



Full wwPDB X-ray Structure Validation Report ⓘ

May 8, 2016 – 11:29 PM EDT

PDB ID : 5E9G
Title : Structural insights of isocitrate lyases from *Magnaporthe oryzae*
Authors : Park, Y.; Cho, Y.; Lee, Y.-H.; Lee, Y.-W.; Rhee, S.
Deposited on : 2015-10-15
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

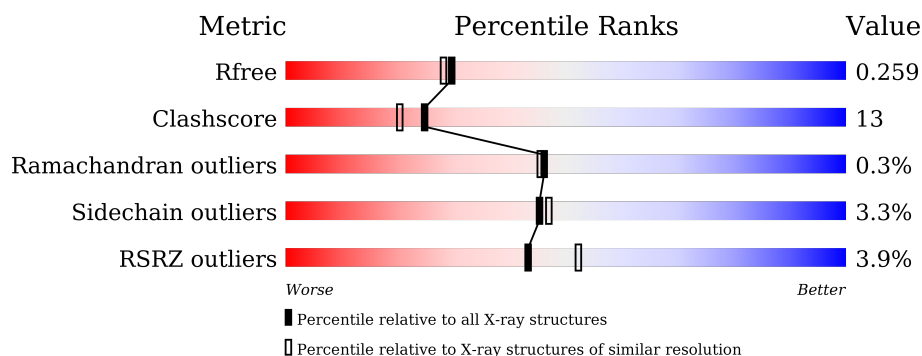
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	560	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>• 6%</div> </div> </div>
1	B	560	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>• 6%</div> </div> </div>
1	C	560	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>22%</div> <div>• 11%</div> </div> </div>
1	D	560	<div> <div>5%</div> <div> <div></div> <div>64%</div> <div>21%</div> <div>• 13%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLV	B	601	-	-	X	-
2	GLV	C	601	-	-	-	X
2	GLV	D	601	-	-	X	-
3	GOL	A	602	-	-	-	X
3	GOL	D	602	-	-	-	X
4	MG	A	603	-	-	-	X
4	MG	B	603	-	-	-	X
4	MG	C	602	-	-	-	X
4	MG	D	603	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16409 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 Isocitrate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			4130	2606	720	783	21			
1	B	525	Total	C	N	O	S	0	0	0
			4134	2608	721	784	21			
1	C	499	Total	C	N	O	S	0	0	0
			3949	2501	686	741	21			
1	D	486	Total	C	N	O	S	0	0	0
			3850	2437	672	720	21			

There are 56 discrepancies between the modelled and reference sequences:

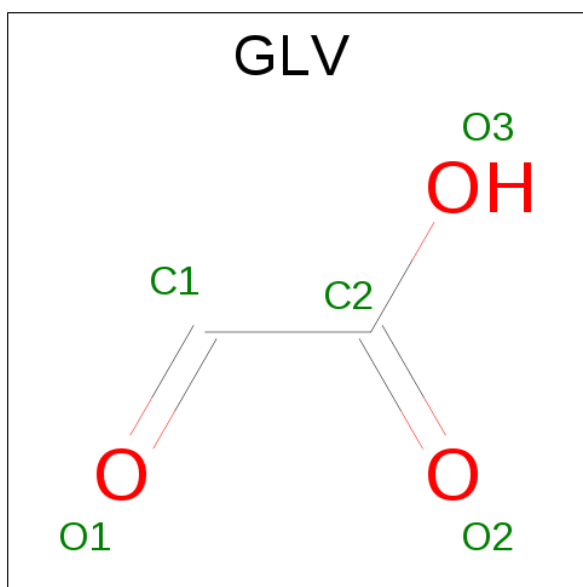
Chain	Residue	Modelled	Actual	Comment	Reference
A	219	GLY	ALA	engineered mutation	UNP P0CT06
A	548	ALA	-	expression tag	UNP P0CT06
A	549	ALA	-	expression tag	UNP P0CT06
A	550	ALA	-	expression tag	UNP P0CT06
A	551	LEU	-	expression tag	UNP P0CT06
A	552	GLU	-	expression tag	UNP P0CT06
A	553	HIS	-	expression tag	UNP P0CT06
A	554	HIS	-	expression tag	UNP P0CT06
A	555	HIS	-	expression tag	UNP P0CT06
A	556	HIS	-	expression tag	UNP P0CT06
A	557	HIS	-	expression tag	UNP P0CT06
A	558	HIS	-	expression tag	UNP P0CT06
A	559	HIS	-	expression tag	UNP P0CT06
A	560	HIS	-	expression tag	UNP P0CT06
B	219	GLY	ALA	engineered mutation	UNP P0CT06
B	548	ALA	-	expression tag	UNP P0CT06
B	549	ALA	-	expression tag	UNP P0CT06
B	550	ALA	-	expression tag	UNP P0CT06
B	551	LEU	-	expression tag	UNP P0CT06
B	552	GLU	-	expression tag	UNP P0CT06
B	553	HIS	-	expression tag	UNP P0CT06

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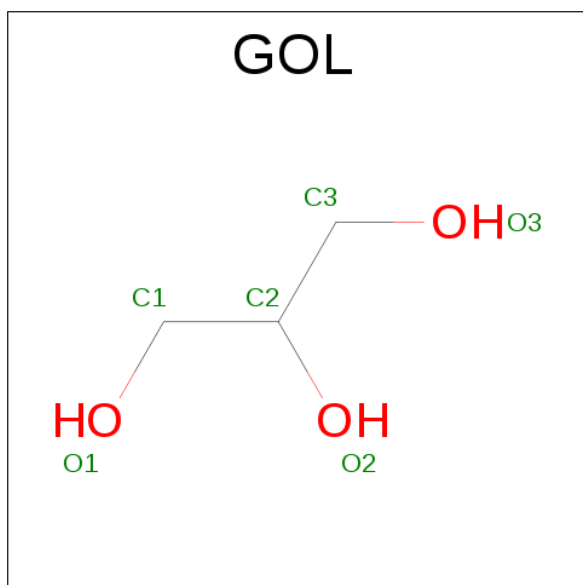
Chain	Residue	Modelled	Actual	Comment	Reference
B	554	HIS	-	expression tag	UNP P0CT06
B	555	HIS	-	expression tag	UNP P0CT06
B	556	HIS	-	expression tag	UNP P0CT06
B	557	HIS	-	expression tag	UNP P0CT06
B	558	HIS	-	expression tag	UNP P0CT06
B	559	HIS	-	expression tag	UNP P0CT06
B	560	HIS	-	expression tag	UNP P0CT06
C	219	GLY	ALA	engineered mutation	UNP P0CT06
C	548	ALA	-	expression tag	UNP P0CT06
C	549	ALA	-	expression tag	UNP P0CT06
C	550	ALA	-	expression tag	UNP P0CT06
C	551	LEU	-	expression tag	UNP P0CT06
C	552	GLU	-	expression tag	UNP P0CT06
C	553	HIS	-	expression tag	UNP P0CT06
C	554	HIS	-	expression tag	UNP P0CT06
C	555	HIS	-	expression tag	UNP P0CT06
C	556	HIS	-	expression tag	UNP P0CT06
C	557	HIS	-	expression tag	UNP P0CT06
C	558	HIS	-	expression tag	UNP P0CT06
C	559	HIS	-	expression tag	UNP P0CT06
C	560	HIS	-	expression tag	UNP P0CT06
D	219	GLY	ALA	engineered mutation	UNP P0CT06
D	548	ALA	-	expression tag	UNP P0CT06
D	549	ALA	-	expression tag	UNP P0CT06
D	550	ALA	-	expression tag	UNP P0CT06
D	551	LEU	-	expression tag	UNP P0CT06
D	552	GLU	-	expression tag	UNP P0CT06
D	553	HIS	-	expression tag	UNP P0CT06
D	554	HIS	-	expression tag	UNP P0CT06
D	555	HIS	-	expression tag	UNP P0CT06
D	556	HIS	-	expression tag	UNP P0CT06
D	557	HIS	-	expression tag	UNP P0CT06
D	558	HIS	-	expression tag	UNP P0CT06
D	559	HIS	-	expression tag	UNP P0CT06
D	560	HIS	-	expression tag	UNP P0CT06

- Molecule 2 is GLYOXYLIC ACID (three-letter code: GLV) (formula: C₂H₂O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			5	2	3		
2	B	1	Total	C	O	0	0
			5	2	3		
2	C	1	Total	C	O	0	0
			5	2	3		
2	D	1	Total	C	O	0	0
			5	2	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

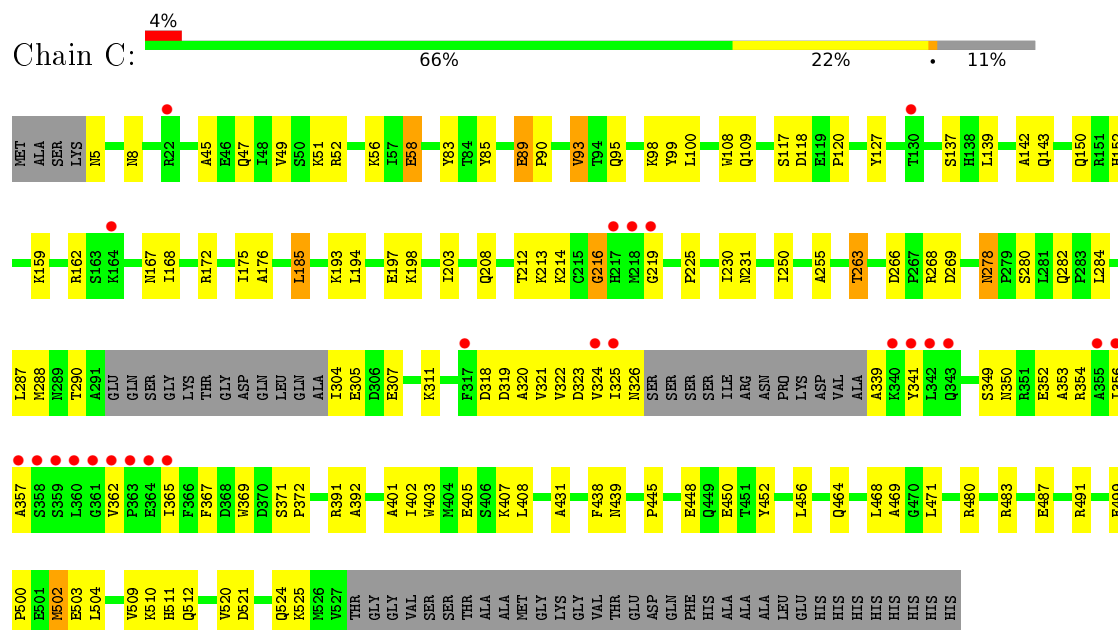
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	89	Total O 89 89	0	0
5	B	82	Total O 82 82	0	0
5	C	73	Total O 73 73	0	0
5	D	60	Total O 60 60	0	0

• Molecule 1: Isocitrate lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.12Å 135.08Å 158.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 47.34 – 2.09	Depositor EDS
% Data completeness (in resolution range)	90.8 (50.00-2.10) 90.4 (47.34-2.09)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.63 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.259 0.224 , 0.259	Depositor DCC
R_{free} test set	13732 reflections (9.96%)	DCC
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16409	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, GLV

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	0.35	0/4224	0.60	0/5723
1	B	0.34	0/4228	0.59	0/5728
1	C	0.34	0/4040	0.58	0/5472
1	D	0.35	0/3938	0.59	0/5327
All	All	0.34	0/16430	0.59	0/22250

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4067	109	0
1	B	4134	0	4070	99	0
1	C	3949	0	3889	111	0
1	D	3850	0	3784	134	0
2	A	5	0	1	0	0
2	B	5	0	1	2	0
2	C	5	0	1	1	0
2	D	5	0	1	2	0
3	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	2	0
3	D	6	0	8	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	89	0	0	3	0
5	B	82	0	0	1	0
5	C	73	0	0	1	0
5	D	60	0	0	2	0
All	All	16409	0	15838	409	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 13.

All (409) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASP:H	1:D:6:MET:HE2	1.04	1.07
2:D:601:GLV:H1	3:D:602:GOL:H31	1.45	0.95
1:A:350:ASN:HD21	1:A:354:ARG:HE	1.16	0.91
5:A:704:HOH:O	1:D:6:MET:HE3	1.70	0.89
1:A:101:ASP:H	1:D:6:MET:CE	1.87	0.87
1:A:101:ASP:N	1:D:6:MET:HE2	1.89	0.87
1:C:150:GLN:HE22	1:C:168:ILE:H	1.22	0.86
1:D:350:ASN:HD21	1:D:354:ARG:HE	1.24	0.85
1:B:150:GLN:HE22	1:B:168:ILE:H	1.22	0.85
1:A:278:ASN:ND2	1:A:280:SER:H	1.77	0.82
1:A:100:LEU:HA	1:D:6:MET:HE1	1.59	0.82
1:A:278:ASN:HD22	1:A:280:SER:H	1.26	0.81
1:A:491:ARG:HD2	1:B:446:ARG:NH1	1.95	0.81
1:C:307:GLU:HG2	1:C:311:LYS:HE2	1.60	0.81
1:D:150:GLN:HE22	1:D:168:ILE:H	1.27	0.80
1:D:282:GLN:HG3	1:D:283:PRO:HD2	1.64	0.79
1:D:278:ASN:ND2	1:D:281:LEU:HG	1.99	0.78
1:D:116:SER:OG	1:D:130:THR:HG23	1.83	0.78
1:D:278:ASN:HD22	1:D:281:LEU:HG	1.50	0.77
1:B:357:ALA:HB1	1:B:362:VAL:HG21	1.65	0.77
1:A:441:LYS:NZ	1:A:446:ARG:HH22	1.83	0.77
1:A:150:GLN:HE22	1:A:168:ILE:H	1.32	0.77
1:C:491:ARG:HD2	1:D:446:ARG:HD2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:491:ARG:HA	1:D:449:GLN:HE21	1.50	0.75
1:C:502:MET:HE3	1:C:509:VAL:HG11	1.70	0.73
1:D:352:GLU:O	1:D:356:ILE:HG12	1.87	0.73
1:B:446:ARG:NH1	1:B:446:ARG:HB3	2.03	0.73
1:A:278:ASN:C	1:A:278:ASN:HD22	1.93	0.71
1:C:216:GLY:HA3	1:C:405:GLU:OE1	1.90	0.71
2:D:601:GLV:C1	3:D:602:GOL:H31	2.18	0.71
1:C:108:TRP:HE1	1:D:512:GLN:NE2	1.89	0.71
1:C:99:TYR:C	1:C:100:LEU:HD12	2.11	0.71
1:B:446:ARG:HH11	1:B:446:ARG:HB3	1.56	0.70
1:A:300:GLN:O	1:A:304:ILE:HG12	1.92	0.70
1:B:278:ASN:C	1:B:278:ASN:HD22	1.95	0.70
1:C:350:ASN:HD21	1:C:354:ARG:HE	1.40	0.69
2:B:601:GLV:H1	3:B:602:GOL:H12	1.75	0.68
1:A:137:SER:HB2	1:A:198:LYS:HD2	1.76	0.68
1:C:445:PRO:HD2	1:C:448:GLU:HG3	1.76	0.68
1:C:137:SER:HB2	1:C:198:LYS:HD2	1.75	0.67
1:C:193:LYS:O	1:C:197:GLU:HG3	1.94	0.67
1:A:440:TRP:H	1:B:498:GLN:HE22	1.41	0.67
1:B:274:LEU:HD21	1:B:382:LYS:HB2	1.77	0.67
1:C:266:ASP:OD1	1:C:268:ARG:HD3	1.96	0.66
1:D:342:LEU:HD12	1:D:342:LEU:H	1.61	0.66
1:D:208:GLN:HE22	1:D:214:LYS:H	1.43	0.66
1:B:500:PRO:O	1:B:504:LEU:HD13	1.96	0.65
1:D:445:PRO:HG2	1:D:448:GLU:HG3	1.78	0.65
1:B:8:ASN:ND2	1:C:172:ARG:HH12	1.94	0.65
1:C:491:ARG:HD2	1:D:446:ARG:CD	2.27	0.65
1:A:215:CYS:HB3	1:A:218:MET:HB2	1.79	0.65
1:C:499:GLU:O	1:C:503:GLU:HG3	1.97	0.64
1:A:491:ARG:HD2	1:B:446:ARG:HH11	1.60	0.64
1:A:158:PRO:HD2	1:A:161:GLU:OE1	1.98	0.64
1:D:407:LYS:O	1:D:408:LEU:HD12	1.98	0.64
1:B:278:ASN:ND2	1:B:280:SER:H	1.97	0.63
1:D:371:SER:OG	1:D:372:PRO:HD3	1.97	0.63
1:D:109:GLN:NE2	1:D:471:LEU:H	1.97	0.62
1:C:322:VAL:HG12	1:C:326:ASN:HD21	1.65	0.62
1:A:446:ARG:HB3	1:B:491:ARG:HD2	1.82	0.62
1:D:350:ASN:HD21	1:D:354:ARG:NE	1.96	0.62
1:A:273:ILE:HA	1:A:381:ILE:HG22	1.81	0.62
1:B:375:ARG:HG3	1:B:376:GLU:OE2	2.01	0.61
1:C:450:GLU:HG3	1:D:488:VAL:HB	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ALA:HB3	1:B:213:LYS:HG2	1.83	0.61
1:C:349:SER:OG	1:C:352:GLU:HG3	2.00	0.61
1:C:108:TRP:HB2	2:C:601:GLV:H1	1.83	0.60
1:A:193:LYS:O	1:A:197:GLU:HG3	2.02	0.60
1:B:172:ARG:HH12	1:C:8:ASN:HD21	1.47	0.60
1:D:342:LEU:H	1:D:342:LEU:CD1	2.13	0.60
1:A:194:LEU:O	1:A:198:LYS:HG2	2.01	0.60
1:B:385:CYS:O	1:B:389:ILE:HG13	2.01	0.60
1:C:230:ILE:HD12	1:C:268:ARG:HH22	1.65	0.60
1:C:365:ILE:HD12	1:C:365:ILE:N	2.16	0.60
1:D:274:LEU:HD21	1:D:382:LYS:HB2	1.82	0.60
1:A:350:ASN:ND2	1:A:354:ARG:HE	1.95	0.60
1:B:216:GLY:HA3	1:B:405:GLU:OE1	2.01	0.60
1:B:453:ILE:HA	1:B:464:GLN:HE22	1.66	0.60
1:B:8:ASN:HD21	1:C:172:ARG:HH12	1.50	0.60
1:B:109:GLN:NE2	1:B:471:LEU:H	2.00	0.60
1:B:137:SER:HB2	1:B:198:LYS:HG3	1.83	0.59
1:A:172:ARG:HH12	1:D:8:ASN:ND2	2.00	0.59
2:B:601:GLV:C1	3:B:602:GOL:H12	2.32	0.59
1:C:89:GLU:HB2	1:C:90:PRO:CD	2.33	0.59
1:A:100:LEU:HA	1:D:6:MET:CE	2.31	0.59
1:A:109:GLN:NE2	1:A:471:LEU:H	1.99	0.59
1:A:89:GLU:HB2	1:A:90:PRO:CD	2.32	0.59
1:D:317:PHE:O	1:D:321:VAL:HG23	2.03	0.58
1:D:354:ARG:NH2	1:D:367:PHE:HB3	2.18	0.58
1:D:185:LEU:HD21	1:D:231:ASN:HB3	1.85	0.58
1:A:172:ARG:HH12	1:D:8:ASN:HD21	1.52	0.58
1:B:357:ALA:HB1	1:B:362:VAL:CG2	2.33	0.58
1:D:287:LEU:CD2	1:D:308:TRP:HB2	2.34	0.58
1:C:89:GLU:HB2	1:C:90:PRO:HD2	1.86	0.58
1:D:498:GLN:HG2	1:D:502:MET:CE	2.34	0.57
1:B:159:LYS:O	1:B:159:LYS:HD3	2.03	0.57
1:C:352:GLU:O	1:C:356:ILE:HG13	2.04	0.57
1:A:446:ARG:HG2	1:A:446:ARG:HH11	1.70	0.57
1:C:108:TRP:HE1	1:D:512:GLN:HE22	1.50	0.57
1:C:365:ILE:H	1:C:365:ILE:HD12	1.70	0.57
1:D:407:LYS:C	1:D:408:LEU:HD12	2.24	0.57
1:A:415:LYS:O	1:A:419:GLU:HG3	2.04	0.57
1:A:527:VAL:O	1:A:527:VAL:HG12	2.05	0.56
1:C:512:GLN:NE2	1:D:108:TRP:HE1	2.03	0.56
1:D:342:LEU:N	1:D:342:LEU:HD12	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:GLY:HA3	1:D:405:GLU:OE1	2.05	0.56
1:B:179:ASP:O	1:B:206:GLU:HG2	2.04	0.56
1:D:283:PRO:HB2	1:D:286:ASP:OD2	2.05	0.56
1:A:292:GLU:C	1:A:294:SER:H	2.09	0.56
1:C:208:GLN:HE22	1:C:214:LYS:H	1.54	0.56
1:A:52:ARG:O	1:D:151:ARG:HD3	2.06	0.56
1:D:343:GLN:HE21	1:D:343:GLN:HA	1.71	0.56
1:D:341:TYR:HD2	1:D:342:LEU:HD12	1.70	0.56
1:A:292:GLU:HA	1:A:292:GLU:OE2	2.06	0.56
1:C:502:MET:CE	1:C:509:VAL:HG11	2.35	0.56
1:D:128:PRO:HB2	1:D:130:THR:HG22	1.88	0.55
1:A:213:LYS:HD3	1:A:214:LYS:N	2.21	0.55
1:D:159:LYS:HD3	1:D:162:ARG:NH1	2.21	0.55
1:C:491:ARG:HA	1:D:449:GLN:NE2	2.21	0.55
1:B:22:ARG:O	1:B:26:GLU:HG3	2.05	0.55
1:B:350:ASN:HD21	1:B:354:ARG:HE	1.54	0.55
1:C:408:LEU:HD23	1:C:438:PHE:CE1	2.41	0.55
1:C:255:ALA:HB2	1:C:391:ARG:HD2	1.89	0.55
1:D:90:PRO:O	1:D:93:VAL:HG12	2.06	0.55
1:B:208:GLN:HE22	1:B:214:LYS:H	1.53	0.55
1:C:100:LEU:HD12	1:C:100:LEU:N	2.22	0.55
1:A:266:ASP:OD1	1:A:268:ARG:HD2	2.07	0.54
1:A:250:ILE:HG12	1:A:401:ALA:HB3	1.89	0.54
1:D:47:GLN:O	1:D:51:LYS:HG2	2.07	0.54
1:C:152:HIS:HD2	5:C:760:HOH:O	1.90	0.54
1:D:150:GLN:NE2	1:D:168:ILE:H	2.03	0.54
1:A:483:ARG:O	1:A:487:GLU:HG3	2.07	0.54
1:C:502:MET:HA	1:C:502:MET:CE	2.38	0.54
1:B:172:ARG:HH12	1:C:8:ASN:ND2	2.06	0.54
1:A:350:ASN:HD21	1:A:354:ARG:NE	1.95	0.54
1:B:150:GLN:NE2	1:B:168:ILE:H	2.01	0.54
1:C:212:THR:O	1:C:214:LYS:HD3	2.08	0.54
1:D:284:LEU:C	1:D:284:LEU:HD13	2.27	0.54
1:C:483:ARG:O	1:C:487:GLU:HG3	2.08	0.54
1:A:440:TRP:H	1:B:498:GLN:NE2	2.04	0.53
1:A:296:LYS:HG2	1:A:300:GLN:HE22	1.73	0.53
1:B:320:ALA:O	1:B:324:VAL:HG23	2.08	0.53
1:A:332:ARG:HB2	1:A:332:ARG:CZ	2.39	0.53
1:B:159:LYS:HD3	1:B:159:LYS:C	2.29	0.53
1:B:357:ALA:O	1:B:362:VAL:HG22	2.08	0.53
1:D:354:ARG:HH22	1:D:367:PHE:HB3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:THR:O	1:B:477:ILE:HD13	2.09	0.53
1:C:278:ASN:HD22	1:C:278:ASN:C	2.11	0.53
1:D:281:LEU:HD12	1:D:312:ALA:HA	1.91	0.53
1:B:152:HIS:HD2	5:B:772:HOH:O	1.91	0.52
1:C:56:LYS:HE2	1:C:58:GLU:OE2	2.09	0.52
1:D:433:ASN:HD22	1:D:433:ASN:C	2.11	0.52
1:D:150:GLN:HE22	1:D:168:ILE:N	2.01	0.52
1:A:150:GLN:HE22	1:A:168:ILE:N	2.06	0.52
1:A:375:ARG:NH2	1:C:231:ASN:HD21	2.07	0.52
1:A:446:ARG:CG	1:A:446:ARG:HH11	2.23	0.52
1:B:118:ASP:O	1:B:120:PRO:HD3	2.10	0.52
1:B:357:ALA:C	1:B:362:VAL:HG22	2.30	0.52
1:C:499:GLU:HB2	1:C:500:PRO:HD3	1.91	0.52
1:D:152:HIS:HD2	5:D:717:HOH:O	1.93	0.52
1:D:343:GLN:NE2	1:D:343:GLN:HA	2.25	0.52
1:C:521:ASP:OD2	1:C:525:LYS:HE2	2.10	0.52
1:D:453:ILE:HA	1:D:464:GLN:HE22	1.75	0.52
1:B:452:TYR:CE2	1:B:456:LEU:HD11	2.45	0.52
1:D:278:ASN:HD22	1:D:281:LEU:CG	2.19	0.52
1:A:175:ILE:HD12	1:A:463:TRP:CE2	2.45	0.51
1:D:194:LEU:O	1:D:198:LYS:HG2	2.10	0.51
1:D:159:LYS:HD3	1:D:162:ARG:HH11	1.74	0.51
1:A:152:HIS:HD2	5:A:754:HOH:O	1.93	0.51
1:A:182:HIS:HD2	5:A:778:HOH:O	1.93	0.51
1:A:22:ARG:O	1:A:26:GLU:HG3	2.11	0.51
1:D:440:TRP:O	1:D:441:LYS:HB3	2.10	0.51
1:C:304:ILE:O	1:C:307:GLU:HB3	2.11	0.51
1:D:282:GLN:HG3	1:D:283:PRO:CD	2.39	0.51
1:B:139:LEU:O	1:B:143:GLN:HG3	2.11	0.51
1:D:341:TYR:CD2	1:D:342:LEU:HD12	2.45	0.51
1:B:278:ASN:HD22	1:B:279:PRO:N	2.09	0.51
1:D:98:LYS:HG2	1:D:168:ILE:HG12	1.93	0.51
1:A:85:TYR:HB2	1:A:469:ALA:HB3	1.94	0.50
1:C:502:MET:HA	1:C:502:MET:HE3	1.92	0.50
1:A:291:ALA:O	1:A:296:LYS:HD2	2.12	0.50
1:A:527:VAL:O	1:A:528:THR:HB	2.11	0.50
1:A:216:GLY:HA3	1:A:405:GLU:OE1	2.12	0.50
1:B:333:ASN:HB3	1:B:336:ASP:HB2	1.94	0.50
1:D:214:LYS:HB3	1:D:218:MET:HG2	1.92	0.50
1:C:403:TRP:HB2	1:C:431:ALA:HB3	1.94	0.50
1:A:118:ASP:O	1:A:120:PRO:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:PRO:HG3	1:D:263:THR:HG23	1.94	0.50
1:B:266:ASP:OD1	1:B:268:ARG:HD3	2.11	0.50
1:C:278:ASN:ND2	1:C:280:SER:H	2.09	0.50
1:D:109:GLN:NE2	1:D:468:LEU:HA	2.27	0.50
1:D:497:VAL:C	1:D:500:PRO:HD2	2.33	0.50
1:A:179:ASP:OD2	1:A:182:HIS:HE1	1.95	0.49
1:A:283:PRO:HG2	1:A:286:ASP:OD1	2.12	0.49
1:D:350:ASN:ND2	1:D:354:ARG:HE	2.02	0.49
1:D:497:VAL:O	1:D:500:PRO:HD2	2.13	0.49
1:A:433:ASN:HD22	1:A:433:ASN:C	2.16	0.49
1:B:278:ASN:C	1:B:278:ASN:ND2	2.63	0.49
1:B:483:ARG:O	1:B:487:GLU:HG3	2.11	0.49
1:B:89:GLU:HB2	1:B:90:PRO:CD	2.42	0.49
1:C:320:ALA:O	1:C:324:VAL:HG23	2.12	0.48
1:A:221:LYS:HE3	1:A:254:ASP:HB3	1.95	0.48
1:C:45:ALA:O	1:C:49:VAL:HG23	2.14	0.48
1:A:176:ALA:O	1:A:203:ILE:HA	2.13	0.48
1:A:56:LYS:HE2	1:A:58:GLU:CG	2.44	0.48
1:D:433:ASN:ND2	1:D:433:ASN:C	2.67	0.48
1:D:67:LYS:O	1:D:71:ILE:HG13	2.13	0.48
1:D:214:LYS:HE3	1:D:218:MET:HB3	1.95	0.48
1:A:325:ILE:HD13	1:A:337:VAL:HG12	1.95	0.48
1:C:99:TYR:HB2	1:C:100:LEU:HD12	1.95	0.48
1:D:441:LYS:C	1:D:443:ALA:N	2.67	0.48
1:C:512:GLN:HE22	1:D:108:TRP:HE1	1.61	0.48
1:D:89:GLU:HB2	1:D:90:PRO:CD	2.44	0.48
1:A:450:GLU:HG3	1:B:488:VAL:HB	1.95	0.48
1:B:292:GLU:C	1:B:294:SER:H	2.17	0.48
1:B:8:ASN:HD21	1:C:172:ARG:NH1	2.10	0.48
1:C:322:VAL:HG12	1:C:326:ASN:ND2	2.28	0.48
1:D:137:SER:HB2	1:D:198:LYS:HD2	1.95	0.48
1:A:422:HIS:HE1	1:A:428:GLN:O	1.97	0.48
1:A:490:MET:SD	1:B:466:ILE:HD11	2.54	0.48
1:C:175:ILE:HD12	1:C:175:ILE:N	2.29	0.47
1:B:9:PRO:HB2	1:C:167:ASN:ND2	2.28	0.47
1:D:225:PRO:CG	1:D:263:THR:HG23	2.44	0.47
1:A:221:LYS:CE	1:A:254:ASP:HB3	2.45	0.47
1:C:142:ALA:HA	1:D:120:PRO:HG2	1.95	0.47
1:D:498:GLN:HG2	1:D:502:MET:HE1	1.96	0.47
1:A:278:ASN:C	1:A:278:ASN:ND2	2.65	0.47
1:A:89:GLU:HB2	1:A:90:PRO:HD2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:GLN:NE2	1:C:471:LEU:H	2.13	0.47
1:D:56:LYS:HB3	1:D:56:LYS:NZ	2.30	0.47
1:D:213:LYS:HD3	1:D:213:LYS:C	2.35	0.47
1:D:83:TYR:HA	1:D:464:GLN:O	2.15	0.47
1:C:318:ASP:O	1:C:322:VAL:HG23	2.15	0.47
1:B:89:GLU:HB2	1:B:90:PRO:HD2	1.97	0.47
1:D:278:ASN:HD21	1:D:280:SER:HB2	1.78	0.47
1:C:392:ALA:HB1	1:C:402:ILE:HG21	1.96	0.47
1:D:218:MET:HA	1:D:218:MET:CE	2.44	0.47
1:D:56:LYS:HE2	1:D:58:GLU:OE2	2.15	0.47
1:A:441:LYS:HZ2	1:A:446:ARG:HH22	1.60	0.47
1:C:350:ASN:HD21	1:C:354:ARG:NE	2.10	0.47
1:D:409:PRO:HD3	1:D:438:PHE:CG	2.50	0.47
1:D:5:ASN:O	1:D:6:MET:HB2	2.15	0.47
1:A:336:ASP:OD1	1:A:340:LYS:HE3	2.14	0.47
1:A:433:ASN:C	1:A:433:ASN:ND2	2.68	0.47
1:C:213:LYS:C	1:C:214:LYS:HD2	2.36	0.46
1:D:132:VAL:HB	1:D:133:PRO:HD3	1.96	0.46
1:C:194:LEU:O	1:C:198:LYS:HG2	2.15	0.46
1:D:278:ASN:ND2	1:D:281:LEU:N	2.63	0.46
1:A:100:LEU:CA	1:D:6:MET:HE1	2.38	0.46
1:D:318:ASP:O	1:D:322:VAL:HG23	2.15	0.46
1:A:511:HIS:HB2	1:B:108:TRP:CH2	2.51	0.46
1:B:524:GLN:HA	1:B:524:GLN:OE1	2.15	0.46
1:B:352:GLU:O	1:B:356:ILE:HG13	2.15	0.46
1:D:159:LYS:HD2	1:D:162:ARG:HD2	1.96	0.46
1:A:499:GLU:HB2	1:A:500:PRO:HD3	1.97	0.46
1:C:47:GLN:O	1:C:51:LYS:HG2	2.14	0.46
1:B:83:TYR:N	1:B:83:TYR:CD1	2.83	0.46
1:D:441:LYS:H	1:D:443:ALA:N	2.14	0.46
1:B:453:ILE:HG23	1:B:464:GLN:NE2	2.31	0.45
1:B:90:PRO:O	1:B:94:THR:HG23	2.16	0.45
1:B:499:GLU:HB2	1:B:500:PRO:HD3	1.98	0.45
1:D:89:GLU:HB2	1:D:90:PRO:HD2	1.98	0.45
1:C:225:PRO:HG3	1:C:263:THR:HG23	1.98	0.45
1:A:333:ASN:O	1:A:337:VAL:HG23	2.15	0.45
1:B:318:ASP:O	1:B:322:VAL:HG23	2.17	0.45
1:D:282:GLN:CG	1:D:283:PRO:HD2	2.42	0.45
1:D:373:ARG:HA	1:D:378:TYR:O	2.17	0.45
1:B:161:GLU:OE2	1:B:164:LYS:HD2	2.17	0.45
1:C:139:LEU:O	1:C:143:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:TYR:HA	1:C:464:GLN:O	2.17	0.45
1:C:500:PRO:O	1:C:504:LEU:HD13	2.16	0.45
1:D:116:SER:CB	1:D:130:THR:HG23	2.46	0.45
1:D:316:ARG:HE	1:D:382:LYS:HB3	1.81	0.45
1:D:494:GLY:O	1:D:499:GLU:HB2	2.17	0.45
1:A:288:MET:HE1	1:A:305:GLU:HB2	1.98	0.45
1:A:292:GLU:OE1	1:A:297:THR:HB	2.17	0.45
1:C:117:SER:O	1:C:118:ASP:HB2	2.17	0.45
1:C:321:VAL:HG21	1:C:341:TYR:CZ	2.52	0.45
1:A:108:TRP:CH2	1:B:511:HIS:HB2	2.52	0.45
1:B:297:THR:O	1:B:300:GLN:HB2	2.17	0.45
1:D:287:LEU:HD23	1:D:308:TRP:HB2	1.98	0.45
1:B:396:ALA:HB3	1:B:397:PRO:HD3	1.98	0.44
1:C:354:ARG:NH2	1:C:367:PHE:HB3	2.32	0.44
1:A:497:VAL:C	1:A:500:PRO:HD2	2.38	0.44
1:B:422:HIS:HE1	1:B:428:GLN:O	1.99	0.44
1:C:250:ILE:HG12	1:C:401:ALA:HB3	1.99	0.44
1:D:85:TYR:HB2	1:D:469:ALA:HB3	1.99	0.44
1:A:278:ASN:ND2	1:A:280:SER:OG	2.45	0.44
1:C:185:LEU:HD21	1:C:231:ASN:HB3	1.98	0.44
1:C:371:SER:N	1:C:372:PRO:CD	2.80	0.44
1:A:296:LYS:HG2	1:A:300:GLN:NE2	2.32	0.44
1:A:381:ILE:O	1:A:381:ILE:HD12	2.18	0.44
1:B:386:ASP:OD1	1:B:387:CYS:N	2.51	0.44
1:D:108:TRP:HB3	1:D:468:LEU:HD21	1.99	0.44
1:B:79:ARG:HD3	1:B:79:ARG:HA	1.71	0.44
1:C:230:ILE:HD12	1:C:268:ARG:NH2	2.31	0.44
1:C:282:GLN:OE1	1:C:287:LEU:HD13	2.17	0.44
1:A:385:CYS:O	1:A:389:ILE:HG13	2.18	0.44
1:C:284:LEU:O	1:C:288:MET:HG2	2.18	0.44
1:D:371:SER:N	1:D:372:PRO:CD	2.81	0.44
1:A:295:GLY:C	1:A:297:THR:H	2.21	0.44
1:B:444:MET:HG3	1:B:449:GLN:HG3	2.00	0.44
1:D:343:GLN:HE21	1:D:343:GLN:CA	2.29	0.44
1:C:109:GLN:NE2	1:C:468:LEU:HA	2.32	0.44
1:C:510:LYS:HE3	1:C:510:LYS:HB2	1.81	0.44
1:B:371:SER:N	1:B:372:PRO:CD	2.81	0.43
1:C:290:THR:HG22	1:C:290:THR:O	2.18	0.43
1:C:339:ALA:C	1:C:341:TYR:H	2.21	0.43
1:D:440:TRP:O	1:D:441:LYS:CB	2.65	0.43
1:D:441:LYS:O	1:D:443:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:TYR:CD1	1:C:469:ALA:HB3	2.52	0.43
1:B:144:LEU:O	1:B:148:ARG:HG3	2.18	0.43
1:B:47:GLN:O	1:B:51:LYS:HG2	2.18	0.43
1:D:284:LEU:HB2	1:D:308:TRP:CE3	2.53	0.43
1:D:281:LEU:HD13	1:D:308:TRP:NE1	2.34	0.43
1:A:275:GLY:HA2	1:A:369:TRP:HA	2.00	0.43
1:D:318:ASP:C	1:D:320:ALA:H	2.20	0.43
1:A:349:SER:OG	1:A:352:GLU:HG3	2.19	0.43
1:B:89:GLU:OE1	1:B:91:THR:HB	2.19	0.43
1:A:446:ARG:CG	1:A:446:ARG:NH1	2.80	0.43
1:A:441:LYS:HZ1	1:A:446:ARG:HH22	1.64	0.43
1:B:9:PRO:HA	1:C:167:ASN:O	2.19	0.43
1:B:206:GLU:OE2	1:B:213:LYS:HE2	2.19	0.43
1:C:100:LEU:CD1	1:C:100:LEU:N	2.81	0.43
1:B:184:GLY:O	1:B:188:VAL:HG23	2.19	0.43
1:D:277:THR:HG21	1:D:315:LYS:HD2	2.00	0.43
1:A:172:ARG:NH1	1:D:8:ASN:HD21	2.17	0.43
1:A:101:ASP:CG	1:D:6:MET:HG2	2.39	0.42
1:A:408:LEU:HG	1:A:409:PRO:HD2	2.00	0.42
1:C:307:GLU:O	1:C:311:LYS:HG3	2.19	0.42
1:C:480:ARG:HH11	1:C:480:ARG:HG3	1.84	0.42
1:B:277:THR:OG1	1:B:313:ASN:HB3	2.19	0.42
1:C:520:VAL:HG21	1:D:122:PRO:HD2	2.01	0.42
1:D:313:ASN:HD22	1:D:315:LYS:HE3	1.84	0.42
1:D:83:TYR:CD1	1:D:83:TYR:N	2.86	0.42
1:B:151:ARG:HD3	1:C:52:ARG:O	2.18	0.42
1:A:13:PRO:HA	1:A:16:GLU:HG3	2.01	0.42
1:A:488:VAL:HB	1:B:450:GLU:HG3	2.01	0.42
1:B:292:GLU:HG2	1:B:301:LEU:HD11	2.01	0.42
1:A:506:VAL:O	1:A:509:VAL:HG12	2.19	0.42
1:A:56:LYS:HE2	1:A:58:GLU:HG2	2.01	0.42
1:C:511:HIS:HB2	1:D:108:TRP:CH2	2.55	0.42
1:C:150:GLN:NE2	1:C:168:ILE:H	2.04	0.42
1:C:307:GLU:CG	1:C:311:LYS:HE2	2.41	0.42
1:A:90:PRO:HD3	1:A:138:HIS:CE1	2.55	0.42
1:B:196:ILE:HD13	1:B:245:VAL:HG21	2.00	0.42
1:B:430:LEU:O	1:B:461:TYR:HA	2.20	0.42
1:B:175:ILE:HD12	1:B:463:TRP:CE2	2.54	0.42
1:C:95:GLN:HA	1:C:98:LYS:HE3	2.02	0.42
1:D:139:LEU:O	1:D:143:GLN:HG3	2.20	0.42
1:A:497:VAL:O	1:A:500:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:VAL:HG21	1:C:365:ILE:HG13	2.01	0.42
1:C:325:ILE:HG12	1:C:362:VAL:HG22	2.02	0.42
1:C:520:VAL:HG21	1:D:122:PRO:CD	2.50	0.42
1:B:84:THR:OG1	1:B:85:TYR:N	2.51	0.41
1:C:284:LEU:HD21	1:C:305:GLU:HG3	2.01	0.41
1:A:371:SER:OG	1:A:372:PRO:HD3	2.19	0.41
1:B:278:ASN:HD22	1:B:280:SER:H	1.66	0.41
1:B:278:ASN:HA	1:B:279:PRO:HD3	1.82	0.41
1:B:371:SER:N	1:B:372:PRO:HD3	2.35	0.41
1:C:159:LYS:HA	1:C:162:ARG:CD	2.49	0.41
1:D:177:ASP:CG	1:D:204:HIS:CE1	2.93	0.41
1:D:422:HIS:HE1	1:D:428:GLN:O	2.03	0.41
1:B:283:PRO:HB2	1:B:286:ASP:OD2	2.20	0.41
1:D:206:GLU:C	1:D:229:HIS:CE1	2.94	0.41
1:A:284:LEU:O	1:A:288:MET:HG2	2.21	0.41
1:B:181:GLY:HA3	1:B:188:VAL:HG22	2.03	0.41
1:D:119:GLU:HA	1:D:120:PRO:HD3	1.93	0.41
1:A:295:GLY:O	1:A:296:LYS:HB2	2.21	0.41
1:C:445:PRO:HD2	1:C:448:GLU:CG	2.48	0.41
1:C:85:TYR:HB2	1:C:469:ALA:HB3	2.01	0.41
1:D:59:TYR:HB3	5:D:723:HOH:O	2.20	0.41
1:B:44:THR:OG1	1:B:47:GLN:HG3	2.21	0.41
1:C:452:TYR:CE2	1:C:456:LEU:HD11	2.54	0.41
1:D:278:ASN:ND2	1:D:281:LEU:H	2.18	0.41
1:D:33:ASP:CG	1:D:34:PRO:HD2	2.41	0.41
1:A:512:GLN:HE22	1:B:108:TRP:HE1	1.68	0.41
1:B:336:ASP:O	1:B:340:LYS:HG3	2.20	0.41
1:C:266:ASP:HB3	1:C:269:ASP:OD2	2.21	0.41
1:C:357:ALA:O	1:C:362:VAL:HB	2.21	0.41
1:D:106:SER:HB3	1:D:109:GLN:HG3	2.03	0.41
1:D:114:ALA:O	1:D:131:THR:HG23	2.21	0.41
1:D:315:LYS:O	1:D:367:PHE:HE1	2.04	0.41
1:A:278:ASN:ND2	1:A:280:SER:N	2.58	0.41
1:A:371:SER:N	1:A:372:PRO:CD	2.84	0.41
1:B:5:ASN:HB2	1:B:6:MET:H	1.68	0.41
1:C:407:LYS:HG3	1:C:408:LEU:H	1.86	0.41
1:A:150:GLN:NE2	1:A:168:ILE:H	2.10	0.41
1:A:524:GLN:HA	1:A:524:GLN:OE1	2.21	0.41
1:B:289:ASN:O	1:B:293:GLN:HG3	2.21	0.41
1:A:446:ARG:O	1:B:491:ARG:HD3	2.20	0.41
1:A:266:ASP:OD1	1:A:268:ARG:CD	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:THR:O	1:A:465:PHE:HA	2.21	0.41
1:B:108:TRP:CD1	1:B:123:ASP:HB2	2.55	0.41
1:B:309:MET:O	1:B:312:ALA:HB3	2.21	0.41
1:C:90:PRO:O	1:C:93:VAL:HG12	2.21	0.41
1:D:117:SER:O	1:D:118:ASP:HB2	2.21	0.41
1:D:498:GLN:HG2	1:D:502:MET:HE2	2.03	0.41
1:A:409:PRO:HD3	1:A:438:PHE:CG	2.56	0.40
1:B:130:THR:HG23	1:D:128:PRO:CG	2.51	0.40
1:C:512:GLN:NE2	1:D:215:CYS:SG	2.95	0.40
1:B:133:PRO:O	1:B:198:LYS:HG2	2.22	0.40
1:B:85:TYR:HB2	1:B:469:ALA:HB3	2.04	0.40
1:C:284:LEU:HD11	1:C:305:GLU:HG3	2.03	0.40
1:A:453:ILE:HA	1:A:464:GLN:HE22	1.87	0.40
1:C:118:ASP:O	1:C:120:PRO:HD3	2.22	0.40
1:C:176:ALA:O	1:C:203:ILE:HA	2.22	0.40
1:C:353:ALA:HA	1:C:356:ILE:HD12	2.02	0.40
1:D:307:GLU:OE2	1:D:307:GLU:N	2.54	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	522/560 (93%)	505 (97%)	14 (3%)	3 (1%)	30	24
1	B	523/560 (93%)	502 (96%)	21 (4%)	0	100	100
1	C	493/560 (88%)	464 (94%)	27 (6%)	2 (0%)	39	37
1	D	476/560 (85%)	451 (95%)	24 (5%)	1 (0%)	52	53
All	All	2014/2240 (90%)	1922 (95%)	86 (4%)	6 (0%)	46	45

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	ASP
1	C	216	GLY
1	D	219	GLY
1	A	293	GLN
1	A	294	SER
1	C	219	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	436/462 (94%)	423 (97%)	13 (3%)	48	51
1	B	436/462 (94%)	421 (97%)	15 (3%)	44	45
1	C	415/462 (90%)	401 (97%)	14 (3%)	44	45
1	D	403/462 (87%)	389 (96%)	14 (4%)	43	44
All	All	1690/1848 (92%)	1634 (97%)	56 (3%)	45	47

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	SER
1	A	93	VAL
1	A	100	LEU
1	A	127	TYR
1	A	185	LEU
1	A	268	ARG
1	A	278	ASN
1	A	302	GLN
1	A	332	ARG
1	A	369	TRP
1	A	433	ASN
1	A	442	THR
1	A	504	LEU
1	B	83	TYR
1	B	93	VAL
1	B	100	LEU

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Mol	Chain	Res	Type
1	B	127	TYR
1	B	185	LEU
1	B	213	LYS
1	B	260	LEU
1	B	278	ASN
1	B	299	ASP
1	B	313	ASN
1	B	336	ASP
1	B	369	TRP
1	B	403	TRP
1	B	433	ASN
1	B	439	ASN
1	C	5	ASN
1	C	58	GLU
1	C	89	GLU
1	C	93	VAL
1	C	127	TYR
1	C	185	LEU
1	C	263	THR
1	C	278	ASN
1	C	319	ASP
1	C	323	ASP
1	C	369	TRP
1	C	439	ASN
1	C	502	MET
1	C	524	GLN
1	D	58	GLU
1	D	83	TYR
1	D	89	GLU
1	D	93	VAL
1	D	100	LEU
1	D	127	TYR
1	D	185	LEU
1	D	268	ARG
1	D	284	LEU
1	D	341	TYR
1	D	369	TRP
1	D	433	ASN
1	D	441	LYS
1	D	447	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	150	GLN
1	A	152	HIS
1	A	182	HIS
1	A	208	GLN
1	A	278	ASN
1	A	282	GLN
1	A	300	GLN
1	A	350	ASN
1	A	422	HIS
1	A	428	GLN
1	A	433	ASN
1	A	464	GLN
1	B	8	ASN
1	B	109	GLN
1	B	150	GLN
1	B	152	HIS
1	B	208	GLN
1	B	217	HIS
1	B	278	ASN
1	B	282	GLN
1	B	293	GLN
1	B	313	ASN
1	B	350	ASN
1	B	422	HIS
1	B	433	ASN
1	B	464	GLN
1	B	498	GLN
1	C	5	ASN
1	C	8	ASN
1	C	29	GLN
1	C	64	GLN
1	C	77	GLN
1	C	109	GLN
1	C	150	GLN
1	C	152	HIS
1	C	166	GLN
1	C	208	GLN
1	C	231	ASN
1	C	278	ASN
1	C	326	ASN
1	C	350	ASN
1	C	413	GLN

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Mol	Chain	Res	Type
1	C	439	ASN
1	C	464	GLN
1	C	511	HIS
1	C	512	GLN
1	D	8	ASN
1	D	77	GLN
1	D	109	GLN
1	D	150	GLN
1	D	152	HIS
1	D	208	GLN
1	D	278	ASN
1	D	282	GLN
1	D	313	ASN
1	D	343	GLN
1	D	350	ASN
1	D	413	GLN
1	D	422	HIS
1	D	433	ASN
1	D	449	GLN
1	D	464	GLN
1	D	512	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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	GLV	A	601	4	1,4,4	0.17	0	0,4,4	0.00	-
3	GOL	A	602	-	5,5,5	0.58	0	5,5,5	0.31	0
2	GLV	B	601	4	1,4,4	0.18	0	0,4,4	0.00	-
3	GOL	B	602	-	5,5,5	0.43	0	5,5,5	0.43	0
2	GLV	C	601	4	1,4,4	0.01	0	0,4,4	0.00	-
2	GLV	D	601	4	1,4,4	0.16	0	0,4,4	0.00	-
3	GOL	D	602	-	5,5,5	0.52	0	5,5,5	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLV	A	601	4	-	0/0/2/2	0/0/0/0
3	GOL	A	602	-	-	0/4/4/4	0/0/0/0
2	GLV	B	601	4	-	0/0/2/2	0/0/0/0
3	GOL	B	602	-	-	0/4/4/4	0/0/0/0
2	GLV	C	601	4	-	0/0/2/2	0/0/0/0
2	GLV	D	601	4	-	0/0/2/2	0/0/0/0
3	GOL	D	602	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	GLV	2	0
3	B	602	GOL	2	0
2	C	601	GLV	1	0
2	D	601	GLV	2	0
3	D	602	GOL	2	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	524/560 (93%)	-0.07	14 (2%) 58 65	22, 32, 55, 90	0
1	B	525/560 (93%)	0.07	13 (2%) 61 67	22, 34, 52, 66	0
1	C	499/560 (89%)	0.11	24 (4%) 34 43	22, 34, 68, 78	0
1	D	486/560 (86%)	0.18	28 (5%) 26 34	23, 35, 68, 84	0
All	All	2034/2240 (90%)	0.07	79 (3%) 43 52	22, 34, 63, 90	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	341	TYR	6.4
1	C	357	ALA	6.1
1	D	322	VAL	5.7
1	D	308	TRP	5.7
1	D	287	LEU	5.5
1	C	217	HIS	5.1
1	C	362	VAL	4.5
1	C	341	TYR	4.0
1	C	361	GLY	4.0
1	D	356	ILE	3.9
1	C	359	SER	3.9
1	C	360	LEU	3.9
1	C	324	VAL	3.7
1	A	300	GLN	3.6
1	A	297	THR	3.5
1	A	7	VAL	3.5
1	D	357	ALA	3.5
1	D	343	GLN	3.4
1	D	281	LEU	3.3
1	D	358	SER	3.3
1	C	219	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	301	LEU	3.3
1	D	321	VAL	3.3
1	D	367	PHE	3.2
1	D	344	ALA	3.1
1	C	340	LYS	3.1
1	C	364	GLU	3.1
1	C	325	ILE	3.1
1	B	331	ILE	3.0
1	A	11	VAL	3.0
1	C	358	SER	2.9
1	D	160	SER	2.8
1	C	356	ILE	2.8
1	D	345	ALA	2.8
1	C	317	PHE	2.8
1	A	290	THR	2.8
1	D	130	THR	2.8
1	D	309	MET	2.8
1	A	302	GLN	2.7
1	A	296	LYS	2.7
1	D	346	LYS	2.7
1	A	332	ARG	2.7
1	D	288	MET	2.6
1	C	22	ARG	2.5
1	B	446	ARG	2.5
1	D	275	GLY	2.5
1	A	293	GLN	2.4
1	B	22	ARG	2.4
1	D	317	PHE	2.4
1	D	158	PRO	2.4
1	B	328	SER	2.4
1	D	446	ARG	2.4
1	C	218	MET	2.4
1	C	355	ALA	2.4
1	D	319	ASP	2.4
1	B	191	LEU	2.3
1	A	131	THR	2.3
1	C	342	LEU	2.3
1	A	294	SER	2.3
1	B	15	MET	2.3
1	B	211	GLY	2.3
1	C	130	THR	2.3
1	B	329	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	375	ARG	2.3
1	B	130	THR	2.2
1	C	363	PRO	2.2
1	C	343	GLN	2.2
1	B	334	PRO	2.2
1	D	315	LYS	2.2
1	C	365	ILE	2.2
1	B	132	VAL	2.1
1	D	351	ARG	2.1
1	D	116	SER	2.1
1	B	447	ASP	2.1
1	C	164	LYS	2.0
1	A	304	ILE	2.0
1	A	18	ASP	2.0
1	D	218	MET	2.0
1	B	131	THR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	B	603	1/1	0.82	0.31	7.70	43,43,43,43	0
4	MG	A	603	1/1	0.95	0.25	4.38	34,34,34,34	0
2	GLV	C	601	5/5	0.76	0.21	3.87	47,49,50,52	0
4	MG	D	603	1/1	0.87	0.22	2.98	46,46,46,46	0
3	GOL	A	602	6/6	0.73	0.18	2.74	32,33,34,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MG	C	602	1/1	0.90	0.20	2.72	41,41,41,41	0
3	GOL	D	602	6/6	0.79	0.18	2.10	34,34,36,36	0
3	GOL	B	602	6/6	0.82	0.16	1.78	29,32,35,37	0
2	GLV	B	601	5/5	0.93	0.17	1.54	30,31,32,35	0
2	GLV	D	601	5/5	0.94	0.14	0.54	34,35,36,37	0
2	GLV	A	601	5/5	0.95	0.12	-0.48	32,32,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.