



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:12 PM GMT

PDB ID : 1EGV
Title : CRYSTAL STRUCTURE OF THE DIOL DEHYDRATASE-ADENINYLPENTYLCOBALAMIN COMPLEX FROM KLEBSIELLA OXYTOCA UNDER THE ILLUMINATED CONDITION.
Authors : Masuda, J.; Shibata, N.; Toraya, T.; Morimoto, Y.; Yasuoka, N.
Deposited on : 2000-02-17
Resolution : 1.75 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:

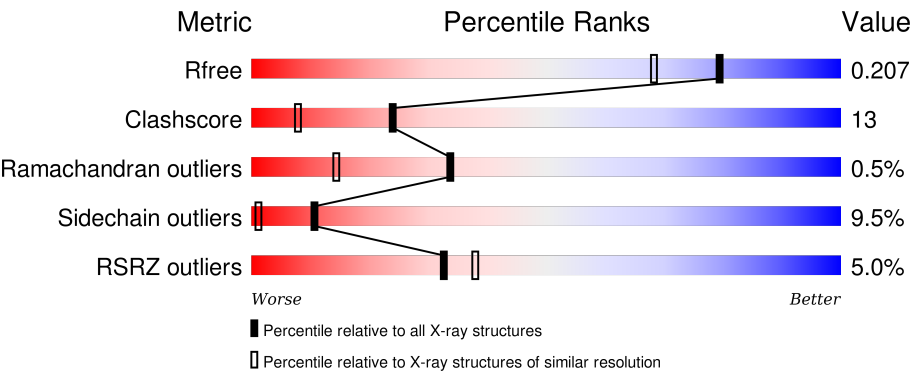
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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 <=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	554	<div><div>%</div><div><div></div><div>85%</div><div>12%</div><div>••</div></div></div>
1	L	554	<div><div>3%</div><div><div></div><div>77%</div><div>18%</div><div>••</div></div></div>
2	B	224	<div><div></div><div><div></div><div>63%</div><div>15%</div><div>•</div><div>21%</div></div></div>
2	E	224	<div><div>21%</div><div><div></div><div>39%</div><div>32%</div><div>8%</div><div>•</div><div>21%</div></div></div>
3	G	173	<div><div>%</div><div><div></div><div>62%</div><div>12%</div><div>5%</div><div>•</div><div>21%</div></div></div>

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Mol	Chain	Length	Quality of chain
3	M	173	

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
5	COY	A	601	X	-	-	-
5	COY	L	601	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15471 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 PROPANEDIOL DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	4	0
			4217	2629	731	828	29			
1	L	551	Total	C	N	O	S	0	7	0
			4225	2632	734	830	29			

- Molecule 2 is a protein called PROPANEDIOL DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	4	0
			1378	871	249	256	2			
2	E	178	Total	C	N	O	S	0	1	0
			1363	863	245	253	2			

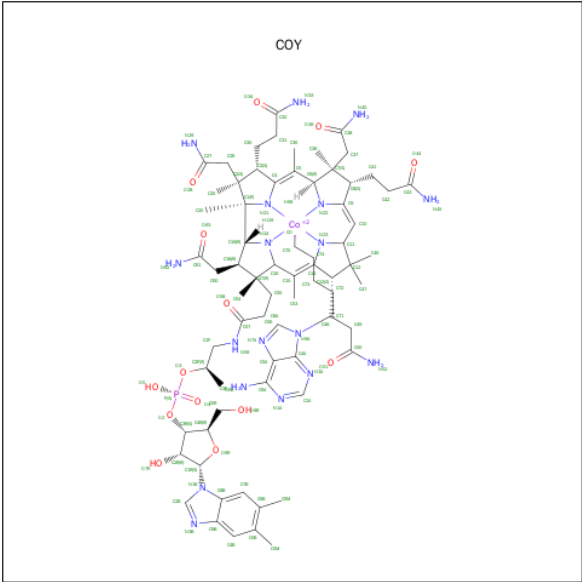
- Molecule 3 is a protein called PROPANEDIOL DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	137	Total	C	N	O	S	0	4	0
			1111	691	200	217	3			
3	M	137	Total	C	N	O	S	0	2	0
			1102	686	196	217	3			

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

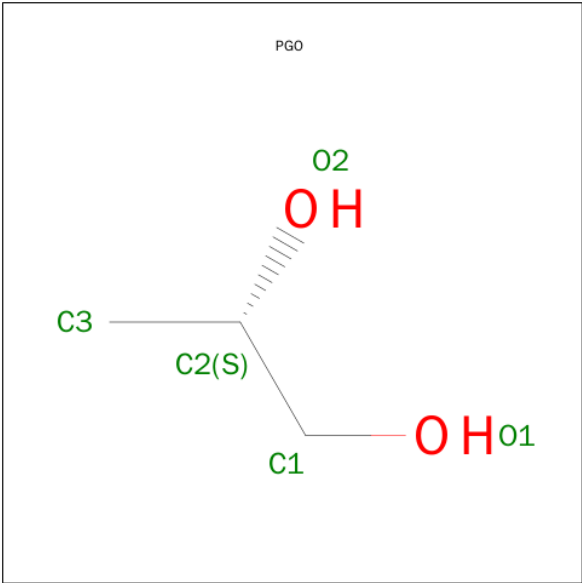
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	K	0	0
			2	2		
4	L	2	Total	K	0	0
			2	2		

- Molecule 5 is CO-(ADENIN-9-YL-PENTYL)-COBALAMIN (three-letter code: COY) (formula: C₇₂H₁₀₆CoN₁₈O₁₄P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	Co	N	O	P	0	0
			106	72	1	18	14	1		
5	L	1	Total	C	Co	N	O	P	0	0
			106	72	1	18	14	1		

- Molecule 6 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: C₃H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			5	3	2		
6	L	1	Total	C	O	0	0
			5	3	2		

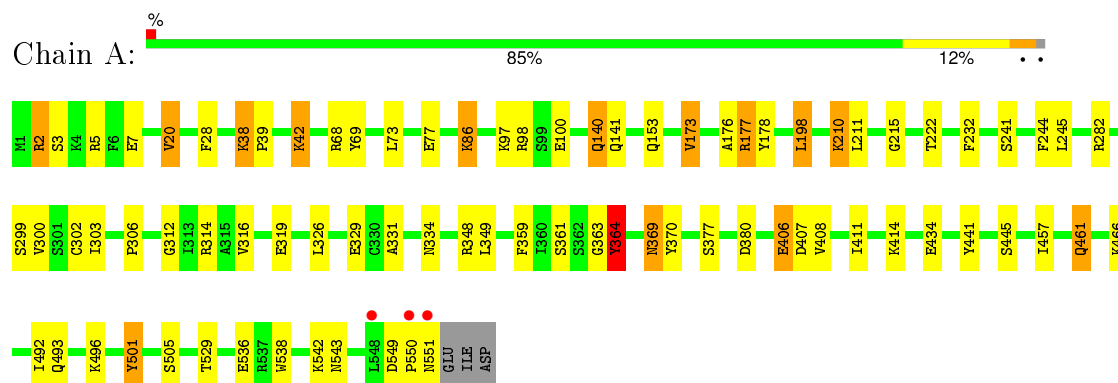
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	675	Total 675	O 675	0	0
7	B	215	Total 215	O 215	0	0
7	E	106	Total 106	O 106	0	0
7	G	204	Total 204	O 204	0	0
7	L	498	Total 498	O 498	0	0
7	M	151	Total 151	O 151	0	0

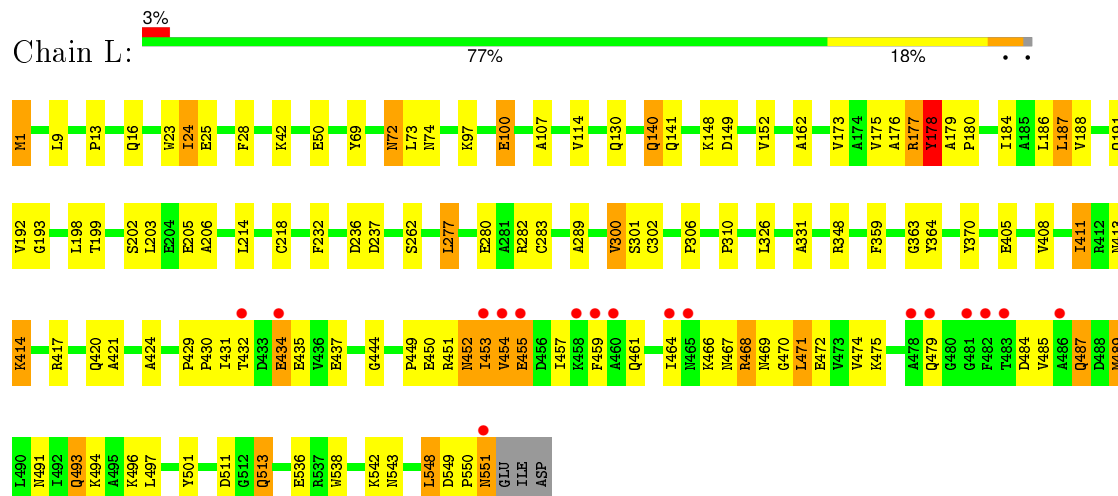
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

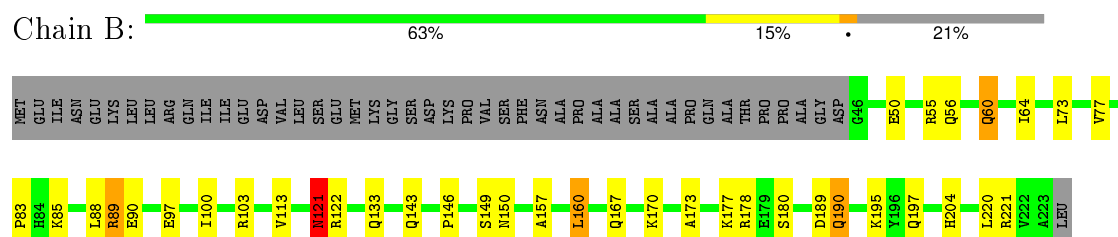
• Molecule 1: PROPANEDIOL DEHYDRATASE



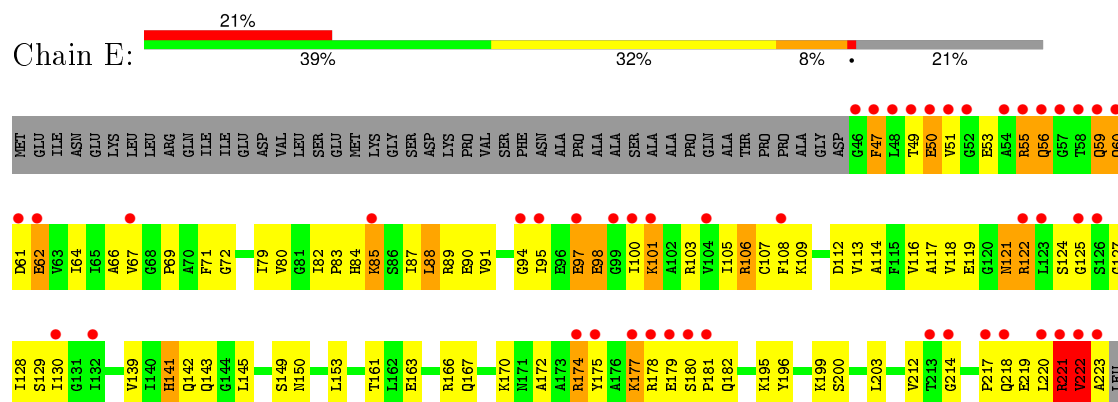
• Molecule 1: PROPANEDIOL DEHYDRATASE



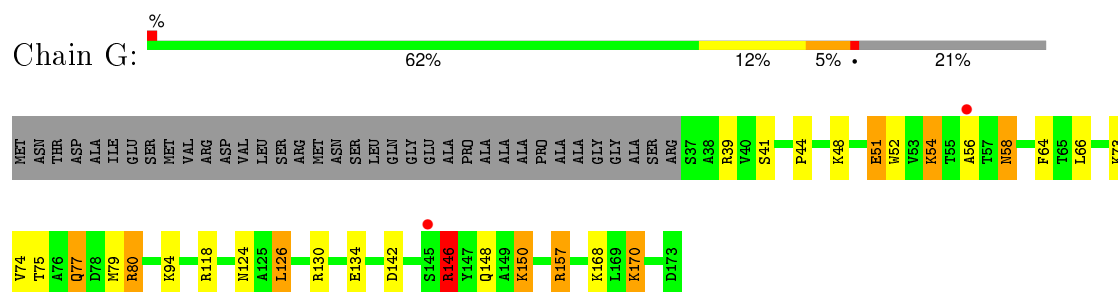
• Molecule 2: PROPANEDIOL DEHYDRATASE



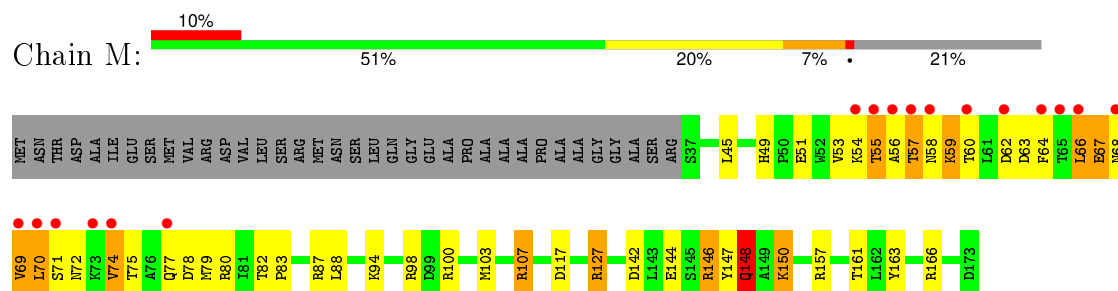
● Molecule 2: PROPANEDIOL DEHYDRATASE



● Molecule 3: PROPANEDIOL DEHYDRATASE



● Molecule 3: PROPANEDIOL DEHYDRATASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.38Å 121.40Å 207.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75 31.54 – 1.74	Depositor EDS
% Data completeness (in resolution range)	80.0 (30.00-1.75) 79.8 (31.54-1.74)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 1.74Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.152 , 0.214 0.152 , 0.207	Depositor DCC
R_{free} test set	7513 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	13.3	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 109.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 151109 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15471	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COY, PGO, K

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	0/4308	1.04	17/5832 (0.3%)
1	L	0.36	0/4328	1.10	10/5858 (0.2%)
2	B	0.35	0/1418	1.02	4/1917 (0.2%)
2	E	0.31	0/1389	0.93	1/1879 (0.1%)
3	G	0.35	0/1145	1.13	5/1545 (0.3%)
3	M	0.33	0/1125	1.09	8/1520 (0.5%)
All	All	0.35	0/13713	1.06	45/18551 (0.2%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	L	282	ARG	CD-NE-CZ	29.11	164.35	123.60
1	L	282	ARG	NE-CZ-NH1	13.06	126.83	120.30
2	B	122	ARG	CD-NE-CZ	8.40	135.36	123.60
1	L	364	TYR	CG-CD1-CE1	8.38	128.01	121.30
1	A	98	ARG	NE-CZ-NH1	8.27	124.43	120.30
1	A	370	TYR	CB-CG-CD1	8.07	125.84	121.00
1	A	364	TYR	CB-CG-CD1	7.31	125.39	121.00
1	L	282	ARG	NE-CZ-NH2	-7.20	116.70	120.30
2	E	221	ARG	C-N-CA	7.18	139.66	121.70
1	A	364	TYR	CG-CD1-CE1	7.03	126.92	121.30
3	M	127	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	L	468	ARG	NE-CZ-NH1	6.65	123.62	120.30
3	M	107	ARG	NE-CZ-NH1	-6.63	116.99	120.30
1	L	468	ARG	NE-CZ-NH2	-6.62	116.99	120.30
3	M	127	ARG	NE-CZ-NH2	-6.48	117.06	120.30
3	M	98	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	L	178	TYR	CB-CG-CD2	6.07	124.64	121.00
1	A	501	TYR	CB-CG-CD1	6.02	124.61	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	L	364	TYR	CB-CG-CD1	5.88	124.53	121.00
1	A	314	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	244	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	A	370	TYR	CG-CD1-CE1	5.79	125.94	121.30
2	B	121	ASN	CA-CB-CG	5.76	126.06	113.40
3	M	166	ARG	NE-CZ-NH1	-5.70	117.45	120.30
2	B	89	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	L	237	ASP	CB-CG-OD2	5.47	123.23	118.30
3	G	146[A]	ARG	CD-NE-CZ	5.42	131.18	123.60
3	G	146[B]	ARG	CD-NE-CZ	5.42	131.18	123.60
1	A	501	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	L	149	ASP	CB-CG-OD1	5.37	123.13	118.30
3	G	80	ARG	CD-NE-CZ	5.33	131.06	123.60
1	A	69	TYR	CB-CG-CD2	-5.30	117.82	121.00
3	G	157	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	2	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	282	ARG	NE-CZ-NH1	5.22	122.91	120.30
3	M	163	TYR	CB-CG-CD1	5.20	124.12	121.00
2	B	189	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	5	ARG	NE-CZ-NH2	-5.16	117.72	120.30
3	M	87	ARG	NE-CZ-NH2	-5.15	117.72	120.30
3	G	80	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	98	ARG	NE-CZ-NH2	-5.13	117.73	120.30
3	M	148	GLN	CA-CB-CG	5.05	124.51	113.40
1	A	380	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	198	LEU	CA-CB-CG	5.03	126.87	115.30

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	4217	0	4161	60	0
1	L	4225	0	4154	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1378	0	1432	20	0
2	E	1363	0	1417	100	0
3	G	1111	0	1115	25	0
3	M	1102	0	1105	50	0
4	A	2	0	0	0	0
4	L	2	0	0	0	0
5	A	106	0	100	11	0
5	L	106	0	100	12	0
6	A	5	0	6	0	0
6	L	5	0	6	0	0
7	A	675	0	0	18	0
7	B	215	0	0	2	0
7	E	106	0	0	6	0
7	G	204	0	0	10	0
7	L	498	0	0	10	0
7	M	151	0	0	12	0
All	All	15471	0	13596	358	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 (358) 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)
2:B:100:ILE:HD11	2:B:177[B]:LYS:HD3	1.51	0.92
1:A:97:LYS:HB2	1:A:100[A]:GLU:HG3	1.53	0.90
1:L:497:LEU:HD21	3:M:79:MET:HA	1.53	0.89
3:M:68:ASN:HB3	3:M:74:VAL:HG13	1.55	0.86
1:L:173:VAL:HG21	1:L:176:ALA:HA	1.57	0.86
2:E:67:VAL:HG13	2:E:71:PHE:HB3	1.58	0.83
2:E:55:ARG:HE	2:E:56:GLN:HB2	1.41	0.83
2:E:174:ARG:HH11	2:E:179:GLU:HG2	1.48	0.78
1:L:42:LYS:HB2	1:L:50:GLU:HB3	1.66	0.78
3:M:69:VAL:HG12	3:M:70:LEU:HD13	1.66	0.77
2:E:55:ARG:HE	2:E:56:GLN:H	1.33	0.77
3:M:54:LYS:HE2	3:M:58:ASN:O	1.86	0.76
3:M:80:ARG:HD2	7:M:214:HOH:O	1.86	0.75
3:M:103:MET:HG3	7:M:258:HOH:O	1.87	0.74
2:E:121:ASN:ND2	2:E:122:ARG:HD3	2.01	0.74
1:L:469:ASN:OD1	1:L:471:LEU:HB2	1.87	0.73
2:E:174:ARG:HD2	2:E:179:GLU:HG2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:142:ASP:HB3	7:M:309:HOH:O	1.87	0.73
1:L:413:ASN:ND2	1:L:417:ARG:HE	1.87	0.73
1:L:455:GLU:HG3	7:L:1041:HOH:O	1.89	0.72
3:M:55:THR:OG1	3:M:57:THR:HG22	1.89	0.72
1:L:475:LYS:O	1:L:479:GLN:HG2	1.90	0.72
1:A:369:ASN:HD21	1:A:377:SER:H	1.35	0.72
3:M:59:LYS:HB2	3:M:63:ASP:OD1	1.90	0.71
2:E:195[B]:LYS:HD2	7:E:288:HOH:O	1.91	0.71
1:L:192:VAL:HG13	1:L:414:LYS:HD2	1.72	0.70
1:A:173:VAL:HG21	1:A:176:ALA:HA	1.74	0.70
2:B:55:ARG:HG3	7:B:325:HOH:O	1.91	0.70
3:M:75:THR:O	3:M:78:ASP:HB2	1.93	0.69
3:G:58:ASN:HA	7:G:332:HOH:O	1.93	0.69
3:M:54:LYS:HB2	7:M:301:HOH:O	1.90	0.69
2:E:121:ASN:HD22	2:E:122:ARG:HD3	1.59	0.68
2:B:97:GLU:OE2	2:B:170:LYS:HD2	1.94	0.68
1:L:493:GLN:O	1:L:496:LYS:HB2	1.92	0.68
1:A:550:PRO:HG3	1:L:23:TRP:HB2	1.77	0.67
2:E:222:VAL:HG22	2:E:223:ALA:H	1.60	0.66
2:E:50:GLU:HA	2:E:220:LEU:HD23	1.79	0.64
1:L:513:GLN:HG3	7:L:825:HOH:O	1.96	0.64
3:G:148:GLN:O	3:G:150:LYS:HE3	1.96	0.64
2:E:122:ARG:NH1	7:E:320:HOH:O	2.31	0.64
2:E:55:ARG:NE	2:E:56:GLN:H	1.95	0.64
2:E:49:THR:O	2:E:220:LEU:HA	1.98	0.63
1:L:551:ASN:ND2	1:L:551:ASN:H	1.97	0.63
1:L:97:LYS:HB2	1:L:100[A]:GLU:HG2	1.79	0.62
2:E:94:GLY:HA2	2:E:97:GLU:OE1	1.98	0.62
2:B:173:ALA:O	2:B:177[A]:LYS:HG3	2.00	0.61
2:E:174:ARG:HB3	2:E:181:PRO:HD3	1.82	0.61
3:M:62:ASP:HA	7:M:324:HOH:O	1.99	0.61
2:E:62:GLU:HB2	2:E:101:LYS:HB2	1.81	0.61
1:A:2:ARG:NH1	1:A:2:ARG:HB3	2.16	0.61
2:E:55:ARG:NE	2:E:56:GLN:HB2	2.13	0.61
2:E:55:ARG:HH21	2:E:56:GLN:HB2	1.66	0.60
1:L:538:TRP:O	1:L:542:LYS:HG3	2.02	0.60
3:M:55:THR:HG22	7:M:322:HOH:O	2.01	0.59
1:L:431:ILE:HA	1:L:451:ARG:NH2	2.17	0.59
5:L:601:COY:H262	5:L:601:COY:H601	1.84	0.59
2:E:105:ILE:HD12	2:E:217:PRO:HB3	1.83	0.59
2:E:177:LYS:O	2:E:177:LYS:HE3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:219:GLU:HG3	2:E:220:LEU:N	2.17	0.59
2:E:59:GLN:O	2:E:125:GLY:HA3	2.02	0.59
1:A:140:GLN:HE21	1:A:141:GLN:H	1.49	0.59
5:A:601:COY:H492	5:A:601:COY:C2B	2.33	0.59
5:L:601:COY:H301	2:E:153:LEU:HD23	1.85	0.59
3:M:67:GLU:HG3	3:M:68:ASN:N	2.19	0.58
2:E:177:LYS:HG2	2:E:179:GLU:OE1	2.02	0.58
1:A:536:GLU:HG2	7:A:1271:HOH:O	2.03	0.58
1:L:414:LYS:O	1:L:414:LYS:HG2	2.02	0.58
1:L:493:GLN:HB3	7:L:815:HOH:O	2.03	0.57
3:M:100:ARG:HD3	3:M:103:MET:CE	2.34	0.57
1:L:431:ILE:HA	1:L:451:ARG:HH21	1.67	0.57
1:L:484:ASP:OD2	1:L:485:VAL:HG23	2.04	0.57
3:G:130:ARG:O	3:G:170:LYS:HE3	2.04	0.57
5:A:601:COY:H351	5:A:601:COY:H362	1.85	0.57
2:E:98:GLU:OE1	2:E:98:GLU:HA	2.04	0.57
2:E:59:GLN:H	2:E:59:GLN:NE2	2.03	0.57
1:A:210[A]:LYS:HD2	7:A:1075:HOH:O	2.05	0.57
1:L:413:ASN:HD21	1:L:417:ARG:HE	1.52	0.56
1:L:42:LYS:HB2	1:L:50:GLU:CB	2.33	0.56
1:A:20:VAL:HG22	1:L:548:LEU:HG	1.86	0.56
5:L:601:COY:H552	5:L:601:COY:H531	1.86	0.56
3:G:54[B]:LYS:HG2	7:G:332:HOH:O	2.05	0.56
1:A:177[B]:ARG:HD2	7:A:1266:HOH:O	2.06	0.56
1:A:441:TYR:CD2	1:L:1:MET:HG2	2.40	0.56
1:L:408:VAL:O	1:L:411:ILE:HG22	2.06	0.56
2:E:55:ARG:HE	2:E:56:GLN:N	2.01	0.56
2:E:72:GLY:H	2:E:84:HIS:HD2	1.53	0.56
1:A:369:ASN:ND2	1:A:377:SER:H	2.03	0.55
5:L:601:COY:C2B	5:L:601:COY:H492	2.36	0.55
2:E:161:THR:HB	7:E:305:HOH:O	2.05	0.55
2:B:146:PRO:HG2	2:B:149:SER:HB2	1.88	0.55
3:M:55:THR:HA	7:M:268:HOH:O	2.06	0.55
2:E:79:ILE:HG13	2:E:199:LYS:HD3	1.88	0.55
2:E:66:ALA:HB1	2:E:107:CYS:SG	2.47	0.55
1:L:421:ALA:O	1:L:424:ALA:HB3	2.07	0.55
1:L:214:LEU:HD21	1:L:467:ASN:HA	1.87	0.54
2:E:71:PHE:HE1	2:E:88:LEU:HD22	1.72	0.54
2:E:87:ILE:O	2:E:91:VAL:HG23	2.07	0.54
1:L:25:GLU:HB3	7:L:862:HOH:O	2.06	0.54
2:E:49:THR:HG22	2:E:51:VAL:HG13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:LYS:HG2	1:L:310:PRO:CG	2.37	0.54
2:E:174:ARG:NH1	2:E:179:GLU:HG2	2.20	0.54
2:B:89:ARG:HD2	2:B:90:GLU:OE1	2.07	0.54
2:E:175:TYR:CD1	2:E:181:PRO:HD2	2.43	0.53
1:A:38:LYS:HD3	7:A:962:HOH:O	2.08	0.53
3:M:146:ARG:HD2	3:M:147:TYR:CZ	2.43	0.53
1:L:152:VAL:HG22	1:L:431:ILE:HD13	1.90	0.53
2:E:106:ARG:HG2	2:E:108:PHE:CZ	2.44	0.53
2:E:59:GLN:HG3	2:E:61:ASP:OD1	2.08	0.53
3:M:54:LYS:HD3	3:M:58:ASN:HA	1.91	0.53
1:A:177[A]:ARG:HB3	1:A:457:ILE:HG23	1.91	0.52
1:A:177[B]:ARG:HB3	1:A:457:ILE:HG23	1.91	0.52
5:L:601:COY:H351	5:L:601:COY:H362	1.92	0.52
2:B:121:ASN:ND2	2:B:143:GLN:HA	2.25	0.52
3:M:66:LEU:O	3:M:70:LEU:HD13	2.08	0.52
1:A:241:SER:HB3	3:G:126:LEU:HB3	1.90	0.52
2:E:128:ILE:HD12	2:E:175:TYR:HB3	1.91	0.52
2:E:50:GLU:HG3	2:E:50:GLU:O	2.09	0.52
1:A:493:GLN:HE22	1:A:496:LYS:NZ	2.08	0.52
2:E:177:LYS:CG	2:E:179:GLU:HB2	2.40	0.51
1:A:42:LYS:HE2	7:A:1174:HOH:O	2.10	0.51
1:L:175:VAL:O	1:L:178:TYR:HB2	2.10	0.51
1:A:38:LYS:HG2	7:A:962:HOH:O	2.11	0.51
1:L:453:ILE:HG23	1:L:457:ILE:HD12	1.93	0.51
1:A:434:GLU:HB2	7:A:1131:HOH:O	2.10	0.51
2:E:119:GLU:OE2	2:E:217:PRO:HD3	2.10	0.51
2:E:109:LYS:HG2	2:E:214:GLY:H	1.76	0.51
1:A:529:THR:HB	7:A:1022:HOH:O	2.09	0.51
1:L:429:PRO:HG2	1:L:455:GLU:O	2.10	0.51
3:M:53:VAL:O	3:M:53:VAL:HG12	2.10	0.51
3:G:51:GLU:O	3:G:54[A]:LYS:HD3	2.09	0.51
1:A:140:GLN:HE21	1:A:141:GLN:N	2.08	0.51
1:A:549:ASP:OD2	1:A:551:ASN:OD1	2.29	0.51
1:L:205:GLU:HG2	7:L:812:HOH:O	2.11	0.50
2:E:219:GLU:O	2:E:220:LEU:HD23	2.10	0.50
2:E:107:CYS:CB	2:E:116:VAL:HB	2.41	0.50
3:M:56:ALA:O	3:M:58:ASN:OD1	2.30	0.50
3:M:100:ARG:HD3	3:M:103:MET:HE2	1.93	0.50
2:E:106:ARG:HB2	2:E:220:LEU:HD11	1.94	0.50
1:A:77:GLU:HG2	7:A:786:HOH:O	2.10	0.50
5:A:601:COY:H361	5:A:601:COY:O39	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:VAL:HB	2:B:133:GLN:HG3	1.94	0.50
2:E:101:LYS:N	2:E:101:LYS:HD2	2.26	0.50
2:E:105:ILE:HD12	2:E:217:PRO:CB	2.41	0.50
3:M:144:GLU:OE1	3:M:150:LYS:HE2	2.11	0.50
1:L:187:LEU:O	1:L:191:GLN:HG2	2.12	0.49
3:M:64:PHE:CE2	3:M:78:ASP:HB3	2.47	0.49
1:L:432:THR:OG1	1:L:434:GLU:OE2	2.30	0.49
2:B:146:PRO:HG2	2:B:149:SER:CB	2.43	0.49
3:M:69:VAL:HG12	3:M:70:LEU:CD1	2.40	0.49
2:E:64:ILE:HD12	2:E:124:SER:HA	1.93	0.49
1:L:236:ASP:O	3:M:127:ARG:HD2	2.12	0.49
1:A:316:VAL:O	1:A:319:GLU:HG2	2.12	0.49
2:E:64:ILE:HD12	2:E:124:SER:CA	2.43	0.49
1:L:206:ALA:HB3	7:L:1048:HOH:O	2.12	0.49
7:L:1093:HOH:O	2:E:195[B]:LYS:HE2	2.13	0.49
1:A:177[B]:ARG:HG2	1:A:461:GLN:NE2	2.28	0.49
3:M:60:THR:HG22	7:M:301:HOH:O	2.12	0.49
1:A:406:GLU:HG3	1:A:407:ASP:N	2.27	0.49
3:M:66:LEU:HD22	3:M:70:LEU:CD1	2.43	0.49
3:M:55:THR:OG1	3:M:59:LYS:O	2.30	0.49
1:A:2:ARG:HB3	1:A:2:ARG:HH11	1.76	0.49
3:M:55:THR:CB	3:M:57:THR:HG22	2.43	0.49
5:L:601:COY:H1R	7:E:229:HOH:O	2.13	0.49
3:M:49:HIS:HA	3:M:51:GLU:OE2	2.13	0.49
2:E:64:ILE:HA	2:E:103:ARG:O	2.13	0.48
2:E:50:GLU:HA	2:E:219:GLU:O	2.13	0.48
1:A:153:GLN:HE22	1:A:445:SER:HB3	1.77	0.48
5:A:601:COY:H531	5:A:601:COY:H552	1.94	0.48
1:L:177[B]:ARG:HG2	1:L:461:GLN:CG	2.43	0.48
1:L:140:GLN:HE21	1:L:141:GLN:H	1.61	0.48
1:A:20:VAL:HG13	1:L:550:PRO:HG3	1.96	0.48
1:A:441:TYR:CG	1:L:1:MET:HG2	2.48	0.48
2:E:69:PRO:HA	2:E:106:ARG:HD3	1.94	0.48
1:L:429:PRO:HA	1:L:430:PRO:HD3	1.77	0.48
1:A:222:THR:HB	5:A:601:COY:H721	1.95	0.48
1:L:461:GLN:HA	1:L:461:GLN:NE2	2.29	0.48
1:L:186:LEU:CD2	1:L:199:THR:HB	2.44	0.48
2:E:109:LYS:HG2	2:E:214:GLY:N	2.29	0.48
1:L:69:TYR:HB2	1:L:289:ALA:HB1	1.95	0.48
2:E:94:GLY:O	2:E:97:GLU:OE2	2.31	0.48
2:B:50:GLU:HG2	2:B:220:LEU:CD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1113:HOH:O	2:B:197:GLN:HG3	2.14	0.47
1:L:452:ASN:ND2	1:L:454:VAL:HG23	2.29	0.47
3:M:66:LEU:HA	3:M:66:LEU:HD23	1.71	0.47
5:L:601:COY:C6	5:L:601:COY:H4B	2.45	0.47
5:L:601:COY:H202	5:L:601:COY:N3B	2.29	0.47
1:A:140:GLN:HE22	1:A:361[B]:SER:HB2	1.78	0.47
1:A:331:ALA:HA	1:A:359:PHE:HB2	1.97	0.47
2:E:112:ASP:O	2:E:116:VAL:HG13	2.15	0.47
2:E:199:LYS:HE2	2:E:203:LEU:HD11	1.97	0.46
1:L:179:ALA:HB3	1:L:180:PRO:HD3	1.96	0.46
2:E:55:ARG:NH2	2:E:56:GLN:HB2	2.29	0.46
1:L:152:VAL:HG21	1:L:431:ILE:HG23	1.97	0.46
2:E:119:GLU:OE2	2:E:217:PRO:HG3	2.15	0.46
3:G:77:GLN:NE2	7:G:226:HOH:O	2.42	0.46
2:E:178:ARG:HG3	2:E:178:ARG:NH1	2.30	0.46
3:M:60:THR:HB	7:M:221:HOH:O	2.15	0.46
5:A:601:COY:H491	5:A:601:COY:H473	1.96	0.46
2:E:212:VAL:HA	7:E:245:HOH:O	2.16	0.46
2:E:177:LYS:HG2	2:E:179:GLU:HB2	1.98	0.46
2:E:178:ARG:HG3	2:E:178:ARG:HH11	1.80	0.46
2:E:174:ARG:HH11	2:E:179:GLU:CG	2.25	0.46
1:A:306:PRO:O	1:A:312:GLY:HA3	2.16	0.46
3:G:54[B]:LYS:HD2	3:G:58:ASN:HD22	1.81	0.46
1:L:262:SER:HA	7:L:606:HOH:O	2.15	0.46
1:A:369:ASN:HD22	1:A:369:ASN:HA	1.57	0.46
1:L:331:ALA:HA	1:L:359:PHE:HB2	1.98	0.45
1:L:429:PRO:HD3	1:L:459:PHE:CG	2.51	0.45
1:A:2:ARG:NH1	1:L:405:GLU:OE1	2.50	0.45
1:A:299:SER:OG	1:A:303:ILE:HA	2.15	0.45
2:E:62:GLU:OE2	2:E:125:GLY:N	2.50	0.45
1:A:466:LYS:NZ	7:A:1277:HOH:O	2.50	0.45
1:L:370:TYR:OH	1:L:444:GLY:HA3	2.17	0.45
3:M:69:VAL:HG23	3:M:74:VAL:HG22	1.98	0.45
1:L:430:PRO:O	1:L:451:ARG:NH2	2.50	0.45
5:L:601:COY:H301	2:E:153:LEU:CD2	2.46	0.45
2:E:51:VAL:HG11	2:E:221:ARG:HD2	1.99	0.45
1:L:549:ASP:OD2	1:L:551:ASN:ND2	2.50	0.45
1:L:192:VAL:CG1	1:L:414:LYS:HD2	2.43	0.45
2:B:60:GLN:NE2	7:B:435:HOH:O	2.48	0.45
3:G:80:ARG:NH2	7:G:325:HOH:O	2.49	0.45
3:M:80:ARG:NH1	7:M:266:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:170:LYS:HE2	7:G:300:HOH:O	2.17	0.45
1:L:487:GLN:NE2	1:L:491:ASN:OD1	2.50	0.45
3:M:71:SER:O	3:M:72:ASN:HB2	2.16	0.45
2:E:163:GLU:N	7:E:301:HOH:O	2.50	0.45
3:M:74:VAL:HA	3:M:78:ASP:OD1	2.16	0.45
3:M:117:ASP:OD1	3:M:117:ASP:N	2.50	0.45
2:B:157:ALA:HA	2:B:160:LEU:HD22	1.98	0.45
1:A:461:GLN:NE2	7:A:1134:HOH:O	2.49	0.45
1:A:414:LYS:NZ	7:A:1240:HOH:O	2.49	0.45
2:B:88:LEU:HD12	2:B:88:LEU:HA	1.89	0.45
2:E:174:ARG:HB2	2:E:181:PRO:HG3	1.99	0.44
3:M:54:LYS:HG2	3:M:55:THR:O	2.16	0.44
1:L:549:ASP:HA	1:L:550:PRO:HD3	1.70	0.44
1:A:177[A]:ARG:NH2	7:A:1181:HOH:O	2.50	0.44
1:A:38:LYS:HE2	7:A:942:HOH:O	2.17	0.44
2:E:47:PHE:CE1	2:E:85:LYS:HA	2.52	0.44
2:E:72:GLY:N	2:E:84:HIS:HD2	2.15	0.44
1:A:550:PRO:CG	1:L:23:TRP:HB2	2.45	0.44
3:G:64:PHE:CE2	3:G:79:MET:HG2	2.52	0.44
3:G:142:ASP:OD1	3:G:146[A]:ARG:NH1	2.50	0.44
1:L:493:GLN:H	1:L:493:GLN:HG2	1.51	0.44
1:L:175:VAL:HG13	1:L:175:VAL:O	2.17	0.44
2:E:127:GLY:O	2:E:142:GLN:HA	2.17	0.44
1:A:302:CYS:O	1:A:306:PRO:HD2	2.17	0.44
2:E:141:HIS:NE2	2:E:149:SER:O	2.50	0.44
1:A:329:GLU:OE2	1:A:505:SER:HA	2.17	0.44
3:G:157:ARG:NH2	7:G:290:HOH:O	2.50	0.44
3:G:39:ARG:NH1	7:G:309:HOH:O	2.50	0.44
1:L:432:THR:OG1	1:L:434:GLU:HG3	2.18	0.44
2:E:62:GLU:CD	2:E:125:GLY:H	2.21	0.44
3:G:168:LYS:NZ	7:G:274:HOH:O	2.50	0.44
1:A:538:TRP:CE2	1:A:542:LYS:HD2	2.52	0.44
2:E:90:GLU:O	2:E:166:ARG:HD2	2.18	0.44
2:E:122:ARG:HD2	2:E:122:ARG:HA	1.66	0.44
1:L:16:GLN:NE2	7:L:1093:HOH:O	2.50	0.44
3:M:107:ARG:HD3	3:M:107:ARG:HH11	1.61	0.44
1:L:468:ARG:HD2	1:L:472:GLU:OE1	2.18	0.44
1:L:429:PRO:HD3	1:L:459:PHE:CD2	2.53	0.43
1:A:177[A]:ARG:NH1	7:A:1265:HOH:O	2.50	0.43
1:L:177[A]:ARG:HG2	1:L:461:GLN:CG	2.48	0.43
1:A:97:LYS:HB2	1:A:100[A]:GLU:CG	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:57:THR:HG21	3:M:59:LYS:HD2	2.00	0.43
2:E:195[A]:LYS:HE3	2:E:196:TYR:OH	2.18	0.43
1:L:435:GLU:OE2	1:L:451:ARG:NE	2.50	0.43
1:A:177[B]:ARG:HG2	1:A:461:GLN:CD	2.38	0.43
1:L:432:THR:OG1	1:L:435:GLU:HG3	2.18	0.43
2:E:90:GLU:O	2:E:166:ARG:HA	2.19	0.43
5:A:601:COY:H601	5:A:601:COY:H262	2.01	0.43
1:L:435:GLU:HG2	1:L:449:PRO:HG2	2.00	0.43
5:A:601:COY:H4B	5:A:601:COY:C6	2.49	0.43
3:G:75:THR:OG1	3:G:77:GLN:HG2	2.18	0.43
1:L:24:ILE:N	1:L:24:ILE:HD13	2.34	0.43
3:M:66:LEU:HD22	3:M:70:LEU:HD13	2.00	0.43
2:E:62:GLU:HA	2:E:100:ILE:HG23	1.99	0.43
1:A:441:TYR:CE2	1:L:1:MET:HG2	2.54	0.43
3:M:94:LYS:NZ	7:M:286:HOH:O	2.50	0.43
2:B:77:VAL:HG12	2:B:83:PRO:HA	2.01	0.43
2:E:49:THR:HG22	2:E:51:VAL:CG1	2.48	0.42
2:E:114:ALA:O	2:E:118:VAL:HG23	2.19	0.42
1:A:215:GLY:HA2	7:A:791:HOH:O	2.19	0.42
5:L:601:COY:HM62	2:E:114:ALA:HB2	2.00	0.42
1:L:173:VAL:CG2	1:L:176:ALA:HA	2.37	0.42
1:A:140:GLN:HE21	1:A:140:GLN:CA	2.32	0.42
5:A:601:COY:H202	5:A:601:COY:N3B	2.34	0.42
3:M:82:THR:HB	3:M:83:PRO:HD2	2.01	0.42
2:E:53:GLU:HG3	2:E:218:GLN:NE2	2.35	0.42
1:L:489:MET:O	1:L:493:GLN:HG2	2.19	0.42
2:E:60:GLN:HA	2:E:125:GLY:O	2.19	0.42
2:E:95:ILE:CG2	2:E:100:ILE:HG22	2.50	0.42
5:L:601:COY:H3P1	2:E:200:SER:HB2	2.01	0.42
5:A:601:COY:H531	5:A:601:COY:C55	2.49	0.42
2:E:117:ALA:HB1	2:E:141:HIS:HB2	2.02	0.42
1:A:408:VAL:HA	1:A:411:ILE:HG22	2.01	0.42
3:M:157:ARG:HD2	7:M:224:HOH:O	2.19	0.42
2:E:177:LYS:HG3	2:E:179:GLU:HB2	2.01	0.42
1:L:97:LYS:HE3	1:L:97:LYS:HB2	1.80	0.42
5:L:601:COY:C2B	5:L:601:COY:H202	2.50	0.42
2:E:59:GLN:HG2	2:E:61:ASP:H	1.85	0.41
3:G:41:SER:O	3:G:48:LYS:HE2	2.20	0.41
2:E:130:ILE:HD11	2:E:172:ALA:CB	2.50	0.41
1:L:280:GLU:O	1:L:283:CYS:HB2	2.20	0.41
1:L:72:ASN:HB3	1:L:107:ALA:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1142:HOH:O	2:B:204:HIS:HE1	2.04	0.41
1:A:86:LYS:HA	1:A:86:LYS:HD3	1.59	0.41
3:G:54[B]:LYS:HB3	3:G:54[B]:LYS:HE3	1.76	0.41
1:A:361[A]:SER:HG	1:A:364:TYR:HB2	1.86	0.41
3:M:144:GLU:O	3:M:148:GLN:HA	2.21	0.41
1:L:162:ALA:HB3	1:L:193:GLY:HA3	2.02	0.41
1:A:334:ASN:OD1	1:A:349:LEU:HA	2.20	0.41
2:B:64:ILE:HD13	2:B:103:ARG:HB3	2.03	0.41
1:L:497:LEU:HD21	3:M:79:MET:CA	2.37	0.41
1:L:175:VAL:HG11	1:L:457:ILE:HD11	2.01	0.41
2:E:82:ILE:HA	2:E:83:PRO:HD3	1.95	0.41
2:E:139:VAL:O	2:E:139:VAL:HG13	2.20	0.41
2:E:90:GLU:HB3	2:E:166:ARG:HB2	2.02	0.41
2:E:221:ARG:O	2:E:222:VAL:O	2.39	0.41
1:L:114:VAL:HG13	1:L:277:LEU:HD13	2.03	0.41
1:L:470:GLY:O	1:L:474:VAL:HG23	2.20	0.41
3:M:100:ARG:HA	3:M:100:ARG:NE	2.36	0.41
1:L:434:GLU:HG3	1:L:434:GLU:H	1.64	0.41
1:L:496:LYS:HB3	1:L:496:LYS:HE2	1.80	0.41
1:L:414:LYS:HZ3	1:L:414:LYS:HB2	1.86	0.40
5:A:601:COY:O28	5:A:601:COY:H3	2.20	0.40
1:A:38:LYS:HG3	1:A:39:PRO:HD2	2.03	0.40
1:L:140:GLN:HE21	1:L:141:GLN:N	2.19	0.40
3:G:52:TRP:O	3:G:54[A]:LYS:HE3	2.21	0.40
1:L:300:VAL:HG12	1:L:301:SER:N	2.36	0.40
1:A:3:SER:O	1:A:7:GLU:HG3	2.21	0.40
1:L:184:ILE:O	1:L:188:VAL:HG23	2.21	0.40
2:E:175:TYR:CE1	2:E:181:PRO:HD2	2.56	0.40
2:E:174:ARG:CD	2:E:179:GLU:HG2	2.48	0.40
2:E:222:VAL:HG13	2:E:223:ALA:N	2.36	0.40
1:L:180:PRO:HG3	1:L:464:ILE:HD11	2.03	0.40
3:G:44:PRO:O	3:G:48:LYS:HG2	2.21	0.40
1:L:202:SER:O	1:L:203:LEU:HD23	2.22	0.40
1:L:302:CYS:O	1:L:306:PRO:HD2	2.21	0.40
2:E:128:ILE:CD1	2:E:175:TYR:HB3	2.52	0.40
1:L:420:GLN:HA	1:L:431:ILE:HD12	2.03	0.40
3:G:118:ARG:NH2	7:G:262:HOH:O	2.50	0.40
1:L:536:GLU:HG2	7:L:1059:HOH:O	2.21	0.40
2:E:122:ARG:NH1	2:E:122:ARG:HG3	2.37	0.40
1:L:152:VAL:HG22	1:L:431:ILE:CD1	2.52	0.40
3:M:146:ARG:HD3	3:M:146:ARG:HH11	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:140:GLN:HE21	1:L:140:GLN:CA	2.34	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	553/554 (100%)	533 (96%)	18 (3%)	2 (0%)	39	19
1	L	555/554 (100%)	536 (97%)	17 (3%)	2 (0%)	39	19
2	B	180/224 (80%)	176 (98%)	4 (2%)	0	100	100
2	E	177/224 (79%)	163 (92%)	12 (7%)	2 (1%)	17	4
3	G	139/173 (80%)	136 (98%)	2 (1%)	1 (1%)	26	10
3	M	137/173 (79%)	134 (98%)	2 (2%)	1 (1%)	26	10
All	All	1741/1902 (92%)	1678 (96%)	55 (3%)	8 (0%)	34	14

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	222	VAL
3	G	56	ALA
3	M	55	THR
1	A	300	VAL
1	L	300	VAL
1	A	363	GLY
1	L	363	GLY
2	E	47	PHE

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	454/453 (100%)	428 (94%)	26 (6%)	25	6
1	L	456/453 (101%)	414 (91%)	42 (9%)	11	1
2	B	150/183 (82%)	135 (90%)	15 (10%)	9	1
2	E	147/183 (80%)	117 (80%)	30 (20%)	1	0
3	G	120/141 (85%)	103 (86%)	17 (14%)	4	0
3	M	118/141 (84%)	104 (88%)	14 (12%)	6	0
All	All	1445/1554 (93%)	1301 (90%)	144 (10%)	11	1

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	28	PHE
1	A	38	LYS
1	A	42	LYS
1	A	73	LEU
1	A	86	LYS
1	A	140	GLN
1	A	173	VAL
1	A	177[A]	ARG
1	A	177[B]	ARG
1	A	178	TYR
1	A	198	LEU
1	A	210[A]	LYS
1	A	210[B]	LYS
1	A	211	LEU
1	A	232	PHE
1	A	245	LEU
1	A	326	LEU
1	A	348	ARG
1	A	364	TYR
1	A	369	ASN
1	A	406	GLU

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Mol	Chain	Res	Type
1	A	461	GLN
1	A	492	ILE
1	A	501	TYR
1	A	543	ASN
2	B	56	GLN
2	B	60	GLN
2	B	73	LEU
2	B	85	LYS
2	B	121	ASN
2	B	150	ASN
2	B	160	LEU
2	B	167	GLN
2	B	178	ARG
2	B	180	SER
2	B	190[A]	GLN
2	B	190[B]	GLN
2	B	195	LYS
2	B	221[A]	ARG
2	B	221[B]	ARG
3	G	51	GLU
3	G	54[A]	LYS
3	G	54[B]	LYS
3	G	58	ASN
3	G	66	LEU
3	G	73	LYS
3	G	74	VAL
3	G	77	GLN
3	G	94	LYS
3	G	124[A]	ASN
3	G	124[B]	ASN
3	G	126	LEU
3	G	134	GLU
3	G	146[A]	ARG
3	G	146[B]	ARG
3	G	150	LYS
3	G	170	LYS
1	L	1	MET
1	L	9	LEU
1	L	13	PRO
1	L	24	ILE
1	L	28	PHE
1	L	72	ASN

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Mol	Chain	Res	Type
1	L	73	LEU
1	L	74	ASN
1	L	100[A]	GLU
1	L	100[B]	GLU
1	L	140	GLN
1	L	148	LYS
1	L	177[A]	ARG
1	L	177[B]	ARG
1	L	178	TYR
1	L	187	LEU
1	L	198	LEU
1	L	218	CYS
1	L	232	PHE
1	L	277	LEU
1	L	326	LEU
1	L	348	ARG
1	L	411	ILE
1	L	414	LYS
1	L	434	GLU
1	L	450	GLU
1	L	452	ASN
1	L	453	ILE
1	L	454	VAL
1	L	455	GLU
1	L	466	LYS
1	L	471	LEU
1	L	487	GLN
1	L	489	MET
1	L	493	GLN
1	L	494	LYS
1	L	501	TYR
1	L	511	ASP
1	L	513	GLN
1	L	543	ASN
1	L	548	LEU
1	L	551	ASN
2	E	50	GLU
2	E	55	ARG
2	E	56	GLN
2	E	59	GLN
2	E	60	GLN
2	E	62	GLU

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Mol	Chain	Res	Type
2	E	80	VAL
2	E	85	LYS
2	E	88	LEU
2	E	89	ARG
2	E	97	GLU
2	E	98	GLU
2	E	101	LYS
2	E	106	ARG
2	E	113	VAL
2	E	121	ASN
2	E	122	ARG
2	E	129	SER
2	E	141	HIS
2	E	143	GLN
2	E	145	LEU
2	E	150	ASN
2	E	167	GLN
2	E	170	LYS
2	E	174	ARG
2	E	177	LYS
2	E	180	SER
2	E	182	GLN
2	E	221	ARG
2	E	222	VAL
3	M	45	LEU
3	M	57	THR
3	M	59	LYS
3	M	66	LEU
3	M	67	GLU
3	M	69	VAL
3	M	70	LEU
3	M	74	VAL
3	M	77	GLN
3	M	88	LEU
3	M	146	ARG
3	M	148	GLN
3	M	150	LYS
3	M	161	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	74	ASN
1	A	140	GLN
1	A	153	GLN
1	A	369	ASN
1	A	388	ASN
1	A	461	GLN
1	A	465	ASN
1	A	467	ASN
1	A	479	GLN
1	A	493	GLN
2	B	59	GLN
2	B	121	ASN
2	B	204	HIS
3	G	58	ASN
3	G	77	GLN
1	L	35	ASN
1	L	45	ASN
1	L	72	ASN
1	L	140	GLN
1	L	267	GLN
1	L	413	ASN
1	L	452	ASN
1	L	465	ASN
1	L	487	GLN
1	L	493	GLN
1	L	534	GLN
1	L	551	ASN
2	E	59	GLN
2	E	60	GLN
2	E	84	HIS
2	E	121	ASN
2	E	143	GLN
2	E	150	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
5	COY	A	601	-	95,118,118	1.00	2 (2%)	116,192,192	1.19	5 (4%)
6	PGO	A	602	4	4,4,4	0.83	0	2,4,4	0.89	0
5	COY	L	601	-	95,118,118	1.01	2 (2%)	116,192,192	1.32	9 (7%)
6	PGO	L	602	4	4,4,4	0.88	0	2,4,4	0.48	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
5	COY	A	601	-	3/3/36/38	0/57/241/241	0/5/13/13
6	PGO	A	602	4	-	0/2/2/2	0/0/0/0
5	COY	L	601	-	2/2/36/38	0/57/241/241	0/5/13/13
6	PGO	L	602	4	-	0/2/2/2	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	COY	C11-C10	-5.20	1.37	1.49
5	L	601	COY	C11-C10	-5.15	1.37	1.49
5	A	601	COY	O58-C57	2.29	1.28	1.23
5	L	601	COY	O58-C57	2.53	1.28	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	601	COY	C53-C15-C14	-6.56	113.50	124.16
5	A	601	COY	C35-C5-C4	-6.38	113.78	124.16
5	A	601	COY	C53-C15-C14	-5.29	115.56	124.16
5	L	601	COY	C35-C5-C4	-4.96	116.10	124.16
5	A	601	COY	O58-C57-C56	-3.14	116.57	121.98
5	L	601	COY	O58-C57-C56	-2.91	116.96	121.98
5	L	601	COY	P-O3-C2P	-2.59	117.53	120.92
5	L	601	COY	C11-N23-C14	-2.44	107.78	112.02
5	L	601	COY	C4B-C9B-C8B	-2.35	118.70	121.10
5	A	601	COY	C10-C11-N23	2.01	122.53	113.76
5	L	601	COY	C47-C12-C13	2.12	119.34	111.75
5	L	601	COY	C60-C61-N62	2.74	122.13	116.08
5	A	601	COY	C47-C12-C13	2.81	121.78	111.75
5	L	601	COY	C56-C57-N59	3.19	122.00	116.46

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	601	COY	C6
5	A	601	COY	C16
5	A	601	COY	C11
5	L	601	COY	C16
5	L	601	COY	C11

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	COY	11	0
5	L	601	COY	12	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	551/554 (99%)	-0.41	3 (0%) 91 93	8, 12, 26, 74	0
1	L	551/554 (99%)	-0.11	17 (3%) 52 58	8, 17, 45, 74	1 (0%)
2	B	178/224 (79%)	-0.20	0 100 100	11, 20, 36, 56	0
2	E	178/224 (79%)	1.40	47 (26%) 1 1	16, 37, 80, 104	0
3	G	137/173 (79%)	-0.21	2 (1%) 76 82	11, 17, 38, 58	0
3	M	137/173 (79%)	0.31	17 (12%) 5 7	14, 21, 63, 108	0
All	All	1732/1902 (91%)	-0.04	86 (4%) 32 38	8, 17, 49, 108	1 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	51	VAL	10.0
2	E	222	VAL	7.3
2	E	58	THR	7.3
2	E	46	GLY	6.9
2	E	47	PHE	6.9
3	M	57	THR	6.5
3	M	58	ASN	6.3
2	E	221	ARG	5.8
3	M	66	LEU	5.7
2	E	59	GLN	5.2
2	E	179	GLU	5.1
2	E	48	LEU	5.1
2	E	49	THR	5.0
2	E	60	GLN	4.7
1	L	454	VAL	4.7
3	G	56	ALA	4.4
2	E	61	ASP	4.4
2	E	95	ILE	4.3
1	L	453	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	L	482	PHE	4.2
3	M	56	ALA	4.2
3	M	74	VAL	4.1
1	L	479	GLN	4.0
2	E	177	LYS	3.9
2	E	54	ALA	3.9
3	M	55	THR	3.9
2	E	122	ARG	3.8
2	E	223	ALA	3.8
2	E	94	GLY	3.8
1	L	434	GLU	3.8
2	E	57	GLY	3.6
3	M	70	LEU	3.6
1	L	458	LYS	3.5
1	L	464	ILE	3.4
2	E	97	GLU	3.4
2	E	178	ARG	3.4
1	L	483	THR	3.4
2	E	50	GLU	3.3
2	E	132	ILE	3.3
3	M	64	PHE	3.2
2	E	52	GLY	3.2
2	E	220	LEU	3.2
1	A	548	LEU	3.2
2	E	181	PRO	3.1
3	M	73	LYS	3.1
1	L	432	THR	3.1
1	A	551	ASN	3.0
2	E	218	GLN	3.0
2	E	213	THR	3.0
2	E	180	SER	2.9
1	L	551	ASN	2.9
2	E	130	ILE	2.8
3	M	77	GLN	2.8
3	M	60	THR	2.7
2	E	174	ARG	2.7
1	L	459	PHE	2.7
2	E	85	LYS	2.7
2	E	125	GLY	2.7
2	E	99	GLY	2.6
2	E	62	GLU	2.6
2	E	55	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
3	M	69	VAL	2.5
2	E	67	VAL	2.5
1	L	455	GLU	2.4
3	M	62	ASP	2.4
2	E	126	SER	2.3
1	L	465	ASN	2.3
3	G	145	SER	2.3
1	L	478	ALA	2.3
2	E	108	PHE	2.3
1	A	550	PRO	2.3
1	L	486	ALA	2.2
2	E	100	ILE	2.2
2	E	175	TYR	2.2
3	M	54	LYS	2.2
2	E	214	GLY	2.2
3	M	71	SER	2.2
3	M	65	THR	2.2
2	E	104	VAL	2.2
2	E	217	PRO	2.1
2	E	56	GLN	2.1
1	L	460	ALA	2.1
2	E	101	LYS	2.1
1	L	481	GLY	2.0
3	M	68	ASN	2.0
2	E	123	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
6	PGO	L	602	5/5	0.96	0.08	1.62	10,11,17,21	0
6	PGO	A	602	5/5	0.97	0.09	1.56	10,10,12,19	0
5	COY	L	601	106/106	0.96	0.09	0.04	10,20,33,53	0
5	COY	A	601	106/106	0.98	0.07	-0.58	5,13,19,29	0
4	K	A	603	1/1	1.00	0.05	-0.90	9,9,9,9	0
4	K	A	604	1/1	1.00	0.07	-1.50	12,12,12,12	0
4	K	L	603	1/1	1.00	0.05	-2.08	12,12,12,12	0
4	K	L	604	1/1	1.00	0.04	-2.82	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.