



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:40 AM UTC

PDB ID : 3JVA / pdb_00003jva
Title : Crystal structure of Dipeptide Epimerase from Enterococcus faecalis V583
Authors : Fedorov, A.A.; Fedorov, E.V.; Sakai, A.; Imker, H.; Gerlt, J.A.; Almo, S.C.
Deposited on : 2009-09-16
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

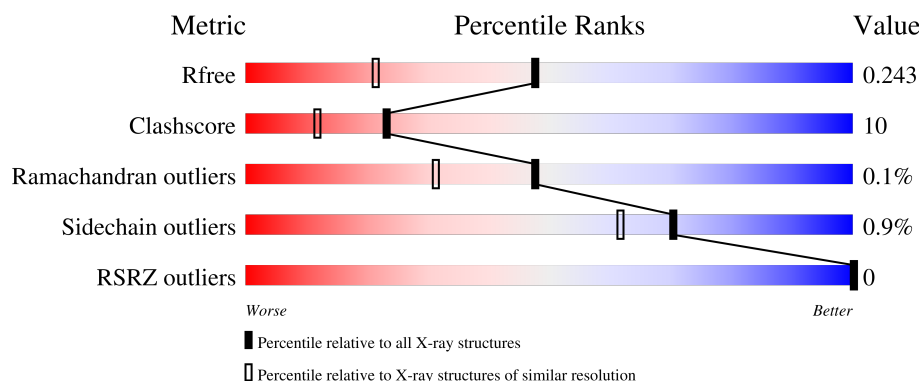
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	354	 79% 20% .
1	B	354	 79% 20% .
1	C	354	 73% 24% . .
1	D	354	 80% 17% . .
1	E	354	 79% 21% .

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Mol	Chain	Length	Quality of chain
1	F	354	 83%17%
1	G	354	 69%27%••
1	H	354	 78%20%•

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21865 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 Dipeptide Epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	0
			2638	1674	434	516	14			
1	B	354	Total	C	N	O	S	0	0	0
			2649	1680	437	518	14			
1	C	344	Total	C	N	O	S	0	0	0
			2576	1632	427	503	14			
1	D	346	Total	C	N	O	S	0	0	0
			2591	1640	429	508	14			
1	E	353	Total	C	N	O	S	0	0	0
			2638	1674	434	516	14			
1	F	354	Total	C	N	O	S	0	0	0
			2649	1680	437	518	14			
1	G	345	Total	C	N	O	S	0	0	0
			2582	1635	428	505	14			
1	H	346	Total	C	N	O	S	0	0	0
			2591	1640	429	508	14			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

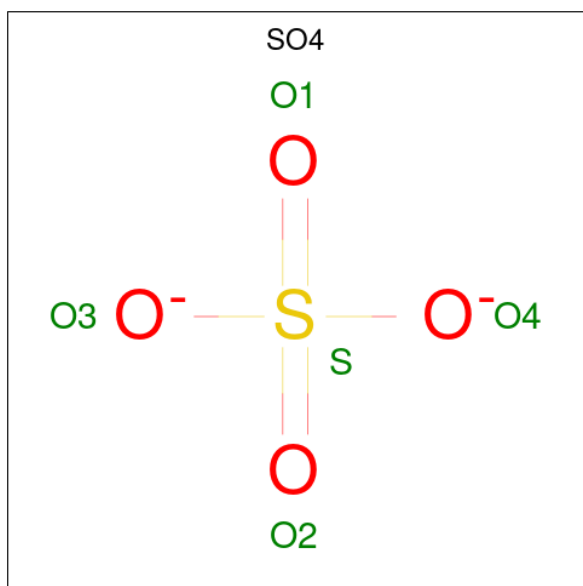
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	97	Total	O	0	0
			97	97		
5	B	153	Total	O	0	0
			153	153		
5	C	78	Total	O	0	0
			78	78		

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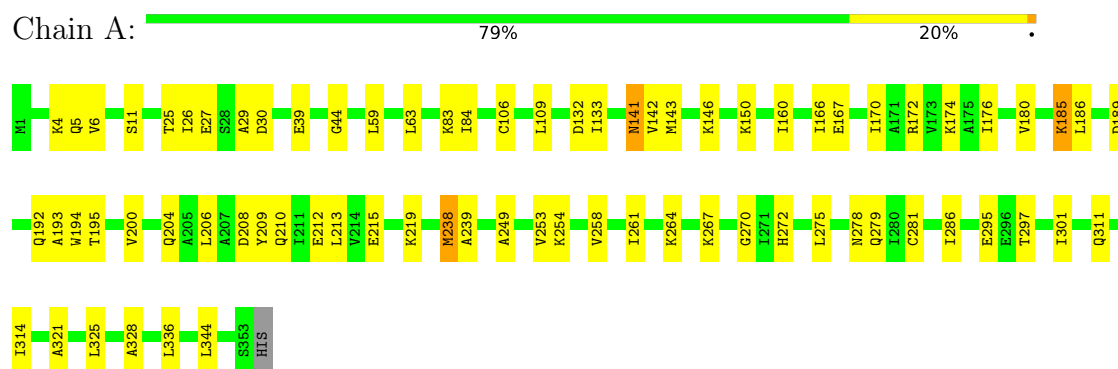
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	131	Total 131	O 131	0	0
5	E	90	Total 90	O 90	0	0
5	F	138	Total 138	O 138	0	0
5	G	76	Total 76	O 76	0	0
5	H	125	Total 125	O 125	0	0

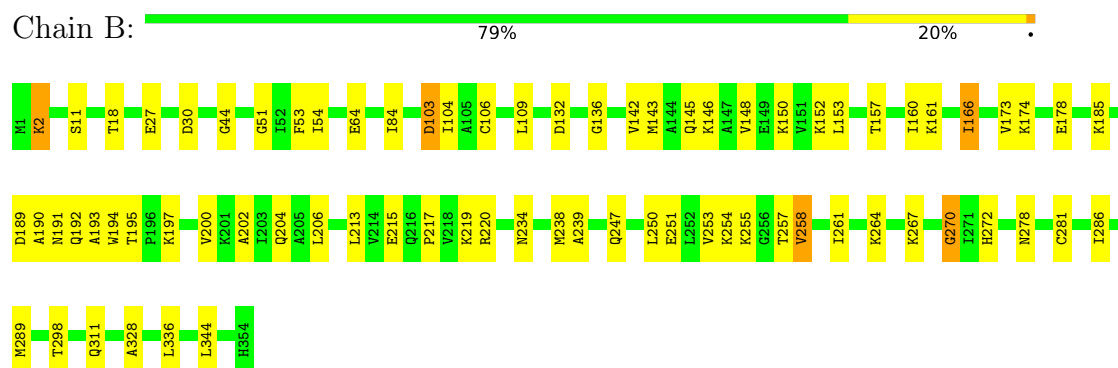
3 Residue-property plots

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

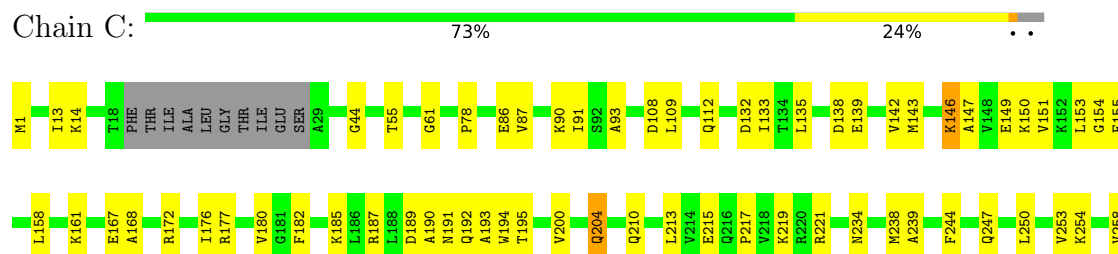
• Molecule 1: Dipeptide Epimerase



• Molecule 1: Dipeptide Epimerase



• Molecule 1: Dipeptide Epimerase





• Molecule 1: Dipeptide Epimerase

Chain D: 80% 17%



• Molecule 1: Dipeptide Epimerase

Chain E: 79% 21%



• Molecule 1: Dipeptide Epimerase

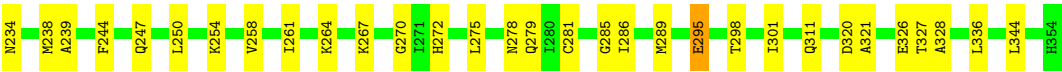
Chain F: 83% 17%



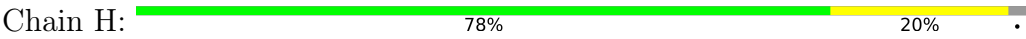
• Molecule 1: Dipeptide Epimerase

Chain G: 69% 27%





● Molecule 1: Dipeptide Epimerase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	162.27 Å 162.27 Å 319.56 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.93 – 1.70 24.93 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (24.93-1.70) 99.2 (24.93-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.70 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.244 0.222 , 0.243	Depositor DCC
R_{free} test set	17272 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 25.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.486 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21865	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: MG, GOL, SO4

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	0.37	1/2667 (0.0%)	0.84	6/3605 (0.2%)
1	B	0.36	0/2679	0.87	11/3620 (0.3%)
1	C	0.32	0/2604	0.83	5/3516 (0.1%)
1	D	0.34	0/2619	0.85	7/3536 (0.2%)
1	E	0.36	0/2667	0.85	5/3605 (0.1%)
1	F	0.36	0/2679	0.86	9/3620 (0.2%)
1	G	0.32	0/2610	0.82	6/3524 (0.2%)
1	H	0.34	0/2619	0.86	9/3536 (0.3%)
All	All	0.35	1/21144 (0.0%)	0.85	58/28562 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	MET	SD-CE	-6.17	1.64	1.79

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	344	LEU	N-CA-C	7.69	119.74	111.36
1	D	270	GLY	N-CA-C	7.51	119.67	112.08
1	D	344	LEU	N-CA-C	7.44	119.47	111.36
1	F	195	THR	N-CA-C	-7.44	99.23	110.39
1	A	344	LEU	N-CA-C	7.27	121.39	112.23
1	B	195	THR	N-CA-C	-7.18	99.61	110.39
1	D	195	THR	N-CA-C	-7.18	99.62	110.39
1	C	195	THR	N-CA-C	-7.17	99.63	110.39
1	A	270	GLY	N-CA-C	7.12	119.30	112.04
1	E	270	GLY	N-CA-C	7.11	119.26	112.08
1	E	344	LEU	N-CA-C	7.07	121.14	112.23
1	G	270	GLY	N-CA-C	7.02	119.17	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	193	ALA	N-CA-C	6.92	119.85	111.82
1	B	193	ALA	N-CA-C	6.89	119.82	111.82
1	H	195	THR	N-CA-C	-6.84	100.13	110.39
1	G	195	THR	N-CA-C	-6.84	100.13	110.39
1	B	270	GLY	N-CA-C	6.80	120.41	111.70
1	B	194	TRP	N-CA-C	6.63	120.42	110.14
1	H	270	GLY	N-CA-C	6.47	119.62	111.85
1	C	270	GLY	N-CA-C	6.46	118.63	112.04
1	F	344	LEU	N-CA-C	6.35	120.23	112.23
1	H	193	ALA	N-CA-C	6.26	120.17	112.54
1	H	194	TRP	N-CA-C	6.23	119.80	110.14
1	F	270	GLY	N-CA-C	6.22	119.66	111.70
1	C	344	LEU	N-CA-C	6.15	119.98	112.23
1	F	194	TRP	N-CA-C	6.15	119.67	110.14
1	D	194	TRP	N-CA-C	6.10	119.59	110.14
1	B	344	LEU	N-CA-C	6.05	120.39	112.89
1	F	193	ALA	N-CA-C	5.98	119.76	112.23
1	G	194	TRP	N-CA-C	5.90	119.18	109.85
1	C	194	TRP	N-CA-C	5.86	119.23	110.14
1	H	257	THR	N-CA-C	5.84	117.65	111.28
1	G	344	LEU	N-CA-C	5.61	120.19	113.23
1	F	257	THR	N-CA-C	5.59	117.45	111.36
1	D	289	MET	N-CA-C	-5.54	101.10	109.85
1	E	195	THR	N-CA-C	-5.52	102.11	110.39
1	A	193	ALA	N-CA-C	5.51	118.21	111.82
1	H	41	GLY	N-CA-C	5.36	121.88	114.92
1	A	314	ILE	N-CA-C	-5.34	98.81	106.55
1	E	257	THR	N-CA-C	5.32	117.08	111.28
1	B	298	THR	N-CA-C	5.32	117.49	111.11
1	C	193	ALA	N-CA-C	5.30	119.46	112.89
1	A	195	THR	N-CA-C	-5.29	102.46	110.39
1	H	220	ARG	N-CA-C	5.26	117.70	111.33
1	B	220	ARG	N-CA-C	5.23	118.45	111.75
1	A	194	TRP	N-CA-C	5.23	118.25	110.14
1	B	289	MET	N-CA-C	-5.19	101.64	109.85
1	F	166	ILE	N-CA-C	5.17	116.51	110.62
1	B	257	THR	N-CA-C	5.15	116.98	111.36
1	F	117	PRO	N-CA-C	-5.12	103.23	111.38
1	E	314	ILE	N-CA-C	-5.12	99.13	106.55
1	G	298	THR	N-CA-C	5.10	117.23	111.11
1	B	166	ILE	N-CA-C	5.09	116.42	110.62
1	F	289	MET	N-CA-C	-5.09	101.81	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	VAL	N-CA-C	5.06	115.99	108.65
1	H	289	MET	N-CA-C	-5.04	101.88	109.85
1	G	193	ALA	N-CA-C	5.03	119.13	112.89
1	D	257	THR	N-CA-C	5.02	116.83	111.36

There are no chirality outliers.

There are no planarity outliers.

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	2638	0	2726	58	0
1	B	2649	0	2733	58	0
1	C	2576	0	2657	67	0
1	D	2591	0	2668	49	0
1	E	2638	0	2726	58	0
1	F	2649	0	2733	38	0
1	G	2582	0	2662	79	0
1	H	2591	0	2668	50	0
2	A	6	0	8	3	0
2	B	18	0	24	2	0
2	F	6	0	8	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	5	0	0	0	0
4	C	10	0	0	1	0
4	E	5	0	0	0	0
4	G	5	0	0	0	0
5	A	97	0	0	2	0
5	B	153	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	78	0	0	3	0
5	D	131	0	0	4	0
5	E	90	0	0	5	0
5	F	138	0	0	2	0
5	G	76	0	0	3	0
5	H	125	0	0	1	0
All	All	21865	0	21613	437	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (437) 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:E:328:ALA:HB2	1:E:336:LEU:HD11	1.39	1.04
1:F:328:ALA:HB2	1:F:336:LEU:HD11	1.40	1.04
1:B:328:ALA:HB2	1:B:336:LEU:HD21	1.42	1.02
1:D:328:ALA:HB2	1:D:336:LEU:HD11	1.42	1.01
1:A:328:ALA:HB2	1:A:336:LEU:HD21	1.45	0.98
1:A:254:LYS:HG2	1:B:254:LYS:HG2	1.51	0.93
1:D:278:ASN:HD22	1:D:311:GLN:HE21	1.11	0.93
1:H:278:ASN:HD22	1:H:311:GLN:HE21	1.13	0.91
2:A:355:GOL:H12	1:E:61:GLY:HA3	1.54	0.89
1:G:133:ILE:HD13	1:G:150:LYS:HD3	1.56	0.87
1:F:278:ASN:HD22	1:F:311:GLN:HE21	1.21	0.87
1:D:1:MET:HG3	1:D:78:PRO:HD2	1.58	0.86
1:B:253:VAL:HG12	1:B:286:ILE:HD12	1.57	0.86
1:A:253:VAL:HG12	1:A:286:ILE:HD12	1.58	0.85
1:A:170:ILE:HG22	1:A:174:LYS:HE2	1.60	0.84
1:E:253:VAL:HG12	1:E:286:ILE:HD12	1.58	0.83
1:G:64:GLU:O	1:G:68:LEU:HD13	1.81	0.81
1:G:150:LYS:HA	1:G:150:LYS:HE2	1.63	0.80
1:B:278:ASN:HD22	1:B:311:GLN:HE21	1.29	0.80
1:G:328:ALA:HB2	1:G:336:LEU:HD11	1.64	0.80
1:D:278:ASN:ND2	1:D:311:GLN:HE21	1.80	0.78
1:H:278:ASN:ND2	1:H:311:GLN:HE21	1.80	0.78
1:G:278:ASN:HD22	1:G:311:GLN:HE21	1.32	0.78
1:A:4:LYS:HE3	1:A:39:GLU:HA	1.64	0.77
1:C:55:THR:HG22	1:C:244:PHE:HE2	1.50	0.77
1:C:143:MET:HE2	1:C:176:ILE:HD11	1.67	0.76
1:C:328:ALA:HB2	1:C:336:LEU:HD11	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:VAL:HG12	1:C:286:ILE:HD12	1.66	0.76
1:A:59:LEU:O	1:A:63:LEU:HD13	1.85	0.76
1:A:278:ASN:HD22	1:A:311:GLN:HE21	1.33	0.75
1:C:278:ASN:HD22	1:C:311:GLN:HE21	1.32	0.75
1:E:278:ASN:HD22	1:E:311:GLN:HE21	1.35	0.75
1:C:143:MET:SD	1:C:172:ARG:HD2	2.26	0.74
1:F:148:VAL:O	1:F:152:LYS:HG3	1.89	0.73
1:E:166:ILE:O	1:E:170:ILE:HD13	1.89	0.73
1:H:215:GLU:HG3	1:H:238:MET:HE3	1.71	0.73
1:A:5:GLN:HE21	1:A:6:VAL:H	1.38	0.72
1:G:55:THR:HG22	1:G:244:PHE:HE2	1.53	0.72
1:C:87:VAL:HA	1:C:90:LYS:NZ	2.05	0.71
1:A:141:ASN:HD22	1:A:142:VAL:H	1.38	0.71
1:B:202:ALA:O	1:B:206:LEU:HD23	1.91	0.71
1:B:234:ASN:HB3	1:E:201:LYS:HE3	1.70	0.71
1:B:215:GLU:HG3	1:B:238:MET:HE3	1.73	0.70
1:C:161:LYS:HD2	1:C:191:ASN:HD21	1.55	0.70
1:A:141:ASN:HD22	1:A:142:VAL:N	1.90	0.69
1:G:226:LEU:O	1:G:229:VAL:HG22	1.92	0.69
1:G:278:ASN:ND2	1:G:311:GLN:HE21	1.91	0.69
1:H:251:GLU:OE1	1:H:255:LYS:HE2	1.93	0.69
1:E:141:ASN:HD22	1:E:141:ASN:N	1.91	0.68
1:F:238:MET:HE2	1:F:260:VAL:HG11	1.76	0.68
1:H:167:GLU:HG3	1:H:168:ALA:H	1.59	0.68
1:E:2:LYS:HD2	1:E:39:GLU:OE2	1.94	0.67
1:F:145:GLN:O	1:F:148:VAL:HG22	1.95	0.67
1:A:185:LYS:HD3	1:A:212:GLU:CD	2.20	0.67
1:C:133:ILE:HD13	1:C:150:LYS:HD2	1.76	0.67
1:B:250:LEU:HG	1:B:254:LYS:HE3	1.76	0.66
1:B:161:LYS:HG3	1:B:191:ASN:HD22	1.60	0.66
1:B:143:MET:HA	1:B:146:LYS:HE2	1.78	0.66
1:A:170:ILE:CG2	1:A:174:LYS:HE2	2.25	0.66
1:F:2:LYS:HE2	1:F:39:GLU:HG3	1.79	0.66
1:D:264:LYS:HB2	1:D:267:LYS:HE2	1.78	0.65
1:A:336:LEU:HD23	5:A:637:HOH:O	1.96	0.65
1:D:1:MET:HE2	1:D:38:THR:HG21	1.77	0.65
1:G:135:LEU:HD21	1:G:158:LEU:HD22	1.77	0.65
1:G:172:ARG:O	1:G:176:ILE:HG12	1.96	0.65
1:E:250:LEU:O	1:E:254:LYS:HG3	1.97	0.65
1:B:145:GLN:O	1:B:148:VAL:HG22	1.97	0.65
1:G:55:THR:HG22	1:G:244:PHE:CE2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:LYS:HD2	1:C:191:ASN:ND2	2.12	0.64
1:C:55:THR:HG22	1:C:244:PHE:CE2	2.32	0.64
1:H:167:GLU:HG3	1:H:168:ALA:N	2.13	0.64
1:B:53:PHE:CD1	1:B:54:ILE:HG13	2.33	0.63
1:E:336:LEU:HD13	5:E:843:HOH:O	1.98	0.63
1:G:13:ILE:HD12	1:G:327:THR:HG23	1.81	0.63
2:A:355:GOL:H11	1:E:58:THR:H	1.64	0.63
1:C:278:ASN:ND2	1:C:311:GLN:HE21	1.97	0.62
1:A:185:LYS:HD3	1:A:212:GLU:OE2	1.98	0.62
1:A:254:LYS:HA	1:B:254:LYS:HE2	1.81	0.62
1:B:250:LEU:O	1:B:254:LYS:HG3	2.00	0.62
1:A:166:ILE:O	1:A:170:ILE:HG13	2.00	0.62
1:D:295:GLU:HG2	5:D:883:HOH:O	1.99	0.62
1:E:196:PRO:HG2	5:E:435:HOH:O	1.99	0.62
1:B:148:VAL:O	1:B:152:LYS:HG3	2.00	0.61
1:B:247:GLN:OE1	1:H:221:ARG:HD3	2.00	0.61
1:F:20:THR:OG1	1:F:137:ILE:HD11	1.99	0.61
1:E:2:LYS:HB2	1:E:2:LYS:NZ	2.16	0.61
1:C:149:GLU:O	1:C:153:LEU:HD23	2.01	0.61
1:D:278:ASN:HD22	1:D:311:GLN:NE2	1.93	0.60
1:C:139:GLU:HB2	1:C:142:VAL:HG23	1.82	0.60
1:F:278:ASN:ND2	1:F:311:GLN:HE21	1.96	0.60
1:C:86:GLU:HG2	1:C:90:LYS:HE3	1.84	0.59
1:G:185:LYS:HD2	1:G:212:GLU:OE1	2.03	0.59
1:B:166:ILE:HB	2:B:355:GOL:H12	1.84	0.59
1:E:133:ILE:HD13	1:E:150:LYS:HG3	1.83	0.59
1:G:116:LEU:HB2	1:G:121:LEU:HD21	1.85	0.59
1:G:40:GLU:HG3	5:G:366:HOH:O	2.02	0.59
1:E:215:GLU:HG3	1:E:238:MET:HE3	1.84	0.58
1:C:250:LEU:O	1:C:254:LYS:HG3	2.02	0.58
1:A:278:ASN:ND2	1:A:311:GLN:HE21	2.02	0.58
1:C:135:LEU:HD11	1:C:158:LEU:HD13	1.86	0.58
1:C:146:LYS:NZ	1:C:146:LYS:HB3	2.18	0.58
1:C:200:VAL:O	1:C:204:GLN:HB2	2.04	0.58
1:F:238:MET:HE2	1:F:260:VAL:CG1	2.34	0.58
1:H:215:GLU:CG	1:H:238:MET:HE3	2.33	0.57
1:H:330:VAL:HG22	1:H:331:THR:N	2.19	0.57
1:B:174:LYS:O	1:B:178:GLU:HG2	2.04	0.57
1:C:168:ALA:HB1	1:C:172:ARG:HH12	1.69	0.57
1:C:247:GLN:HB2	1:G:221:ARG:HH21	1.70	0.57
1:E:278:ASN:ND2	1:E:311:GLN:HE21	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:VAL:O	1:A:204:GLN:HG3	2.03	0.57
1:D:127:ASN:C	1:D:127:ASN:HD22	2.11	0.57
1:H:239:ALA:HB2	1:H:258:VAL:HG11	1.87	0.57
1:C:190:ALA:HB3	1:C:217:PRO:HA	1.86	0.57
1:E:200:VAL:O	1:E:204:GLN:HG3	2.05	0.56
1:G:146:LYS:O	1:G:150:LYS:HG2	2.04	0.56
1:A:185:LYS:HB2	1:A:185:LYS:NZ	2.21	0.56
1:C:132:ASP:OD2	1:C:187:ARG:HD2	2.06	0.56
1:C:154:GLY:C	1:C:340:PRO:HG2	2.31	0.56
1:G:50:PRO:O	1:G:295:GLU:HG3	2.06	0.56
1:G:239:ALA:HB2	1:G:258:VAL:HG11	1.87	0.56
1:C:146:LYS:O	1:C:150:LYS:HG2	2.05	0.56
1:F:161:LYS:HG3	1:F:191:ASN:HD22	1.70	0.56
1:H:278:ASN:HD22	1:H:311:GLN:NE2	1.93	0.56
1:H:184:ILE:HD12	1:H:184:ILE:N	2.20	0.56
1:C:87:VAL:HA	1:C:90:LYS:HZ1	1.71	0.56
1:C:176:ILE:O	1:C:180:VAL:HG22	2.06	0.56
1:F:53:PHE:CD1	1:F:54:ILE:HG13	2.41	0.56
1:F:295:GLU:HG2	5:F:404:HOH:O	2.06	0.56
1:G:134:THR:HG22	1:G:320:ASP:OD2	2.06	0.56
1:H:133:ILE:HD13	1:H:323:PHE:HD2	1.69	0.55
1:B:264:LYS:HB2	1:B:267:LYS:HE2	1.87	0.55
1:G:54:ILE:N	1:G:54:ILE:HD12	2.21	0.55
1:H:330:VAL:HG21	1:H:352:ILE:CG2	2.37	0.55
1:B:213:LEU:C	1:B:213:LEU:HD12	2.32	0.55
1:G:144:ALA:HA	1:G:176:ILE:HD13	1.88	0.55
1:G:137:ILE:HA	1:G:143:MET:HE3	1.89	0.55
1:E:161:LYS:NZ	1:E:191:ASN:HD21	2.05	0.55
1:E:197:LYS:HG2	1:E:201:LYS:HZ3	1.71	0.54
1:E:220:ARG:HG3	1:E:221:ARG:HG3	1.88	0.54
1:H:154:GLY:C	1:H:340:PRO:HG2	2.32	0.54
1:H:161:LYS:HG3	1:H:191:ASN:HD22	1.72	0.54
1:B:157:THR:OG1	1:B:185:LYS:HE3	2.07	0.54
1:C:189:ASP:HA	1:C:215:GLU:HB3	1.89	0.54
1:B:215:GLU:CG	1:B:238:MET:HE3	2.37	0.54
1:C:192:GLN:HB3	1:C:219:LYS:HA	1.90	0.54
1:G:135:LEU:HD23	1:G:158:LEU:HB3	1.89	0.54
1:G:147:ALA:O	1:G:151:VAL:HG23	2.08	0.54
1:B:261:ILE:HD12	1:B:281:CYS:SG	2.48	0.54
1:B:2:LYS:NZ	1:B:2:LYS:HB2	2.23	0.54
1:C:172:ARG:O	1:C:176:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:272:HIS:HD2	5:H:389:HOH:O	1.92	0.53
1:H:330:VAL:HG22	1:H:331:THR:H	1.72	0.53
1:A:275:LEU:O	1:A:279:GLN:HG3	2.09	0.53
1:B:278:ASN:ND2	1:B:311:GLN:HE21	2.04	0.53
1:E:141:ASN:N	1:E:141:ASN:ND2	2.54	0.53
1:G:250:LEU:HG	1:G:254:LYS:HE3	1.90	0.53
1:F:264:LYS:HB2	1:F:267:LYS:HE2	1.90	0.53
1:C:264:LYS:HB2	1:C:267:LYS:HE2	1.90	0.53
1:H:1:MET:HE1	1:H:113:LYS:HB2	1.90	0.53
1:C:247:GLN:HB2	1:G:221:ARG:NH2	2.24	0.52
1:D:238:MET:HE2	1:D:260:VAL:HG11	1.91	0.52
1:A:84:ILE:HD13	1:A:106:CYS:SG	2.49	0.52
1:E:143:MET:SD	1:E:172:ARG:HD3	2.49	0.52
1:F:2:LYS:HG3	1:F:39:GLU:CG	2.39	0.52
1:E:54:ILE:HD13	5:E:368:HOH:O	2.10	0.52
1:E:215:GLU:CG	1:E:238:MET:HE3	2.40	0.52
1:G:143:MET:HB3	1:G:176:ILE:HD11	1.90	0.52
1:B:161:LYS:HG3	1:B:191:ASN:ND2	2.23	0.52
1:H:174:LYS:O	1:H:178:GLU:HG2	2.10	0.52
1:A:166:ILE:HG23	1:A:167:GLU:N	2.25	0.51
1:E:239:ALA:HB2	1:E:258:VAL:HG11	1.92	0.51
1:A:143:MET:SD	1:A:172:ARG:HD3	2.51	0.51
1:B:146:LYS:O	1:B:150:LYS:HG2	2.09	0.51
1:C:247:GLN:OE1	1:G:221:ARG:HD2	2.10	0.51
1:F:278:ASN:HD22	1:F:311:GLN:NE2	2.01	0.51
1:F:336:LEU:N	1:F:336:LEU:HD12	2.25	0.51
1:D:238:MET:HE2	1:D:260:VAL:CG1	2.41	0.51
1:B:142:VAL:O	1:B:145:GLN:HG2	2.10	0.51
1:D:58:THR:HB	1:F:64:GLU:OE1	2.10	0.51
1:H:57:GLU:OE1	1:H:96:PRO:HG2	2.11	0.51
1:C:90:LYS:NZ	1:C:90:LYS:HB2	2.25	0.51
1:G:200:VAL:O	1:G:204:GLN:HG3	2.11	0.51
1:H:264:LYS:HB2	1:H:267:LYS:HE2	1.93	0.51
1:D:138:ASP:OD1	1:D:142:VAL:HG11	2.11	0.51
1:G:192:GLN:HB3	1:G:219:LYS:HA	1.93	0.51
1:B:234:ASN:CB	1:E:201:LYS:HE3	2.40	0.50
1:E:141:ASN:ND2	1:E:141:ASN:H	2.08	0.50
1:H:145:GLN:O	1:H:148:VAL:HG12	2.11	0.50
1:G:150:LYS:HE2	1:G:150:LYS:CA	2.39	0.50
1:C:14:LYS:HE3	1:C:326:GLU:OE1	2.10	0.50
1:D:182:PHE:HD1	1:D:210:GLN:HE21	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:MET:HE1	1:C:289:MET:CE	2.42	0.50
1:H:176:ILE:O	1:H:180:VAL:HG22	2.11	0.50
1:D:182:PHE:HB3	1:D:210:GLN:HE22	1.77	0.50
1:A:213:LEU:HD12	1:A:213:LEU:C	2.37	0.50
1:E:261:ILE:HD12	1:E:281:CYS:SG	2.52	0.50
1:H:146:LYS:O	1:H:150:LYS:HG2	2.11	0.50
1:H:215:GLU:CD	1:H:238:MET:HE3	2.37	0.50
1:D:239:ALA:HB2	1:D:258:VAL:HG11	1.94	0.49
1:B:18:THR:HG22	1:B:27:GLU:HB3	1.94	0.49
1:F:84:ILE:HD13	1:F:106:CYS:SG	2.52	0.49
1:G:190:ALA:HB3	1:G:217:PRO:HA	1.93	0.49
1:D:223:LEU:N	1:D:223:LEU:HD22	2.28	0.49
1:B:336:LEU:N	1:B:336:LEU:HD22	2.28	0.49
1:C:177:ARG:NH1	1:C:182:PHE:HA	2.27	0.49
1:E:86:GLU:HG2	1:E:90:LYS:HE2	1.95	0.49
1:A:29:ALA:HA	1:A:295:GLU:HA	1.94	0.49
1:D:15:LEU:HG	1:D:28:SER:HA	1.95	0.49
1:D:213:LEU:HD12	1:D:213:LEU:C	2.36	0.49
1:F:141:ASN:O	1:F:145:GLN:HG3	2.12	0.49
1:G:177:ARG:HH11	1:G:182:PHE:HA	1.77	0.49
1:C:272:HIS:HD2	5:C:413:HOH:O	1.95	0.49
1:E:84:ILE:HD13	1:E:106:CYS:SG	2.53	0.49
1:C:132:ASP:C	1:C:132:ASP:OD1	2.56	0.48
1:D:53:PHE:CD1	1:D:54:ILE:HG13	2.48	0.48
1:D:141:ASN:N	1:D:141:ASN:HD22	2.10	0.48
1:E:197:LYS:HG2	1:E:201:LYS:NZ	2.27	0.48
1:G:143:MET:SD	1:G:172:ARG:HD2	2.53	0.48
1:A:133:ILE:HD13	1:A:150:LYS:HD2	1.95	0.48
1:D:176:ILE:O	1:D:180:VAL:HG22	2.13	0.48
1:E:166:ILE:HG23	1:E:167:GLU:N	2.27	0.48
1:E:167:GLU:H	1:E:167:GLU:CD	2.22	0.48
1:G:189:ASP:HA	1:G:215:GLU:HB3	1.95	0.48
1:A:192:GLN:HB3	1:A:219:LYS:HA	1.95	0.48
1:A:210:GLN:O	1:A:210:GLN:HG2	2.13	0.48
1:G:1:MET:HE3	1:G:78:PRO:HB2	1.96	0.48
1:H:1:MET:HE2	1:H:38:THR:HG21	1.96	0.48
1:A:264:LYS:HB2	1:A:267:LYS:HE2	1.94	0.48
1:D:167:GLU:CD	1:D:167:GLU:H	2.22	0.48
1:C:147:ALA:O	1:C:151:VAL:HG23	2.14	0.48
1:G:219:LYS:HG3	5:G:473:HOH:O	2.13	0.48
1:G:229:VAL:HG23	1:G:230:THR:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:LYS:NZ	1:B:255:LYS:HB3	2.29	0.48
1:C:336:LEU:N	1:C:336:LEU:HD12	2.28	0.48
1:G:272:HIS:HD2	5:G:377:HOH:O	1.95	0.48
1:C:13:ILE:HD12	1:C:327:THR:HG23	1.95	0.48
1:C:213:LEU:C	1:C:213:LEU:HD12	2.39	0.48
1:D:336:LEU:HD12	1:D:336:LEU:N	2.27	0.48
1:A:141:ASN:ND2	1:A:142:VAL:N	2.59	0.47
1:A:336:LEU:N	1:A:336:LEU:HD22	2.29	0.47
1:C:221:ARG:NH2	1:G:247:GLN:OE1	2.47	0.47
1:G:176:ILE:O	1:G:180:VAL:HG22	2.14	0.47
1:A:132:ASP:C	1:A:132:ASP:OD1	2.57	0.47
1:B:132:ASP:OD1	1:B:132:ASP:C	2.57	0.47
1:C:167:GLU:CD	1:C:167:GLU:H	2.22	0.47
1:D:146:LYS:O	1:D:150:LYS:HG2	2.13	0.47
1:E:29:ALA:HA	1:E:295:GLU:HA	1.96	0.47
1:F:213:LEU:HD12	1:F:213:LEU:C	2.39	0.47
1:G:135:LEU:CD2	1:G:158:LEU:HB3	2.44	0.47
1:G:213:LEU:C	1:G:213:LEU:HD12	2.39	0.47
1:F:18:THR:HG22	1:F:27:GLU:HG2	1.96	0.47
1:G:15:LEU:HG	1:G:28:SER:N	2.29	0.47
1:G:167:GLU:H	1:G:167:GLU:CD	2.22	0.47
1:C:90:LYS:HG3	5:C:449:HOH:O	2.14	0.47
1:G:102:ILE:N	1:G:102:ILE:HD12	2.30	0.47
1:E:213:LEU:C	1:E:213:LEU:HD12	2.38	0.47
1:E:215:GLU:CD	1:E:238:MET:HE3	2.40	0.47
1:C:146:LYS:NZ	1:C:150:LYS:HE3	2.28	0.47
1:A:239:ALA:HB2	1:A:258:VAL:HG11	1.97	0.47
1:B:103:ASP:CG	1:B:104:ILE:N	2.72	0.47
1:B:200:VAL:O	1:B:204:GLN:HG3	2.15	0.47
1:D:132:ASP:OD1	1:D:132:ASP:C	2.57	0.47
1:G:177:ARG:HD2	1:G:182:PHE:CD1	2.50	0.47
1:B:64:GLU:OE1	1:H:58:THR:HB	2.15	0.47
1:D:275:LEU:O	1:D:279:GLN:HG3	2.14	0.47
1:E:11:SER:O	1:E:30:ASP:HA	2.15	0.47
1:G:146:LYS:HD2	1:G:149:GLU:OE2	2.15	0.47
1:H:12:LYS:HB2	1:H:12:LYS:NZ	2.29	0.47
1:C:239:ALA:HB2	1:C:258:VAL:HG11	1.96	0.47
1:C:61:GLY:HA3	4:C:356:SO4:O2	2.15	0.47
1:H:200:VAL:O	1:H:204:GLN:HG3	2.15	0.47
1:H:330:VAL:HG23	1:H:354:HIS:HB2	1.96	0.47
1:G:192:GLN:HE22	1:G:220:ARG:HH21	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ILE:HG23	1:A:167:GLU:H	1.80	0.46
1:A:253:VAL:HG12	1:A:286:ILE:CD1	2.39	0.46
1:D:336:LEU:HD13	5:D:374:HOH:O	2.15	0.46
1:F:146:LYS:O	1:F:150:LYS:HG2	2.15	0.46
1:E:275:LEU:O	1:E:279:GLN:HG3	2.15	0.46
1:E:327:THR:HG23	5:E:386:HOH:O	2.15	0.46
1:F:44:GLY:HA3	1:F:109:LEU:HG	1.98	0.46
1:G:132:ASP:OD1	1:G:132:ASP:C	2.58	0.46
1:D:159:LYS:NZ	1:D:189:ASP:HB2	2.30	0.46
1:F:132:ASP:OD1	1:F:132:ASP:C	2.59	0.46
1:F:261:ILE:HD12	1:F:281:CYS:SG	2.54	0.46
1:B:84:ILE:HD13	1:B:106:CYS:SG	2.56	0.46
1:D:127:ASN:C	1:D:127:ASN:ND2	2.73	0.46
1:G:98:ALA:O	1:G:102:ILE:HD13	2.16	0.46
1:G:177:ARG:NH1	1:G:182:PHE:HA	2.30	0.46
1:C:1:MET:HE3	1:C:78:PRO:HB2	1.98	0.46
1:B:197:LYS:HD3	1:G:234:ASN:O	2.16	0.46
1:C:293:MET:HB2	1:C:296:GLU:HG3	1.97	0.46
1:D:339:LYS:HD3	1:D:339:LYS:N	2.31	0.45
1:A:27:GLU:CD	1:A:27:GLU:H	2.25	0.45
1:C:336:LEU:HD13	5:C:364:HOH:O	2.16	0.45
1:A:215:GLU:HG3	1:A:238:MET:HE3	1.98	0.45
1:B:103:ASP:OD1	1:B:270:GLY:HA3	2.16	0.45
1:E:210:GLN:O	1:E:210:GLN:HG2	2.15	0.45
1:H:132:ASP:C	1:H:132:ASP:OD1	2.59	0.45
1:D:142:VAL:O	1:D:146:LYS:HG3	2.16	0.45
1:D:200:VAL:O	1:D:204:GLN:HG3	2.17	0.45
1:E:189:ASP:HA	1:E:215:GLU:HB3	1.99	0.45
1:A:249:ALA:O	1:A:253:VAL:HG22	2.17	0.45
1:H:161:LYS:HG3	1:H:191:ASN:ND2	2.31	0.45
1:A:185:LYS:HB2	1:A:185:LYS:HZ2	1.82	0.45
1:C:275:LEU:O	1:C:279:GLN:HG3	2.17	0.45
1:G:286:ILE:N	1:G:286:ILE:HD12	2.31	0.45
1:H:330:VAL:CG2	1:H:353:SER:O	2.64	0.45
1:B:136:GLY:O	1:B:146:LYS:NZ	2.50	0.45
1:E:272:HIS:HD2	5:E:383:HOH:O	2.00	0.45
2:A:355:GOL:C1	1:E:58:THR:H	2.28	0.45
1:D:57:GLU:OE1	1:D:96:PRO:HG2	2.17	0.45
1:E:161:LYS:HZ3	1:E:191:ASN:HD21	1.63	0.45
1:E:264:LYS:HB2	1:E:267:LYS:HE2	1.99	0.45
1:E:279:GLN:OE1	1:F:279:GLN:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:ILE:HD12	1:E:293:MET:SD	2.57	0.44
1:C:108:ASP:O	1:C:112:GLN:HG3	2.16	0.44
1:A:11:SER:O	1:A:30:ASP:HA	2.17	0.44
1:E:132:ASP:C	1:E:132:ASP:OD1	2.60	0.44
1:B:239:ALA:HB2	1:B:258:VAL:HG11	2.00	0.44
1:D:64:GLU:OE1	1:F:58:THR:HB	2.17	0.44
1:G:121:LEU:HD22	1:G:121:LEU:N	2.33	0.44
1:G:138:ASP:CG	1:G:139:GLU:H	2.26	0.44
1:D:182:PHE:HD1	1:D:210:GLN:NE2	2.15	0.44
1:A:83:LYS:HD2	5:B:783:HOH:O	2.17	0.44
1:C:146:LYS:HB3	1:C:146:LYS:HZ3	1.82	0.44
1:A:261:ILE:HD12	1:A:281:CYS:SG	2.57	0.44
1:E:26:ILE:HD12	1:E:295:GLU:OE2	2.17	0.44
1:G:285:GLY:C	1:G:286:ILE:HD12	2.43	0.44
1:G:336:LEU:HD12	1:G:336:LEU:N	2.33	0.44
1:H:330:VAL:HG22	1:H:353:SER:O	2.18	0.44
1:A:5:GLN:NE2	1:A:6:VAL:H	2.10	0.44
1:C:139:GLU:HB2	1:C:142:VAL:CG2	2.45	0.44
1:H:275:LEU:O	1:H:279:GLN:HG3	2.18	0.44
1:D:48:GLY:O	1:D:50:PRO:HD3	2.18	0.43
1:F:2:LYS:HG3	1:F:39:GLU:HG3	1.99	0.43
1:D:1:MET:CG	1:D:78:PRO:HD2	2.39	0.43
1:F:160:ILE:HD11	1:F:173:VAL:HG22	2.00	0.43
1:H:133:ILE:HD13	1:H:323:PHE:CD2	2.51	0.43
1:B:103:ASP:OD1	1:B:270:GLY:CA	2.66	0.43
1:F:149:GLU:HA	1:F:152:LYS:HD2	2.00	0.43
1:G:14:LYS:HD3	1:G:326:GLU:OE2	2.18	0.43
1:A:146:LYS:O	1:A:150:LYS:HG2	2.18	0.43
1:D:339:LYS:NZ	5:D:412:HOH:O	2.50	0.43
1:E:192:GLN:HB3	1:E:219:LYS:HA	2.01	0.43
1:G:238:MET:HE1	1:G:289:MET:CE	2.48	0.43
1:D:190:ALA:HB3	1:D:217:PRO:HA	2.00	0.43
1:B:44:GLY:HA3	1:B:109:LEU:HG	2.01	0.43
1:C:155:PHE:CG	1:C:340:PRO:HG3	2.54	0.43
1:G:254:LYS:HA	1:H:254:LYS:HE2	1.99	0.43
1:D:233:VAL:O	1:G:197:LYS:HE3	2.19	0.43
1:E:176:ILE:O	1:E:180:VAL:HG22	2.18	0.43
1:H:149:GLU:O	1:H:152:LYS:HB3	2.18	0.43
1:F:272:HIS:HD2	5:F:394:HOH:O	2.02	0.43
1:A:5:GLN:HG3	1:A:6:VAL:N	2.33	0.43
1:G:143:MET:CB	1:G:176:ILE:HD11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:GLN:CD	1:G:221:ARG:HD2	2.44	0.43
1:G:169:ASP:O	1:G:173:VAL:HG23	2.19	0.43
1:A:189:ASP:HA	1:A:215:GLU:HB3	2.01	0.42
1:A:325:LEU:HB2	1:A:336:LEU:HD12	2.01	0.42
1:E:331:THR:HG22	1:E:332:GLY:N	2.34	0.42
1:H:330:VAL:CG2	1:H:352:ILE:HG23	2.49	0.42
1:B:160:ILE:HD11	1:B:173:VAL:HG22	2.01	0.42
1:B:145:GLN:O	1:B:148:VAL:CG2	2.67	0.42
1:B:202:ALA:HB2	2:B:355:GOL:H31	2.01	0.42
1:G:166:ILE:HG23	1:G:167:GLU:N	2.34	0.42
1:B:11:SER:O	1:B:30:ASP:HA	2.20	0.42
1:B:178:GLU:HG3	5:B:484:HOH:O	2.19	0.42
1:F:189:ASP:HA	1:F:215:GLU:HB3	2.01	0.42
1:A:215:GLU:CD	1:A:238:MET:HE3	2.44	0.42
1:B:189:ASP:HA	1:B:215:GLU:HB3	2.01	0.42
1:C:87:VAL:O	1:C:91:ILE:HG12	2.20	0.42
1:G:44:GLY:HA3	1:G:109:LEU:HG	2.01	0.42
1:H:44:GLY:HA3	1:H:109:LEU:HG	2.01	0.42
1:A:297:THR:HA	1:A:325:LEU:HD11	2.01	0.42
1:G:264:LYS:HB2	1:G:267:LYS:HE2	2.02	0.42
1:B:103:ASP:CG	1:B:270:GLY:HA3	2.45	0.42
1:B:250:LEU:CG	1:B:254:LYS:HE3	2.46	0.42
1:C:93:ALA:HB2	1:G:53:PHE:O	2.20	0.42
1:C:177:ARG:HD3	1:C:177:ARG:HA	1.86	0.42
1:C:234:ASN:O	1:F:197:LYS:HD3	2.20	0.42
1:E:2:LYS:HB2	1:E:2:LYS:HZ2	1.84	0.42
1:A:174:LYS:HG2	1:A:209:TYR:CZ	2.55	0.42
1:D:157:THR:HG21	1:D:187:ARG:CZ	2.50	0.42
1:A:206:LEU:C	1:A:208:ASP:H	2.28	0.41
1:B:173:VAL:HG21	1:B:206:LEU:HD12	2.02	0.41
1:D:223:LEU:HD22	1:D:223:LEU:H	1.84	0.41
1:E:13:ILE:HD12	1:E:297:THR:HG21	2.02	0.41
1:G:6:VAL:HG21	1:G:70:GLY:HA2	2.02	0.41
1:H:213:LEU:C	1:H:213:LEU:HD12	2.44	0.41
1:A:25:THR:HG22	1:A:26:ILE:N	2.34	0.41
1:D:157:THR:OG1	1:D:185:LYS:HE3	2.19	0.41
1:F:143:MET:SD	1:F:172:ARG:HD3	2.59	0.41
1:H:261:ILE:HD12	1:H:281:CYS:SG	2.61	0.41
1:A:272:HIS:HD2	5:A:370:HOH:O	2.03	0.41
1:C:44:GLY:HA3	1:C:109:LEU:HG	2.03	0.41
1:C:138:ASP:CG	1:C:139:GLU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:137:ILE:HA	1:G:143:MET:CE	2.49	0.41
1:D:221:ARG:HG2	1:F:247:GLN:NE2	2.35	0.41
1:G:229:VAL:CG2	1:G:230:THR:N	2.84	0.41
1:G:261:ILE:HD12	1:G:281:CYS:SG	2.61	0.41
1:C:261:ILE:HD12	1:C:281:CYS:SG	2.61	0.41
1:C:238:MET:HE1	1:C:289:MET:HE2	2.02	0.41
1:D:182:PHE:CD1	1:D:210:GLN:NE2	2.88	0.41
1:H:184:ILE:N	1:H:184:ILE:CD1	2.83	0.41
1:A:44:GLY:HA3	1:A:109:LEU:HG	2.02	0.41
1:E:146:LYS:O	1:E:150:LYS:HD3	2.20	0.41
1:H:15:LEU:HG	1:H:28:SER:HA	2.02	0.41
1:H:339:LYS:HA	1:H:340:PRO:HD3	1.91	0.41
1:A:176:ILE:O	1:A:180:VAL:HG22	2.20	0.41
1:B:192:GLN:HB3	1:B:219:LYS:HA	2.01	0.41
1:B:251:GLU:OE2	1:B:255:LYS:HD2	2.20	0.41
1:B:272:HIS:HD2	5:B:398:HOH:O	2.03	0.41
1:C:323:PHE:N	1:C:323:PHE:CD1	2.89	0.41
1:D:299:ILE:HG13	5:D:387:HOH:O	2.21	0.41
1:E:336:LEU:N	1:E:336:LEU:HD12	2.36	0.41
1:F:238:MET:SD	1:F:262:ASN:HB2	2.61	0.41
1:G:144:ALA:O	1:G:148:VAL:HG23	2.21	0.41
1:H:133:ILE:HD12	1:H:320:ASP:HB2	2.02	0.41
1:H:190:ALA:HB3	1:H:217:PRO:HA	2.02	0.41
1:H:330:VAL:HG21	1:H:352:ILE:HG23	2.03	0.41
1:A:160:ILE:HD11	1:A:186:LEU:HD22	2.03	0.41
1:B:53:PHE:CE1	1:B:54:ILE:HG13	2.56	0.41
1:B:213:LEU:HD13	1:B:238:MET:HE2	2.02	0.41
1:E:117:PRO:HG2	1:E:120:GLN:HG2	2.03	0.41
1:G:275:LEU:O	1:G:279:GLN:HG3	2.21	0.41
1:B:190:ALA:HB3	1:B:217:PRO:HA	2.03	0.40
1:D:141:ASN:N	1:D:141:ASN:ND2	2.69	0.40
1:G:301:ILE:HD11	1:G:321:ALA:HB3	2.04	0.40
1:A:26:ILE:HD12	1:A:295:GLU:OE2	2.20	0.40
1:E:168:ALA:O	1:E:172:ARG:HG3	2.22	0.40
1:F:19:PHE:HB3	1:F:26:ILE:HB	2.03	0.40
1:F:145:GLN:O	1:F:148:VAL:CG2	2.67	0.40
1:G:250:LEU:O	1:G:254:LYS:HG3	2.20	0.40
1:H:147:ALA:O	1:H:151:VAL:HG23	2.21	0.40
1:A:301:ILE:HD11	1:A:321:ALA:HB3	2.03	0.40
1:D:221:ARG:O	1:D:221:ARG:HG3	2.22	0.40
1:G:84:ILE:HD13	1:G:106:CYS:SG	2.62	0.40

There are no symmetry-related clashes.

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	351/354 (99%)	333 (95%)	18 (5%)	0	100	100
1	B	352/354 (99%)	339 (96%)	12 (3%)	1 (0%)	36	22
1	C	340/354 (96%)	327 (96%)	12 (4%)	1 (0%)	36	22
1	D	342/354 (97%)	327 (96%)	14 (4%)	1 (0%)	36	22
1	E	351/354 (99%)	335 (95%)	16 (5%)	0	100	100
1	F	352/354 (99%)	340 (97%)	11 (3%)	1 (0%)	36	22
1	G	341/354 (96%)	328 (96%)	13 (4%)	0	100	100
1	H	342/354 (97%)	326 (95%)	16 (5%)	0	100	100
All	All	2771/2832 (98%)	2655 (96%)	112 (4%)	4 (0%)	48	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	210	GLN
1	F	51	GLY
1	B	51	GLY
1	D	51	GLY

5.3.2 Protein sidechains [i](#)

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	277/278 (100%)	275 (99%)	2 (1%)	76	69
1	B	278/278 (100%)	275 (99%)	3 (1%)	65	54
1	C	270/278 (97%)	267 (99%)	3 (1%)	65	54
1	D	272/278 (98%)	269 (99%)	3 (1%)	65	54
1	E	277/278 (100%)	273 (99%)	4 (1%)	59	46
1	F	278/278 (100%)	276 (99%)	2 (1%)	76	69
1	G	271/278 (98%)	269 (99%)	2 (1%)	76	69
1	H	272/278 (98%)	271 (100%)	1 (0%)	84	80
All	All	2195/2224 (99%)	2175 (99%)	20 (1%)	70	62

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	ASN
1	A	185	LYS
1	B	2	LYS
1	B	103	ASP
1	B	153	LEU
1	C	146	LYS
1	C	185	LYS
1	C	204	GLN
1	D	127	ASN
1	D	191	ASN
1	D	339	LYS
1	E	2	LYS
1	E	27	GLU
1	E	141	ASN
1	E	145	GLN
1	F	71	GLN
1	F	251	GLU
1	G	139	GLU
1	G	295	GLU
1	H	12	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	112	GLN

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Mol	Chain	Res	Type
1	A	141	ASN
1	A	204	GLN
1	A	272	HIS
1	A	279	GLN
1	A	311	GLN
1	B	115	GLN
1	B	128	GLN
1	B	191	ASN
1	B	262	ASN
1	B	272	HIS
1	B	311	GLN
1	B	354	HIS
1	C	112	GLN
1	C	191	ASN
1	C	210	GLN
1	C	234	ASN
1	C	272	HIS
1	C	279	GLN
1	C	311	GLN
1	D	5	GLN
1	D	71	GLN
1	D	112	GLN
1	D	127	ASN
1	D	141	ASN
1	D	204	GLN
1	D	210	GLN
1	D	234	ASN
1	D	262	ASN
1	D	272	HIS
1	D	311	GLN
1	E	5	GLN
1	E	7	HIS
1	E	141	ASN
1	E	145	GLN
1	E	191	ASN
1	E	262	ASN
1	E	272	HIS
1	E	279	GLN
1	E	311	GLN
1	F	5	GLN
1	F	71	GLN
1	F	145	GLN

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Mol	Chain	Res	Type
1	F	191	ASN
1	F	232	GLN
1	F	247	GLN
1	F	262	ASN
1	F	272	HIS
1	F	279	GLN
1	F	311	GLN
1	F	354	HIS
1	G	7	HIS
1	G	115	GLN
1	G	191	ASN
1	G	204	GLN
1	G	210	GLN
1	G	234	ASN
1	G	272	HIS
1	G	279	GLN
1	G	311	GLN
1	H	5	GLN
1	H	112	GLN
1	H	145	GLN
1	H	191	ASN
1	H	272	HIS
1	H	311	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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
4	SO4	A	357	3	4,4,4	0.41	0	6,6,6	0.08	0
2	GOL	A	355	-	5,5,5	0.24	0	5,5,5	0.38	0
2	GOL	F	355	-	5,5,5	0.37	0	5,5,5	0.34	0
2	GOL	B	357	-	5,5,5	0.31	0	5,5,5	0.29	0
4	SO4	C	356	-	4,4,4	0.37	0	6,6,6	0.12	0
4	SO4	C	357	-	4,4,4	0.36	0	6,6,6	0.10	0
4	SO4	E	356	3	4,4,4	0.41	0	6,6,6	0.10	0
4	SO4	G	356	-	4,4,4	0.37	0	6,6,6	0.07	0
2	GOL	B	355	-	5,5,5	0.30	0	5,5,5	0.29	0
2	GOL	B	356	-	5,5,5	0.32	0	5,5,5	0.29	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	GOL	A	355	-	-	4/4/4/4	-
2	GOL	F	355	-	-	4/4/4/4	-
2	GOL	B	357	-	-	4/4/4/4	-
2	GOL	B	355	-	-	0/4/4/4	-
2	GOL	B	356	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	355	GOL	C1-C2-C3-O3
2	A	355	GOL	O2-C2-C3-O3
2	B	357	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	F	355	GOL	C1-C2-C3-O3
2	F	355	GOL	O2-C2-C3-O3
2	A	355	GOL	O1-C1-C2-C3
2	B	357	GOL	C1-C2-C3-O3
2	F	355	GOL	O1-C1-C2-C3
2	B	357	GOL	O1-C1-C2-O2
2	B	357	GOL	O2-C2-C3-O3
2	A	355	GOL	O1-C1-C2-O2
2	F	355	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	355	GOL	3	0
4	C	356	SO4	1	0
2	B	355	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	353/354 (99%)	-1.01	0 100 100	18, 27, 44, 53	0
1	B	354/354 (100%)	-1.14	0 100 100	17, 24, 37, 47	0
1	C	344/354 (97%)	-0.91	0 100 100	19, 31, 62, 70	0
1	D	346/354 (97%)	-1.08	0 100 100	19, 26, 45, 55	0
1	E	353/354 (99%)	-1.00	0 100 100	18, 28, 45, 53	0
1	F	354/354 (100%)	-1.13	0 100 100	17, 25, 37, 47	0
1	G	345/354 (97%)	-0.90	0 100 100	19, 31, 63, 71	0
1	H	346/354 (97%)	-1.08	0 100 100	19, 26, 44, 54	0
All	All	2795/2832 (98%)	-1.03	0 100 100	17, 27, 48, 71	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	355	6/6	0.98	0.05	32,33,36,37	0
2	GOL	B	355	6/6	0.98	0.06	57,58,59,59	0
2	GOL	B	357	6/6	0.98	0.07	53,54,54,55	0
2	GOL	F	355	6/6	0.98	0.06	53,54,55,56	0
4	SO4	C	357	5/5	0.98	0.06	70,70,70,70	0
4	SO4	G	356	5/5	0.98	0.05	69,69,70,70	0
3	MG	E	355	1/1	0.99	0.02	28,28,28,28	0
3	MG	G	355	1/1	0.99	0.05	30,30,30,30	0
4	SO4	A	357	5/5	0.99	0.04	35,37,39,40	0
4	SO4	C	356	5/5	0.99	0.04	52,53,54,54	0
2	GOL	B	356	6/6	0.99	0.04	32,33,36,37	0
4	SO4	E	356	5/5	0.99	0.04	35,37,39,40	0
3	MG	C	355	1/1	0.99	0.04	30,30,30,30	0
3	MG	D	355	1/1	1.00	0.02	24,24,24,24	0
3	MG	B	358	1/1	1.00	0.03	20,20,20,20	0
3	MG	F	356	1/1	1.00	0.03	19,19,19,19	0
3	MG	A	356	1/1	1.00	0.02	29,29,29,29	0
3	MG	H	355	1/1	1.00	0.02	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.