



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:40 PM UTC

PDB ID : 1EC8 / pdb_00001ec8
Title : E. COLI GLUCARATE DEHYDRATASE BOUND TO PRODUCT 2,3-DIHYDROXY-5-OXO-HEXANEDIOATE
Authors : Gulick, A.M.; Hubbard, B.K.; Gerlt, J.A.; Rayment, I.
Deposited on : 2000-01-25
Resolution : 1.90 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

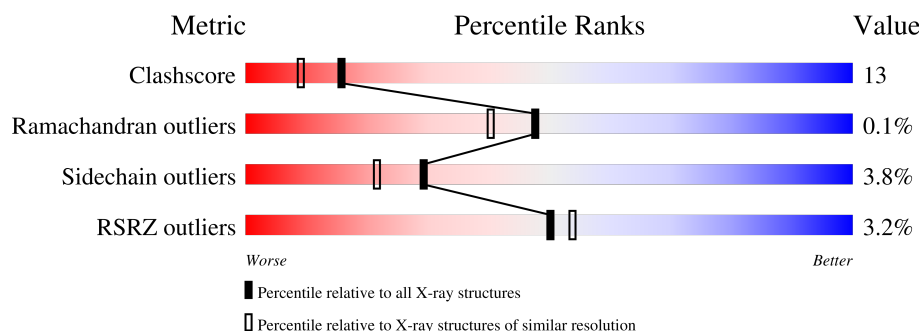
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 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	446	2% 70% 25% ..
1	B	446	4% 68% 27% ..
1	C	446	2% 74% 22% ..
1	D	446	5% 70% 26% ..

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
4	IPA	A	603	-	-	X	-
4	IPA	D	602	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14943 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.

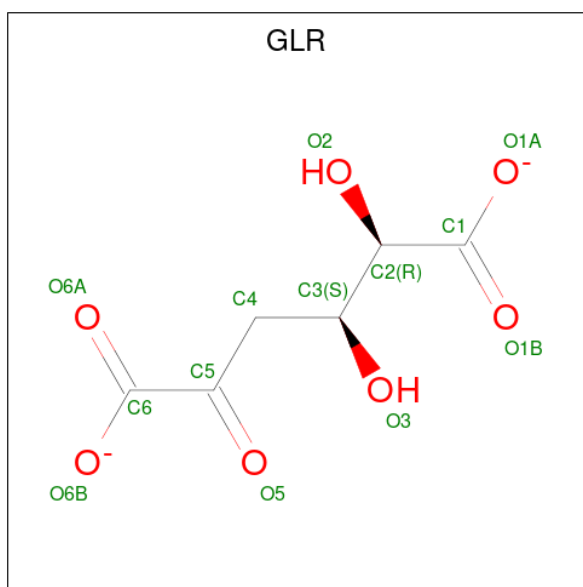
- Molecule 1 is a protein called GLUCARATE DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3419	2161	599	638	21			
1	B	442	Total	C	N	O	S	0	0	0
			3408	2156	596	635	21			
1	C	442	Total	C	N	O	S	0	0	0
			3407	2154	595	637	21			
1	D	442	Total	C	N	O	S	0	0	0
			3403	2151	597	634	21			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

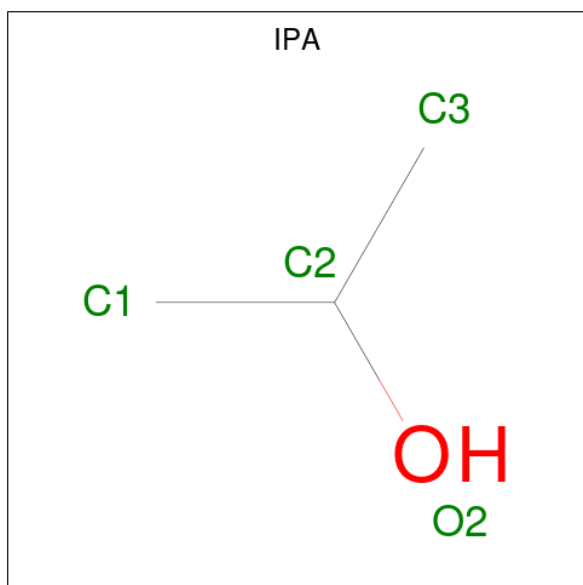
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2,3-DIHYDROXY-5-OXO-HEXANEDIOATE (CCD ID: GLR) (formula: C₆H₆O₇).



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	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



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

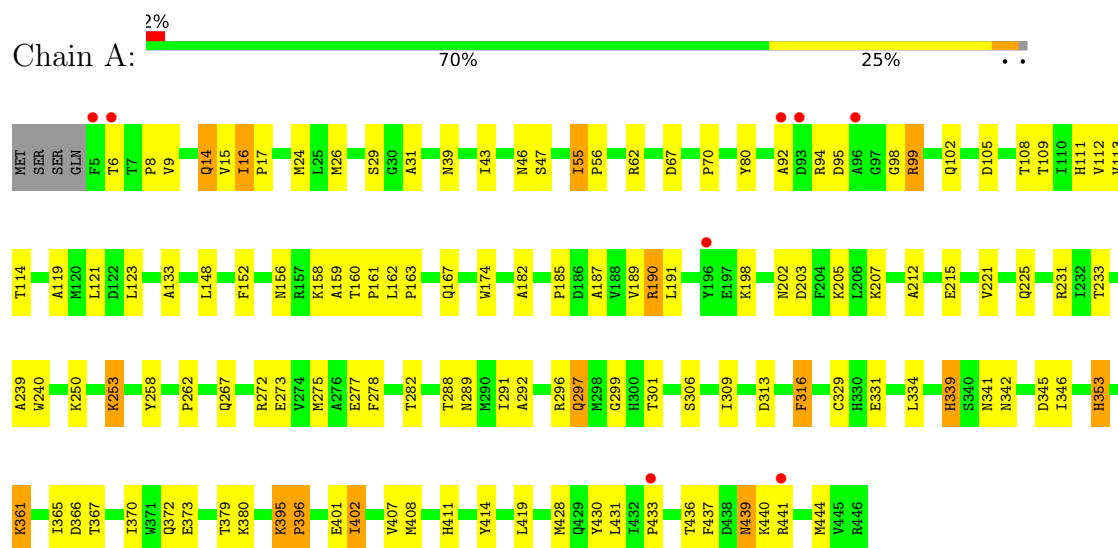
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	342	Total O 342 342	0	0
5	B	259	Total O 259 259	0	0
5	C	344	Total O 344 344	0	0
5	D	289	Total O 289 289	0	0

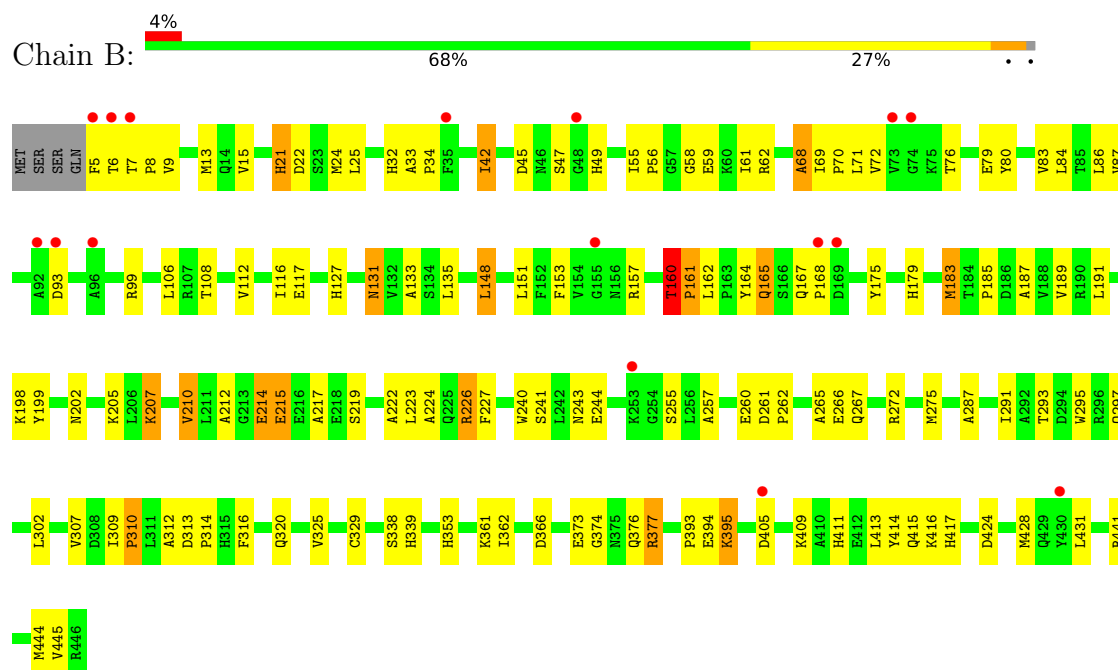
3 Residue-property plots [i](#)

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

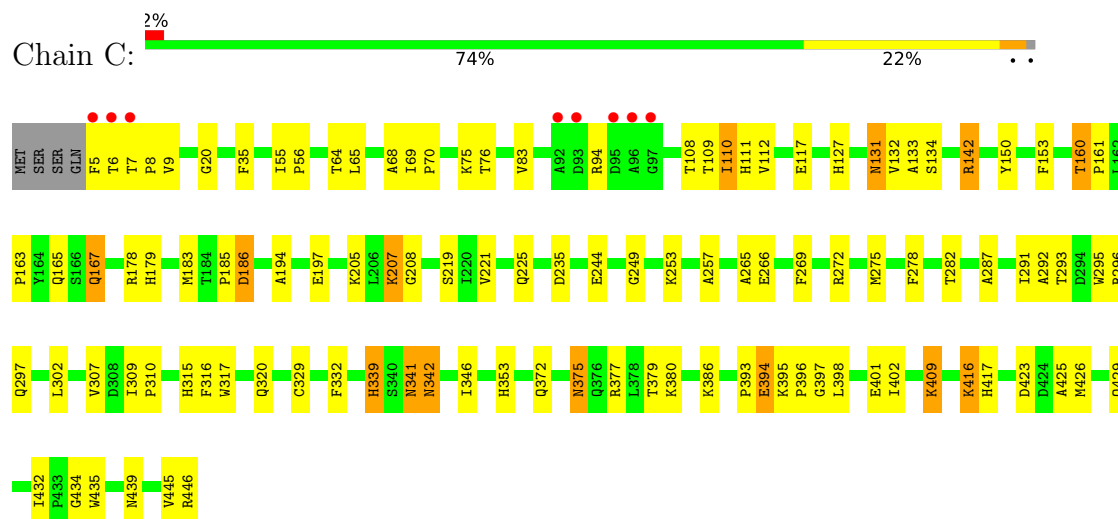
• Molecule 1: GLUCARATE DEHYDRATASE



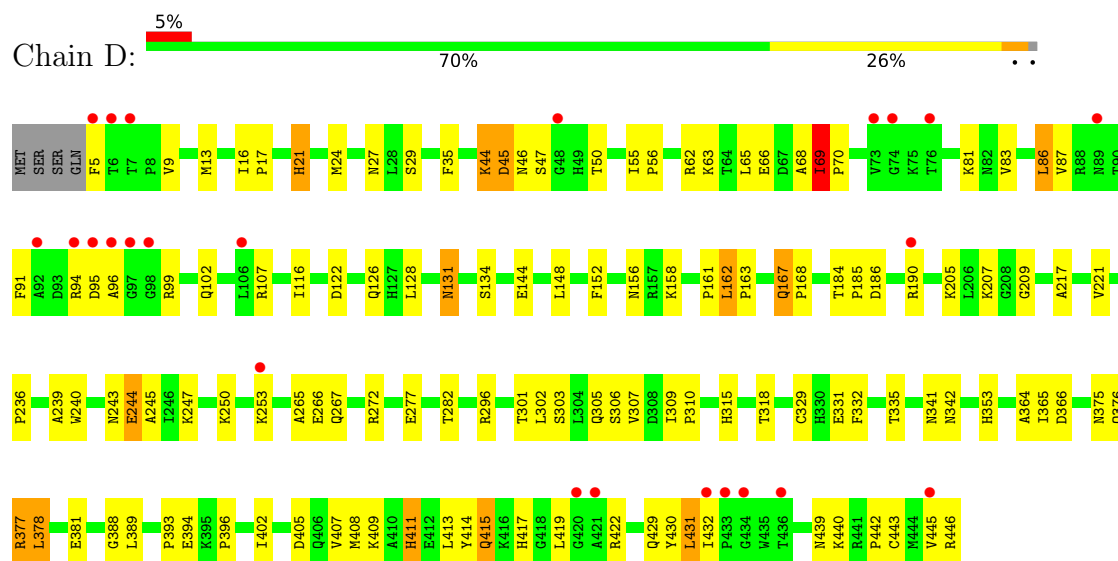
• Molecule 1: GLUCARATE DEHYDRATASE



• Molecule 1: GLUCARATE DEHYDRATASE



• Molecule 1: GLUCARATE DEHYDRATASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.09Å 84.61Å 98.86Å 103.42° 93.99° 113.06°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (30.00-1.90) 96.1 (30.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.69 (at 1.70Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.196 , (Not available) 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 96.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14943	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: GLR, MG, IPA

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	1.39	8/3498 (0.2%)	1.46	23/4741 (0.5%)
1	B	1.29	6/3487 (0.2%)	1.47	19/4728 (0.4%)
1	C	1.40	6/3486 (0.2%)	1.49	17/4728 (0.4%)
1	D	1.35	4/3482 (0.1%)	1.49	26/4722 (0.6%)
All	All	1.36	24/13953 (0.2%)	1.48	85/18919 (0.4%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	160	THR	C-N	-6.63	1.28	1.33
1	D	95	ASP	CG-OD2	6.46	1.37	1.25
1	B	189	VAL	CA-CB	-6.31	1.46	1.54
1	A	16	ILE	CA-C	-6.03	1.47	1.52
1	B	261	ASP	C-O	-5.95	1.21	1.23
1	B	161	PRO	N-CA	-5.78	1.43	1.47
1	C	208	GLY	CA-C	5.77	1.58	1.51
1	A	14	GLN	N-CA	-5.65	1.38	1.45
1	C	194	ALA	N-CA	-5.63	1.39	1.46
1	D	244	GLU	CA-C	-5.58	1.45	1.52
1	A	95	ASP	CG-OD2	5.58	1.35	1.25
1	C	249	GLY	C-N	-5.55	1.26	1.34
1	A	297	GLN	CA-C	5.51	1.59	1.52
1	D	245	ALA	N-CA	-5.48	1.39	1.46
1	A	31	ALA	CA-C	-5.41	1.46	1.52
1	D	277	GLU	N-CA	-5.38	1.39	1.46
1	A	202	ASN	C-N	5.37	1.40	1.33
1	C	183	MET	CA-C	-5.34	1.46	1.52
1	B	21	HIS	CA-C	-5.34	1.46	1.52
1	B	226	ARG	N-CA	-5.25	1.40	1.46
1	A	114	THR	C-N	5.19	1.40	1.33
1	C	108	THR	CA-C	5.16	1.56	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	THR	CA-C	-5.15	1.46	1.52
1	C	235	ASP	CA-C	5.05	1.57	1.52

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	393	PRO	N-CA-CB	7.89	110.21	103.35
1	D	411	HIS	CA-CB-CG	-7.68	106.12	113.80
1	C	109	THR	N-CA-C	7.20	119.13	111.28
1	C	94	ARG	N-CA-C	6.99	121.39	113.01
1	C	153	PHE	N-CA-C	-6.86	100.12	110.28
1	D	239	ALA	N-CA-C	6.85	118.83	111.36
1	B	314	PRO	CB-CA-C	-6.74	102.28	111.85
1	D	167	GLN	CA-C-N	6.72	128.23	119.84
1	D	167	GLN	C-N-CA	6.72	128.23	119.84
1	C	257	ALA	N-CA-C	-6.70	103.79	112.23
1	B	202	ASN	N-CA-C	-6.55	105.83	113.88
1	B	243	ASN	CA-CB-CG	-6.42	106.18	112.60
1	D	307	VAL	N-CA-C	6.25	117.11	108.12
1	D	318	THR	N-CA-CB	6.18	120.94	110.49
1	B	214	GLU	N-CA-CB	6.16	119.71	110.22
1	B	424	ASP	CA-CB-CG	6.09	118.69	112.60
1	C	341	ASN	CA-CB-CG	-6.08	106.52	112.60
1	C	393	PRO	N-CA-CB	6.08	108.99	103.33
1	D	315	HIS	CA-CB-CG	-6.08	107.72	113.80
1	C	163	PRO	N-CA-CB	6.05	106.82	102.28
1	D	381	GLU	O-C-N	6.04	125.46	121.23
1	A	80	TYR	N-CA-C	6.03	118.63	111.33
1	D	21	HIS	CA-CB-CG	-6.02	107.78	113.80
1	A	98	GLY	CA-C-N	5.96	128.27	120.28
1	A	98	GLY	C-N-CA	5.96	128.27	120.28
1	B	153	PHE	N-CA-C	-5.96	100.28	109.76
1	B	148	LEU	N-CA-CB	5.94	119.55	110.70
1	C	342	ASN	N-CA-CB	5.90	118.36	109.34
1	A	161	PRO	CB-CA-C	-5.88	102.69	110.27
1	D	396	PRO	N-CA-CB	5.77	108.37	103.35
1	B	312	ALA	N-CA-C	5.76	118.26	109.62
1	A	411	HIS	CA-CB-CG	-5.76	108.04	113.80
1	A	433	PRO	N-CA-CB	5.75	108.29	103.17
1	D	443	CYS	N-CA-C	5.74	118.27	111.33
1	B	307	VAL	N-CA-C	5.72	116.36	108.12
1	B	257	ALA	N-CA-C	-5.71	105.03	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	142	ARG	CD-NE-CZ	-5.69	116.43	124.40
1	A	202	ASN	N-CA-C	-5.67	106.03	113.12
1	D	69	ILE	N-CA-C	5.67	121.13	108.88
1	D	393	PRO	N-CA-CB	5.66	108.59	103.33
1	A	159	ALA	N-CA-C	-5.64	106.38	113.20
1	C	317	TRP	N-CA-C	-5.63	107.05	114.31
1	D	422	ARG	N-CA-C	5.62	118.39	110.23
1	D	364	ALA	CA-C-N	5.60	128.59	120.98
1	D	364	ALA	C-N-CA	5.60	128.59	120.98
1	D	162	LEU	CA-C-N	5.59	126.83	119.84
1	D	162	LEU	C-N-CA	5.59	126.83	119.84
1	A	152	PHE	CB-CA-C	-5.58	97.79	110.07
1	A	353	HIS	N-CA-CB	5.58	118.32	110.12
1	A	92	ALA	N-CA-C	5.57	117.79	111.11
1	D	152	PHE	CA-CB-CG	5.56	119.36	113.80
1	A	395	LYS	CA-C-N	5.54	125.48	119.78
1	A	395	LYS	C-N-CA	5.54	125.48	119.78
1	A	365	ILE	N-CA-CB	-5.52	103.52	110.31
1	B	310	PRO	N-CA-CB	5.50	106.91	103.23
1	B	93	ASP	CA-CB-CG	5.44	118.04	112.60
1	D	45	ASP	CA-CB-CG	5.42	118.02	112.60
1	C	315	HIS	CA-C-N	-5.41	114.16	122.60
1	C	315	HIS	C-N-CA	-5.41	114.16	122.60
1	A	316	PHE	N-CA-CB	5.39	118.75	110.61
1	D	272	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	B	214	GLU	CB-CG-CD	5.34	121.67	112.60
1	C	186	ASP	CA-CB-CG	5.33	117.92	112.60
1	D	162	LEU	N-CA-C	5.31	116.58	109.83
1	C	307	VAL	N-CA-C	5.31	115.76	108.12
1	A	121	LEU	N-CA-C	-5.31	105.50	111.28
1	C	7	THR	CB-CA-C	5.29	116.33	108.87
1	A	309	ILE	N-CA-C	5.27	113.37	108.15
1	A	367	THR	N-CA-CB	5.26	120.30	110.99
1	B	68	ALA	N-CA-C	5.26	119.41	112.89
1	C	167	GLN	CA-C-N	5.25	126.41	119.84
1	C	167	GLN	C-N-CA	5.25	126.41	119.84
1	B	325	VAL	N-CA-C	-5.24	105.43	110.72
1	A	239	ALA	N-CA-C	5.21	116.96	111.28
1	A	167	GLN	CA-C-N	5.20	125.00	119.28
1	A	167	GLN	C-N-CA	5.20	125.00	119.28
1	D	184	THR	O-C-N	5.20	125.03	121.71
1	B	261	ASP	CA-C-N	5.19	124.81	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	261	ASP	C-N-CA	5.19	124.81	119.05
1	B	210	VAL	O-C-N	5.16	125.77	121.85
1	D	388	GLY	N-CA-C	-5.12	107.94	115.30
1	A	396	PRO	N-CA-CB	5.08	107.77	103.35
1	D	96	ALA	N-CA-C	5.05	116.48	111.07
1	A	198	LYS	N-CA-C	5.05	117.90	111.69
1	D	236	PRO	N-CA-CB	5.01	107.43	102.17

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	3419	0	3345	96	0
1	B	3408	0	3327	101	0
1	C	3407	0	3324	71	0
1	D	3403	0	3312	104	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	13	0	6	0	0
3	B	13	0	6	0	0
3	C	13	0	6	2	0
3	D	13	0	6	0	0
4	A	8	0	16	4	0
4	D	8	0	16	7	0
5	A	342	0	0	9	0
5	B	259	0	0	4	0
5	C	344	0	0	3	0
5	D	289	0	0	10	0
All	All	14943	0	13364	360	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 (360) 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:D:402:ILE:HD11	1:D:407:VAL:HG21	1.42	1.01
1:A:407:VAL:HG12	1:A:408:MET:CE	1.96	0.96
1:D:408:MET:HA	1:D:408:MET:HE2	1.46	0.95
1:A:26:MET:CE	1:A:444:MET:HE3	1.98	0.94
1:A:428:MET:HE1	1:A:444:MET:CE	1.99	0.93
1:D:250:LYS:HA	1:D:253:LYS:HG3	1.50	0.91
1:D:415:GLN:HA	1:D:415:GLN:NE2	1.87	0.90
1:D:402:ILE:HD11	1:D:407:VAL:CG2	2.05	0.86
1:A:428:MET:HE1	1:A:444:MET:HE2	1.57	0.85
1:A:55:ILE:HB	1:A:56:PRO:HD2	1.61	0.83
1:B:165:GLN:H	1:B:165:GLN:NE2	1.76	0.82
1:C:346:ILE:HD11	1:C:402:ILE:HD13	1.61	0.82
1:D:405:ASP:O	1:D:409:LYS:HG3	1.80	0.82
1:B:293:THR:H	1:B:297:GLN:HE21	1.25	0.81
1:D:24:MET:HE1	1:D:431:LEU:HD21	1.63	0.81
1:B:21:HIS:H	1:B:376:GLN:HE22	1.25	0.81
1:C:346:ILE:HD11	1:C:402:ILE:CD1	2.11	0.80
1:D:377:ARG:HG3	1:D:377:ARG:HH11	1.46	0.80
1:B:262:PRO:HD2	1:B:275:MET:CE	2.12	0.80
1:A:47:SER:HA	1:C:5:PHE:CE1	2.18	0.78
1:D:407:VAL:HG12	1:D:408:MET:HE3	1.66	0.78
1:D:63:LYS:O	1:D:66:GLU:HB3	1.83	0.77
1:C:167:GLN:HE22	1:C:178:ARG:HH21	1.32	0.76
1:C:375:ASN:H	1:C:375:ASN:HD22	1.31	0.76
1:A:436:THR:HG22	5:A:1630:HOH:O	1.86	0.76
1:B:240:TRP:HB3	1:B:244:GLU:HG3	1.67	0.76
1:A:408:MET:HE2	1:A:408:MET:HA	1.69	0.75
1:A:250:LYS:HE2	5:A:2141:HOH:O	1.87	0.74
1:B:293:THR:H	1:B:297:GLN:NE2	1.84	0.74
1:A:203:ASP:OD1	1:A:231:ARG:HB2	1.87	0.74
1:B:68:ALA:C	1:B:70:PRO:HD2	2.12	0.74
1:B:24:MET:CE	1:B:431:LEU:HD11	2.18	0.74
1:A:428:MET:HE1	1:A:444:MET:HE1	1.69	0.73
1:D:44:LYS:HE2	1:D:50:THR:OG1	1.87	0.73
1:D:415:GLN:HA	1:D:415:GLN:HE21	1.51	0.73
1:A:26:MET:HE2	1:A:444:MET:HE3	1.69	0.72
1:B:262:PRO:HD2	1:B:275:MET:HE1	1.71	0.72
1:C:394:GLU:CD	1:C:394:GLU:H	1.98	0.72
1:D:122:ASP:O	1:D:126:GLN:HG3	1.89	0.72
1:D:408:MET:HA	1:D:408:MET:CE	2.18	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:LYS:NZ	1:A:366:ASP:OD2	2.22	0.72
1:B:394:GLU:CD	1:B:394:GLU:H	1.96	0.71
1:D:21:HIS:H	1:D:376:GLN:HE22	1.38	0.71
1:D:429:GLN:HA	1:D:429:GLN:OE1	1.91	0.70
1:B:55:ILE:HD12	1:B:61:ILE:HG21	1.73	0.70
1:D:267:GLN:NE2	5:D:1121:HOH:O	2.18	0.69
1:A:55:ILE:HB	1:A:56:PRO:CD	2.22	0.69
1:A:267:GLN:OE1	5:A:1431:HOH:O	2.11	0.69
1:C:293:THR:H	1:C:297:GLN:HE21	1.39	0.69
1:D:253:LYS:HE2	1:D:282:THR:O	1.91	0.68
1:C:375:ASN:H	1:C:375:ASN:ND2	1.91	0.68
1:A:407:VAL:HG12	1:A:408:MET:HE2	1.76	0.68
1:B:21:HIS:H	1:B:376:GLN:NE2	1.91	0.68
1:C:293:THR:H	1:C:297:GLN:NE2	1.92	0.67
1:A:408:MET:HE2	1:A:408:MET:N	2.09	0.67
1:A:408:MET:HE2	1:A:408:MET:CA	2.24	0.67
1:A:253:LYS:HE2	1:A:282:THR:O	1.95	0.66
1:A:14:GLN:HB3	5:A:1996:HOH:O	1.95	0.66
1:C:150:TYR:CE1	1:C:205:LYS:HD3	2.31	0.65
1:D:156:ASN:HD21	1:D:158:LYS:HB2	1.60	0.65
1:B:13:MET:HA	1:B:42:ILE:O	1.96	0.64
1:B:207:LYS:HE3	1:B:207:LYS:HA	1.78	0.64
1:B:157:ARG:HD3	1:B:179:HIS:O	1.97	0.64
1:A:439:ASN:ND2	5:A:1472:HOH:O	2.29	0.64
1:D:408:MET:HE2	1:D:408:MET:CA	2.22	0.64
1:C:55:ILE:HB	1:C:56:PRO:HD2	1.79	0.64
1:D:332:PHE:CD2	4:D:604:IPA:H32	2.34	0.63
1:B:55:ILE:HB	1:B:56:PRO:HD2	1.78	0.63
1:B:58:GLY:HA3	5:B:1221:HOH:O	1.99	0.63
1:B:414:TYR:HD1	1:B:415:GLN:HE21	1.47	0.63
1:D:247:LYS:HE3	5:D:2101:HOH:O	1.98	0.63
1:B:205:LYS:HE3	1:B:260:GLU:OE1	1.97	0.63
1:D:162:LEU:HD11	1:D:430:TYR:CE1	2.34	0.63
1:D:205:LYS:NZ	1:D:366:ASP:OD2	2.32	0.63
1:C:342:ASN:HD22	1:C:372:GLN:HE22	1.45	0.63
1:A:407:VAL:HG12	1:A:408:MET:HE3	1.77	0.62
1:A:29:SER:OG	1:A:102:GLN:OE1	2.16	0.62
4:A:603:IPA:H13	1:C:332:PHE:CD2	2.34	0.62
1:A:43:ILE:HD12	1:A:119:ALA:HB3	1.82	0.62
1:B:219:SER:O	1:B:222:ALA:HB3	2.00	0.61
1:C:55:ILE:HB	1:C:56:PRO:CD	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:VAL:HG12	1:A:46:ASN:CG	2.26	0.60
1:A:299:GLY:O	4:A:603:IPA:H33	2.01	0.60
1:A:162:LEU:HD11	1:A:430:TYR:CE1	2.37	0.60
1:B:395:LYS:NZ	5:B:1984:HOH:O	2.32	0.60
1:A:156:ASN:ND2	1:A:158:LYS:H	1.99	0.60
1:A:342:ASN:HD22	1:A:372:GLN:HE22	1.49	0.60
1:D:13:MET:HG2	1:D:69:ILE:HD13	1.83	0.60
1:B:366:ASP:OD2	5:B:1767:HOH:O	2.16	0.60
1:B:394:GLU:HG2	1:B:395:LYS:N	2.15	0.60
1:A:24:MET:HE1	1:A:431:LEU:HD21	1.83	0.59
1:C:131:ASN:ND2	1:C:134:SER:OG	2.35	0.59
1:A:102:GLN:NE2	1:A:437:PHE:CD1	2.71	0.59
1:B:21:HIS:N	1:B:376:GLN:HE22	1.99	0.59
1:B:265:ALA:O	1:B:266:GLU:HB3	2.00	0.59
1:C:55:ILE:HD11	1:C:65:LEU:HD11	1.83	0.59
1:D:16:ILE:HG21	1:D:408:MET:HE1	1.85	0.58
1:D:431:LEU:C	1:D:432:ILE:HG13	2.29	0.58
1:C:375:ASN:HD22	1:C:375:ASN:N	1.94	0.58
1:D:250:LYS:HA	1:D:253:LYS:HE3	1.86	0.58
1:A:162:LEU:HD11	1:A:430:TYR:HE1	1.69	0.58
1:B:117:GLU:OE1	1:B:320:GLN:HG3	2.04	0.58
1:D:250:LYS:CA	1:D:253:LYS:HG3	2.30	0.58
1:A:102:GLN:NE2	1:A:437:PHE:CG	2.72	0.58
1:A:174:TRP:CZ2	1:A:370:ILE:HD12	2.39	0.57
1:A:203:ASP:CG	1:A:231:ARG:HB2	2.28	0.57
1:D:332:PHE:CD2	4:D:604:IPA:C3	2.87	0.57
1:D:66:GLU:O	1:D:69:ILE:HG13	2.05	0.57
1:A:407:VAL:C	1:A:408:MET:HE2	2.30	0.57
1:A:190:ARG:NE	1:A:190:ARG:HA	2.18	0.56
1:A:190:ARG:HA	1:A:190:ARG:HE	1.69	0.56
1:A:414:TYR:HA	1:A:419:LEU:HD12	1.85	0.56
1:D:411:HIS:O	1:D:414:TYR:HB3	2.06	0.56
1:A:440:LYS:NZ	5:A:1413:HOH:O	2.38	0.56
1:A:67:ASP:O	1:A:70:PRO:HD2	2.06	0.56
1:C:342:ASN:HD22	1:C:372:GLN:NE2	2.03	0.56
1:A:39:ASN:O	1:A:55:ILE:HD13	2.05	0.56
1:C:445:VAL:O	1:C:446:ARG:HD3	2.05	0.55
1:D:162:LEU:HB3	1:D:163:PRO:HD2	1.87	0.55
1:A:55:ILE:HD13	1:A:55:ILE:N	2.21	0.55
1:A:342:ASN:HD22	1:A:372:GLN:NE2	2.05	0.55
1:A:408:MET:CE	1:A:408:MET:HA	2.33	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:HIS:HB2	1:D:419:LEU:HD11	1.89	0.55
1:D:431:LEU:O	1:D:432:ILE:HG13	2.07	0.55
1:B:69:ILE:N	1:B:70:PRO:CD	2.70	0.55
1:B:71:LEU:HD13	1:B:86:LEU:HG	1.89	0.55
1:A:47:SER:HB2	1:C:5:PHE:CD1	2.42	0.55
1:A:148:LEU:HD12	1:A:148:LEU:C	2.32	0.55
1:A:55:ILE:HD13	1:A:55:ILE:H	1.72	0.54
1:D:377:ARG:HG3	1:D:377:ARG:NH1	2.17	0.54
1:A:221:VAL:HG12	1:A:225:GLN:HE21	1.73	0.54
4:A:603:IPA:H2	1:C:302:LEU:HB3	1.88	0.54
1:B:413:LEU:O	1:B:417:HIS:HD2	1.91	0.54
1:D:55:ILE:HD11	1:D:65:LEU:HD11	1.90	0.54
1:D:305:GLN:NE2	5:D:1004:HOH:O	2.40	0.54
1:D:156:ASN:ND2	1:D:158:LYS:HB2	2.22	0.54
1:B:55:ILE:CD1	1:B:61:ILE:HG21	2.38	0.54
1:B:45:ASP:OD2	1:B:47:SER:N	2.33	0.53
1:B:47:SER:HB3	1:D:5:PHE:CD2	2.43	0.53
1:C:275:MET:HG3	1:C:291:ILE:HD13	1.90	0.53
1:D:168:PRO:HD2	5:D:1115:HOH:O	2.07	0.53
1:B:165:GLN:H	1:B:165:GLN:CD	2.17	0.53
1:D:91:PHE:O	1:D:94:ARG:HG3	2.07	0.53
1:B:394:GLU:OE2	1:B:395:LYS:HE3	2.09	0.53
4:D:602:IPA:H13	5:D:1324:HOH:O	2.08	0.53
1:B:160:THR:HB	1:B:161:PRO:HD2	1.91	0.52
1:D:86:LEU:C	1:D:86:LEU:HD12	2.33	0.52
1:D:29:SER:OG	1:D:102:GLN:NE2	2.42	0.52
1:D:250:LYS:HG2	1:D:253:LYS:HE3	1.90	0.52
1:B:302:LEU:O	4:D:602:IPA:H12	2.09	0.52
1:A:17:PRO:HG3	1:A:62:ARG:HD3	1.92	0.52
1:D:265:ALA:O	1:D:266:GLU:HB3	2.09	0.52
1:B:313:ASP:HB3	1:B:316:PHE:CE1	2.45	0.52
1:D:302:LEU:HD22	4:D:604:IPA:H33	1.91	0.52
1:B:59:GLU:OE1	1:B:62:ARG:NE	2.29	0.52
1:A:99:ARG:HG3	1:A:105:ASP:OD2	2.10	0.51
1:B:428:MET:HA	1:B:431:LEU:HD13	1.92	0.51
1:C:253:LYS:HE2	1:C:282:THR:O	2.10	0.51
1:D:405:ASP:OD1	1:D:409:LYS:HE2	2.11	0.51
1:B:135:LEU:O	1:D:81:LYS:NZ	2.43	0.51
1:B:262:PRO:CD	1:B:275:MET:HE1	2.39	0.51
1:A:133:ALA:H	1:A:353:HIS:CD2	2.28	0.51
1:D:303:SER:OG	4:D:602:IPA:H13	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ILE:N	1:B:70:PRO:HD2	2.25	0.51
1:D:156:ASN:ND2	1:D:158:LYS:H	2.09	0.51
1:D:407:VAL:HG12	1:D:408:MET:CE	2.38	0.51
1:D:55:ILE:HB	1:D:56:PRO:CD	2.42	0.50
1:C:296:ARG:HH12	1:D:267:GLN:NE2	2.09	0.50
1:A:6:THR:O	1:C:5:PHE:HA	2.11	0.50
1:C:380:LYS:HG3	1:C:401:GLU:HB2	1.94	0.50
1:B:287:ALA:HB2	1:B:309:ILE:HB	1.94	0.50
1:B:55:ILE:HB	1:B:56:PRO:CD	2.41	0.50
1:D:55:ILE:HB	1:D:56:PRO:HD2	1.92	0.50
1:C:75:LYS:HG3	1:C:83:VAL:CG2	2.42	0.49
1:A:272:ARG:HA	1:A:291:ILE:HD12	1.94	0.49
1:C:265:ALA:O	1:C:266:GLU:HB3	2.12	0.49
1:A:341:ASN:O	1:A:342:ASN:C	2.55	0.49
1:B:24:MET:HE1	1:B:431:LEU:HD11	1.94	0.49
1:B:80:TYR:O	1:B:84:LEU:HG	2.12	0.49
1:D:365:ILE:HD13	1:D:365:ILE:N	2.27	0.49
1:D:144:GLU:HG3	1:D:389:LEU:HD22	1.94	0.49
1:D:417:HIS:HB2	1:D:419:LEU:CD1	2.43	0.49
1:A:133:ALA:H	1:A:353:HIS:HD2	1.60	0.49
1:D:107:ARG:NH1	5:D:2046:HOH:O	2.46	0.49
1:B:272:ARG:HA	1:B:291:ILE:HD12	1.95	0.49
1:D:240:TRP:HB3	1:D:244:GLU:HB2	1.95	0.49
1:D:440:LYS:NZ	5:D:1683:HOH:O	2.37	0.49
1:A:26:MET:CE	1:A:444:MET:CE	2.84	0.49
1:C:64:THR:HB	1:C:112:VAL:HG21	1.95	0.49
1:A:361:LYS:HD3	5:A:1809:HOH:O	2.12	0.48
1:B:99:ARG:O	1:B:106:LEU:HB2	2.13	0.48
1:D:17:PRO:HB2	1:D:414:TYR:CE1	2.48	0.48
1:A:292:ALA:HA	1:A:297:GLN:HB3	1.95	0.48
1:B:212:ALA:O	1:B:215:GLU:HB3	2.13	0.48
1:C:423:ASP:OD2	1:C:425:ALA:HB3	2.12	0.48
4:A:603:IPA:H11	5:C:1384:HOH:O	2.13	0.48
1:C:416:LYS:HD3	1:C:417:HIS:CE1	2.48	0.48
1:A:380:LYS:HG3	1:A:401:GLU:HB2	1.96	0.48
1:B:76:THR:OG1	1:B:79:GLU:HG3	2.14	0.48
1:D:148:LEU:HD12	1:D:148:LEU:C	2.38	0.48
1:B:24:MET:HG3	1:B:164:TYR:CZ	2.49	0.48
1:D:131:ASN:ND2	1:D:134:SER:H	2.12	0.48
1:D:402:ILE:O	1:D:402:ILE:HG23	2.13	0.48
1:B:25:LEU:HB2	1:B:32:HIS:CG	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLU:OE2	5:A:1173:HOH:O	2.20	0.47
1:C:165:GLN:HG3	1:C:179:HIS:CE1	2.49	0.47
1:A:109:THR:O	1:A:113:VAL:HG23	2.14	0.47
1:B:7:THR:HG21	1:D:128:LEU:HA	1.96	0.47
1:B:49:HIS:HA	5:B:1220:HOH:O	2.14	0.47
1:C:377:ARG:HD2	1:C:379:THR:O	2.15	0.47
1:D:445:VAL:C	1:D:446:ARG:HG2	2.40	0.47
1:B:7:THR:HA	1:B:8:PRO:HD3	1.74	0.47
1:D:310:PRO:HG2	1:D:329:CYS:SG	2.55	0.47
1:C:69:ILE:N	1:C:70:PRO:CD	2.77	0.47
1:D:301:THR:HG23	1:D:306:SER:HB2	1.96	0.47
1:A:185:PRO:O	1:A:189:VAL:HG23	2.14	0.47
1:B:7:THR:HG22	1:B:127:HIS:HE2	1.80	0.47
1:C:8:PRO:HD3	1:C:127:HIS:CE1	2.50	0.47
1:C:409:LYS:HB2	1:C:409:LYS:HE3	1.79	0.47
1:A:16:ILE:HD13	1:A:408:MET:HE1	1.97	0.46
1:A:345:ASP:OD1	1:A:379:THR:OG1	2.29	0.46
1:A:43:ILE:HG22	1:A:123:LEU:HD11	1.96	0.46
1:B:45:ASP:OD2	1:B:45:ASP:C	2.57	0.46
1:D:83:VAL:O	1:D:87:VAL:HG23	2.15	0.46
1:D:217:ALA:O	1:D:221:VAL:HG23	2.15	0.46
1:C:142:ARG:HH11	1:C:142:ARG:HD3	1.53	0.46
1:D:378:LEU:HG	1:D:407:VAL:HG22	1.98	0.46
1:D:167:GLN:N	1:D:168:PRO:HD3	2.29	0.46
1:B:148:LEU:HD11	1:B:366:ASP:HA	1.96	0.46
1:A:331:GLU:HB3	1:C:295:TRP:HB3	1.97	0.46
1:A:148:LEU:HD12	1:A:148:LEU:O	2.16	0.46
1:B:59:GLU:CD	1:B:62:ARG:HE	2.22	0.46
1:C:117:GLU:OE1	1:C:320:GLN:HG3	2.15	0.46
1:B:224:ALA:HB2	1:B:255:SER:HB3	1.98	0.45
1:B:405:ASP:O	1:B:409:LYS:HG3	2.17	0.45
1:A:108:THR:O	1:A:112:VAL:HG23	2.16	0.45
1:B:394:GLU:OE2	1:B:395:LYS:HG2	2.15	0.45
1:B:416:LYS:HD3	1:B:417:HIS:NE2	2.32	0.45
1:C:353:HIS:HE1	1:C:398:LEU:O	1.99	0.45
1:A:262:PRO:HD2	1:A:275:MET:SD	2.57	0.45
1:B:55:ILE:CD1	1:B:61:ILE:CG2	2.94	0.45
1:C:429:GLN:OE1	1:C:434:GLY:N	2.48	0.45
1:A:233:THR:HG21	1:A:258:TYR:CE2	2.51	0.45
1:A:395:LYS:HB2	1:A:396:PRO:HD2	1.99	0.45
1:B:241:SER:N	1:B:244:GLU:HG2	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:ASN:HB2	1:D:353:HIS:CE1	2.51	0.45
1:C:269:PHE:CZ	1:D:296:ARG:HG2	2.51	0.45
1:D:86:LEU:HD12	1:D:86:LEU:O	2.17	0.45
1:B:338:SER:O	1:B:366:ASP:HB2	2.16	0.45
1:D:375:ASN:OD1	1:D:376:GLN:HG3	2.17	0.45
1:D:394:GLU:OE2	1:D:394:GLU:HA	2.15	0.45
1:A:408:MET:CE	1:A:408:MET:CA	2.94	0.45
1:B:7:THR:HG21	1:D:128:LEU:HD23	1.99	0.45
1:B:9:VAL:HG12	1:B:76:THR:HG22	1.99	0.45
1:B:175:TYR:CZ	1:B:198:LYS:HE2	2.51	0.45
1:B:33:ALA:HB1	1:B:34:PRO:HD2	1.98	0.45
1:C:160:THR:HB	1:C:161:PRO:HD2	1.98	0.45
1:A:174:TRP:HZ3	1:A:191:LEU:HD22	1.82	0.45
1:B:13:MET:HE2	1:B:69:ILE:HG12	1.99	0.45
1:C:150:TYR:CZ	1:C:205:LYS:HD3	2.52	0.45
1:C:310:PRO:HG2	1:C:329:CYS:SG	2.57	0.45
1:D:209:GLY:O	1:D:442:PRO:HA	2.17	0.45
1:D:24:MET:CE	1:D:431:LEU:HD21	2.43	0.45
1:B:167:GLN:N	1:B:168:PRO:HD3	2.32	0.44
1:C:395:LYS:HB2	1:C:396:PRO:HD2	1.99	0.44
1:A:174:TRP:CZ3	1:A:191:LEU:HD22	2.52	0.44
1:C:278:PHE:CD1	1:C:278:PHE:C	2.93	0.44
1:B:241:SER:H	1:B:244:GLU:HG2	1.82	0.44
1:B:361:LYS:HE2	1:B:362:ILE:O	2.17	0.44
1:B:441:ARG:HD3	1:B:445:VAL:O	2.18	0.44
1:B:72:VAL:HG21	1:B:116:ILE:HD13	1.99	0.44
1:C:339:HIS:HD2	3:C:501:GLR:C6	2.31	0.44
1:C:375:ASN:ND2	1:C:375:ASN:N	2.54	0.44
1:C:131:ASN:C	1:C:131:ASN:HD22	2.26	0.44
1:D:62:ARG:NH1	5:D:2188:HOH:O	2.40	0.44
1:B:133:ALA:H	1:B:353:HIS:CD2	2.36	0.43
1:B:165:GLN:CD	1:B:165:GLN:N	2.75	0.43
1:C:110:ILE:HD12	1:C:110:ILE:HA	1.60	0.43
1:B:295:TRP:HB3	1:D:331:GLU:HB3	1.99	0.43
1:C:131:ASN:ND2	1:C:134:SER:H	2.15	0.43
1:C:402:ILE:HD12	1:C:402:ILE:HA	1.84	0.43
1:D:69:ILE:N	1:D:70:PRO:CD	2.80	0.43
1:D:131:ASN:C	1:D:131:ASN:HD22	2.25	0.43
1:D:243:ASN:ND2	5:D:1909:HOH:O	2.50	0.43
1:B:187:ALA:O	1:B:191:LEU:HB2	2.18	0.43
1:C:68:ALA:C	1:C:70:PRO:HD2	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:HIS:CD2	3:C:501:GLR:C6	3.01	0.43
1:D:45:ASP:C	1:D:47:SER:H	2.25	0.43
1:A:26:MET:HE1	1:A:444:MET:HE3	1.96	0.43
1:A:346:ILE:HD11	1:A:402:ILE:HD12	2.00	0.43
1:B:210:VAL:O	1:B:444:MET:HB2	2.18	0.43
1:D:131:ASN:HB2	1:D:353:HIS:HE1	1.82	0.43
1:C:207:LYS:HE3	1:C:207:LYS:HA	2.00	0.43
1:C:316:PHE:HD2	5:C:1995:HOH:O	2.01	0.43
1:B:22:ASP:O	1:B:165:GLN:OE1	2.36	0.43
1:B:376:GLN:O	1:B:377:ARG:HB3	2.19	0.43
1:C:221:VAL:O	1:C:225:GLN:HG3	2.17	0.43
1:C:432:ILE:O	1:C:435:TRP:HB2	2.19	0.43
1:A:8:PRO:HG3	1:A:47:SER:HB3	2.01	0.42
1:A:329:CYS:HA	1:A:334:LEU:HB2	2.01	0.42
1:A:331:GLU:HB3	1:C:295:TRP:CB	2.49	0.42
1:C:20:GLY:O	1:C:35:PHE:HA	2.20	0.42
1:A:16:ILE:HG21	1:A:408:MET:HE1	2.01	0.42
1:D:68:ALA:C	1:D:70:PRO:HD2	2.44	0.42
1:D:185:PRO:HD3	5:D:2058:HOH:O	2.19	0.42
1:A:56:PRO:HG2	1:A:111:HIS:CD2	2.54	0.42
1:C:426:MET:HG2	5:C:1649:HOH:O	2.20	0.42
1:D:250:LYS:HG2	1:D:253:LYS:CE	2.48	0.42
1:A:313:ASP:HB3	1:A:316:PHE:CE1	2.54	0.42
1:D:21:HIS:H	1:D:376:GLN:NE2	2.11	0.42
1:A:296:ARG:HH12	1:B:267:GLN:NE2	2.17	0.42
1:D:402:ILE:CD1	1:D:407:VAL:HG21	2.30	0.42
1:D:417:HIS:HB2	1:D:419:LEU:HG	2.02	0.42
1:A:395:LYS:HA	1:A:396:PRO:HD3	1.88	0.42
1:B:83:VAL:O	1:B:87:VAL:HG23	2.19	0.42
1:D:186:ASP:O	1:D:190:ARG:HG3	2.19	0.42
1:B:185:PRO:HB3	1:B:219:SER:HA	2.01	0.42
1:C:110:ILE:CG2	1:C:111:HIS:N	2.83	0.42
1:A:212:ALA:O	1:A:215:GLU:HB3	2.20	0.41
1:B:7:THR:HG22	1:B:127:HIS:NE2	2.35	0.41
1:B:199:TYR:OH	1:B:373:GLU:OE1	2.34	0.41
1:B:226:ARG:HG3	1:B:227:PHE:CE1	2.55	0.41
1:A:162:LEU:HA	1:A:163:PRO:HD3	1.86	0.41
1:B:373:GLU:CD	1:B:374:GLY:N	2.78	0.41
1:C:287:ALA:HA	1:C:309:ILE:O	2.20	0.41
1:B:302:LEU:HB3	4:D:602:IPA:H33	2.03	0.41
1:B:310:PRO:HG2	1:B:329:CYS:SG	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:LEU:N	1:B:431:LEU:HD12	2.34	0.41
1:C:132:VAL:HG23	1:C:397:GLY:C	2.44	0.41
1:C:272:ARG:HA	1:C:291:ILE:HD12	2.03	0.41
1:C:341:ASN:O	1:C:342:ASN:C	2.63	0.41
1:A:301:THR:HG23	1:A:306:SER:HB2	2.03	0.41
1:B:162:LEU:HB2	1:B:164:TYR:CE1	2.56	0.41
1:B:183:MET:HE3	1:B:183:MET:HB3	1.70	0.41
1:C:133:ALA:H	1:C:353:HIS:HD2	1.68	0.41
1:B:411:HIS:O	1:B:414:TYR:HB3	2.21	0.41
1:A:278:PHE:CD1	1:A:278:PHE:C	2.98	0.41
1:A:289:ASN:CG	1:A:339:HIS:CD2	2.99	0.41
1:A:182:ALA:HA	1:A:187:ALA:HB1	2.03	0.41
1:A:273:GLU:O	1:A:277:GLU:HG3	2.21	0.41
1:A:275:MET:HG3	1:A:291:ILE:HD13	2.03	0.41
1:A:440:LYS:HE3	5:A:1702:HOH:O	2.20	0.41
1:B:151:LEU:CD1	1:B:223:LEU:HD11	2.51	0.41
1:C:292:ALA:HA	1:C:297:GLN:HB3	2.01	0.41
1:D:250:LYS:HG2	1:D:253:LYS:NZ	2.35	0.41
1:D:309:ILE:HA	1:D:335:THR:O	2.21	0.41
1:A:9:VAL:HG12	1:A:46:ASN:ND2	2.36	0.41
1:B:6:THR:O	1:D:5:PHE:HA	2.21	0.41
1:D:35:PHE:CD1	1:D:413:LEU:HD21	2.56	0.41
1:D:417:HIS:HB2	1:D:419:LEU:CG	2.51	0.41
1:B:214:GLU:O	1:B:217:ALA:HB3	2.21	0.40
1:C:9:VAL:HA	1:C:76:THR:HA	2.03	0.40
1:D:162:LEU:HA	1:D:163:PRO:HD3	1.81	0.40
1:A:240:TRP:HB2	1:A:262:PRO:O	2.21	0.40
1:B:131:ASN:HD22	1:B:131:ASN:C	2.29	0.40
1:D:161:PRO:CD	1:D:430:TYR:CE2	3.05	0.40
1:B:108:THR:O	1:B:112:VAL:HG23	2.22	0.40
1:C:185:PRO:O	1:C:186:ASP:C	2.64	0.40
1:D:45:ASP:C	1:D:47:SER:N	2.80	0.40
1:D:341:ASN:O	1:D:342:ASN:C	2.63	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	440/446 (99%)	425 (97%)	15 (3%)	0	100	100
1	B	440/446 (99%)	425 (97%)	15 (3%)	0	100	100
1	C	440/446 (99%)	425 (97%)	15 (3%)	0	100	100
1	D	440/446 (99%)	424 (96%)	15 (3%)	1 (0%)	43	36
All	All	1760/1784 (99%)	1699 (96%)	60 (3%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	46	ASN

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	356/362 (98%)	343 (96%)	13 (4%)	30	22
1	B	353/362 (98%)	341 (97%)	12 (3%)	32	25
1	C	354/362 (98%)	339 (96%)	15 (4%)	26	19
1	D	351/362 (97%)	337 (96%)	14 (4%)	28	20
All	All	1414/1448 (98%)	1360 (96%)	54 (4%)	29	21

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	55	ILE
1	A	94	ARG
1	A	99	ARG
1	A	160	THR
1	A	190	ARG
1	A	207	LYS
1	A	253	LYS
1	A	339	HIS
1	A	361	LYS
1	A	402	ILE
1	A	439	ASN
1	A	441	ARG
1	B	5	PHE
1	B	15	VAL
1	B	42	ILE
1	B	131	ASN
1	B	160	THR
1	B	165	GLN
1	B	183	MET
1	B	207	LYS
1	B	215	GLU
1	B	339	HIS
1	B	377	ARG
1	B	395	LYS
1	C	6	THR
1	C	110	ILE
1	C	131	ASN
1	C	160	THR
1	C	197	GLU
1	C	207	LYS
1	C	219	SER
1	C	244	GLU
1	C	339	HIS
1	C	375	ASN
1	C	386	LYS
1	C	394	GLU
1	C	409	LYS
1	C	416	LYS
1	C	439	ASN
1	D	9	VAL
1	D	27	ASN
1	D	44	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	69	ILE
1	D	86	LEU
1	D	99	ARG
1	D	116	ILE
1	D	131	ASN
1	D	207	LYS
1	D	377	ARG
1	D	378	LEU
1	D	415	GLN
1	D	431	LEU
1	D	439	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	156	ASN
1	A	225	GLN
1	A	353	HIS
1	A	372	GLN
1	A	417	HIS
1	B	102	GLN
1	B	131	ASN
1	B	140	GLN
1	B	165	GLN
1	B	243	ASN
1	B	297	GLN
1	B	320	GLN
1	B	341	ASN
1	B	353	HIS
1	B	376	GLN
1	B	415	GLN
1	B	417	HIS
1	C	39	ASN
1	C	102	GLN
1	C	131	ASN
1	C	140	GLN
1	C	165	GLN
1	C	167	GLN
1	C	229	GLN
1	C	243	ASN
1	C	297	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	353	HIS
1	C	372	GLN
1	C	375	ASN
1	C	417	HIS
1	C	439	ASN
1	D	102	GLN
1	D	131	ASN
1	D	140	GLN
1	D	141	GLN
1	D	156	ASN
1	D	243	ASN
1	D	267	GLN
1	D	305	GLN
1	D	320	GLN
1	D	341	ASN
1	D	376	GLN
1	D	391	GLN
1	D	411	HIS
1	D	415	GLN
1	D	417	HIS

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	IPA	A	601	-	3,3,3	0.59	0	3,3,3	0.17	0
3	GLR	D	502	2	12,12,12	1.73	2 (16%)	13,16,16	1.28	1 (7%)
3	GLR	C	501	2	12,12,12	2.08	3 (25%)	13,16,16	1.03	0
4	IPA	D	602	-	3,3,3	0.67	0	3,3,3	0.50	0
3	GLR	A	499	2	12,12,12	1.48	2 (16%)	13,16,16	1.40	3 (23%)
4	IPA	A	603	-	3,3,3	0.52	0	3,3,3	0.35	0
4	IPA	D	604	-	3,3,3	0.54	0	3,3,3	0.32	0
3	GLR	B	500	2	12,12,12	1.98	2 (16%)	13,16,16	1.65	2 (15%)

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
3	GLR	C	501	2	-	0/16/16/16	-
3	GLR	B	500	2	-	0/16/16/16	-
3	GLR	D	502	2	-	1/16/16/16	-
3	GLR	A	499	2	-	0/16/16/16	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	GLR	C5-C6	-5.15	1.45	1.53
3	C	501	GLR	C5-C6	-4.89	1.46	1.53
3	D	502	GLR	C5-C6	-3.76	1.47	1.53
3	C	501	GLR	C2-C1	-2.96	1.48	1.52
3	D	502	GLR	O6B-C6	-2.38	1.24	1.30
3	A	499	GLR	C5-C6	-2.21	1.50	1.53
3	B	500	GLR	O1A-C1	-2.10	1.24	1.30
3	A	499	GLR	O5-C5	2.08	1.27	1.23
3	C	501	GLR	C4-C3	2.04	1.56	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	GLR	O6A-C6-C5	-3.48	117.48	121.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	499	GLR	O5-C5-C6	2.71	123.54	119.67
3	A	499	GLR	O6A-C6-C5	-2.61	118.57	121.81
3	B	500	GLR	O6B-C6-C5	2.54	120.64	113.59
3	D	502	GLR	O1A-C1-C2	2.45	120.13	113.31
3	A	499	GLR	O6B-C6-C5	2.39	120.21	113.59

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	502	GLR	C3-C4-C5-C6

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	GLR	2	0
4	D	602	IPA	4	0
4	A	603	IPA	4	0
4	D	604	IPA	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	442/446 (99%)	-0.13	8 (1%) 67 71	11, 21, 44, 86	0
1	B	442/446 (99%)	0.17	16 (3%) 46 49	10, 27, 55, 85	0
1	C	442/446 (99%)	-0.25	8 (1%) 67 71	9, 20, 42, 86	0
1	D	442/446 (99%)	0.02	24 (5%) 31 33	9, 22, 54, 85	0
All	All	1768/1784 (99%)	-0.05	56 (3%) 50 54	9, 22, 50, 86	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	THR	5.2
1	D	5	PHE	5.1
1	D	6	THR	4.9
1	B	48	GLY	4.7
1	D	106	LEU	4.7
1	D	434	GLY	4.6
1	B	92	ALA	4.5
1	A	92	ALA	4.5
1	B	5	PHE	4.2
1	A	96	ALA	4.2
1	C	5	PHE	4.2
1	C	96	ALA	4.1
1	A	433	PRO	4.0
1	B	168	PRO	4.0
1	C	95	ASP	3.8
1	D	432	ILE	3.7
1	D	253	LYS	3.7
1	D	96	ALA	3.6
1	D	97	GLY	3.6
1	C	92	ALA	3.5
1	B	73	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	436	THR	3.4
1	A	6	THR	3.3
1	C	93	ASP	3.3
1	D	420	GLY	3.3
1	B	74	GLY	3.2
1	B	405	ASP	3.1
1	C	6	THR	3.1
1	B	96	ALA	3.0
1	D	92	ALA	3.0
1	A	196	TYR	2.9
1	C	97	GLY	2.9
1	D	421	ALA	2.8
1	C	7	THR	2.8
1	D	76	THR	2.6
1	B	93	ASP	2.6
1	B	155	GLY	2.6
1	D	74	GLY	2.6
1	A	93	ASP	2.6
1	B	169	ASP	2.5
1	B	7	THR	2.5
1	D	190	ARG	2.4
1	A	5	PHE	2.3
1	B	430	TYR	2.3
1	D	48	GLY	2.3
1	D	7	THR	2.3
1	D	98	GLY	2.2
1	D	94	ARG	2.2
1	D	445	VAL	2.1
1	B	35	PHE	2.1
1	D	73	VAL	2.1
1	D	89	ASN	2.1
1	D	433	PRO	2.0
1	A	441	ARG	2.0
1	D	95	ASP	2.0
1	B	253	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 [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(Å ²)	Q<0.9
4	IPA	A	603	4/4	0.91	0.18	14,28,39,82	0
4	IPA	D	604	4/4	0.93	0.09	11,17,28,29	0
4	IPA	D	602	4/4	0.95	0.09	10,32,34,40	0
3	GLR	D	502	13/13	0.97	0.09	12,19,34,100	0
4	IPA	A	601	4/4	0.97	0.07	5,23,36,40	0
2	MG	A	498	1/1	0.97	0.03	15,15,15,15	0
3	GLR	B	500	13/13	0.97	0.07	12,22,39,42	0
3	GLR	C	501	13/13	0.97	0.07	14,20,35,43	0
3	GLR	A	499	13/13	0.98	0.07	10,18,34,84	0
2	MG	D	498	1/1	0.98	0.02	15,15,15,15	0
2	MG	C	498	1/1	0.99	0.02	13,13,13,13	0
2	MG	B	498	1/1	0.99	0.02	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.