H:584:VAL:HG23	2.12	0.49
1:A:773:ARG:NE	2:A:1001:SO4:O4	2.37	0.49
1:A:728:TYR:O	1:A:732:VAL:HG12	2.13	0.49
1:C:53:HIS:CE1	1:C:97:LEU:HD11	2.47	0.49
1:D:385:THR:HG22	1:D:405:SER:HB2	1.93	0.49
1:E:74:LYS:O	1:E:76:ASP:N	2.46	0.49
1:G:529:PHE:HB2	1:G:559:LEU:HD21	1.93	0.49
1:H:568:LEU:CD2	1:H:572:GLN:OE1	2.60	0.49
1:F:775:ILE:HB	1:F:776:PRO:HD3	1.94	0.49
1:G:599:VAL:HB	1:G:617:LEU:HD21	1.95	0.49
1:H:969:THR:OG1	1:H:970:GLY:N	2.35	0.49
1:F:74:LYS:O	1:F:76:ASP:N	2.45	0.49
1:G:121:ARG:HH22	1:H:204:ASP:HB3	1.78	0.49
1:B:339:LEU:CD2	1:B:370:PRO:HB2	2.41	0.49
1:D:243:TYR:O	1:D:246:SER:OG	2.31	0.49
1:D:919:VAL:HG22	1:D:920:THR:H	1.78	0.49
1:F:756:ILE:HD11	1:F:956:ILE:HG12	1.95	0.49
1:A:969:THR:OG1	1:A:970:GLY:N	2.45	0.49
1:B:737:ARG:HB3	1:B:853:LEU:HD21	1.94	0.49
1:F:146:THR:O	1:F:150:LEU:HD23	2.13	0.49
1:G:110:ASN:O	1:G:114:GLU:HG3	2.13	0.49
1:C:162:PHE:O	1:C:166:LYS:HG3	2.13	0.49
1:D:888:LYS:O	1:D:892:VAL:HG13	2.13	0.49
3:E:1004:FLC:OG2	3:E:1004:FLC:OHB	2.29	0.49
1:A:185:SER:OG	2:A:1002:SO4:S	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:O	1:A:44:ARG:HG2	2.13	0.48
1:A:574:ALA:O	1:A:578:VAL:HG23	2.13	0.48
1:A:835:LYS:HB3	1:A:966:MET:CE	2.43	0.48
1:F:390:ARG:HH21	1:F:391:HIS:CD2	2.30	0.48
1:G:395:SER:OG	1:G:397:VAL:O	2.31	0.48
1:B:808:ASN:O	1:B:811:VAL:HG12	2.13	0.48
1:C:385:THR:HG22	1:C:406:PHE:H	1.77	0.48
1:D:29:SER:OG	1:D:31:ASP:OD1	2.31	0.48
1:D:872:LEU:HD21	1:D:880:ILE:HD12	1.94	0.48
1:F:369:GLU:O	1:F:373:VAL:HG23	2.13	0.48
1:G:192:ARG:NH1	1:G:220:GLU:OE2	2.47	0.48
1:H:602:SER:HB3	1:H:778:ILE:HD11	1.95	0.48
1:A:94:ASP:O	1:A:98:VAL:HG23	2.13	0.48
1:E:180:GLN:HB3	1:E:960:LYS:NZ	2.28	0.48
1:D:288:TRP:CD1	1:D:454:ASP:HB2	2.47	0.48
1:D:651:PRO:HD2	4:D:1001:PG0:H53	1.95	0.48
1:D:531:PRO:HG3	1:D:669:ARG:HH12	1.78	0.48
1:E:813:LYS:HG2	1:E:874:ILE:O	2.12	0.48
1:F:798:PHE:O	1:F:802:ILE:HG12	2.14	0.48
1:A:138:THR:HG21	1:A:886:PHE:CG	2.49	0.48
1:A:775:ILE:HB	1:A:776:PRO:HD3	1.95	0.48
1:C:370:PRO:HA	1:C:373:VAL:HG12	1.96	0.48
1:H:952:GLU:O	1:H:956:ILE:HG13	2.14	0.48
1:A:835:LYS:HB3	1:A:966:MET:HE1	1.95	0.48
1:G:381:LYS:O	1:G:385:THR:HG23	2.12	0.48
1:G:715:LYS:O	1:G:719:GLU:HG3	2.14	0.48
1:F:382:LEU:O	1:F:385:THR:OG1	2.27	0.48
1:A:217:LEU:O	1:A:221:ILE:HG13	2.14	0.48
1:D:256:VAL:CG2	1:D:257:PRO:HD3	2.43	0.48
1:D:599:VAL:HB	1:D:617:LEU:HD21	1.96	0.48
1:E:349:SER:O	1:E:350:SER:HB2	2.13	0.48
1:B:337:ASP:O	1:B:341:VAL:HG13	2.14	0.48
1:E:356:LYS:HD3	1:F:390:ARG:NH1	2.28	0.48
1:A:147:LEU:HD22	1:A:161:VAL:HG11	1.96	0.48
1:C:335:CYS:SG	1:C:340:ARG:HB2	2.54	0.48
1:C:84:GLY:O	1:C:88:THR:HG23	2.13	0.48
1:A:356:LYS:HA	1:A:356:LYS:HD3	1.70	0.47
1:A:611:LEU:HB2	1:A:794:VAL:HG12	1.96	0.47
1:C:52:LEU:HD11	1:C:226:ARG:CZ	2.44	0.47
1:D:743:ARG:HD2	1:D:749:THR:CG2	2.44	0.47
1:H:339:LEU:HD21	1:H:370:PRO:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:58:ARG:NH2	1:H:62:GLN:OE1	2.42	0.47
1:A:855:PRO:O	1:A:859:GLN:HG3	2.14	0.47
1:C:968:ASN:OD1	3:C:1003:FLC:HG1	2.15	0.47
1:D:53:HIS:CD2	1:D:97:LEU:HD21	2.49	0.47
1:F:194:ARG:O	1:F:198:THR:HG23	2.13	0.47
1:G:508:THR:HG23	1:G:511:ILE:H	1.78	0.47
1:H:647:ARG:C	1:H:652:THR:HG23	2.35	0.47
1:B:775:ILE:HB	1:B:776:PRO:HD3	1.97	0.47
1:E:148:LYS:O	1:E:152:SER:HB3	2.15	0.47
1:E:807:ARG:O	1:E:811:VAL:HG23	2.15	0.47
1:G:194:ARG:O	1:G:198:THR:HG23	2.14	0.47
1:G:316:ALA:O	1:G:320:ILE:HG12	2.14	0.47
1:H:731:VAL:CG2	1:H:792:LEU:HD21	2.44	0.47
1:D:660:PRO:HB2	1:D:663:THR:HG21	1.96	0.47
1:H:147:LEU:O	1:H:151:VAL:HG23	2.14	0.47
1:C:713:TRP:CD1	1:C:815:MET:HE2	2.50	0.47
1:G:585:ASP:OD1	1:G:586:TRP:N	2.47	0.47
1:H:606:LYS:HD3	1:H:777:TRP:CG	2.49	0.47
1:C:52:LEU:HD11	1:C:226:ARG:NE	2.29	0.47
1:F:319:TYR:CE1	1:F:443:VAL:HG12	2.48	0.47
1:G:226:ARG:CZ	1:H:334:ARG:HH11	2.27	0.47
1:C:952:GLU:O	1:C:956:ILE:HG12	2.15	0.47
1:E:804:LYS:HA	1:E:804:LYS:HD3	1.59	0.47
1:E:844:TYR:OH	1:E:905:GLN:NE2	2.48	0.47
1:H:365:ILE:O	1:H:365:ILE:HD12	2.14	0.47
1:H:55:PRO:O	1:H:57:LEU:N	2.47	0.47
1:B:288:TRP:CD1	1:B:454:ASP:HB2	2.49	0.47
1:E:355:THR:O	1:E:355:THR:HG22	2.14	0.47
1:F:911:ARG:HE	1:F:919:VAL:HG22	1.74	0.47
1:G:401:SER:O	1:G:404:SER:OG	2.20	0.47
1:G:955:LEU:O	1:G:958:THR:HB	2.15	0.47
1:G:969:THR:OG1	1:G:970:GLY:N	2.42	0.47
1:A:954:THR:O	1:A:958:THR:HG23	2.15	0.47
1:D:44:ARG:NE	1:D:214:ASP:OD1	2.48	0.47
1:D:181:SER:HB2	1:D:243:TYR:CD2	2.50	0.47
1:F:186:LEU:HD13	1:F:229:GLU:HG3	1.97	0.47
1:H:84:GLY:O	1:H:88:THR:OG1	2.33	0.47
1:B:76:ASP:OD1	1:B:77:THR:N	2.46	0.47
1:D:94:ASP:O	1:D:98:VAL:HG23	2.14	0.47
1:E:303:VAL:O	1:E:307:VAL:HG23	2.14	0.47
1:G:674:GLY:HA2	1:G:677:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:GLN:HG3	1:A:870:LEU:N	2.31	0.46
1:D:465:VAL:HG22	1:D:511:ILE:HG23	1.97	0.46
1:A:845:ASP:HA	1:A:849:VAL:HG23	1.97	0.46
1:D:401:SER:O	1:D:404:SER:OG	2.21	0.46
1:E:660:PRO:HB2	1:E:663:THR:HG21	1.97	0.46
1:F:332:MET:N	1:F:332:MET:SD	2.88	0.46
1:F:401:SER:O	1:F:404:SER:OG	2.27	0.46
1:G:94:ASP:O	1:G:98:VAL:HG23	2.15	0.46
1:B:185:SER:HG	3:B:1003:FLC:CAC	2.28	0.46
1:F:73:GLY:O	1:F:74:LYS:HG2	2.15	0.46
1:H:44:ARG:HG2	1:H:218:GLN:HG2	1.98	0.46
1:B:336:ASN:HB2	1:B:422:SER:HB2	1.96	0.46
1:C:151:VAL:HG13	1:C:156:LYS:O	2.15	0.46
1:D:241:MET:HG3	1:D:242:ARG:N	2.29	0.46
1:D:850:ALA:HB3	1:D:853:LEU:HD12	1.97	0.46
1:D:835:LYS:HG2	1:D:891:LEU:HD13	1.98	0.46
1:E:288:TRP:CD1	1:E:454:ASP:HB2	2.50	0.46
1:G:409:ILE:H	1:G:409:ILE:HD12	1.81	0.46
1:H:64:CYS:SG	1:H:83:LEU:HD11	2.56	0.46
1:H:231:ARG:HG2	1:H:960:LYS:HE3	1.97	0.46
1:A:568:LEU:O	1:A:572:GLN:HG3	2.15	0.46
1:B:458:GLU:HA	1:B:535:SER:HB2	1.97	0.46
1:C:775:ILE:HB	1:C:776:PRO:HD3	1.97	0.46
1:E:366:PRO:HB2	1:E:368:ASN:OD1	2.16	0.46
1:H:742:PHE:CZ	1:H:748:GLU:HG3	2.49	0.46
1:A:608:ALA:HB1	1:A:725:THR:HG23	1.97	0.46
1:C:177:HIS:CE1	1:C:179:THR:HG22	2.51	0.46
1:C:185:SER:HB2	1:D:372:ARG:HH22	1.81	0.46
1:D:895:ASN:O	1:D:899:THR:HG23	2.15	0.46
1:F:481:TRP:HB3	1:F:485:LYS:HB3	1.97	0.46
1:F:103:LEU:HD13	1:F:961:GLY:HA2	1.98	0.46
1:G:852:GLU:HG3	1:G:853:LEU:HG	1.97	0.46
1:H:763:ARG:HG2	1:H:773:ARG:NH2	2.30	0.46
1:H:785:ARG:HD2	1:H:902:ASN:OD1	2.16	0.46
1:E:203:LYS:HG3	1:E:204:ASP:H	1.81	0.46
1:E:851:GLU:HA	1:E:854:LYS:HD2	1.97	0.46
1:G:912:ILE:HD12	1:G:955:LEU:HD22	1.97	0.46
1:B:608:ALA:HB1	1:B:725:THR:HG23	1.98	0.46
1:D:12:LYS:O	1:D:58:ARG:NH1	2.49	0.46
1:E:638:PHE:CE1	1:E:671:THR:HG22	2.51	0.46
1:F:647:ARG:HE	3:F:1004:FLC:CGC	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:VAL:HG21	1:D:83:LEU:HD13	1.96	0.46
1:D:787:HIS:CE1	1:D:835:LYS:O	2.69	0.46
1:F:916:ASN:O	1:F:917:PHE:HB2	2.16	0.46
1:H:143:ILE:O	1:H:147:LEU:HG	2.15	0.46
1:H:799:LYS:HE2	1:H:803:ASP:OD1	2.16	0.46
1:A:189:LYS:O	1:A:193:ILE:HG13	2.16	0.45
1:A:228:ASP:N	1:A:228:ASP:OD1	2.49	0.45
1:B:234:GLN:HG2	1:B:235:PRO:HD2	1.98	0.45
1:B:772:LEU:CD1	1:B:773:ARG:O	2.62	0.45
1:C:283:ILE:O	1:C:445:THR:HG23	2.16	0.45
1:F:676:VAL:HG12	1:F:680:CYS:SG	2.56	0.45
1:F:914:ASP:HB2	1:F:916:ASN:OD1	2.16	0.45
1:G:143:ILE:O	1:G:147:LEU:HD13	2.16	0.45
1:H:339:LEU:HD23	1:H:339:LEU:C	2.35	0.45
1:H:775:ILE:HB	1:H:776:PRO:HD3	1.98	0.45
1:E:811:VAL:HA	1:E:814:GLU:HG2	1.97	0.45
1:F:574:ALA:O	1:F:578:VAL:HG23	2.15	0.45
1:G:508:THR:OG1	1:G:509:GLU:N	2.49	0.45
1:B:147:LEU:HD22	1:B:161:VAL:HG11	1.98	0.45
1:B:773:ARG:O	1:B:776:PRO:HD2	2.15	0.45
1:C:74:LYS:O	1:C:76:ASP:N	2.49	0.45
3:E:1004:FLC:OA2	3:E:1004:FLC:OHB	2.33	0.45
1:E:673:GLN:NE2	1:E:675:GLU:OE2	2.50	0.45
1:F:610:ARG:NH2	1:F:642:GLY:O	2.48	0.45
1:G:186:LEU:CD2	1:G:186:LEU:C	2.85	0.45
1:H:782:THR:HG22	1:H:787:HIS:ND1	2.32	0.45
1:B:59:GLU:O	1:B:63:GLU:HG3	2.16	0.45
3:F:1004:FLC:OHB	3:F:1004:FLC:OG1	2.34	0.45
1:F:414:GLU:HB3	1:F:415:PRO:HD3	1.98	0.45
1:G:955:LEU:O	1:G:959:MET:HG3	2.16	0.45
1:H:243:TYR:O	1:H:246:SER:OG	2.32	0.45
1:A:177:HIS:ND1	1:A:180:GLN:HB2	2.31	0.45
1:F:403:GLU:OE1	1:F:403:GLU:N	2.42	0.45
1:A:133:ASP:O	1:A:139:THR:OG1	2.35	0.45
1:E:599:VAL:HB	1:E:617:LEU:HD21	1.99	0.45
1:H:16:ILE:HB	1:H:65:TYR:CE2	2.48	0.45
1:A:358:TYR:OH	1:A:380:ASP:OD1	2.12	0.45
1:B:934:LYS:HB2	1:B:935:PRO:HD3	1.99	0.45
1:C:647:ARG:C	1:C:652:THR:HG23	2.37	0.45
1:F:276:LEU:HG	1:F:280:VAL:HG21	1.99	0.45
1:H:754:MET:HB2	1:H:756:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:LYS:HG2	1:D:404:SER:O	2.16	0.45
1:E:134:GLU:O	1:E:653:HIS:HB3	2.17	0.45
1:F:911:ARG:NH1	1:F:951:LEU:HD21	2.31	0.45
1:C:293:ARG:HG2	1:C:456:ARG:O	2.17	0.45
1:F:421:LYS:HE3	1:F:421:LYS:HB2	1.55	0.45
1:F:674:GLY:O	1:F:677:ILE:HG22	2.16	0.45
1:G:16:ILE:HD12	1:G:65:TYR:CE2	2.52	0.45
1:A:102:ILE:HD13	1:A:105:MET:HE1	1.99	0.44
1:A:231:ARG:HD3	1:A:231:ARG:O	2.16	0.44
1:C:288:TRP:CD1	1:C:454:ASP:HB2	2.52	0.44
1:C:61:VAL:HG22	1:C:98:VAL:HG23	1.99	0.44
1:F:580:ARG:HH11	1:F:580:ARG:CG	2.29	0.44
1:G:21:ARG:HE	1:G:35:ILE:HG21	1.81	0.44
1:G:764:ARG:HH21	1:G:766:GLY:CA	2.28	0.44
1:H:16:ILE:HD13	1:H:42:VAL:HG21	1.98	0.44
1:A:547:GLU:OE1	1:A:590:ARG:NH2	2.49	0.44
1:E:762:LYS:HB3	1:E:762:LYS:HE3	1.78	0.44
1:C:481:TRP:HB3	1:C:485:LYS:HB3	1.99	0.44
1:D:812:LEU:HD23	1:D:815:MET:CE	2.47	0.44
1:G:284:ARG:HB3	1:G:452:LYS:NZ	2.32	0.44
1:H:409:ILE:HD12	1:H:409:ILE:H	1.82	0.44
1:B:126:LEU:O	1:B:128:LYS:HE3	2.18	0.44
1:B:87:LEU:HD22	1:B:904:PHE:CE2	2.52	0.44
1:D:811:VAL:O	1:D:815:MET:HG3	2.17	0.44
1:F:606:LYS:HE2	1:F:769:ILE:HG22	1.99	0.44
1:G:24:VAL:HG21	1:G:889:GLN:HG3	1.99	0.44
1:B:342:ARG:HG3	1:B:346:LEU:CD1	2.47	0.44
1:B:399:GLU:HG3	1:D:399:GLU:HG3	2.00	0.44
1:A:71:TYR:OH	1:A:837:ASP:OD1	2.35	0.44
1:B:337:ASP:HA	1:B:340:ARG:NH1	2.33	0.44
1:C:148:LYS:O	1:C:152:SER:HB3	2.18	0.44
1:C:919:VAL:O	1:C:921:PRO:HD3	2.18	0.44
1:E:346:LEU:HD12	1:E:374:ILE:HD13	2.00	0.44
1:F:499:PRO:HB2	1:G:499:PRO:HB2	1.99	0.44
1:G:775:ILE:HB	1:G:776:PRO:HD3	1.99	0.44
1:H:256:VAL:HG22	1:H:257:PRO:HD3	1.99	0.44
1:H:647:ARG:O	1:H:649:GLY:N	2.51	0.44
1:A:737:ARG:NH2	1:A:852:GLU:HG3	2.33	0.44
1:B:171:ASP:OD2	1:B:669:ARG:HD2	2.18	0.44
1:E:162:PHE:O	1:E:166:LYS:HG3	2.18	0.44
1:F:205:ILE:HD11	1:F:210:LYS:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:293:ARG:HG2	1:F:456:ARG:O	2.17	0.44
1:A:878:LYS:N	1:A:878:LYS:HD2	2.33	0.44
1:B:138:THR:HG21	1:B:886:PHE:CG	2.53	0.44
1:C:41:LEU:HD22	1:C:108:LEU:HD22	2.00	0.44
1:C:59:GLU:O	1:C:63:GLU:HG3	2.18	0.44
1:C:622:GLU:O	1:C:626:GLN:HG3	2.18	0.44
1:D:726:GLU:O	1:D:730:SER:HB3	2.17	0.44
1:E:878:LYS:HA	1:E:878:LYS:HD2	1.71	0.44
1:F:454:ASP:OD1	1:F:531:PRO:HD2	2.18	0.44
1:H:764:ARG:O	1:H:766:GLY:N	2.50	0.44
1:H:858:LYS:HD2	1:H:861:ARG:HH21	1.82	0.44
1:A:229:GLU:OE2	1:A:229:GLU:HA	2.18	0.43
1:A:477:SER:HB3	1:A:480:GLU:CD	2.38	0.43
1:A:813:LYS:O	1:A:817:ASN:ND2	2.47	0.43
1:F:579:GLU:HB2	1:F:627:VAL:HG21	2.00	0.43
1:G:44:ARG:HD2	1:G:218:GLN:HG2	2.00	0.43
1:H:683:GLU:OE1	1:H:685:HIS:N	2.51	0.43
1:A:298:ARG:CZ	1:A:758:SER:HB3	2.48	0.43
1:E:27:LYS:HB3	1:E:32:ASP:HB3	1.99	0.43
1:E:314:MET:HB2	1:E:314:MET:HE2	1.63	0.43
1:G:449:SER:O	1:G:451:VAL:N	2.52	0.43
1:G:458:GLU:HA	1:G:535:SER:HB2	2.00	0.43
1:B:169:THR:HG23	1:B:281:SER:O	2.18	0.43
1:B:267:LEU:HA	1:B:270:ILE:HG12	2.00	0.43
1:C:94:ASP:O	1:C:98:VAL:HG12	2.19	0.43
1:C:954:THR:O	1:C:958:THR:HG23	2.17	0.43
1:G:86:LYS:HD3	1:G:86:LYS:HA	1.76	0.43
1:D:79:LYS:HD3	1:D:79:LYS:HA	1.78	0.43
1:F:762:LYS:HG3	1:F:772:LEU:HD12	2.01	0.43
1:G:171:ASP:HB3	1:G:669:ARG:HG2	1.99	0.43
1:E:171:ASP:HB3	1:E:669:ARG:HG2	2.00	0.43
1:F:500:LEU:N	1:F:552:GLU:OE1	2.52	0.43
1:A:288:TRP:CD1	1:A:454:ASP:HB2	2.54	0.43
1:C:231:ARG:HH12	1:C:960:LYS:HZ1	1.67	0.43
1:G:256:VAL:CG2	1:G:257:PRO:HD3	2.49	0.43
1:H:630:ARG:HG2	1:H:631:TYR:CD2	2.54	0.43
1:E:694:PHE:O	1:E:698:THR:HG23	2.19	0.43
1:F:184:ARG:NH2	2:F:1003:SO4:O4	2.52	0.43
1:F:807:ARG:O	1:F:811:VAL:HG23	2.19	0.43
1:G:293:ARG:HG2	1:G:456:ARG:O	2.18	0.43
1:G:530:GLY:O	1:G:559:LEU:HD22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:673:GLN:O	1:G:676:VAL:HG22	2.19	0.43
1:B:103:LEU:HD23	1:B:230:ILE:HG21	2.01	0.43
1:F:55:PRO:O	1:F:59:GLU:HG3	2.18	0.43
1:A:171:ASP:HB3	1:A:669:ARG:HG2	2.00	0.43
1:D:602:SER:OG	1:D:970:GLY:O	2.27	0.43
1:E:128:LYS:HE2	1:E:128:LYS:HB3	1.85	0.43
1:G:403:GLU:CD	1:G:403:GLU:H	2.22	0.43
1:G:905:GLN:CG	1:G:958:THR:HG21	2.49	0.43
1:A:339:LEU:CD1	1:A:374:ILE:HG13	2.44	0.42
1:A:481:TRP:HB3	1:A:485:LYS:HB3	2.00	0.42
1:A:870:LEU:O	1:A:874:ILE:HG13	2.19	0.42
1:G:103:LEU:HA	1:G:106:LEU:HD13	2.01	0.42
1:G:889:GLN:O	1:G:893:LEU:HG	2.19	0.42
1:H:381:LYS:HE2	1:H:381:LYS:HB3	1.89	0.42
1:H:812:LEU:HD23	1:H:815:MET:CE	2.48	0.42
1:A:101:SER:O	1:A:105:MET:HG3	2.20	0.42
1:A:487:GLN:O	1:A:491:LEU:HD13	2.19	0.42
1:A:579:GLU:HG3	1:A:627:VAL:HG13	2.01	0.42
1:A:579:GLU:HG2	1:A:631:TYR:HE2	1.84	0.42
1:A:63:GLU:O	1:A:67:VAL:HG23	2.19	0.42
1:B:454:ASP:OD2	1:B:669:ARG:NH2	2.42	0.42
1:E:450:LEU:HA	1:E:450:LEU:HD23	1.86	0.42
1:G:336:ASN:O	1:G:340:ARG:HG3	2.18	0.42
1:H:660:PRO:HB2	1:H:663:THR:HG21	2.01	0.42
1:A:144:GLU:OE1	1:A:269:ASN:ND2	2.46	0.42
1:D:525:PRO:O	1:D:528:SER:OG	2.35	0.42
1:E:835:LYS:HB3	1:E:966:MET:CE	2.45	0.42
1:H:185:SER:HB3	2:H:1002:SO4:O3	2.19	0.42
1:D:473:LEU:HD21	1:D:502:PRO:HG3	2.01	0.42
1:D:720:MET:CE	1:D:798:PHE:HD1	2.32	0.42
1:F:911:ARG:NH2	1:F:919:VAL:CG1	2.77	0.42
1:G:115:VAL:HG13	1:G:198:THR:HG22	2.01	0.42
1:G:849:VAL:HG12	1:G:850:ALA:O	2.19	0.42
1:H:232:ARG:CZ	1:H:232:ARG:HB3	2.49	0.42
1:A:63:GLU:OE1	1:A:86:LYS:NZ	2.53	0.42
1:D:481:TRP:HB3	1:D:485:LYS:HB3	2.02	0.42
1:D:728:TYR:CD1	1:D:792:LEU:HD23	2.55	0.42
1:E:800:PHE:O	1:E:804:LYS:HG2	2.19	0.42
1:H:858:LYS:CD	1:H:861:ARG:HH21	2.32	0.42
1:B:651:PRO:HG2	3:B:1004:FLC:OA1	2.19	0.42
1:C:241:MET:HE2	1:C:307:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:VAL:HA	1:D:156:LYS:O	2.19	0.42
1:G:249:HIS:ND1	1:G:318:LEU:HD11	2.34	0.42
1:G:121:ARG:NH1	1:H:204:ASP:HB3	2.32	0.42
1:B:585:ASP:OD1	1:B:586:TRP:N	2.52	0.42
1:C:17:ASP:OD1	1:C:21:ARG:HD2	2.20	0.42
1:E:230:ILE:HD12	1:E:230:ILE:H	1.84	0.42
1:H:764:ARG:HA	1:H:765:PRO:HD3	1.73	0.42
1:A:568:LEU:CD1	1:A:608:ALA:CB	2.97	0.42
1:A:572:GLN:HG2	1:A:616:GLN:OE1	2.20	0.42
1:H:288:TRP:CD1	1:H:454:ASP:HB2	2.55	0.42
1:H:888:LYS:HE2	1:H:888:LYS:HB3	1.82	0.42
1:A:505:LEU:O	1:A:507:GLN:HG3	2.20	0.42
1:B:386:ARG:NH2	1:B:387:GLU:OE2	2.53	0.42
1:B:602:SER:HB3	1:B:778:ILE:HD11	2.02	0.42
1:C:342:ARG:O	1:C:346:LEU:HG	2.19	0.42
1:E:449:SER:O	1:E:451:VAL:N	2.49	0.42
1:E:624:MET:HE2	1:E:624:MET:HB3	1.94	0.42
1:F:847:LEU:HD11	1:F:907:TYR:CE1	2.55	0.42
1:H:728:TYR:CD1	1:H:792:LEU:HD23	2.55	0.42
1:A:837:ASP:OD1	1:A:840:ILE:HG13	2.20	0.42
1:B:863:LYS:HA	1:B:866:GLU:HG2	2.01	0.42
1:C:157:SER:OG	1:C:159:GLU:OE1	2.37	0.42
1:F:268:LYS:HA	1:F:272:ILE:O	2.20	0.42
1:F:948:PRO:HA	1:F:949:PRO:HD3	1.92	0.42
1:G:147:LEU:HD22	1:G:266:ALA:HB1	2.02	0.42
1:H:919:VAL:HG12	1:H:920:THR:N	2.35	0.42
1:A:256:VAL:CG2	1:A:257:PRO:HD3	2.49	0.41
1:F:330:LEU:HA	1:F:330:LEU:HD23	1.80	0.41
1:G:335:CYS:SG	1:G:340:ARG:HG2	2.60	0.41
1:G:452:LYS:HE2	1:G:452:LYS:HB2	1.84	0.41
1:G:610:ARG:NH2	1:G:642:GLY:O	2.53	0.41
1:C:156:LYS:HE3	1:C:703:MET:HB3	2.00	0.41
1:D:923:PRO:HA	1:D:924:PRO:HD3	1.96	0.41
1:E:247:TYR:O	1:E:251:THR:HG22	2.20	0.41
1:F:340:ARG:HH11	1:F:340:ARG:HG2	1.85	0.41
1:F:288:TRP:CD1	1:F:454:ASP:HB2	2.55	0.41
1:F:485:LYS:HA	1:F:488:GLU:HG2	2.01	0.41
1:H:645:VAL:O	1:H:652:THR:HG22	2.20	0.41
1:A:363:LYS:HE2	1:B:242:ARG:NH1	2.36	0.41
1:B:582:PHE:CZ	1:B:633:VAL:HG21	2.55	0.41
1:C:402:ALA:HB1	1:C:407:THR:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:LYS:HD2	1:C:421:LYS:HA	1.86	0.41
1:E:673:GLN:O	1:E:677:ILE:HG13	2.20	0.41
1:A:731:VAL:HG11	1:A:860:LEU:HD21	2.02	0.41
1:A:821:PHE:O	1:A:825:THR:OG1	2.32	0.41
1:B:338:GLU:O	1:B:341:VAL:HG22	2.20	0.41
1:C:258:LYS:HB3	1:C:258:LYS:HE2	1.67	0.41
1:D:177:HIS:CE1	1:D:675:GLU:HA	2.55	0.41
1:E:97:LEU:O	1:E:101:SER:OG	2.29	0.41
1:H:945:SER:OG	1:H:952:GLU:OE1	2.27	0.41
1:A:579:GLU:HG2	1:A:631:TYR:CE2	2.56	0.41
1:C:673:GLN:O	1:C:676:VAL:HG22	2.20	0.41
1:F:277:PRO:O	1:F:280:VAL:HG22	2.20	0.41
1:F:327:MET:CE	1:F:379:ARG:HD3	2.51	0.41
1:F:773:ARG:O	1:F:776:PRO:HD2	2.20	0.41
1:G:755:ASN:OD1	1:G:758:SER:HA	2.21	0.41
1:B:374:ILE:O	1:B:378:VAL:HG23	2.21	0.41
1:F:134:GLU:OE2	1:F:141:SER:OG	2.37	0.41
1:G:141:SER:OG	1:G:149:ARG:NH2	2.45	0.41
1:G:52:LEU:HD13	1:G:226:ARG:HD3	2.03	0.41
1:A:200:LEU:HD23	1:A:200:LEU:HA	1.82	0.41
1:A:473:LEU:HD22	1:C:498:ARG:HB2	2.03	0.41
1:B:134:GLU:O	1:B:653:HIS:HB3	2.20	0.41
1:B:767:GLY:O	1:B:770:THR:OG1	2.35	0.41
1:C:638:PHE:CE1	1:C:671:THR:HG22	2.56	0.41
1:A:223:ALA:O	1:A:227:THR:HG23	2.21	0.41
1:B:395:SER:OG	1:B:397:VAL:O	2.39	0.41
1:C:181:SER:HB3	1:C:231:ARG:NE	2.35	0.41
1:C:642:GLY:H	1:C:673:GLN:NE2	2.19	0.41
1:D:125:LYS:HG3	1:D:125:LYS:O	2.21	0.41
1:G:29:SER:OG	1:G:31:ASP:OD1	2.37	0.41
1:G:611:LEU:HB2	1:G:794:VAL:HG22	2.03	0.41
1:H:295:GLY:HA3	1:H:773:ARG:HH22	1.85	0.41
1:H:830:GLU:HG3	1:H:880:ILE:CG1	2.51	0.41
1:B:866:GLU:O	1:B:870:LEU:HD13	2.21	0.41
1:C:439:LEU:O	1:C:443:VAL:HG23	2.21	0.41
1:C:851:GLU:HA	1:C:854:LYS:HG3	2.02	0.41
1:G:927:LYS:HD3	1:G:927:LYS:HA	1.88	0.41
1:H:103:LEU:HD13	1:H:961:GLY:HA2	2.03	0.41
1:H:762:LYS:HD2	1:H:765:PRO:CA	2.51	0.41
1:H:820:PRO:O	1:H:824:VAL:HG13	2.21	0.41
1:A:601:TYR:CD2	1:A:643:GLY:HA2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:950:GLY:O	1:C:954:THR:HG22	2.21	0.41
1:D:147:LEU:O	1:D:151:VAL:HG22	2.20	0.41
1:D:638:PHE:CE1	1:D:671:THR:HG22	2.56	0.41
1:E:241:MET:HG3	1:E:307:VAL:CG1	2.49	0.41
1:G:300:THR:O	1:G:303:VAL:HG22	2.20	0.41
1:G:87:LEU:HD22	1:G:904:PHE:CE2	2.56	0.41
1:H:200:LEU:HD23	1:H:210:LYS:HG3	2.01	0.41
1:C:649:GLY:HA3	3:C:1003:FLC:OB2	2.21	0.41
1:E:611:LEU:HB2	1:E:794:VAL:HG12	2.03	0.41
1:E:923:PRO:HA	1:E:924:PRO:HD3	1.98	0.41
1:F:16:ILE:HG23	1:F:65:TYR:CZ	2.56	0.41
1:G:604:SER:HB2	1:G:613:ALA:HB1	2.01	0.41
1:H:317:ASN:OD1	1:H:386:ARG:HD3	2.21	0.41
1:H:716:LEU:HD12	1:H:716:LEU:HA	1.86	0.41
1:B:449:SER:O	1:B:451:VAL:N	2.47	0.40
1:C:85:ALA:HA	1:C:88:THR:CG2	2.51	0.40
1:D:391:HIS:HB2	1:D:398:SER:HB2	2.03	0.40
1:D:494:LEU:HD23	1:D:494:LEU:HA	1.95	0.40
1:G:158:PRO:HB2	1:G:272:ILE:HD11	2.03	0.40
1:G:414:GLU:HB3	1:G:415:PRO:HD3	2.02	0.40
1:G:502:PRO:HA	1:G:503:PRO:HD3	1.99	0.40
1:A:185:SER:OG	2:A:1002:SO4:O1	2.26	0.40
1:D:568:LEU:HD21	1:D:613:ALA:HA	2.02	0.40
1:E:835:LYS:HD3	1:E:966:MET:HE3	2.02	0.40
1:F:327:MET:HE1	1:F:379:ARG:HD3	2.02	0.40
1:F:385:THR:HG22	1:F:405:SER:HB2	2.02	0.40
1:H:177:HIS:CE1	1:H:179:THR:HG22	2.56	0.40
1:A:881:LEU:HB2	1:A:888:LYS:HD3	2.03	0.40
1:C:412:PHE:O	1:C:415:PRO:HD2	2.22	0.40
1:D:597:VAL:HG23	1:D:635:LEU:HD11	2.03	0.40
1:E:907:TYR:O	1:E:911:ARG:HG3	2.20	0.40
1:F:858:LYS:HD3	1:F:858:LYS:HA	1.88	0.40
1:H:812:LEU:HD23	1:H:815:MET:HE1	2.03	0.40
1:H:138:THR:HG21	1:H:886:PHE:CD2	2.56	0.40
1:D:138:THR:HG21	1:D:886:PHE:CG	2.56	0.40
1:A:239:ASP:OD1	1:A:242:ARG:NH1	2.54	0.40
1:C:16:ILE:HD13	1:C:42:VAL:HG21	2.03	0.40
1:G:180:GLN:OE1	1:G:960:LYS:NZ	2.55	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:VAL:O	1:G:810:GLN:NE2[1_655]	2.09	0.11

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	934/970 (96%)	897 (96%)	31 (3%)	6 (1%)	25	58
1	B	938/970 (97%)	905 (96%)	31 (3%)	2 (0%)	47	78
1	C	924/970 (95%)	897 (97%)	24 (3%)	3 (0%)	41	71
1	D	921/970 (95%)	886 (96%)	31 (3%)	4 (0%)	34	66
1	E	936/970 (96%)	905 (97%)	27 (3%)	4 (0%)	34	66
1	F	940/970 (97%)	904 (96%)	31 (3%)	5 (0%)	29	61
1	G	919/970 (95%)	879 (96%)	34 (4%)	6 (1%)	22	54
1	H	924/970 (95%)	883 (96%)	34 (4%)	7 (1%)	19	51
All	All	7436/7760 (96%)	7156 (96%)	243 (3%)	37 (0%)	29	61

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	806	VAL
1	C	75	GLY
1	C	181	SER
1	D	75	GLY
1	D	231	ARG
1	D	926	SER
1	E	75	GLY
1	E	181	SER
1	E	182	ALA
1	E	349	SER
1	F	25	PRO
1	F	75	GLY

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Mol	Chain	Res	Type
1	F	917	PHE
1	F	918	LYS
1	G	228	ASP
1	H	75	GLY
1	H	127	LYS
1	A	228	ASP
1	D	648	GLY
1	G	75	GLY
1	G	555	VAL
1	H	128	LYS
1	A	229	GLU
1	A	356	LYS
1	B	77	THR
1	C	232	ARG
1	H	55	PRO
1	H	943	PRO
1	A	179	THR
1	H	765	PRO
1	B	929	PHE
1	G	230	ILE
1	G	233	ALA
1	G	450	LEU
1	H	648	GLY
1	F	929	PHE
1	A	75	GLY

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	809/832 (97%)	797 (98%)	12 (2%)	65	87
1	B	808/832 (97%)	793 (98%)	15 (2%)	57	84
1	C	800/832 (96%)	787 (98%)	13 (2%)	62	86
1	D	797/832 (96%)	781 (98%)	16 (2%)	55	82
1	E	811/832 (98%)	799 (98%)	12 (2%)	65	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	810/832 (97%)	793 (98%)	17 (2%)	53	81
1	G	796/832 (96%)	782 (98%)	14 (2%)	59	85
1	H	800/832 (96%)	783 (98%)	17 (2%)	53	81
All	All	6431/6656 (97%)	6315 (98%)	116 (2%)	59	85

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ARG
1	A	79	LYS
1	A	121	ARG
1	A	181	SER
1	A	231	ARG
1	A	492	SER
1	A	556	ARG
1	A	590	ARG
1	A	667	SER
1	A	869	GLN
1	A	904	PHE
1	A	946	GLU
1	B	15	SER
1	B	76	ASP
1	B	163	GLU
1	B	254	LYS
1	B	328	PHE
1	B	398	SER
1	B	403	GLU
1	B	404	SER
1	B	492	SER
1	B	580	ARG
1	B	617	LEU
1	B	730	SER
1	B	764	ARG
1	B	904	PHE
1	B	926	SER
1	C	33	LYS
1	C	58	ARG
1	C	183	ARG
1	C	184	ARG
1	C	185	SER
1	C	186	LEU

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Mol	Chain	Res	Type
1	C	332	MET
1	C	398	SER
1	C	422	SER
1	C	556	ARG
1	C	712	GLU
1	C	715	LYS
1	C	904	PHE
1	D	33	LYS
1	D	70	ASP
1	D	100	SER
1	D	201	ASN
1	D	234	GLN
1	D	287	SER
1	D	332	MET
1	D	488	GLU
1	D	541	SER
1	D	662	ASP
1	D	730	SER
1	D	734	LYS
1	D	800	PHE
1	D	869	GLN
1	D	904	PHE
1	D	953	ASP
1	E	17	ASP
1	E	58	ARG
1	E	68	SER
1	E	74	LYS
1	E	133	ASP
1	E	152	SER
1	E	210	LYS
1	E	287	SER
1	E	298	ARG
1	E	904	PHE
1	E	926	SER
1	E	942	ASN
1	F	29	SER
1	F	58	ARG
1	F	122	ARG
1	F	203	LYS
1	F	332	MET
1	F	379	ARG
1	F	460	GLU

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Mol	Chain	Res	Type
1	F	505	LEU
1	F	610	ARG
1	F	641	ARG
1	F	743	ARG
1	F	799	LYS
1	F	904	PHE
1	F	925	LEU
1	F	926	SER
1	F	929	PHE
1	F	953	ASP
1	G	58	ARG
1	G	121	ARG
1	G	122	ARG
1	G	289	MET
1	G	332	MET
1	G	492	SER
1	G	501	LEU
1	G	556	ARG
1	G	662	ASP
1	G	667	SER
1	G	869	GLN
1	G	904	PHE
1	G	926	SER
1	G	960	LYS
1	H	22	GLN
1	H	58	ARG
1	H	74	LYS
1	H	152	SER
1	H	186	LEU
1	H	203	LYS
1	H	328	PHE
1	H	342	ARG
1	H	363	LYS
1	H	580	ARG
1	H	583	SER
1	H	590	ARG
1	H	667	SER
1	H	708	SER
1	H	762	LYS
1	H	904	PHE
1	H	927	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	755	ASN
1	B	472	HIS
1	C	19	GLN
1	C	269	ASN
1	C	557	GLN
1	C	616	GLN
1	C	621	GLN
1	C	673	GLN
1	C	787	HIS
1	C	810	GLN
1	D	177	HIS
1	D	572	GLN
1	D	895	ASN
1	E	269	ASN
1	E	621	GLN
1	E	659	GLN
1	E	905	GLN
1	E	942	ASN
1	F	269	ASN
1	F	869	GLN
1	G	50	GLN
1	G	116	GLN
1	G	177	HIS
1	H	621	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 monosaccharides in this entry.

5.6 Ligand geometry

31 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	SO4	F	1001	-	4,4,4	0.13	0	6,6,6	0.24	0
2	SO4	D	1002	-	4,4,4	0.18	0	6,6,6	0.30	0
2	SO4	H	1004	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	G	1004	-	4,4,4	0.12	0	6,6,6	0.24	0
2	SO4	E	1003	-	4,4,4	0.12	0	6,6,6	0.21	0
2	SO4	H	1002	-	4,4,4	0.19	0	6,6,6	0.30	0
3	FLC	B	1003	-	3,12,12	1.06	0	3,17,17	1.41	1 (33%)
3	FLC	E	1004	-	3,12,12	1.48	0	3,17,17	1.88	1 (33%)
2	SO4	B	1001	-	4,4,4	0.11	0	6,6,6	0.22	0
2	SO4	D	1003	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	C	1002	-	4,4,4	0.14	0	6,6,6	0.22	0
2	SO4	G	1003	-	4,4,4	0.14	0	6,6,6	0.18	0
5	GOL	H	1001	-	5,5,5	0.87	0	5,5,5	0.96	0
2	SO4	G	1002	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	E	1002	-	4,4,4	0.11	0	6,6,6	0.14	0
4	PG0	D	1001	-	7,7,7	0.46	0	6,6,6	0.38	0
2	SO4	B	1002	-	4,4,4	0.11	0	6,6,6	0.24	0
3	FLC	C	1003	-	3,12,12	1.49	0	3,17,17	2.05	1 (33%)
2	SO4	A	1003	-	4,4,4	0.19	0	6,6,6	0.20	0
5	GOL	G	1001	-	5,5,5	0.90	0	5,5,5	0.99	0
3	FLC	F	1004	-	3,12,12	1.84	1 (33%)	3,17,17	2.66	2 (66%)
2	SO4	H	1003	-	4,4,4	0.12	0	6,6,6	0.18	0
2	SO4	D	1004	-	4,4,4	0.14	0	6,6,6	0.19	0
2	SO4	F	1003	-	4,4,4	0.19	0	6,6,6	0.17	0
2	SO4	C	1001	-	4,4,4	0.14	0	6,6,6	0.19	0
3	FLC	B	1004	-	3,12,12	1.85	0	3,17,17	2.37	1 (33%)
2	SO4	E	1001	-	4,4,4	0.14	0	6,6,6	0.15	0
2	SO4	A	1001	-	4,4,4	0.19	0	6,6,6	0.28	0
2	SO4	F	1002	-	4,4,4	0.18	0	6,6,6	0.15	0
2	SO4	A	1002	-	4,4,4	0.15	0	6,6,6	0.19	0
3	FLC	A	1004	-	3,12,12	1.36	0	3,17,17	1.66	1 (33%)

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
5	GOL	H	1001	-	-	2/4/4/4	-
5	GOL	G	1001	-	-	2/4/4/4	-
3	FLC	B	1004	-	-	3/6/16/16	-
3	FLC	B	1003	-	-	4/6/16/16	-
3	FLC	E	1004	-	-	6/6/16/16	-
4	PG0	D	1001	-	-	3/5/5/5	-
3	FLC	F	1004	-	-	3/6/16/16	-
3	FLC	A	1004	-	-	3/6/16/16	-
3	FLC	C	1003	-	-	3/6/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1004	FLC	CG-CB	-2.23	1.51	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1004	FLC	CB-CG-CGC	-4.12	108.38	114.98
3	B	1004	FLC	CB-CA-CAC	-3.89	108.75	114.98
3	C	1003	FLC	CB-CA-CAC	-3.29	109.72	114.98
3	E	1004	FLC	CB-CG-CGC	-3.23	109.82	114.98
3	A	1004	FLC	CB-CA-CAC	-2.41	111.12	114.98
3	B	1003	FLC	CB-CA-CAC	-2.07	111.67	114.98
3	F	1004	FLC	CB-CA-CAC	-2.04	111.72	114.98

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1003	FLC	CAC-CA-CB-CBC
3	B	1003	FLC	CAC-CA-CB-CG
3	B	1003	FLC	CAC-CA-CB-OHB
3	E	1004	FLC	CAC-CA-CB-CBC
3	E	1004	FLC	CAC-CA-CB-CG
3	E	1004	FLC	CAC-CA-CB-OHB

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Mol	Chain	Res	Type	Atoms
3	E	1004	FLC	CBC-CB-CG-CGC
3	C	1003	FLC	CA-CB-CG-CGC
3	C	1003	FLC	CBC-CB-CG-CGC
3	C	1003	FLC	OHB-CB-CG-CGC
5	G	1001	GOL	O1-C1-C2-C3
3	F	1004	FLC	CBC-CB-CG-CGC
3	B	1004	FLC	CA-CB-CG-CGC
3	B	1004	FLC	CBC-CB-CG-CGC
3	B	1004	FLC	OHB-CB-CG-CGC
3	A	1004	FLC	CA-CB-CG-CGC
3	A	1004	FLC	CBC-CB-CG-CGC
3	A	1004	FLC	OHB-CB-CG-CGC
4	D	1001	PG0	OTT-C1-C2-O1
5	H	1001	GOL	O1-C1-C2-C3
5	G	1001	GOL	O1-C1-C2-O2
3	F	1004	FLC	OHB-CB-CG-CGC
3	E	1004	FLC	CA-CB-CG-CGC
3	E	1004	FLC	OHB-CB-CG-CGC
3	F	1004	FLC	CA-CB-CG-CGC
5	H	1001	GOL	O1-C1-C2-O2
3	B	1003	FLC	OHB-CB-CG-CGC
4	D	1001	PG0	C3-C4-O2-C5
4	D	1001	PG0	O1-C3-C4-O2

There are no ring outliers.

11 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1002	SO4	2	0
3	B	1003	FLC	2	0
3	E	1004	FLC	2	0
4	D	1001	PG0	1	0
3	C	1003	FLC	4	0
3	F	1004	FLC	3	0
2	F	1003	SO4	1	0
3	B	1004	FLC	2	0
2	A	1001	SO4	1	0
2	A	1002	SO4	2	0
3	A	1004	FLC	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	940/970 (96%)	0.13	3 (0%) 94 94	41, 58, 79, 98	0
1	B	942/970 (97%)	0.10	4 (0%) 92 93	40, 55, 77, 104	0
1	C	930/970 (95%)	0.15	6 (0%) 89 89	37, 55, 84, 105	0
1	D	927/970 (95%)	0.18	10 (1%) 80 80	41, 61, 86, 109	0
1	E	942/970 (97%)	0.12	2 (0%) 95 95	42, 58, 76, 99	0
1	F	944/970 (97%)	0.11	2 (0%) 95 95	43, 56, 78, 107	0
1	G	925/970 (95%)	0.23	11 (1%) 79 79	42, 66, 91, 111	0
1	H	930/970 (95%)	0.19	11 (1%) 79 79	40, 58, 89, 106	0
All	All	7480/7760 (96%)	0.15	49 (0%) 87 87	37, 58, 84, 111	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	13	HIS	4.5
1	H	764	ARG	3.6
1	G	365	ILE	3.6
1	B	917	PHE	3.5
1	H	365	ILE	3.2
1	H	765	PRO	3.2
1	G	756	ILE	3.0
1	F	917	PHE	3.0
1	D	229	GLU	3.0
1	H	233	ALA	3.0
1	C	765	PRO	2.9
1	G	765	PRO	2.8
1	G	453	LEU	2.7
1	D	234	GLN	2.7
1	C	20	LEU	2.7
1	D	756	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	764	ARG	2.6
1	F	761	ALA	2.6
1	D	232	ARG	2.6
1	G	177	HIS	2.5
1	G	20	LEU	2.5
1	H	917	PHE	2.4
1	B	920	THR	2.4
1	A	944	ALA	2.4
1	D	13	HIS	2.4
1	E	65	TYR	2.4
1	G	243	TYR	2.4
1	G	180	GLN	2.4
1	A	74	LYS	2.3
1	D	80	LEU	2.3
1	D	187	LEU	2.3
1	H	229	GLU	2.3
1	C	29	SER	2.2
1	D	20	LEU	2.2
1	G	450	LEU	2.2
1	B	73	GLY	2.2
1	D	233	ALA	2.2
1	H	753	ARG	2.2
1	B	428	ASP	2.1
1	E	233	ALA	2.1
1	H	755	ASN	2.1
1	H	243	TYR	2.1
1	G	923	PRO	2.1
1	C	229	GLU	2.1
1	G	761	ALA	2.1
1	D	21	ARG	2.1
1	H	231	ARG	2.0
1	H	383	TYR	2.0
1	A	356	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands [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(\AA^2)	Q<0.9
2	SO4	F	1003	5/5	0.83	0.16	84,84,84,84	0
3	FLC	B	1003	13/13	0.87	0.20	54,54,54,54	0
3	FLC	E	1004	13/13	0.90	0.26	62,62,62,62	0
2	SO4	F	1002	5/5	0.90	0.21	82,82,82,82	0
3	FLC	A	1004	13/13	0.90	0.21	62,62,62,62	0
2	SO4	A	1001	5/5	0.91	0.17	73,73,73,73	0
4	PG0	D	1001	8/8	0.91	0.21	54,59,66,69	0
2	SO4	G	1004	5/5	0.91	0.12	93,93,93,93	0
3	FLC	B	1004	13/13	0.92	0.22	53,53,53,53	0
2	SO4	H	1002	5/5	0.92	0.16	92,92,92,92	0
2	SO4	H	1003	5/5	0.92	0.22	79,79,79,79	0
2	SO4	E	1002	5/5	0.92	0.22	79,79,79,79	0
2	SO4	A	1003	5/5	0.93	0.15	63,63,63,63	0
3	FLC	F	1004	13/13	0.93	0.31	59,59,59,59	0
5	GOL	H	1001	6/6	0.94	0.13	55,65,70,71	0
2	SO4	H	1004	5/5	0.94	0.17	82,82,82,82	0
5	GOL	G	1001	6/6	0.94	0.15	63,63,64,64	0
2	SO4	C	1001	5/5	0.94	0.18	66,66,66,66	0
2	SO4	G	1002	5/5	0.95	0.14	80,80,80,80	0
2	SO4	F	1001	5/5	0.95	0.12	73,73,73,73	0
2	SO4	D	1003	5/5	0.95	0.11	94,94,94,94	0
3	FLC	C	1003	13/13	0.95	0.24	58,58,58,58	0
2	SO4	E	1001	5/5	0.95	0.14	74,74,74,74	0
2	SO4	C	1002	5/5	0.95	0.09	91,91,91,91	0
2	SO4	G	1003	5/5	0.95	0.13	82,82,82,82	0
2	SO4	E	1003	5/5	0.95	0.17	70,70,70,70	0
2	SO4	B	1001	5/5	0.96	0.15	74,74,74,74	0
2	SO4	A	1002	5/5	0.96	0.15	74,74,74,74	0
2	SO4	D	1002	5/5	0.96	0.13	71,71,71,71	0
2	SO4	B	1002	5/5	0.97	0.11	77,77,77,77	0
2	SO4	D	1004	5/5	0.97	0.12	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.