



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:33 AM UTC

PDB ID : 2CW6 / pdb_00002cw6
Title : Crystal Structure of Human HMG-CoA Lyase: Insights into Catalysis and the Molecular Basis for Hydroxymethylglutaric Aciduria
Authors : Fu, Z.; Runquist, J.A.; Hunt, J.F.; Mizioro, H.M.; Kim, J.-J.P.
Deposited on : 2005-06-17
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

<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

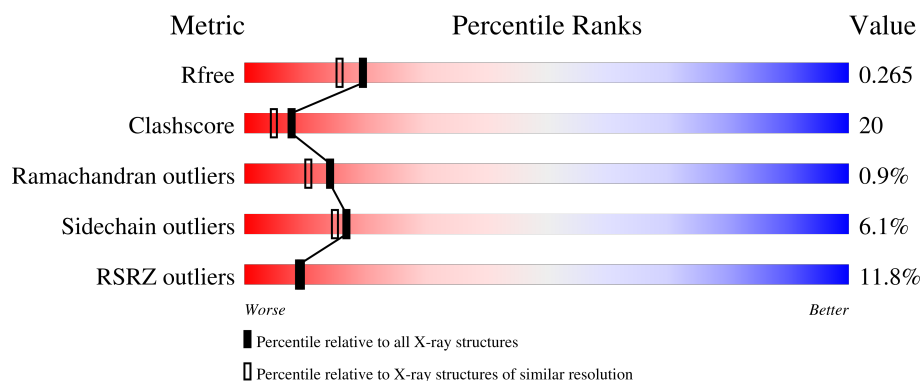
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	298	 4% 70% 25% . .
1	B	298	 10% 68% 26% . .
1	C	298	 5% 62% 33% . .
1	D	298	 15% 55% 35% . 5%
1	E	298	 7% 70% 26% . .

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Mol	Chain	Length	Quality of chain
1	F	298	

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
3	3HG	A	399	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13543 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.

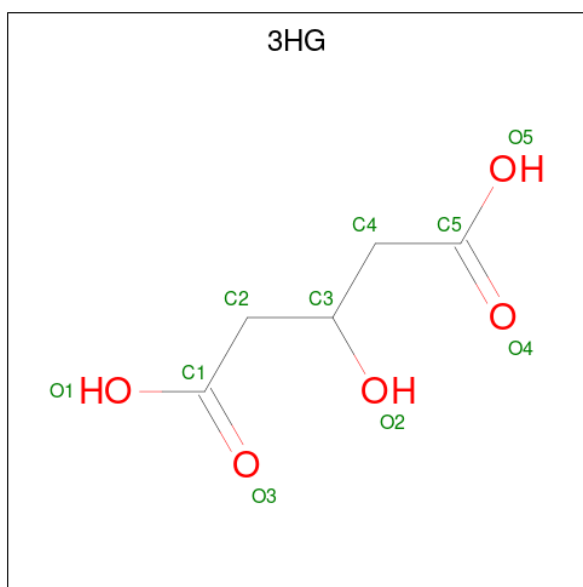
- Molecule 1 is a protein called Hydroxymethylglutaryl-CoA lyase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2189	1390	365	417	17			
1	B	296	Total	C	N	O	S	0	0	0
			2189	1390	365	417	17			
1	C	294	Total	C	N	O	S	0	0	0
			2176	1383	363	414	16			
1	D	282	Total	C	N	O	S	0	0	0
			2089	1330	348	396	15			
1	E	296	Total	C	N	O	S	0	0	0
			2189	1390	365	417	17			
1	F	288	Total	C	N	O	S	0	0	0
			2130	1353	355	406	16			

- 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		
2	E	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 3-HYDROXPENTANEDIOIC ACID (CCD ID: 3HG) (formula: C₅H₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		

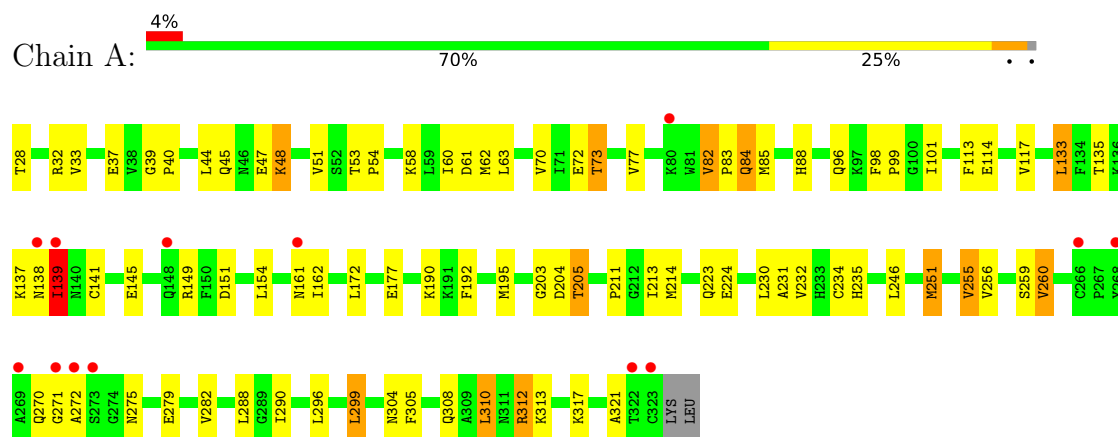
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		
4	B	95	Total	O	0	0
			95	95		
4	C	96	Total	O	0	0
			96	96		
4	D	56	Total	O	0	0
			56	56		
4	E	104	Total	O	0	0
			104	104		
4	F	53	Total	O	0	0
			53	53		

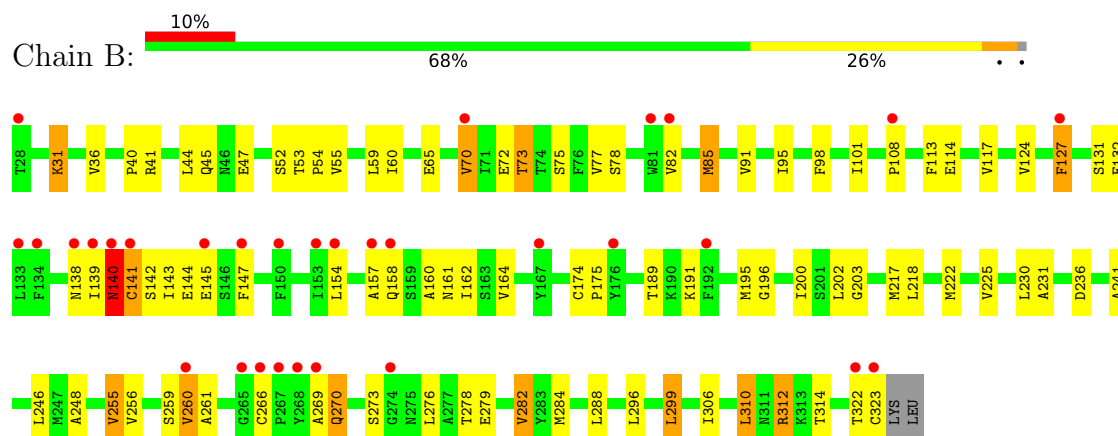
3 Residue-property plots

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.

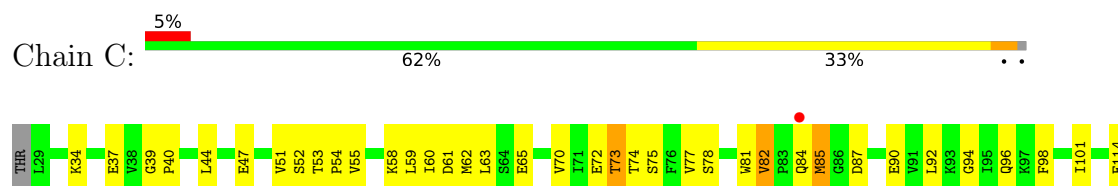
- Molecule 1: Hydroxymethylglutaryl-CoA lyase, mitochondrial

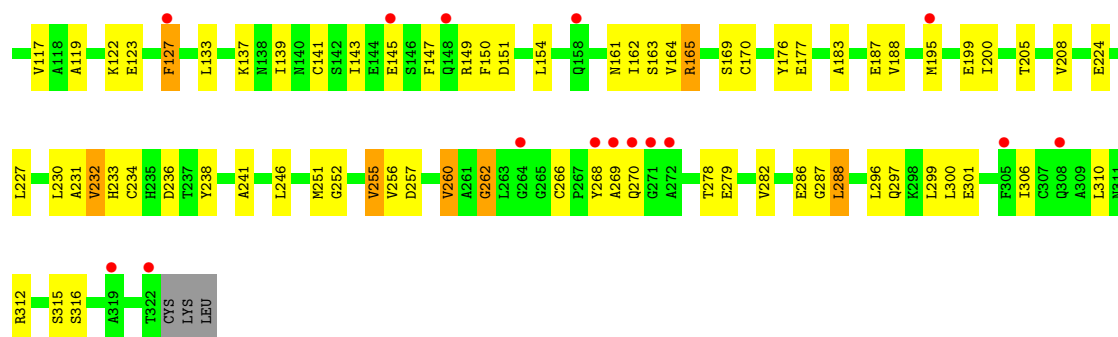


- Molecule 1: Hydroxymethylglutaryl-CoA lyase, mitochondrial

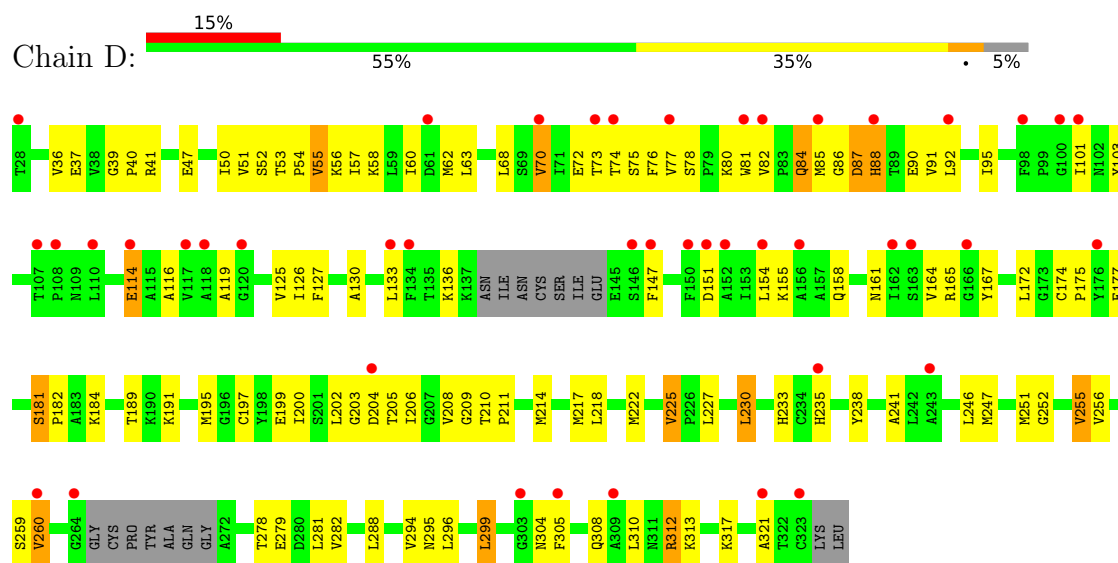


- Molecule 1: Hydroxymethylglutaryl-CoA lyase, mitochondrial

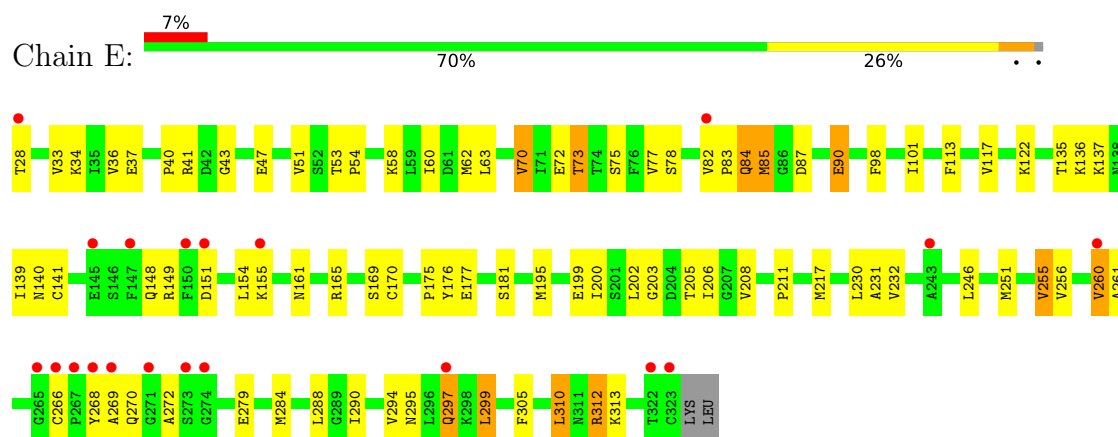




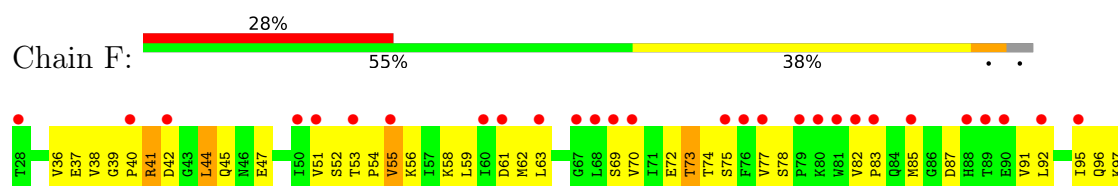
• Molecule 1: Hydroxymethylglutaryl-CoA lyase, mitochondrial

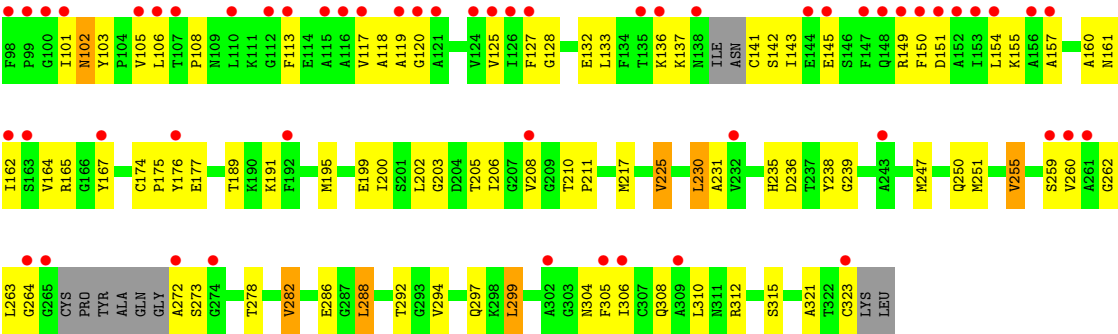


• Molecule 1: Hydroxymethylglutaryl-CoA lyase, mitochondrial



• Molecule 1: Hydroxymethylglutaryl-CoA lyase, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.99Å 117.08Å 86.83Å 90.00° 112.50° 90.00°	Depositor
Resolution (Å)	30.44 – 2.10 30.44 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.44-2.10) 98.3 (30.44-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.265 0.227 , 0.265	Depositor DCC
R_{free} test set	10457 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13543	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: 3HG, MG

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	0.54	0/2224	0.96	5/3011 (0.2%)
1	B	0.44	0/2224	0.93	8/3011 (0.3%)
1	C	0.43	0/2211	0.91	6/2993 (0.2%)
1	D	0.37	0/2120	0.86	4/2866 (0.1%)
1	E	0.44	0/2224	0.90	3/3011 (0.1%)
1	F	0.59	4/2161 (0.2%)	0.91	5/2921 (0.2%)
All	All	0.47	4/13164 (0.0%)	0.91	31/17813 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	272	ALA	C-O	-12.85	0.97	1.23
1	F	272	ALA	C-N	10.53	1.46	1.33
1	F	273	SER	CA-C	10.08	1.65	1.52
1	F	264	GLY	CA-C	5.88	1.59	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	264	GLY	CA-C-O	-10.78	114.79	122.23
1	B	141	CYS	N-CA-C	7.49	121.28	109.81
1	F	272	ALA	O-C-N	7.42	134.86	123.00
1	B	73	THR	N-CA-C	7.00	119.94	111.40
1	F	264	GLY	O-C-N	6.90	130.65	122.64
1	A	73	THR	N-CA-C	6.78	121.88	112.45
1	E	73	THR	N-CA-C	6.48	121.37	112.04
1	D	225	VAL	N-CA-C	6.34	114.80	107.89
1	B	196	GLY	N-CA-C	6.19	120.20	113.58
1	C	73	THR	N-CA-C	6.03	119.02	111.24
1	C	241	ALA	N-CA-C	5.95	118.28	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	94	GLY	N-CA-C	5.75	121.08	113.37
1	A	275	ASN	N-CA-C	5.72	118.08	110.53
1	A	205	THR	N-CA-C	5.61	118.93	111.75
1	B	241	ALA	N-CA-C	5.47	117.69	111.02
1	E	203	GLY	N-CA-C	5.44	120.40	110.71
1	A	204	ASP	N-CA-C	-5.27	99.39	108.56
1	D	209	GLY	N-CA-C	5.26	117.97	111.93
1	C	262	GLY	N-CA-C	-5.17	107.12	115.08
1	C	224	GLU	N-CA-C	5.16	119.85	113.50
1	F	225	VAL	N-CA-C	5.16	113.75	107.61
1	A	203	GLY	N-CA-C	5.14	118.58	110.71
1	B	127	PHE	N-CA-C	5.14	116.78	108.41
1	C	127	PHE	N-CA-C	5.13	117.19	109.23
1	D	241	ALA	N-CA-C	5.12	117.25	111.11
1	B	203	GLY	N-CA-C	5.09	120.05	111.04
1	B	140	ASN	N-CA-C	5.09	121.64	110.80
1	E	294	VAL	N-CA-C	5.07	115.21	108.11
1	D	88	HIS	N-CA-C	5.03	117.49	111.71
1	B	276	LEU	N-CA-C	-5.01	102.96	110.23
1	F	203	GLY	N-CA-C	5.01	119.91	111.04

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	2189	0	2244	78	0
1	B	2189	0	2244	74	0
1	C	2176	0	2232	91	0
1	D	2089	0	2152	99	0
1	E	2189	0	2244	82	0
1	F	2130	0	2188	116	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	10	0	5	4	0
4	A	161	0	0	4	0
4	B	95	0	0	4	0
4	C	96	0	0	0	0
4	D	56	0	0	3	0
4	E	104	0	0	2	0
4	F	53	0	0	0	0
All	All	13543	0	13309	522	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 20.

All (522) 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:288:LEU:HD11	1:F:211:PRO:HG2	1.39	0.99
1:A:48:LYS:H	1:A:48:LYS:HD2	1.28	0.98
1:F:51:VAL:HB	1:F:55:VAL:HG11	1.45	0.96
1:C:288:LEU:HD11	1:D:211:PRO:HG2	1.47	0.95
1:B:142:SER:HB3	1:B:145:GLU:HG3	1.49	0.93
1:C:139:ILE:HB	1:C:149:ARG:HH22	1.33	0.91
1:A:84:GLN:H	1:A:84:GLN:NE2	1.68	0.90
1:D:58:LYS:HG2	1:D:62:MET:HE2	1.52	0.89
1:C:47:GLU:HG2	1:C:310:LEU:HD21	1.53	0.88
1:A:58:LYS:HG2	1:A:62:MET:HE2	1.55	0.88
1:D:75:SER:HB3	1:D:85:MET:HG2	1.58	0.86
1:C:40:PRO:HA	1:C:44:LEU:HD23	1.56	0.86
1:D:125:VAL:HG22	1:D:165:ARG:HB3	1.60	0.84
1:A:211:PRO:HG2	1:B:288:LEU:HD21	1.59	0.84
1:B:75:SER:HB3	1:B:85:MET:HG2	1.57	0.84
1:F:191:LYS:HG3	1:F:195:MET:HE2	1.61	0.83
1:F:292:THR:HG23	1:F:294:VAL:H	1.42	0.83
1:E:297:GLN:H	1:E:297:GLN:CD	1.88	0.81
1:F:47:GLU:HG2	1:F:310:LEU:HD21	1.63	0.79
1:F:247:MET:HE2	1:F:251:MET:HE3	1.65	0.79
1:F:142:SER:HB3	1:F:145:GLU:HG3	1.66	0.78
1:B:98:PHE:HB2	1:B:101:ILE:HD12	1.66	0.78
1:F:51:VAL:CB	1:F:55:VAL:HG11	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ILE:HD13	1:B:73:THR:HG23	1.66	0.77
1:A:84:GLN:H	1:A:84:GLN:HE21	1.30	0.77
1:A:48:LYS:HD2	1:A:48:LYS:N	1.98	0.77
1:B:266:CYS:SG	1:B:269:ALA:HB3	2.24	0.77
1:C:279:GLU:HG3	1:C:299:LEU:HD12	1.66	0.76
1:E:270:GLN:HB2	1:F:321:ALA:HA	1.66	0.76
1:F:77:VAL:HG22	1:F:78:SER:H	1.51	0.76
1:D:50:ILE:HG22	1:D:84:GLN:HG3	1.68	0.74
1:A:138:ASN:O	1:A:139:ILE:HG23	1.87	0.74
1:D:36:VAL:HG22	1:D:70:VAL:HG11	1.68	0.74
1:A:58:LYS:HG2	1:A:62:MET:CE	2.18	0.74
1:E:260:VAL:HG23	1:E:261:ALA:H	1.52	0.74
1:E:260:VAL:O	1:E:279:GLU:OE1	2.06	0.74
1:F:113:PHE:O	1:F:117:VAL:HG23	1.89	0.73
1:E:295:ASN:OD1	1:E:297:GLN:HG2	1.89	0.73
1:E:58:LYS:NZ	1:E:62:MET:HE2	2.03	0.72
1:C:154:LEU:HD23	1:C:164:VAL:HG21	1.71	0.72
1:A:260:VAL:O	1:A:279:GLU:OE1	2.07	0.72
1:F:59:LEU:HD13	1:F:306:ILE:HB	1.72	0.72
1:D:39:GLY:HA3	1:D:260:VAL:HG23	1.71	0.72
1:D:172:LEU:HD11	1:D:214:MET:HE2	1.72	0.71
1:D:91:VAL:O	1:D:95:ILE:HG23	1.90	0.71
1:A:172:LEU:HD22	1:A:213:ILE:HG22	1.71	0.70
1:E:36:VAL:HA	1:E:70:VAL:HG13	1.72	0.70
1:C:52:SER:OG	1:C:55:VAL:HG23	1.90	0.70
1:C:282:VAL:HG21	1:C:296:LEU:HD13	1.73	0.69
1:F:247:MET:CE	1:F:251:MET:HE3	2.22	0.69
1:F:278:THR:O	1:F:282:VAL:HG13	1.92	0.69
1:F:36:VAL:HA	1:F:70:VAL:HG13	1.75	0.69
1:F:77:VAL:HG22	1:F:78:SER:N	2.08	0.68
1:A:154:LEU:HD13	1:A:195:MET:HG2	1.75	0.68
1:B:31:LYS:HB2	1:B:31:LYS:NZ	2.08	0.68
1:D:47:GLU:HG2	1:D:310:LEU:HD21	1.74	0.68
1:E:51:VAL:HG13	1:E:310:LEU:HD13	1.76	0.68
1:A:161:ASN:ND2	1:F:149:ARG:HH12	1.92	0.67
1:B:113:PHE:O	1:B:117:VAL:HG23	1.94	0.67
1:E:297:GLN:H	1:E:297:GLN:NE2	1.91	0.67
1:F:62:MET:HE1	1:F:305:PHE:CG	2.29	0.67
1:A:161:ASN:CG	1:F:149:ARG:HH12	2.02	0.67
1:B:139:ILE:O	1:B:140:ASN:HB2	1.94	0.67
1:D:62:MET:HE1	1:D:305:PHE:CG	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:ASP:O	1:E:155:LYS:HD3	1.95	0.67
1:F:262:GLY:HA3	1:F:315:SER:HB2	1.77	0.67
1:C:96:GLN:HB2	1:C:98:PHE:HE1	1.59	0.66
1:D:36:VAL:HA	1:D:70:VAL:HG13	1.76	0.66
1:D:172:LEU:HD12	1:D:204:ASP:HB2	1.76	0.66
1:C:123:GLU:HG3	1:C:163:SER:OG	1.95	0.66
1:C:282:VAL:CG2	1:C:296:LEU:HD13	2.25	0.66
1:F:55:VAL:HG12	1:F:56:LYS:N	2.09	0.66
1:C:96:GLN:HB2	1:C:98:PHE:CE1	2.31	0.66
1:A:270:GLN:O	1:A:272:ALA:N	2.27	0.66
1:F:87:ASP:O	1:F:91:VAL:HG23	1.95	0.66
1:C:133:LEU:O	1:C:137:LYS:HB2	1.94	0.66
1:D:62:MET:HE1	1:D:305:PHE:CD2	2.30	0.65
1:A:60:ILE:HD13	1:A:73:THR:HG23	1.78	0.65
1:C:251:MET:HE2	1:C:251:MET:HA	1.78	0.65
1:C:279:GLU:HG2	1:C:300:LEU:HD23	1.79	0.65
1:E:251:MET:HE2	1:E:251:MET:HA	1.79	0.65
1:D:76:PHE:CE2	1:D:116:ALA:HA	2.30	0.65
1:B:45:GLN:HG3	1:B:82:VAL:HG21	1.76	0.65
1:A:282:VAL:CG2	1:A:296:LEU:HD13	2.26	0.65
1:E:58:LYS:HZ2	1:E:62:MET:HE2	1.61	0.65
1:E:284:MET:O	1:E:288:LEU:HD13	1.97	0.65
1:D:60:ILE:HD13	1:D:73:THR:HG23	1.79	0.64
1:E:62:MET:HE1	1:E:305:PHE:CG	2.32	0.64
1:E:154:LEU:CD1	1:E:195:MET:HB3	2.28	0.64
1:D:74:THR:OG1	1:D:85:MET:HE2	1.97	0.64
1:C:154:LEU:HD13	1:C:195:MET:HB3	1.78	0.64
1:D:154:LEU:HD13	1:D:195:MET:O	1.98	0.64
1:D:154:LEU:HD23	1:D:164:VAL:HG21	1.78	0.64
1:A:62:MET:HE1	1:A:305:PHE:CG	2.33	0.64
1:B:36:VAL:HA	1:B:70:VAL:HG13	1.79	0.64
1:C:278:THR:O	1:C:282:VAL:HG13	1.97	0.64
1:B:322:THR:O	1:B:323:CYS:HB2	1.96	0.63
1:C:260:VAL:O	1:C:279:GLU:OE1	2.16	0.63
1:E:40:PRO:HG2	1:E:72:GLU:O	1.99	0.63
1:F:154:LEU:HD23	1:F:164:VAL:HG21	1.80	0.63
1:B:278:THR:HG22	1:B:299:LEU:HD11	1.80	0.63
1:A:139:ILE:HG13	1:A:141:CYS:SG	2.39	0.63
1:A:40:PRO:HG2	1:A:72:GLU:O	1.99	0.63
1:A:137:LYS:HE2	4:A:536:HOH:O	1.98	0.63
1:B:231:ALA:CB	1:B:255:VAL:HG22	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:MET:HA	1:D:251:MET:HE2	1.81	0.62
1:E:60:ILE:HD13	1:E:73:THR:HG23	1.81	0.62
1:A:45:GLN:HE22	3:A:399:3HG:H42	1.64	0.62
1:D:40:PRO:HG2	1:D:72:GLU:O	1.98	0.62
1:E:84:GLN:H	1:E:84:GLN:NE2	1.96	0.62
1:C:297:GLN:O	1:C:301:GLU:HG3	1.99	0.62
1:B:144:GLU:HB2	4:B:770:HOH:O	1.99	0.62
1:C:75:SER:HB3	1:C:85:MET:HG2	1.80	0.62
1:E:83:PRO:HG2	1:E:84:GLN:HE21	1.64	0.62
1:F:36:VAL:HG22	1:F:70:VAL:HG11	1.82	0.62
1:E:231:ALA:CB	1:E:255:VAL:HG22	2.29	0.62
1:C:139:ILE:HD12	1:C:149:ARG:NH2	2.15	0.62
1:A:62:MET:HE1	1:A:305:PHE:CD2	2.35	0.62
1:B:31:LYS:HD3	4:B:1030:HOH:O	2.00	0.62
1:F:74:THR:H	1:F:105:VAL:HG12	1.65	0.61
1:B:113:PHE:CZ	1:B:162:ILE:HD12	2.35	0.61
1:D:84:GLN:H	1:D:84:GLN:NE2	1.98	0.61
1:E:33:VAL:HG23	1:E:290:ILE:HG21	1.82	0.61
1:E:98:PHE:HB2	1:E:101:ILE:HD12	1.82	0.61
1:F:55:VAL:CG1	1:F:56:LYS:N	2.64	0.61
1:B:202:LEU:HD13	1:B:217:MET:SD	2.41	0.61
1:C:231:ALA:CB	1:C:255:VAL:HG22	2.30	0.61
1:D:230:LEU:O	1:D:255:VAL:HG13	2.01	0.61
1:D:53:THR:N	1:D:54:PRO:HD2	2.16	0.61
1:D:167:TYR:HE1	1:D:233:HIS:HD1	1.49	0.61
1:B:36:VAL:HG22	1:B:70:VAL:HG11	1.83	0.60
1:A:172:LEU:HD11	1:A:214:MET:HE2	1.83	0.60
1:B:47:GLU:HG2	1:B:310:LEU:HD21	1.83	0.60
1:E:75:SER:HB3	1:E:85:MET:HG2	1.81	0.60
1:E:139:ILE:HG21	1:E:149:ARG:HH12	1.65	0.60
1:D:130:ALA:O	1:D:184:LYS:HD2	2.02	0.60
1:F:202:LEU:HD13	1:F:217:MET:SD	2.41	0.60
1:D:87:ASP:O	1:D:91:VAL:HG23	2.01	0.59
1:D:278:THR:HG22	1:D:299:LEU:HD11	1.83	0.59
1:C:151:ASP:OD1	1:C:195:MET:HE3	2.02	0.59
1:C:266:CYS:HB3	1:C:269:ALA:HB3	1.85	0.59
1:E:266:CYS:HB3	1:E:269:ALA:HB3	1.85	0.59
1:B:53:THR:N	1:B:54:PRO:HD2	2.18	0.59
1:B:278:THR:O	1:B:282:VAL:HG13	2.03	0.59
1:D:304:ASN:O	1:D:308:GLN:HG3	2.03	0.59
1:D:52:SER:HB2	1:D:54:PRO:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:VAL:HG22	1:E:70:VAL:HG11	1.86	0.58
1:F:47:GLU:CG	1:F:310:LEU:HD21	2.32	0.58
1:D:85:MET:HA	1:D:85:MET:HE3	1.85	0.58
1:D:165:ARG:NH2	1:D:199:GLU:OE2	2.37	0.58
1:D:202:LEU:HD13	1:D:217:MET:SD	2.43	0.58
1:F:102:ASN:N	1:F:102:ASN:HD22	2.01	0.58
1:F:53:THR:N	1:F:54:PRO:HD2	2.19	0.58
1:F:133:LEU:HD13	1:F:136:LYS:HE2	1.86	0.58
1:A:51:VAL:HG13	1:A:310:LEU:HD13	1.86	0.58
1:C:154:LEU:HD12	1:C:195:MET:HE2	1.85	0.58
1:C:279:GLU:OE1	1:C:279:GLU:N	2.36	0.58
1:C:98:PHE:HB2	1:C:101:ILE:HD12	1.86	0.58
1:E:63:LEU:HD21	1:E:260:VAL:CG1	2.33	0.58
1:E:60:ILE:CD1	1:E:73:THR:HG23	2.33	0.58
1:E:154:LEU:HD13	1:E:195:MET:HB3	1.86	0.58
1:F:75:SER:HB3	1:F:85:MET:HG2	1.84	0.57
1:F:157:ALA:HB1	1:F:162:ILE:O	2.04	0.57
1:A:135:THR:O	1:A:139:ILE:HG12	2.05	0.57
1:F:40:PRO:HA	1:F:44:LEU:HD23	1.87	0.57
1:A:47:GLU:HG3	4:A:641:HOH:O	2.05	0.57
1:B:52:SER:OG	1:B:55:VAL:HG23	2.05	0.57
1:A:279:GLU:HG3	1:A:299:LEU:HD13	1.87	0.57
1:C:77:VAL:HG11	1:C:82:VAL:HG11	1.86	0.57
1:C:279:GLU:HG2	1:C:300:LEU:CD2	2.35	0.57
1:B:260:VAL:O	1:B:279:GLU:OE1	2.24	0.56
1:E:155:LYS:N	1:E:155:LYS:HD2	2.20	0.56
1:A:231:ALA:CB	1:A:255:VAL:HG22	2.35	0.56
1:C:154:LEU:CD1	1:C:195:MET:HB3	2.35	0.56
1:F:199:GLU:C	1:F:200:ILE:HD12	2.30	0.56
1:B:282:VAL:CG2	1:B:296:LEU:HD13	2.35	0.56
1:C:150:PHE:HB2	1:C:195:MET:HE1	1.86	0.56
1:D:37:GLU:HG2	1:D:63:LEU:HD13	1.86	0.56
1:B:138:ASN:C	1:B:138:ASN:HD22	2.13	0.56
1:A:84:GLN:HE21	1:A:84:GLN:N	2.01	0.56
1:C:92:LEU:HD23	1:C:119:ALA:HB3	1.87	0.56
1:D:206:ILE:HG13	1:D:208:VAL:HG22	1.88	0.56
1:D:174:CYS:SG	1:D:175:PRO:HD2	2.46	0.56
1:E:58:LYS:HG2	1:E:62:MET:HE2	1.87	0.56
1:B:222:MET:HE1	4:B:685:HOH:O	2.05	0.56
1:D:151:ASP:O	1:D:155:LYS:HD3	2.06	0.56
1:E:137:LYS:HG2	1:E:176:TYR:OH	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ALA:HB2	1:C:255:VAL:HG22	1.88	0.55
1:A:139:ILE:HB	1:A:149:ARG:HH22	1.72	0.55
1:D:51:VAL:HB	1:D:55:VAL:HG11	1.88	0.55
1:C:47:GLU:HG2	1:C:310:LEU:CD2	2.33	0.55
1:C:60:ILE:CD1	1:C:73:THR:HG23	2.37	0.55
1:F:101:ILE:C	1:F:102:ASN:HD22	2.15	0.55
1:D:282:VAL:HG21	1:D:296:LEU:HD13	1.89	0.55
1:B:138:ASN:C	1:B:138:ASN:ND2	2.65	0.55
1:C:176:TYR:OH	1:C:268:TYR:HE2	1.89	0.54
1:E:165:ARG:HD2	1:E:199:GLU:OE2	2.07	0.54
1:E:231:ALA:HB2	1:E:255:VAL:HG22	1.88	0.54
1:A:58:LYS:HZ3	1:A:62:MET:HE2	1.72	0.54
1:A:83:PRO:HG2	1:A:84:GLN:HE21	1.71	0.54
1:A:190:LYS:HD3	1:A:224:GLU:HB3	1.88	0.54
1:B:59:LEU:HD13	1:B:306:ILE:HB	1.89	0.54
1:C:39:GLY:HA3	1:C:260:VAL:HG23	1.88	0.54
1:E:288:LEU:HD11	1:F:211:PRO:CG	2.26	0.54
1:D:82:VAL:O	1:D:82:VAL:HG13	2.08	0.54
1:D:260:VAL:O	1:D:279:GLU:OE1	2.25	0.54
1:E:51:VAL:CG1	1:E:310:LEU:HD13	2.37	0.54
1:F:231:ALA:CB	1:F:255:VAL:HG22	2.38	0.54
1:C:183:ALA:O	1:C:187:GLU:HG3	2.08	0.54
1:F:251:MET:HA	1:F:251:MET:HE2	1.88	0.54
1:C:40:PRO:HG2	1:C:72:GLU:O	2.08	0.54
1:B:160:ALA:O	1:B:161:ASN:HB3	2.08	0.54
1:B:147:PHE:CE1	1:B:191:LYS:HG2	2.42	0.53
1:C:266:CYS:SG	1:C:269:ALA:CB	2.96	0.53
1:D:256:VAL:CG2	1:D:281:LEU:HD21	2.38	0.53
1:F:278:THR:HG22	1:F:299:LEU:HD11	1.90	0.53
1:B:174:CYS:SG	1:B:175:PRO:HD2	2.47	0.53
1:D:50:ILE:CG2	1:D:84:GLN:HG3	2.37	0.53
1:B:117:VAL:HG22	1:B:162:ILE:CD1	2.38	0.53
1:A:98:PHE:HB2	1:A:101:ILE:HD12	1.89	0.53
1:C:147:PHE:HD2	1:C:195:MET:SD	2.31	0.53
1:E:279:GLU:HG3	1:E:299:LEU:HD13	1.91	0.53
1:F:37:GLU:HG2	1:F:63:LEU:HD13	1.90	0.53
1:B:124:VAL:CG2	1:B:164:VAL:HG22	2.39	0.53
1:C:200:ILE:N	1:C:200:ILE:HD12	2.24	0.53
1:C:60:ILE:HD13	1:C:73:THR:HG23	1.90	0.53
1:F:41:ARG:HB2	1:F:72:GLU:O	2.09	0.53
1:F:73:THR:OG1	1:F:103:TYR:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:GLY:N	1:D:40:PRO:HD2	2.24	0.53
1:D:92:LEU:HD23	1:D:119:ALA:HB3	1.90	0.53
1:D:126:ILE:HD11	1:D:197:CYS:SG	2.49	0.53
1:A:251:MET:HA	1:A:251:MET:HE2	1.90	0.52
1:D:78:SER:HG	1:D:81:TRP:CD1	2.26	0.52
1:F:52:SER:C	1:F:54:PRO:HD2	2.33	0.52
1:B:77:VAL:HG23	4:B:944:HOH:O	2.09	0.52
1:C:87:ASP:O	1:C:90:GLU:HG2	2.09	0.52
1:F:62:MET:HE1	1:F:305:PHE:CD2	2.44	0.52
1:A:304:ASN:O	1:A:308:GLN:HG3	2.08	0.52
1:C:266:CYS:SG	1:C:269:ALA:HB3	2.49	0.52
1:E:135:THR:HG23	1:E:139:ILE:HD11	1.91	0.52
1:F:77:VAL:HG23	1:F:108:PRO:HG3	1.91	0.52
1:B:154:LEU:HD13	1:B:195:MET:HG2	1.91	0.52
1:B:231:ALA:HB2	1:B:255:VAL:HG22	1.90	0.52
1:F:58:LYS:O	1:F:61:ASP:HB2	2.10	0.52
1:A:82:VAL:HG22	1:A:82:VAL:O	2.08	0.52
1:F:154:LEU:CD1	1:F:195:MET:HB3	2.39	0.52
1:F:191:LYS:CG	1:F:195:MET:HE2	2.36	0.52
1:A:58:LYS:NZ	1:A:62:MET:HE2	2.25	0.52
1:B:31:LYS:HB2	1:B:31:LYS:HZ3	1.74	0.51
1:E:62:MET:HE1	1:E:305:PHE:CD2	2.45	0.51
1:F:133:LEU:O	1:F:137:LYS:HB2	2.11	0.51
1:C:139:ILE:HB	1:C:149:ARG:NH2	2.15	0.51
1:E:90:GLU:CD	1:E:90:GLU:H	2.16	0.51
1:F:51:VAL:HB	1:F:55:VAL:CG1	2.29	0.51
1:E:58:LYS:HG2	1:E:62:MET:CE	2.41	0.51
1:E:63:LEU:HD21	1:E:260:VAL:HG11	1.93	0.51
1:E:148:GLN:HA	1:E:151:ASP:OD2	2.10	0.51
1:D:133:LEU:HD23	1:D:177:GLU:HG2	1.92	0.51
1:E:175:PRO:HG2	1:E:176:TYR:CD1	2.46	0.51
1:B:310:LEU:HB3	1:B:312:ARG:HG2	1.93	0.50
1:A:161:ASN:ND2	1:F:149:ARG:NH1	2.57	0.50
1:D:41:ARG:HD2	1:D:41:ARG:C	2.36	0.50
1:D:256:VAL:HG21	1:D:281:LEU:HD21	1.92	0.50
1:F:38:VAL:O	1:F:42:ASP:HB3	2.12	0.50
1:D:312:ARG:O	1:D:312:ARG:HD3	2.11	0.50
1:E:41:ARG:C	1:E:41:ARG:HD2	2.37	0.50
1:B:279:GLU:HG3	1:B:299:LEU:HD13	1.94	0.50
1:C:287:GLY:HA3	1:D:210:THR:HG21	1.94	0.50
1:D:147:PHE:CE1	1:D:191:LYS:HG2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:VAL:CG2	1:F:78:SER:H	2.24	0.50
1:B:142:SER:HB3	1:B:145:GLU:CG	2.33	0.50
1:B:200:ILE:N	1:B:200:ILE:HD12	2.27	0.50
1:A:317:LYS:NZ	1:B:236:ASP:OD2	2.45	0.50
1:B:189:THR:HG22	1:B:225:VAL:HG21	1.93	0.49
1:F:82:VAL:HG13	1:F:82:VAL:O	2.12	0.49
1:F:154:LEU:HD13	1:F:195:MET:HB3	1.95	0.49
1:C:37:GLU:HG2	1:C:63:LEU:HD13	1.95	0.49
1:C:169:SER:HB2	1:C:205:THR:OG1	2.12	0.49
1:D:36:VAL:HG22	1:D:70:VAL:CG1	2.41	0.49
1:E:58:LYS:HD3	1:E:305:PHE:CZ	2.47	0.49
1:E:113:PHE:O	1:E:117:VAL:HG23	2.12	0.49
1:C:117:VAL:HG22	1:C:162:ILE:CD1	2.43	0.49
1:E:266:CYS:HB3	1:E:269:ALA:CB	2.42	0.49
1:D:172:LEU:HD11	1:D:214:MET:CE	2.41	0.49
1:F:39:GLY:N	1:F:40:PRO:HD2	2.28	0.49
1:B:139:ILE:O	1:B:140:ASN:CB	2.60	0.49
1:C:133:LEU:HD12	1:C:177:GLU:HG2	1.94	0.49
1:E:51:VAL:HG13	1:E:310:LEU:CD1	2.41	0.49
1:F:92:LEU:HD23	1:F:119:ALA:HB3	1.94	0.49
1:B:40:PRO:HG2	1:B:72:GLU:O	2.13	0.49
1:B:284:MET:O	1:B:288:LEU:HD23	2.13	0.48
1:F:102:ASN:N	1:F:102:ASN:ND2	2.61	0.48
1:D:86:GLY:C	1:D:88:HIS:H	2.21	0.48
1:A:85:MET:O	1:A:88:HIS:HD2	1.96	0.48
1:E:202:LEU:HD13	1:E:217:MET:SD	2.53	0.48
1:E:139:ILE:HG13	1:E:141:CYS:SG	2.53	0.48
1:E:297:GLN:NE2	1:E:297:GLN:N	2.58	0.48
1:F:69:SER:HA	1:F:101:ILE:HD12	1.96	0.48
1:C:262:GLY:HA3	1:C:315:SER:HB2	1.96	0.48
1:D:282:VAL:CG2	1:D:296:LEU:HD13	2.44	0.48
1:E:84:GLN:O	1:E:85:MET:HE3	2.14	0.48
1:E:154:LEU:HD12	1:E:195:MET:HE2	1.96	0.48
1:A:58:LYS:HD3	1:A:305:PHE:CZ	2.49	0.48
1:B:161:ASN:CG	1:B:161:ASN:O	2.56	0.48
1:C:282:VAL:O	1:C:286:GLU:HG3	2.13	0.48
1:E:78:SER:HB2	4:E:852:HOH:O	2.14	0.48
1:E:154:LEU:HD13	1:E:195:MET:O	2.14	0.48
1:E:260:VAL:HG23	1:E:261:ALA:N	2.26	0.48
1:C:279:GLU:HB2	1:C:316:SER:OG	2.14	0.48
1:F:200:ILE:HD12	1:F:200:ILE:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LYS:O	1:B:195:MET:HB2	2.14	0.47
1:C:61:ASP:O	1:C:65:GLU:HG3	2.13	0.47
1:E:53:THR:N	1:E:54:PRO:HD2	2.29	0.47
1:B:282:VAL:HG22	1:B:296:LEU:HD13	1.96	0.47
1:C:143:ILE:O	1:C:147:PHE:HD1	1.98	0.47
1:D:218:LEU:O	1:D:222:MET:HG3	2.15	0.47
1:A:51:VAL:CG1	1:A:310:LEU:HD13	2.43	0.47
1:A:270:GLN:OE1	1:B:323:CYS:HA	2.15	0.47
1:B:41:ARG:HD2	1:B:41:ARG:C	2.39	0.47
1:D:77:VAL:HG22	1:D:78:SER:N	2.28	0.47
1:D:92:LEU:HD23	1:D:119:ALA:CB	2.45	0.47
1:F:74:THR:OG1	1:F:75:SER:N	2.48	0.47
1:A:117:VAL:HG22	1:A:162:ILE:HD12	1.96	0.47
1:F:136:LYS:HG3	1:F:137:LYS:N	2.29	0.47
1:F:259:SER:OG	1:F:263:LEU:HB2	2.14	0.47
1:A:133:LEU:HB2	1:A:177:GLU:HG3	1.96	0.47
1:D:114:GLU:OE1	1:D:114:GLU:HA	2.15	0.47
1:F:175:PRO:HG2	1:F:176:TYR:CD1	2.50	0.47
1:C:176:TYR:HH	1:C:268:TYR:HE2	1.55	0.47
1:F:133:LEU:HD23	1:F:177:GLU:CG	2.45	0.47
1:F:230:LEU:O	1:F:255:VAL:HG13	2.14	0.47
1:C:208:VAL:HG12	1:C:238:TYR:CE2	2.49	0.47
1:F:236:ASP:OD1	1:F:239:GLY:HA2	2.14	0.47
1:D:167:TYR:HE1	1:D:233:HIS:ND1	2.11	0.47
1:F:297:GLN:HA	1:F:297:GLN:NE2	2.29	0.47
1:D:189:THR:HG22	1:D:225:VAL:HG21	1.97	0.47
1:F:92:LEU:HD23	1:F:119:ALA:CB	2.45	0.46
1:F:133:LEU:N	1:F:133:LEU:HD22	2.30	0.46
1:B:113:PHE:CZ	1:B:157:ALA:HA	2.50	0.46
1:C:51:VAL:HG13	1:C:310:LEU:HD13	1.97	0.46
1:C:270:GLN:CG	1:D:321:ALA:O	2.63	0.46
1:F:247:MET:HE3	1:F:250:GLN:HB2	1.96	0.46
1:A:53:THR:N	1:A:54:PRO:HD2	2.30	0.46
1:D:227:LEU:HD21	1:D:252:GLY:HA3	1.98	0.46
1:D:279:GLU:O	1:D:282:VAL:HG22	2.15	0.46
1:F:51:VAL:CG2	1:F:55:VAL:HG11	2.45	0.46
1:F:58:LYS:HD3	1:F:305:PHE:CZ	2.50	0.46
1:F:125:VAL:HG22	1:F:165:ARG:HB3	1.96	0.46
1:C:82:VAL:HG22	1:C:82:VAL:O	2.16	0.46
1:D:51:VAL:O	1:D:56:LYS:NZ	2.48	0.46
1:D:191:LYS:O	1:D:195:MET:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:CYS:HB3	4:A:503:HOH:O	2.16	0.46
1:D:73:THR:OG1	1:D:103:TYR:HB3	2.15	0.46
1:E:270:GLN:C	1:E:272:ALA:H	2.24	0.46
1:A:83:PRO:CD	1:A:84:GLN:NE2	2.79	0.46
1:E:211:PRO:HG2	1:F:288:LEU:HD21	1.97	0.46
1:C:53:THR:N	1:C:54:PRO:HD2	2.30	0.46
1:C:77:VAL:HG11	1:C:82:VAL:CG1	2.45	0.46
1:C:127:PHE:O	1:C:150:PHE:HZ	1.99	0.46
1:E:77:VAL:HG11	1:E:82:VAL:HG11	1.97	0.46
1:F:55:VAL:HG12	1:F:56:LYS:H	1.80	0.46
1:B:261:ALA:HB1	1:B:314:THR:OG1	2.16	0.46
1:D:278:THR:CG2	1:D:299:LEU:HD11	2.45	0.46
1:E:37:GLU:OE2	1:E:260:VAL:HG13	2.16	0.46
1:F:77:VAL:CG2	1:F:78:SER:N	2.77	0.46
1:D:133:LEU:HD23	1:D:177:GLU:CG	2.47	0.45
1:F:160:ALA:O	1:F:161:ASN:HB3	2.16	0.45
1:A:83:PRO:HD2	1:A:84:GLN:HE22	1.82	0.45
1:D:90:GLU:OE1	1:D:90:GLU:N	2.44	0.45
1:D:80:LYS:HE2	4:D:1049:HOH:O	2.16	0.45
1:D:127:PHE:CD1	1:D:127:PHE:N	2.85	0.45
1:F:52:SER:HB2	1:F:54:PRO:HD2	1.97	0.45
1:F:127:PHE:O	1:F:150:PHE:CZ	2.70	0.45
1:F:205:THR:O	1:F:235:HIS:ND1	2.49	0.45
1:C:149:ARG:NH1	1:E:161:ASN:HD21	2.14	0.45
1:D:154:LEU:O	1:D:158:GLN:HG3	2.17	0.45
1:D:259:SER:O	1:D:260:VAL:C	2.58	0.45
1:E:37:GLU:HG2	1:E:63:LEU:HD13	1.98	0.45
1:B:82:VAL:O	1:B:82:VAL:HG13	2.16	0.45
1:B:127:PHE:CD1	1:B:127:PHE:N	2.84	0.45
1:D:58:LYS:HG2	1:D:62:MET:CE	2.34	0.45
1:F:45:GLN:HG3	1:F:82:VAL:HG21	1.98	0.45
1:F:210:THR:HB	1:F:211:PRO:HD2	1.99	0.45
1:A:135:THR:HG22	1:A:141:CYS:O	2.17	0.45
1:D:208:VAL:HG12	1:D:238:TYR:CE2	2.52	0.45
1:F:189:THR:HG22	1:F:225:VAL:HG21	1.97	0.45
1:D:205:THR:O	1:D:235:HIS:ND1	2.43	0.45
1:D:247:MET:CE	1:D:251:MET:HE3	2.46	0.45
1:E:136:LYS:O	1:E:140:ASN:HA	2.16	0.45
1:F:206:ILE:HG13	1:F:208:VAL:HG22	1.98	0.45
1:A:45:GLN:NE2	3:A:399:3HG:H42	2.28	0.45
1:A:282:VAL:HG21	1:A:296:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLY:HA2	1:A:259:SER:OG	2.17	0.44
1:C:147:PHE:HZ	1:C:188:VAL:HG13	1.81	0.44
1:C:236:ASP:OD2	1:D:317:LYS:NZ	2.51	0.44
1:D:313:LYS:HE3	4:D:908:HOH:O	2.17	0.44
1:E:200:ILE:N	1:E:200:ILE:HD12	2.31	0.44
1:A:60:ILE:CD1	1:A:73:THR:HG23	2.47	0.44
1:C:52:SER:O	1:C:55:VAL:HB	2.17	0.44
1:C:141:CYS:HB2	1:C:145:GLU:OE1	2.16	0.44
1:F:128:GLY:N	1:F:167:TYR:O	2.49	0.44
1:F:208:VAL:HG12	1:F:238:TYR:CE2	2.52	0.44
1:A:223:GLN:NE2	4:A:759:HOH:O	2.50	0.44
1:D:203:GLY:HA2	1:D:233:HIS:O	2.17	0.44
1:E:206:ILE:HG13	1:E:208:VAL:HG22	1.99	0.44
1:F:91:VAL:O	1:F:95:ILE:HG23	2.17	0.44
1:C:270:GLN:HG3	1:D:321:ALA:O	2.17	0.44
1:D:210:THR:HB	1:D:211:PRO:HD2	1.98	0.44
1:F:133:LEU:H	1:F:133:LEU:CD2	2.29	0.44
1:D:37:GLU:OE2	1:D:260:VAL:N	2.46	0.44
1:B:53:THR:N	1:B:54:PRO:CD	2.80	0.44
1:A:62:MET:CE	1:A:305:PHE:CD2	3.00	0.44
1:A:138:ASN:O	1:A:139:ILE:HD13	2.18	0.44
1:F:165:ARG:NH2	1:F:199:GLU:OE2	2.51	0.44
1:A:141:CYS:HB2	1:A:145:GLU:HB2	1.99	0.44
1:A:231:ALA:HB1	1:A:255:VAL:HG22	1.99	0.44
1:E:28:THR:HG23	1:E:28:THR:O	2.17	0.44
1:B:77:VAL:HG22	1:B:78:SER:N	2.33	0.43
1:D:53:THR:O	1:D:57:ILE:HG13	2.18	0.43
1:B:131:SER:C	1:B:143:ILE:HD11	2.43	0.43
1:D:51:VAL:HG23	1:D:56:LYS:HG3	2.01	0.43
1:E:84:GLN:H	1:E:84:GLN:HE21	1.64	0.43
1:F:53:THR:N	1:F:54:PRO:CD	2.81	0.43
1:F:77:VAL:HG11	1:F:82:VAL:CG1	2.48	0.43
1:A:45:GLN:NE2	3:A:399:3HG:H21	2.33	0.43
1:F:96:GLN:O	1:F:97:LYS:HD3	2.18	0.43
1:F:282:VAL:O	1:F:286:GLU:HB2	2.19	0.43
1:D:182:PRO:HD2	4:D:671:HOH:O	2.18	0.43
1:E:169:SER:HB2	1:E:205:THR:OG1	2.18	0.43
1:A:33:VAL:HG23	1:A:290:ILE:HG21	2.00	0.43
1:A:195:MET:HE3	1:A:195:MET:HB2	1.95	0.43
1:A:98:PHE:HA	1:A:99:PRO:HD3	1.90	0.43
1:C:74:THR:HA	1:C:85:MET:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:CYS:CB	1:C:269:ALA:HB3	2.48	0.43
1:B:144:GLU:HA	1:B:144:GLU:OE1	2.19	0.43
1:F:41:ARG:HD2	1:F:41:ARG:C	2.44	0.43
1:F:62:MET:HE1	1:F:305:PHE:CB	2.48	0.43
1:F:106:LEU:HD12	1:F:106:LEU:N	2.33	0.43
1:F:41:ARG:CZ	1:F:106:LEU:HD21	2.49	0.43
1:C:232:VAL:CG2	1:C:234:CYS:SG	3.07	0.42
1:D:60:ILE:CD1	1:D:73:THR:HG23	2.48	0.42
1:D:247:MET:HE3	1:D:247:MET:O	2.18	0.42
1:A:77:VAL:CG1	1:A:82:VAL:HG13	2.49	0.42
1:C:58:LYS:HD3	1:C:62:MET:CE	2.49	0.42
1:D:53:THR:N	1:D:54:PRO:CD	2.82	0.42
1:E:176:TYR:OH	1:E:268:TYR:HE2	2.02	0.42
1:F:161:ASN:O	1:F:161:ASN:ND2	2.53	0.42
1:A:231:ALA:HB2	1:A:255:VAL:HG22	2.01	0.42
1:A:312:ARG:HD3	1:A:313:LYS:O	2.19	0.42
1:E:43:GLY:O	1:E:47:GLU:HG2	2.19	0.42
1:E:312:ARG:HD3	1:E:313:LYS:O	2.19	0.42
1:F:151:ASP:OD1	1:F:155:LYS:HD3	2.19	0.42
1:A:85:MET:O	1:A:88:HIS:CD2	2.71	0.42
1:A:113:PHE:O	1:A:117:VAL:HG23	2.19	0.42
1:B:91:VAL:O	1:B:95:ILE:HG23	2.19	0.42
1:F:304:ASN:O	1:F:308:GLN:HG3	2.20	0.42
1:F:175:PRO:HG2	1:F:176:TYR:CE1	2.55	0.42
1:F:231:ALA:HB1	1:F:255:VAL:HG22	2.01	0.42
1:B:218:LEU:CD1	1:B:248:ALA:HA	2.49	0.42
1:B:147:PHE:CD1	1:B:191:LYS:HG2	2.55	0.42
1:C:77:VAL:HG22	1:C:78:SER:N	2.35	0.42
1:F:118:ALA:C	1:F:120:GLY:N	2.77	0.42
1:F:306:ILE:O	1:F:310:LEU:HB2	2.20	0.42
1:D:181:SER:HA	1:D:182:PRO:HD3	1.95	0.42
1:A:321:ALA:O	1:B:270:GLN:HG2	2.20	0.41
1:E:87:ASP:HA	1:E:90:GLU:OE1	2.20	0.41
1:E:137:LYS:HG2	1:E:176:TYR:CZ	2.55	0.41
1:B:36:VAL:HG22	1:B:70:VAL:CG1	2.50	0.41
1:E:169:SER:O	1:E:170:CYS:HB2	2.20	0.41
1:A:37:GLU:HG2	1:A:63:LEU:HD13	2.02	0.41
1:C:117:VAL:HG22	1:C:162:ILE:HD11	2.02	0.41
1:F:52:SER:CB	1:F:54:PRO:HD2	2.51	0.41
1:F:141:CYS:SG	1:F:145:GLU:HB2	2.60	0.41
1:A:45:GLN:HE22	3:A:399:3HG:H21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:GLU:N	1:B:143:ILE:HD11	2.35	0.41
1:F:132:GLU:OE2	1:F:132:GLU:HA	2.20	0.41
1:A:259:SER:O	1:A:260:VAL:C	2.64	0.41
1:B:47:GLU:HG2	1:B:310:LEU:CD2	2.51	0.41
1:C:199:GLU:C	1:C:200:ILE:HD12	2.45	0.41
1:C:227:LEU:HD21	1:C:252:GLY:HA3	2.03	0.41
1:D:51:VAL:HG13	1:D:310:LEU:HD13	2.02	0.41
1:E:199:GLU:C	1:E:200:ILE:HD12	2.45	0.41
1:F:206:ILE:H	1:F:206:ILE:HG12	1.68	0.41
1:B:218:LEU:HD11	1:B:248:ALA:HA	2.03	0.41
1:B:259:SER:O	1:B:260:VAL:C	2.63	0.41
1:C:161:ASN:HD22	1:C:161:ASN:HA	1.65	0.41
1:E:279:GLU:OE1	1:E:279:GLU:N	2.46	0.41
1:C:122:LYS:HE2	1:C:122:LYS:HB3	1.93	0.41
1:C:150:PHE:O	1:C:151:ASP:C	2.64	0.41
1:F:132:GLU:OE2	1:F:143:ILE:HG13	2.21	0.41
1:F:174:CYS:SG	1:F:175:PRO:HD2	2.61	0.41
1:B:98:PHE:CB	1:B:101:ILE:HD12	2.46	0.41
1:B:154:LEU:HD13	1:B:195:MET:O	2.21	0.41
1:B:154:LEU:O	1:B:158:GLN:HG3	2.21	0.41
1:C:81:TRP:CG	1:E:122:LYS:HE3	2.56	0.41
1:D:51:VAL:HB	1:D:55:VAL:CG1	2.49	0.41
1:F:41:ARG:HD3	1:F:75:SER:HB2	2.02	0.41
1:F:63:LEU:HD21	1:F:260:VAL:HG22	2.03	0.41
1:C:34:LYS:HD3	1:C:70:VAL:HG21	2.03	0.40
1:C:58:LYS:HD3	1:C:62:MET:HE1	2.02	0.40
1:C:59:LEU:HD22	1:C:306:ILE:HD13	2.02	0.40
1:C:233:HIS:C	1:C:233:HIS:CD2	2.99	0.40
1:C:299:LEU:HD13	1:C:299:LEU:C	2.45	0.40
1:D:294:VAL:HG12	1:D:295:ASN:N	2.36	0.40
1:C:53:THR:HG21	1:C:90:GLU:HG3	2.03	0.40
1:F:36:VAL:HG22	1:F:70:VAL:CG1	2.50	0.40
1:A:77:VAL:HG11	1:A:82:VAL:CG1	2.51	0.40
1:A:139:ILE:HB	1:A:141:CYS:SG	2.62	0.40
1:A:205:THR:O	1:A:235:HIS:ND1	2.53	0.40
1:C:306:ILE:O	1:C:310:LEU:HB2	2.21	0.40
1:D:68:LEU:O	1:D:101:ILE:HD12	2.21	0.40
1:D:200:ILE:HD12	1:D:200:ILE:N	2.36	0.40
1:F:82:VAL:HA	1:F:83:PRO:HD2	1.96	0.40
1:B:191:LYS:HD2	1:B:191:LYS:HA	1.85	0.40
1:B:260:VAL:HB	1:B:261:ALA:H	1.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:SER:O	1:C:170:CYS:HB2	2.21	0.40
1:A:48:LYS:N	1:A:48:LYS:CD	2.76	0.40
1:A:61:ASP:CG	1:A:96:GLN:HE21	2.30	0.40
1:C:165:ARG:NH1	1:C:257:ASP:OD1	2.55	0.40
1:D:278:THR:O	1:D:282:VAL:HG13	2.21	0.40
1:E:34:LYS:HD3	1:E:70:VAL:HG11	2.03	0.40
1:E:85:MET:HE2	4:E:611:HOH:O	2.20	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	294/298 (99%)	287 (98%)	4 (1%)	3 (1%)	12	9
1	B	294/298 (99%)	281 (96%)	8 (3%)	5 (2%)	7	3
1	C	292/298 (98%)	279 (96%)	12 (4%)	1 (0%)	36	36
1	D	276/298 (93%)	261 (95%)	12 (4%)	3 (1%)	11	8
1	E	294/298 (99%)	281 (96%)	11 (4%)	2 (1%)	18	15
1	F	282/298 (95%)	265 (94%)	15 (5%)	2 (1%)	18	15
All	All	1732/1788 (97%)	1654 (96%)	62 (4%)	16 (1%)	14	10

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	ILE
1	A	260	VAL
1	A	271	GLY
1	B	260	VAL
1	B	270	GLN

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Mol	Chain	Res	Type
1	C	260	VAL
1	D	260	VAL
1	E	260	VAL
1	B	140	ASN
1	D	87	ASP
1	F	41	ARG
1	B	273	SER
1	D	136	LYS
1	E	177	GLU
1	F	73	THR
1	B	108	PRO

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	238/240 (99%)	216 (91%)	22 (9%)	8	6
1	B	238/240 (99%)	222 (93%)	16 (7%)	15	12
1	C	236/240 (98%)	224 (95%)	12 (5%)	21	21
1	D	227/240 (95%)	215 (95%)	12 (5%)	20	19
1	E	238/240 (99%)	224 (94%)	14 (6%)	18	16
1	F	232/240 (97%)	222 (96%)	10 (4%)	26	27
All	All	1409/1440 (98%)	1323 (94%)	86 (6%)	17	15

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	32	ARG
1	A	44	LEU
1	A	48	LYS
1	A	70	VAL
1	A	82	VAL
1	A	84	GLN

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Mol	Chain	Res	Type
1	A	114	GLU
1	A	133	LEU
1	A	139	ILE
1	A	151	ASP
1	A	192	PHE
1	A	230	LEU
1	A	232	VAL
1	A	246	LEU
1	A	251	MET
1	A	255	VAL
1	A	256	VAL
1	A	288	LEU
1	A	299	LEU
1	A	310	LEU
1	A	312	ARG
1	B	31	LYS
1	B	44	LEU
1	B	65	GLU
1	B	70	VAL
1	B	85	MET
1	B	114	GLU
1	B	140	ASN
1	B	141	CYS
1	B	230	LEU
1	B	246	LEU
1	B	255	VAL
1	B	256	VAL
1	B	282	VAL
1	B	299	LEU
1	B	310	LEU
1	B	312	ARG
1	C	82	VAL
1	C	84	GLN
1	C	85	MET
1	C	114	GLU
1	C	165	ARG
1	C	230	LEU
1	C	232	VAL
1	C	246	LEU
1	C	255	VAL
1	C	256	VAL
1	C	288	LEU

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Mol	Chain	Res	Type
1	C	312	ARG
1	D	55	VAL
1	D	70	VAL
1	D	84	GLN
1	D	114	GLU
1	D	161	ASN
1	D	181	SER
1	D	230	LEU
1	D	246	LEU
1	D	255	VAL
1	D	288	LEU
1	D	299	LEU
1	D	312	ARG
1	E	70	VAL
1	E	84	GLN
1	E	85	MET
1	E	90	GLU
1	E	181	SER
1	E	230	LEU
1	E	232	VAL
1	E	246	LEU
1	E	255	VAL
1	E	256	VAL
1	E	297	GLN
1	E	299	LEU
1	E	310	LEU
1	E	312	ARG
1	F	44	LEU
1	F	55	VAL
1	F	102	ASN
1	F	230	LEU
1	F	255	VAL
1	F	282	VAL
1	F	288	LEU
1	F	299	LEU
1	F	312	ARG
1	F	323	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN

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Mol	Chain	Res	Type
1	A	84	GLN
1	A	88	HIS
1	A	96	GLN
1	A	102	ASN
1	A	140	ASN
1	A	161	ASN
1	A	223	GLN
1	A	244	ASN
1	A	250	GLN
1	A	297	GLN
1	A	311	ASN
1	A	320	GLN
1	B	46	ASN
1	B	138	ASN
1	B	161	ASN
1	B	223	GLN
1	B	244	ASN
1	B	250	GLN
1	B	297	GLN
1	B	311	ASN
1	C	109	ASN
1	C	138	ASN
1	C	148	GLN
1	C	161	ASN
1	C	223	GLN
1	C	244	ASN
1	C	250	GLN
1	C	297	GLN
1	C	304	ASN
1	C	311	ASN
1	D	46	ASN
1	D	84	GLN
1	D	158	GLN
1	D	161	ASN
1	D	244	ASN
1	D	250	GLN
1	D	311	ASN
1	E	46	ASN
1	E	84	GLN
1	E	88	HIS
1	E	102	ASN
1	E	138	ASN

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Mol	Chain	Res	Type
1	E	140	ASN
1	E	148	GLN
1	E	161	ASN
1	E	223	GLN
1	E	244	ASN
1	E	250	GLN
1	E	297	GLN
1	E	308	GLN
1	E	311	ASN
1	F	102	ASN
1	F	161	ASN
1	F	223	GLN
1	F	244	ASN
1	F	250	GLN
1	F	297	GLN
1	F	311	ASN
1	F	320	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 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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
3	3HG	A	399	-	9,9,9	1.95	3 (33%)	8,11,11	1.67	1 (12%)

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	3HG	A	399	-	-	5/8/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	399	3HG	O4-C5	3.76	1.34	1.22
3	A	399	3HG	O2-C3	-3.25	1.33	1.43
3	A	399	3HG	C4-C5	-2.25	1.45	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	399	3HG	O5-C5-C4	3.13	123.72	114.00

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	399	3HG	C1-C2-C3-O2
3	A	399	3HG	C1-C2-C3-C4
3	A	399	3HG	C3-C4-C5-O5
3	A	399	3HG	O1-C1-C2-C3
3	A	399	3HG	C3-C4-C5-O4

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	399	3HG	4	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	296/298 (99%)	0.15	13 (4%)	39 41	19, 28, 56, 72	0
1	B	296/298 (99%)	0.61	31 (10%)	11 12	22, 38, 75, 95	0
1	C	294/298 (98%)	0.45	16 (5%)	31 33	22, 38, 62, 74	0
1	D	282/298 (94%)	1.14	44 (15%)	5 5	30, 56, 85, 95	0
1	E	296/298 (99%)	0.49	20 (6%)	23 25	23, 36, 72, 84	0
1	F	288/298 (96%)	1.40	83 (28%)	1 1	20, 60, 87, 95	0
All	All	1752/1788 (97%)	0.70	207 (11%)	9 9	19, 40, 79, 95	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	265	GLY	5.6
1	F	76	PHE	5.1
1	F	127	PHE	5.1
1	B	138	ASN	4.4
1	B	147	PHE	4.4
1	E	269	ALA	4.4
1	E	266	CYS	4.3
1	F	81	TRP	4.3
1	D	81	TRP	4.2
1	F	115	ALA	3.8
1	D	85	MET	3.8
1	B	139	ILE	3.8
1	B	266	CYS	3.8
1	C	268	TYR	3.7
1	C	269	ALA	3.7
1	F	153	ILE	3.7
1	F	68	LEU	3.6
1	F	119	ALA	3.6
1	C	264	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	158	GLN	3.6
1	F	79	PRO	3.6
1	D	147	PHE	3.5
1	F	77	VAL	3.5
1	F	107	THR	3.4
1	F	95	ILE	3.4
1	F	113	PHE	3.4
1	D	146	SER	3.4
1	F	70	VAL	3.4
1	F	92	LEU	3.4
1	F	147	PHE	3.4
1	B	323	CYS	3.3
1	F	82	VAL	3.3
1	F	106	LEU	3.3
1	A	269	ALA	3.2
1	B	176	TYR	3.2
1	C	127	PHE	3.2
1	E	151	ASP	3.2
1	F	98	PHE	3.2
1	A	322	THR	3.2
1	B	141	CYS	3.2
1	F	156	ALA	3.2
1	C	148	GLN	3.2
1	B	322	THR	3.2
1	D	264	GLY	3.2
1	E	273	SER	3.1
1	C	322	THR	3.1
1	D	151	ASP	3.1
1	F	55	VAL	3.1
1	D	154	LEU	3.1
1	E	297	GLN	3.1
1	B	140	ASN	3.0
1	E	323	CYS	3.0
1	D	98	PHE	3.0
1	F	138	ASN	3.0
1	C	271	GLY	3.0
1	A	272	ALA	2.9
1	A	323	CYS	2.9
1	E	265	GLY	2.9
1	B	133	LEU	2.9
1	F	110	LEU	2.9
1	F	323	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	162	ILE	2.9
1	F	176	TYR	2.9
1	F	121	ALA	2.9
1	D	133	LEU	2.8
1	D	260	VAL	2.8
1	F	101	ILE	2.8
1	E	268	TYR	2.8
1	F	88	HIS	2.8
1	F	274	GLY	2.8
1	F	154	LEU	2.8
1	D	163	SER	2.8
1	B	81	TRP	2.8
1	D	152	ALA	2.8
1	F	117	VAL	2.7
1	F	61	ASP	2.7
1	D	309	ALA	2.7
1	F	302	ALA	2.7
1	F	83	PRO	2.7
1	D	74	THR	2.7
1	B	260	VAL	2.7
1	F	50	ILE	2.7
1	F	152	ALA	2.6
1	D	134	PHE	2.6
1	E	28	THR	2.6
1	B	167	TYR	2.6
1	F	112	GLY	2.6
1	D	88	HIS	2.6
1	E	322	THR	2.6
1	F	28	THR	2.6
1	D	156	ALA	2.6
1	F	157	ALA	2.6
1	A	268	TYR	2.5
1	C	195	MET	2.5
1	F	116	ALA	2.5
1	B	154	LEU	2.5
1	B	145	GLU	2.5
1	C	305	PHE	2.5
1	E	147	PHE	2.5
1	E	243	ALA	2.5
1	F	85	MET	2.5
1	F	120	GLY	2.5
1	B	70	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	162	ILE	2.5
1	F	232	VAL	2.5
1	F	306	ILE	2.5
1	F	135	THR	2.5
1	C	272	ALA	2.5
1	F	67	GLY	2.5
1	F	125	VAL	2.4
1	C	270	GLN	2.4
1	B	268	TYR	2.4
1	D	120	GLY	2.4
1	A	148	GLN	2.4
1	D	114	GLU	2.4
1	F	144	GLU	2.4
1	D	70	VAL	2.4
1	F	40	PRO	2.4
1	B	269	ALA	2.4
1	F	53	THR	2.4
1	F	243	ALA	2.4
1	F	261	ALA	2.4
1	C	84	GLN	2.4
1	E	150	PHE	2.4
1	A	80	LYS	2.4
1	F	75	SER	2.4
1	A	266	CYS	2.4
1	F	100	GLY	2.3
1	D	150	PHE	2.3
1	A	138	ASN	2.3
1	F	192	PHE	2.3
1	F	69	SER	2.3
1	F	259	SER	2.3
1	A	139	ILE	2.3
1	B	157	ALA	2.3
1	F	136	LYS	2.3
1	F	151	ASP	2.3
1	A	271	GLY	2.3
1	F	264	GLY	2.3
1	C	158	GLN	2.2
1	F	60	ILE	2.2
1	E	267	PRO	2.2
1	E	155	LYS	2.2
1	D	61	ASP	2.2
1	D	100	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	90	GLU	2.2
1	F	167	TYR	2.2
1	B	82	VAL	2.2
1	B	108	PRO	2.2
1	B	153	ILE	2.2
1	D	107	THR	2.2
1	D	82	VAL	2.2
1	E	82	VAL	2.2
1	D	118	ALA	2.2
1	D	321	ALA	2.2
1	E	145	GLU	2.2
1	C	308	GLN	2.2
1	D	101	ILE	2.2
1	E	260	VAL	2.2
1	F	124	VAL	2.2
1	C	319	ALA	2.2
1	F	148	GLN	2.2
1	F	272	ALA	2.2
1	D	323	CYS	2.2
1	A	273	SER	2.2
1	F	80	LYS	2.2
1	A	161	ASN	2.2
1	B	267	PRO	2.1
1	D	28	THR	2.2
1	B	150	PHE	2.1
1	F	145	GLU	2.1
1	D	77	VAL	2.1
1	F	51	VAL	2.1
1	B	274	GLY	2.1
1	D	166	GLY	2.1
1	F	309	ALA	2.1
1	D	92	LEU	2.1
1	F	63	LEU	2.1
1	D	176	TYR	2.1
1	D	73	THR	2.1
1	D	108	PRO	2.1
1	B	134	PHE	2.1
1	B	192	PHE	2.1
1	D	303	GLY	2.1
1	F	149	ARG	2.1
1	F	163	SER	2.1
1	C	145	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	204	ASP	2.1
1	F	42	ASP	2.1
1	B	28	THR	2.1
1	F	126	ILE	2.1
1	B	127	PHE	2.1
1	F	208	VAL	2.1
1	F	260	VAL	2.1
1	D	110	LEU	2.1
1	D	235	HIS	2.1
1	F	89	THR	2.1
1	F	99	PRO	2.1
1	B	265	GLY	2.1
1	E	271	GLY	2.1
1	E	274	GLY	2.1
1	D	117	VAL	2.1
1	D	305	PHE	2.1
1	D	243	ALA	2.1
1	F	105	VAL	2.0
1	F	150	PHE	2.0
1	F	305	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
2	MG	A	401	1/1	0.45	0.22	35,35,35,35	0
3	3HG	A	399	10/10	0.76	0.12	66,66,67,67	0
2	MG	F	406	1/1	0.77	0.13	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	E	402	1/1	0.78	0.12	44,44,44,44	0
2	MG	B	404	1/1	0.81	0.10	48,48,48,48	0
2	MG	C	403	1/1	0.88	0.09	37,37,37,37	0
2	MG	D	405	1/1	0.97	0.07	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.