



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:59 PM UTC

PDB ID : 2EEZ / pdb_00002eez
Title : Crystal structure of alanine dehydrogenase from *Thermophilus*
Authors : Kumarevel, T.S.; Karthe, P.; Kuramitsu, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-02-19
Resolution : 2.71 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
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

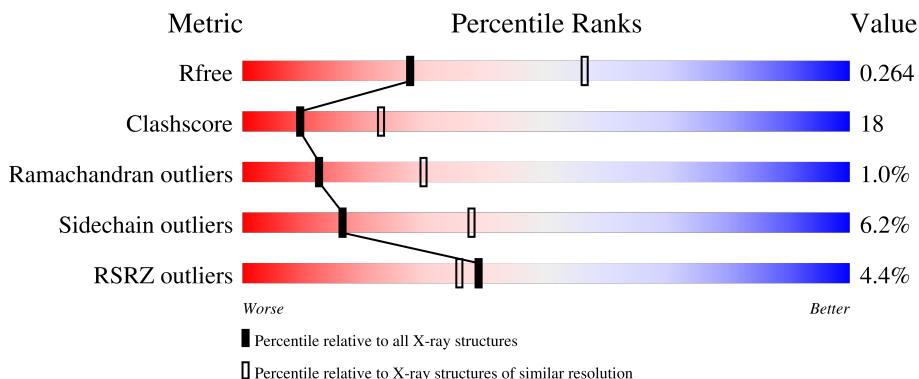
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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.



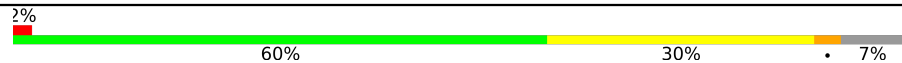
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	369	
1	C	369	
1	D	369	
1	E	369	
1	F	369	

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Mol	Chain	Length	Quality of chain
1	G	369	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment at the beginning labeled '2%', a large green segment labeled '60%', a yellow segment labeled '30%', and a small grey segment at the end labeled '7%'.</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 15522 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 Alanine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	343	2523	1604	438	472	9	0	0	0
1	C	343	2523	1604	438	472	9	0	0	0
1	D	343	2523	1604	438	472	9	0	0	0
1	E	343	2523	1604	438	472	9	0	0	0
1	F	343	2523	1604	438	472	9	0	0	0
1	G	343	2523	1604	438	472	9	0	0	0

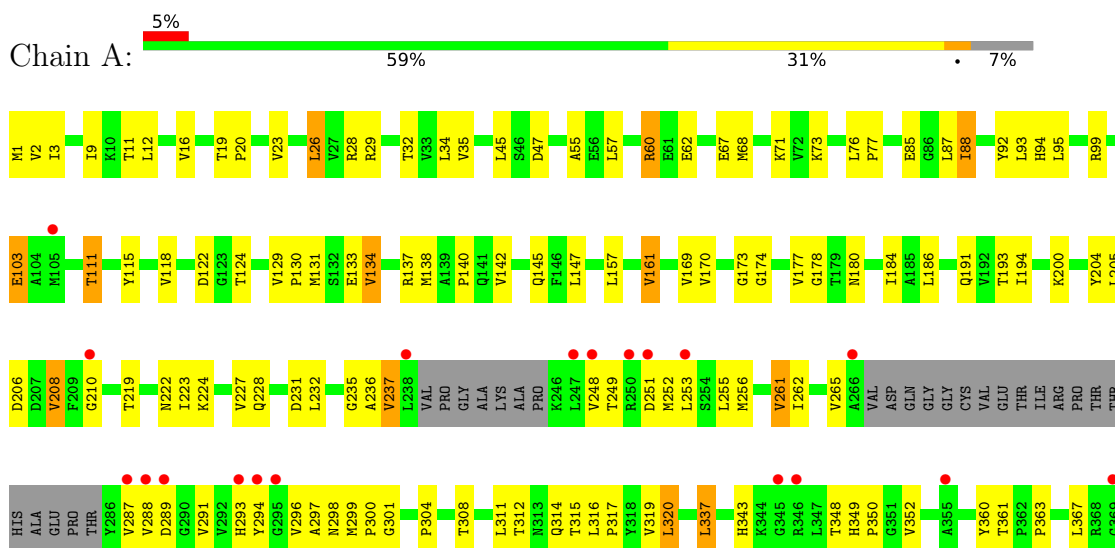
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	65	Total 65	O 65	0	0
2	C	65	Total 65	O 65	0	0
2	D	65	Total 65	O 65	0	0
2	E	59	Total 59	O 59	0	0
2	F	64	Total 64	O 64	0	0
2	G	66	Total 66	O 66	0	0

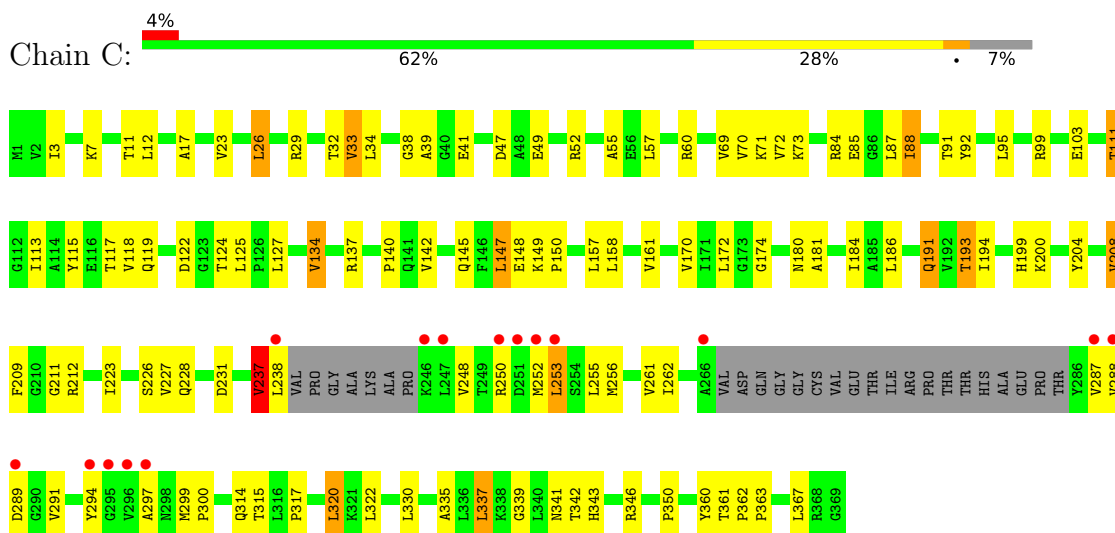
3 Residue-property plots i

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: Alanine dehydrogenase

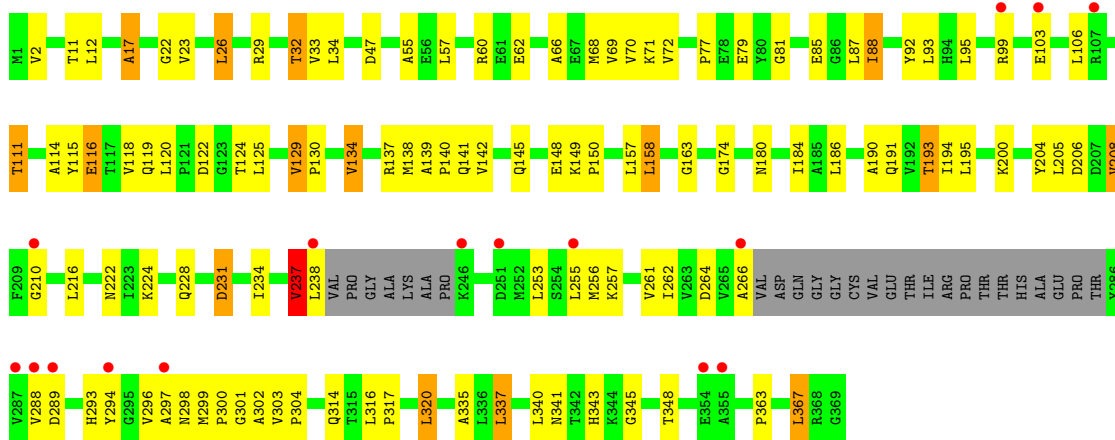


- Molecule 1: Alanine dehydrogenase

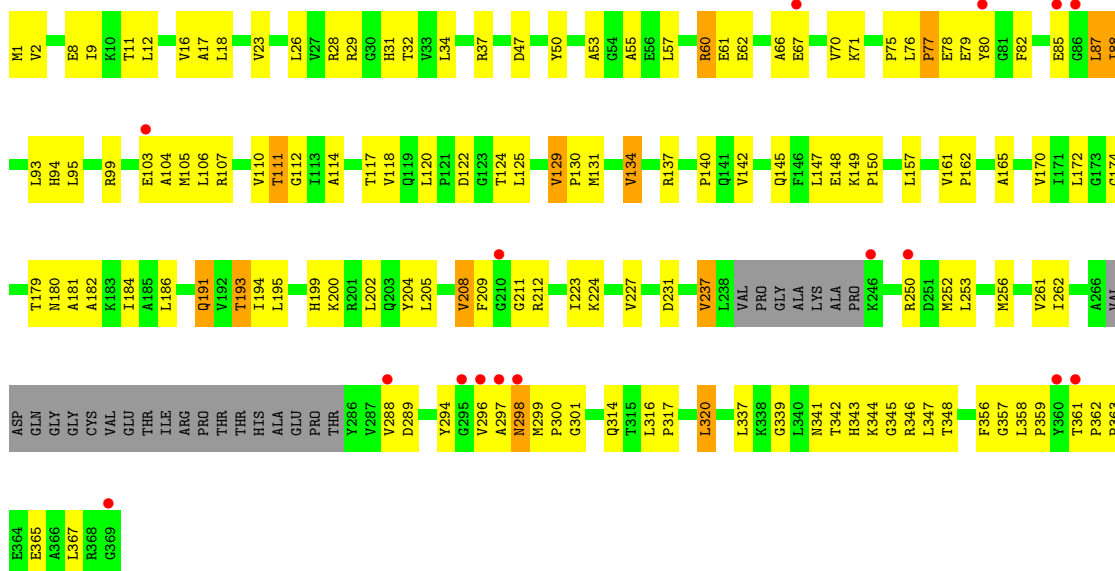


- Molecule 1: Alanine dehydrogenase

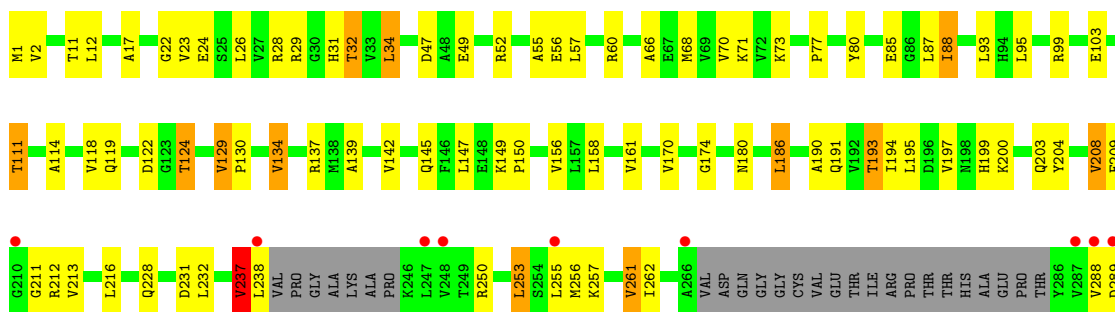


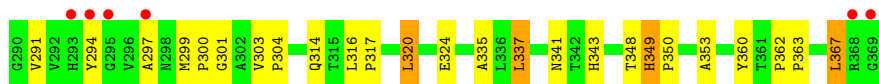


- Molecule 1: Alanine dehydrogenase

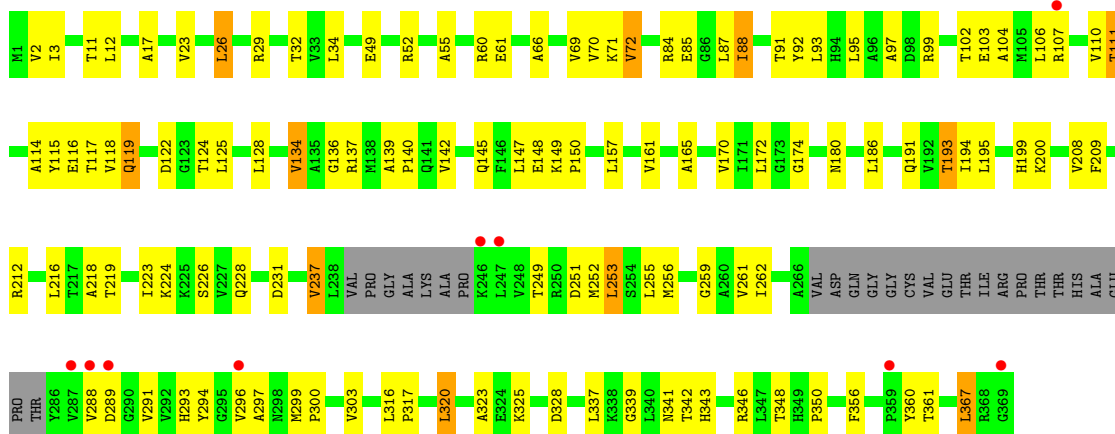


- Molecule 1: Alanine dehydrogenase





- Molecule 1: Alanine dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	133.94Å 133.24Å 147.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.71 19.95 – 2.71	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.95-2.71) 98.7 (19.95-2.71)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.66 (at 2.73Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.264 0.219 , 0.264	Depositor DCC
R_{free} test set	3612 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtrriage
Anisotropy	0.272	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.013 for k,h,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15522	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.48	0/2562	0.94	5/3476 (0.1%)
1	C	0.49	0/2562	0.96	9/3476 (0.3%)
1	D	0.49	0/2562	0.98	9/3476 (0.3%)
1	E	0.48	0/2562	0.97	8/3476 (0.2%)
1	F	0.49	0/2562	1.01	12/3476 (0.3%)
1	G	0.46	0/2562	0.96	10/3476 (0.3%)
All	All	0.48	0/15372	0.97	53/20856 (0.3%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	GLU	N-CA-C	8.59	120.26	111.07
1	A	231	ASP	N-CA-C	-8.22	103.38	113.41
1	E	231	ASP	N-CA-C	-8.04	103.60	113.41
1	G	147	LEU	N-CA-C	-7.44	104.18	113.18
1	F	85	GLU	N-CA-C	7.32	119.15	111.03
1	A	118	VAL	N-CA-C	-7.13	99.75	109.37
1	D	85	GLU	N-CA-C	6.81	119.33	111.02
1	E	118	VAL	N-CA-C	-6.77	99.80	108.93
1	F	349	HIS	CA-C-N	6.77	127.03	119.32
1	F	349	HIS	C-N-CA	6.77	127.03	119.32
1	C	33	VAL	N-CA-C	6.76	117.60	107.80
1	E	129	VAL	CB-CA-C	-6.62	107.41	113.70
1	D	129	VAL	CB-CA-C	-6.59	107.36	114.35
1	C	147	LEU	N-CA-C	-6.50	105.31	113.18
1	G	85	GLU	N-CA-C	6.49	118.04	110.97
1	F	348	THR	N-CA-C	6.48	120.19	112.93
1	E	147	LEU	N-CA-C	-6.43	105.44	113.28
1	F	118	VAL	N-CA-C	-6.42	100.27	108.93
1	E	181	ALA	N-CA-C	-6.33	104.38	111.28
1	E	85	GLU	N-CA-C	6.18	118.53	111.11
1	C	191	GLN	N-CA-C	-6.02	98.72	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	231	ASP	N-CA-C	-5.99	104.13	112.45
1	F	231	ASP	N-CA-C	-5.97	105.08	112.90
1	C	231	ASP	N-CA-C	-5.95	105.11	112.90
1	F	156	VAL	N-CA-C	5.91	117.35	108.96
1	G	118	VAL	N-CA-C	-5.89	101.42	109.37
1	F	147	LEU	N-CA-C	-5.76	106.08	113.23
1	C	85	GLU	N-CA-C	5.73	117.33	111.14
1	G	72	VAL	CB-CA-C	-5.70	106.86	111.71
1	G	303	VAL	CA-C-N	5.60	125.07	119.24
1	G	303	VAL	C-N-CA	5.60	125.07	119.24
1	C	125	LEU	CA-C-N	5.59	126.83	119.84
1	C	125	LEU	C-N-CA	5.59	126.83	119.84
1	E	191	GLN	N-CA-C	-5.57	100.03	108.67
1	F	139	ALA	CA-C-N	-5.57	113.94	119.56
1	F	139	ALA	C-N-CA	-5.57	113.94	119.56
1	D	116	GLU	N-CA-C	5.45	119.55	113.01
1	C	118	VAL	N-CA-C	-5.36	101.76	108.84
1	D	17	ALA	N-CA-C	5.36	119.44	113.01
1	D	118	VAL	N-CA-C	-5.34	102.62	109.30
1	G	119	GLN	N-CA-C	5.33	117.06	108.32
1	D	303	VAL	CA-C-N	5.31	125.37	119.32
1	D	303	VAL	C-N-CA	5.31	125.37	119.32
1	G	259	GLY	N-CA-C	-5.30	107.69	114.37
1	D	158	LEU	N-CA-C	5.29	117.46	111.11
1	F	324	GLU	N-CA-C	5.28	117.11	111.36
1	F	129	VAL	CB-CA-C	-5.26	108.70	113.70
1	G	231	ASP	N-CA-C	-5.20	106.09	112.90
1	A	147	LEU	N-CA-C	-5.06	107.11	113.28
1	A	287	VAL	N-CA-C	5.06	115.25	108.17
1	E	87	LEU	N-CA-C	5.02	117.42	109.24
1	G	165	ALA	N-CA-C	5.01	116.00	109.64
1	C	181	ALA	N-CA-C	-5.01	105.90	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2523	0	2600	112	0
1	C	2523	0	2600	87	0
1	D	2523	0	2600	95	0
1	E	2523	0	2600	120	0
1	F	2523	0	2600	88	0
1	G	2523	0	2600	95	0
2	A	65	0	0	4	0
2	C	65	0	0	3	0
2	D	65	0	0	5	0
2	E	59	0	0	9	0
2	F	64	0	0	4	0
2	G	66	0	0	2	0
All	All	15522	0	15600	551	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 18.

All (551) 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:F:256:MET:HE1	1:F:262:ILE:HD11	1.34	1.08
1:D:256:MET:HE1	1:D:262:ILE:HD11	1.29	1.07
1:G:256:MET:HE1	1:G:262:ILE:HD11	1.37	1.06
1:E:256:MET:HE1	1:E:262:ILE:HD11	1.36	1.03
1:C:256:MET:HE1	1:C:262:ILE:HD11	1.37	1.03
1:A:137:ARG:HE	1:A:180:ASN:HD22	1.07	1.01
1:A:256:MET:HE1	1:A:262:ILE:HD11	1.45	0.97
1:E:137:ARG:HE	1:E:180:ASN:HD22	1.09	0.93
1:D:137:ARG:HE	1:D:180:ASN:HD22	1.14	0.91
1:G:137:ARG:HE	1:G:180:ASN:HD22	0.92	0.89
1:F:137:ARG:HE	1:F:180:ASN:HD22	1.10	0.89
1:A:191:GLN:NE2	1:C:191:GLN:NE2	2.22	0.88
1:G:17:ALA:HB1	1:G:70:VAL:HG12	1.57	0.87
1:G:174:GLY:HA2	1:G:194:ILE:HD11	1.57	0.87
1:E:145:GLN:NE2	2:E:376:HOH:O	2.09	0.86
1:D:142:VAL:HG21	1:D:299:MET:HE2	1.58	0.85
1:A:137:ARG:NE	1:A:180:ASN:HD22	1.75	0.85
1:G:137:ARG:NE	1:G:180:ASN:HD22	1.75	0.84
1:C:95:LEU:HD12	1:C:341:ASN:HD22	1.43	0.84
1:A:200:LYS:NZ	1:E:124:THR:HG21	1.93	0.83
1:E:111:THR:HB	1:E:343:HIS:HD2	1.43	0.83
1:A:191:GLN:HE21	1:C:191:GLN:HE21	1.25	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ARG:HE	1:C:180:ASN:HD22	1.28	0.81
1:A:191:GLN:NE2	1:C:191:GLN:HE21	1.78	0.81
1:G:256:MET:HE3	1:G:291:VAL:HG21	1.62	0.81
1:G:111:THR:HB	1:G:343:HIS:HD2	1.44	0.81
1:C:124:THR:HG21	1:F:200:LYS:HZ1	1.45	0.81
1:C:124:THR:HG21	1:F:200:LYS:NZ	1.96	0.81
1:F:161:VAL:HG11	1:G:134:VAL:HG12	1.64	0.80
1:E:137:ARG:HE	1:E:180:ASN:ND2	1.81	0.79
1:C:228:GLN:HG3	1:C:255:LEU:HB3	1.65	0.78
1:D:191:GLN:NE2	1:G:191:GLN:HE21	1.84	0.76
1:G:193:THR:HG22	2:G:395:HOH:O	1.84	0.76
1:D:23:VAL:HG11	1:D:55:ALA:HB2	1.68	0.75
1:C:134:VAL:HG12	1:E:161:VAL:HG11	1.67	0.75
1:D:191:GLN:NE2	1:G:191:GLN:NE2	2.35	0.75
1:F:17:ALA:HB1	1:F:70:VAL:HG12	1.69	0.75
1:F:23:VAL:HG11	1:F:55:ALA:HB2	1.69	0.75
1:C:193:THR:HG22	2:C:380:HOH:O	1.86	0.74
1:G:142:VAL:HG21	1:G:299:MET:HE2	1.67	0.74
1:F:228:GLN:HG3	1:F:255:LEU:HB3	1.69	0.74
1:D:174:GLY:HA2	1:D:194:ILE:HD11	1.68	0.74
1:E:193:THR:HG22	2:E:385:HOH:O	1.87	0.73
1:F:337:LEU:CD2	1:F:363:PRO:HB2	2.19	0.72
1:E:23:VAL:HG11	1:E:55:ALA:HB2	1.71	0.72
1:D:122:ASP:OD1	1:D:124:THR:HG23	1.89	0.72
1:D:191:GLN:HE21	1:G:191:GLN:HE21	1.39	0.71
1:C:142:VAL:HG21	1:C:299:MET:HE2	1.73	0.70
1:D:26:LEU:HD13	1:D:320:LEU:HD12	1.73	0.70
1:A:62:GLU:HB2	2:A:404:HOH:O	1.92	0.70
1:E:200:LYS:NZ	1:G:124:THR:HG21	2.08	0.69
1:F:111:THR:HB	1:F:343:HIS:CD2	2.28	0.69
1:A:124:THR:HG21	1:G:200:LYS:NZ	2.08	0.68
1:C:26:LEU:HD13	1:C:320:LEU:HD12	1.74	0.68
1:E:137:ARG:NE	1:E:180:ASN:HD22	1.88	0.68
1:G:137:ARG:HE	1:G:180:ASN:ND2	1.78	0.68
1:D:314:GLN:O	1:D:317:PRO:HD2	1.92	0.68
1:F:111:THR:HB	1:F:343:HIS:HD2	1.57	0.68
1:A:134:VAL:HG22	1:A:300:PRO:HG3	1.77	0.67
1:A:200:LYS:HZ2	1:E:124:THR:HG21	1.56	0.67
1:D:200:LYS:NZ	1:F:124:THR:HG21	2.08	0.67
1:G:29:ARG:HH11	1:G:29:ARG:HG3	1.59	0.67
1:A:256:MET:HE3	1:A:291:VAL:HG11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:GLY:HA2	1:F:194:ILE:HD11	1.77	0.67
1:A:191:GLN:HE22	1:C:191:GLN:NE2	1.92	0.67
1:E:191:GLN:HE21	1:F:191:GLN:NE2	1.93	0.67
1:A:145:GLN:NE2	2:A:426:HOH:O	2.28	0.66
1:C:47:ASP:HB3	1:C:57:LEU:HD13	1.78	0.66
1:D:142:VAL:CG2	1:D:299:MET:HE2	2.24	0.66
1:G:122:ASP:OD1	1:G:124:THR:HG23	1.95	0.65
1:F:256:MET:HE3	1:F:291:VAL:HG21	1.79	0.65
1:D:145:GLN:NE2	2:D:376:HOH:O	2.29	0.65
1:G:346:ARG:HG3	1:G:346:ARG:HH11	1.62	0.65
1:G:145:GLN:NE2	2:G:386:HOH:O	2.29	0.65
1:D:193:THR:HG22	2:D:388:HOH:O	1.96	0.64
1:E:99:ARG:O	1:E:103:GLU:HG3	1.98	0.64
1:G:26:LEU:CD1	1:G:320:LEU:HD12	2.28	0.64
1:G:122:ASP:CG	1:G:124:THR:HG23	2.22	0.64
1:A:137:ARG:HE	1:A:180:ASN:ND2	1.87	0.64
1:E:18:LEU:HD12	2:E:393:HOH:O	1.97	0.64
1:F:134:VAL:HG12	1:G:161:VAL:HG11	1.80	0.63
1:D:99:ARG:O	1:D:103:GLU:HG3	1.98	0.63
1:G:119:GLN:HB2	1:G:125:LEU:HD23	1.80	0.63
1:F:93:LEU:HD12	1:F:114:ALA:HB2	1.80	0.63
1:C:145:GLN:NE2	2:C:431:HOH:O	2.31	0.63
1:E:117:THR:OG1	1:E:339:GLY:HA2	1.98	0.63
1:D:17:ALA:HB1	1:D:70:VAL:HG12	1.80	0.63
1:G:253:LEU:HA	1:G:256:MET:HE2	1.81	0.63
1:A:249:THR:C	1:A:251:ASP:H	2.07	0.62
1:C:253:LEU:HD12	1:C:256:MET:HE2	1.81	0.62
1:G:3:ILE:HD11	1:G:323:ALA:HB2	1.81	0.62
1:F:47:ASP:HB3	1:F:57:LEU:HD13	1.80	0.62
1:G:23:VAL:HG11	1:G:55:ALA:HB2	1.82	0.62
1:A:111:THR:HB	1:A:343:HIS:HD2	1.64	0.62
1:E:106:LEU:O	1:E:345:GLY:HA2	2.00	0.62
1:G:26:LEU:HD13	1:G:320:LEU:HD12	1.81	0.62
1:F:122:ASP:OD1	1:F:124:THR:HG23	2.00	0.62
1:D:228:GLN:HG3	1:D:255:LEU:HB3	1.81	0.62
1:D:122:ASP:CG	1:D:124:THR:HG23	2.25	0.61
1:E:294:TYR:CZ	1:E:296:VAL:HB	2.35	0.61
1:F:204:TYR:O	1:F:208:VAL:HG13	2.00	0.61
1:G:2:VAL:O	1:G:66:ALA:HB1	2.00	0.61
1:E:67:GLU:O	1:E:88:ILE:HG23	1.99	0.61
1:A:174:GLY:HA2	1:A:194:ILE:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:MET:N	1:D:300:PRO:CD	2.63	0.61
1:A:47:ASP:HB3	1:A:57:LEU:CD1	2.31	0.61
1:A:337:LEU:CD2	1:A:363:PRO:HB2	2.31	0.61
1:G:69:VAL:HG23	1:G:87:LEU:HD11	1.83	0.61
1:E:95:LEU:HD12	1:E:341:ASN:HD22	1.66	0.60
1:F:87:LEU:O	1:F:111:THR:HG23	2.01	0.60
1:G:294:TYR:CZ	1:G:296:VAL:HB	2.34	0.60
1:C:29:ARG:HG3	1:C:29:ARG:HH11	1.66	0.60
1:F:99:ARG:O	1:F:103:GLU:HG3	2.01	0.60
1:D:26:LEU:CD1	1:D:320:LEU:HD12	2.31	0.60
1:D:95:LEU:HD12	1:D:341:ASN:HD22	1.67	0.60
1:G:26:LEU:HD13	1:G:320:LEU:CD1	2.31	0.60
1:A:170:VAL:HG22	1:A:193:THR:CG2	2.31	0.60
1:C:111:THR:HA	1:C:342:THR:O	2.00	0.60
1:A:93:LEU:HB3	1:A:95:LEU:CD2	2.32	0.60
1:E:191:GLN:NE2	1:F:191:GLN:NE2	2.49	0.60
1:C:157:LEU:HD21	1:E:137:ARG:HB2	1.84	0.60
1:A:256:MET:CE	1:A:291:VAL:HG11	2.32	0.59
1:E:122:ASP:OD1	1:E:124:THR:HG23	2.02	0.59
1:A:219:THR:O	1:A:223:ILE:HG13	2.02	0.59
1:A:294:TYR:CZ	1:A:296:VAL:HB	2.37	0.59
1:C:17:ALA:HB1	1:C:70:VAL:HG12	1.84	0.59
1:C:26:LEU:HD13	1:C:320:LEU:CD1	2.32	0.59
1:A:124:THR:HG21	1:G:200:LYS:HZ3	1.68	0.59
1:A:191:GLN:HE22	1:C:191:GLN:HE22	1.50	0.59
1:C:299:MET:N	1:C:300:PRO:CD	2.65	0.59
1:G:145:GLN:O	1:G:148:GLU:HB2	2.02	0.59
1:A:142:VAL:HG21	1:A:299:MET:HE2	1.85	0.58
1:D:29:ARG:HG3	1:D:29:ARG:HH11	1.67	0.58
1:E:2:VAL:O	1:E:66:ALA:HB1	2.03	0.58
1:G:172:LEU:HD23	1:G:195:LEU:HD13	1.86	0.58
1:A:99:ARG:O	1:A:103:GLU:HG3	2.02	0.58
1:A:93:LEU:HB3	1:A:95:LEU:HD21	1.85	0.58
1:D:191:GLN:HE22	1:G:191:GLN:NE2	2.01	0.58
1:E:140:PRO:HG3	1:E:184:ILE:HB	1.85	0.58
1:E:29:ARG:HG3	1:E:29:ARG:HH11	1.68	0.58
1:F:68:MET:HG3	1:F:88:ILE:HG13	1.84	0.58
1:F:209:PHE:O	1:F:212:ARG:HD3	2.03	0.58
1:C:111:THR:HB	1:C:343:HIS:CD2	2.39	0.58
1:G:111:THR:HB	1:G:343:HIS:CD2	2.33	0.58
1:E:62:GLU:HB2	2:E:408:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LYS:HZ1	1:E:124:THR:HG21	1.69	0.57
1:F:170:VAL:HG22	1:F:193:THR:HG23	1.85	0.57
1:E:224:LYS:HA	1:E:252:MET:HE2	1.86	0.57
1:E:87:LEU:O	1:E:111:THR:HG23	2.04	0.57
1:G:139:ALA:HA	1:G:299:MET:HE1	1.86	0.57
1:G:299:MET:N	1:G:300:PRO:CD	2.68	0.57
1:F:22:GLY:O	1:F:26:LEU:HD23	2.05	0.57
1:F:95:LEU:HD12	1:F:341:ASN:HB3	1.87	0.57
1:A:133:GLU:OE1	1:G:199:HIS:HE1	1.88	0.56
1:E:299:MET:N	1:E:300:PRO:CD	2.68	0.56
1:A:11:THR:O	1:A:12:LEU:HB2	2.04	0.56
1:A:194:ILE:HD13	1:A:205:LEU:HD13	1.87	0.56
1:A:288:VAL:HB	1:A:293:HIS:CE1	2.39	0.56
1:C:99:ARG:O	1:C:103:GLU:HG3	2.05	0.56
1:E:253:LEU:HA	1:E:256:MET:HE2	1.88	0.56
1:F:137:ARG:NE	1:F:180:ASN:HD22	1.91	0.56
1:F:337:LEU:HD22	1:F:363:PRO:HB2	1.88	0.56
1:G:99:ARG:O	1:G:103:GLU:HG3	2.04	0.56
1:G:316:LEU:HB3	1:G:317:PRO:HD3	1.87	0.56
1:D:194:ILE:HD13	1:D:205:LEU:HD13	1.87	0.56
1:G:228:GLN:HG3	1:G:255:LEU:HB3	1.87	0.56
1:D:140:PRO:HG3	1:D:184:ILE:HB	1.88	0.56
1:D:47:ASP:HB3	1:D:57:LEU:HD13	1.86	0.56
1:A:348:THR:HA	1:A:361:THR:O	2.04	0.56
1:D:2:VAL:HG22	1:D:32:THR:HG23	1.88	0.55
1:E:47:ASP:HB3	1:E:57:LEU:HD13	1.88	0.55
1:E:316:LEU:HB3	1:E:317:PRO:HD3	1.88	0.55
1:F:170:VAL:HG22	1:F:193:THR:CG2	2.35	0.55
1:F:299:MET:N	1:F:300:PRO:CD	2.70	0.55
1:C:122:ASP:OD1	1:C:124:THR:HG23	2.06	0.55
1:E:200:LYS:HZ1	1:G:124:THR:HG21	1.72	0.55
1:G:142:VAL:CG2	1:G:299:MET:HE2	2.34	0.55
1:D:69:VAL:HG23	1:D:87:LEU:HD11	1.89	0.55
1:E:99:ARG:HB2	1:E:356:PHE:CE1	2.42	0.55
1:C:111:THR:HB	1:C:343:HIS:HD2	1.71	0.55
1:C:87:LEU:O	1:C:111:THR:HG23	2.07	0.55
1:C:200:LYS:NZ	1:D:124:THR:HG21	2.21	0.55
1:C:174:GLY:HA2	1:C:194:ILE:HD11	1.90	0.54
1:E:47:ASP:HB3	1:E:57:LEU:CD1	2.38	0.54
1:A:23:VAL:HG11	1:A:55:ALA:HB2	1.89	0.54
1:A:87:LEU:O	1:A:111:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:VAL:CG2	1:E:300:PRO:HG3	2.37	0.54
1:F:193:THR:HG22	2:F:386:HOH:O	2.07	0.54
1:A:140:PRO:HG3	1:A:184:ILE:HB	1.90	0.54
1:A:249:THR:C	1:A:251:ASP:N	2.63	0.54
1:F:253:LEU:HA	1:F:256:MET:HE2	1.88	0.54
1:D:158:LEU:HB3	1:D:190:ALA:HB2	1.88	0.54
1:A:19:THR:O	1:A:20:PRO:C	2.49	0.54
1:E:204:TYR:O	1:E:208:VAL:HG13	2.08	0.54
1:A:299:MET:N	1:A:300:PRO:CD	2.71	0.53
1:D:231:ASP:OD1	1:D:257:LYS:HE3	2.08	0.53
1:A:26:LEU:HD13	1:A:320:LEU:HD12	1.91	0.53
1:A:26:LEU:HD13	1:A:320:LEU:CD1	2.38	0.53
1:A:337:LEU:HD22	1:A:363:PRO:HB2	1.90	0.53
1:C:3:ILE:HD12	1:C:26:LEU:HG	1.91	0.53
1:D:88:ILE:HG13	1:D:88:ILE:O	2.07	0.53
1:E:11:THR:O	1:E:12:LEU:HB2	2.07	0.53
1:E:170:VAL:HG22	1:E:193:THR:HG23	1.90	0.53
1:G:346:ARG:HG3	1:G:346:ARG:NH1	2.24	0.53
1:D:93:LEU:HB2	1:D:114:ALA:HB2	1.90	0.53
1:F:158:LEU:HB3	1:F:190:ALA:HB2	1.91	0.53
1:A:111:THR:HB	1:A:343:HIS:CD2	2.42	0.53
1:A:177:VAL:HB	1:A:236:ALA:HB1	1.89	0.53
1:C:26:LEU:CD1	1:C:320:LEU:HD12	2.38	0.53
1:F:288:VAL:O	1:F:289:ASP:HB2	2.08	0.53
1:F:316:LEU:HB3	1:F:317:PRO:HD3	1.90	0.53
1:E:8:GLU:HA	2:E:383:HOH:O	2.09	0.53
1:C:88:ILE:HG13	1:C:88:ILE:O	2.09	0.53
1:D:119:GLN:O	1:D:335:ALA:HA	2.09	0.53
1:E:202:LEU:HD12	2:E:424:HOH:O	2.09	0.53
1:C:161:VAL:HG11	1:E:134:VAL:HG12	1.89	0.53
1:G:343:HIS:CE1	1:G:367:LEU:HD12	2.44	0.53
1:A:294:TYR:OH	1:A:296:VAL:HB	2.09	0.53
1:E:26:LEU:HD13	1:E:320:LEU:HD12	1.92	0.52
1:G:29:ARG:HG3	1:G:29:ARG:NH1	2.22	0.52
1:G:299:MET:HB2	1:G:300:PRO:HD3	1.91	0.52
1:E:363:PRO:O	1:E:367:LEU:HB2	2.08	0.52
1:E:356:PHE:O	1:E:358:LEU:HG	2.09	0.52
1:A:161:VAL:HG11	1:D:134:VAL:HG12	1.91	0.52
1:C:71:LYS:HE3	1:C:73:LYS:O	2.10	0.52
1:A:47:ASP:HB3	1:A:57:LEU:HD13	1.92	0.52
1:E:142:VAL:HG21	1:E:299:MET:CE	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:LEU:HD11	1:E:347:LEU:HD13	1.92	0.52
1:D:2:VAL:O	1:D:66:ALA:HB1	2.09	0.52
1:G:88:ILE:O	1:G:88:ILE:HG13	2.10	0.51
1:C:23:VAL:HG22	1:C:33:VAL:HG11	1.92	0.51
1:C:137:ARG:HB2	1:E:157:LEU:HD21	1.92	0.51
1:D:92:TYR:CD1	1:D:115:TYR:HB2	2.44	0.51
1:D:253:LEU:HD12	1:D:256:MET:HE2	1.92	0.51
1:E:134:VAL:HG22	1:E:300:PRO:HG3	1.92	0.51
1:F:145:GLN:NE2	2:F:433:HOH:O	2.43	0.51
1:F:26:LEU:HD13	1:F:320:LEU:HD12	1.92	0.51
1:F:337:LEU:HD21	1:F:363:PRO:HB2	1.91	0.51
1:A:350:PRO:HD3	1:A:360:TYR:CE1	2.46	0.51
1:E:16:VAL:HG22	1:E:18:LEU:H	1.76	0.51
1:G:348:THR:HA	1:G:361:THR:O	2.11	0.51
1:D:26:LEU:HD13	1:D:320:LEU:CD1	2.41	0.51
1:D:139:ALA:HB1	1:D:234:ILE:HD13	1.93	0.51
1:C:149:LYS:HB3	1:C:150:PRO:HD3	1.92	0.51
1:A:232:LEU:HD13	1:A:261:VAL:HG22	1.93	0.50
1:D:149:LYS:HB3	1:D:150:PRO:HD3	1.92	0.50
1:E:111:THR:HB	1:E:343:HIS:CD2	2.35	0.50
1:C:142:VAL:HG11	1:C:294:TYR:CE2	2.45	0.50
1:D:120:LEU:HD12	1:D:124:THR:OG1	2.11	0.50
1:F:142:VAL:HG21	1:F:299:MET:HE2	1.92	0.50
1:A:35:VAL:HG23	1:A:55:ALA:HB1	1.94	0.50
1:E:191:GLN:NE2	1:F:191:GLN:HE22	2.09	0.50
1:E:200:LYS:HZ2	1:G:124:THR:HG21	1.73	0.50
1:C:288:VAL:O	1:C:289:ASP:HB2	2.12	0.50
1:G:170:VAL:HG21	1:G:226:SER:O	2.12	0.50
1:E:93:LEU:O	1:E:94:HIS:C	2.55	0.50
1:E:288:VAL:O	1:E:289:ASP:HB2	2.12	0.50
1:D:288:VAL:HB	1:D:293:HIS:CE1	2.47	0.50
1:D:294:TYR:CZ	1:D:296:VAL:HB	2.47	0.50
1:A:60:ARG:HG3	1:A:60:ARG:NH1	2.27	0.50
1:E:93:LEU:HD12	1:E:114:ALA:HB2	1.94	0.50
1:D:299:MET:HB2	1:D:300:PRO:HD3	1.94	0.50
1:D:253:LEU:HD12	1:D:256:MET:CE	2.42	0.49
1:F:24:GLU:O	1:F:28:ARG:HB2	2.12	0.49
1:C:170:VAL:HG22	1:C:193:THR:CG2	2.42	0.49
1:F:250:ARG:HA	1:F:253:LEU:HB2	1.94	0.49
1:C:47:ASP:HB3	1:C:57:LEU:CD1	2.41	0.49
1:G:224:LYS:HA	1:G:252:MET:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:ALA:HA	1:E:107:ARG:NH1	2.27	0.49
1:G:116:GLU:HG2	1:G:117:THR:HG23	1.95	0.49
1:G:288:VAL:O	1:G:289:ASP:HB2	2.12	0.49
1:A:67:GLU:O	1:A:87:LEU:HD12	2.12	0.49
1:A:124:THR:HG21	1:G:200:LYS:HZ1	1.77	0.49
1:C:199:HIS:HD2	2:C:371:HOH:O	1.94	0.49
1:A:29:ARG:HG3	1:A:29:ARG:HH11	1.78	0.49
1:A:288:VAL:O	1:A:289:ASP:HB2	2.12	0.49
1:C:29:ARG:HG3	1:C:29:ARG:NH1	2.27	0.49
1:C:314:GLN:O	1:C:317:PRO:HD2	2.13	0.49
1:D:29:ARG:HG3	1:D:29:ARG:NH1	2.25	0.49
1:C:117:THR:OG1	1:C:339:GLY:HA2	2.13	0.49
1:E:358:LEU:HB3	1:E:359:PRO:CD	2.42	0.49
1:G:117:THR:OG1	1:G:339:GLY:HA2	2.13	0.49
1:A:206:ASP:O	1:A:210:GLY:O	2.31	0.48
1:G:87:LEU:O	1:G:110:VAL:HG23	2.13	0.48
1:G:125:LEU:HD12	1:G:128:LEU:HD23	1.95	0.48
1:F:137:ARG:HB2	1:G:157:LEU:HD21	1.95	0.48
1:E:179:THR:O	1:E:182:ALA:HB3	2.13	0.48
1:E:105:MET:HE1	1:E:112:GLY:HA3	1.95	0.48
1:G:61:GLU:CD	1:G:61:GLU:H	2.21	0.48
1:F:2:VAL:O	1:F:66:ALA:HB1	2.14	0.48
1:A:301:GLY:O	1:A:304:PRO:HD3	2.13	0.48
1:F:34:LEU:HD12	1:F:56:GLU:HB2	1.95	0.48
1:G:111:THR:HA	1:G:342:THR:O	2.14	0.48
1:D:253:LEU:HA	1:D:256:MET:HE2	1.94	0.48
1:F:130:PRO:HG3	1:F:314:GLN:HG3	1.96	0.48
1:G:93:LEU:HD12	1:G:114:ALA:HB2	1.95	0.48
1:G:294:TYR:OH	1:G:296:VAL:HB	2.13	0.48
1:A:95:LEU:HB2	1:A:352:VAL:HG21	1.96	0.48
1:A:131:MET:HE3	1:A:311:LEU:HB2	1.96	0.48
1:C:294:TYR:HE2	1:C:299:MET:HE3	1.79	0.48
1:F:1:MET:N	1:F:31:HIS:HD2	2.12	0.48
1:A:169:VAL:HG22	1:A:232:LEU:HB3	1.95	0.48
1:C:204:TYR:O	1:C:208:VAL:HG13	2.11	0.48
1:C:287:VAL:HG13	1:C:291:VAL:O	2.14	0.48
1:G:149:LYS:HB3	1:G:150:PRO:HD3	1.94	0.48
1:A:68:MET:HA	1:A:88:ILE:HG23	1.95	0.48
1:D:11:THR:O	1:D:12:LEU:HB2	2.13	0.48
1:F:353:ALA:CB	1:F:360:TYR:HB2	2.43	0.48
1:E:362:PRO:HB2	1:E:365:GLU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:VAL:O	1:F:197:VAL:HG12	2.13	0.47
1:G:102:THR:O	1:G:106:LEU:HG	2.13	0.47
1:A:47:ASP:HB3	1:A:57:LEU:HD11	1.96	0.47
1:C:127:LEU:HD22	1:C:315:THR:HG22	1.96	0.47
1:A:67:GLU:O	1:A:88:ILE:HG23	2.14	0.47
1:E:209:PHE:O	1:E:212:ARG:HD3	2.14	0.47
1:A:224:LYS:HZ2	1:E:28:ARG:HH12	1.60	0.47
1:D:71:LYS:NZ	2:D:386:HOH:O	2.41	0.47
1:D:72:VAL:O	1:D:92:TYR:HB2	2.14	0.47
1:D:200:LYS:HZ1	1:F:124:THR:HG21	1.78	0.47
1:E:17:ALA:HB1	1:E:70:VAL:HG12	1.96	0.47
1:E:103:GLU:O	1:E:107:ARG:HG3	2.15	0.47
1:E:253:LEU:HD12	1:E:256:MET:CE	2.44	0.47
1:E:362:PRO:HB2	1:E:365:GLU:CB	2.44	0.47
1:D:2:VAL:HG22	1:D:32:THR:CG2	2.45	0.47
1:G:350:PRO:HD3	1:G:360:TYR:CE1	2.49	0.47
1:C:23:VAL:HG11	1:C:55:ALA:HB2	1.96	0.47
1:E:134:VAL:HG21	1:E:300:PRO:HB3	1.96	0.47
1:C:11:THR:O	1:C:12:LEU:HB2	2.15	0.46
1:C:294:TYR:CE2	1:C:299:MET:HE3	2.50	0.46
1:A:316:LEU:HB3	1:A:317:PRO:HD3	1.97	0.46
1:A:224:LYS:NZ	1:E:28:ARG:HH12	2.14	0.46
1:C:209:PHE:O	1:C:212:ARG:HD3	2.15	0.46
1:C:248:VAL:HA	1:C:252:MET:SD	2.55	0.46
1:D:22:GLY:O	1:D:26:LEU:HD22	2.16	0.46
1:D:106:LEU:O	1:D:345:GLY:HA2	2.15	0.46
1:D:145:GLN:O	1:D:148:GLU:HB2	2.14	0.46
1:A:68:MET:HA	1:A:88:ILE:O	2.16	0.46
1:A:204:TYR:O	1:A:208:VAL:HG13	2.16	0.46
1:A:204:TYR:O	1:A:208:VAL:CG1	2.64	0.46
1:C:200:LYS:HZ1	1:D:124:THR:HG21	1.79	0.46
1:F:1:MET:HG2	1:F:2:VAL:N	2.31	0.46
1:F:95:LEU:CD1	1:F:341:ASN:HB3	2.46	0.46
1:C:142:VAL:CG2	1:C:299:MET:HE2	2.44	0.46
1:D:111:THR:HB	1:D:343:HIS:CD2	2.51	0.46
1:D:138:MET:O	1:D:141:GLN:HB3	2.16	0.46
1:E:60:ARG:NH1	1:E:60:ARG:HG3	2.30	0.46
1:A:93:LEU:O	1:A:94:HIS:C	2.59	0.46
1:A:170:VAL:HG22	1:A:193:THR:HG21	1.97	0.46
1:A:235:GLY:O	1:A:265:VAL:HG23	2.16	0.46
1:C:122:ASP:CG	1:C:124:THR:HG23	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:VAL:HG21	1:F:299:MET:CE	2.46	0.46
1:F:186:LEU:HG	1:F:213:VAL:HG23	1.98	0.46
1:G:99:ARG:HD2	1:G:356:PHE:CD1	2.51	0.46
1:A:26:LEU:CD1	1:A:320:LEU:HD12	2.47	0.45
1:A:71:LYS:HE3	1:A:73:LYS:O	2.16	0.45
1:C:119:GLN:O	1:C:335:ALA:HA	2.16	0.45
1:C:337:LEU:CD2	1:C:363:PRO:HB2	2.46	0.45
1:D:129:VAL:N	1:D:130:PRO:CD	2.79	0.45
1:D:301:GLY:O	1:D:304:PRO:HD3	2.16	0.45
1:A:248:VAL:HA	1:A:252:MET:SD	2.56	0.45
1:C:346:ARG:HH11	1:C:346:ARG:HG3	1.81	0.45
1:D:137:ARG:NE	1:D:180:ASN:HD22	1.97	0.45
1:E:125:LEU:O	1:E:129:VAL:HG23	2.16	0.45
1:G:256:MET:CE	1:G:291:VAL:HG11	2.46	0.45
1:F:11:THR:O	1:F:12:LEU:HB2	2.16	0.45
1:D:237:VAL:HB	1:D:238:LEU:H	1.57	0.45
1:A:134:VAL:CG2	1:A:300:PRO:HG3	2.44	0.45
1:E:223:ILE:O	1:E:227:VAL:HG23	2.17	0.45
1:D:195:LEU:HG	1:D:216:LEU:HB2	1.99	0.45
1:E:131:MET:HE2	1:E:131:MET:HA	1.99	0.45
1:E:149:LYS:HB3	1:E:150:PRO:HD3	1.98	0.45
1:F:49:GLU:HA	1:F:52:ARG:NH1	2.32	0.45
1:A:228:GLN:HG3	1:A:255:LEU:HB3	1.98	0.45
1:A:299:MET:HB2	1:A:300:PRO:HD3	1.99	0.45
1:D:114:ALA:HB1	1:D:116:GLU:CD	2.42	0.45
1:D:200:LYS:HZ3	1:F:124:THR:HG21	1.79	0.45
1:A:130:PRO:CG	1:A:314:GLN:HG3	2.47	0.45
1:C:147:LEU:HD12	1:C:158:LEU:HD21	1.98	0.45
1:D:134:VAL:HG21	1:D:300:PRO:HB3	1.99	0.45
1:A:157:LEU:HD21	1:D:137:ARG:HB2	1.98	0.45
1:E:130:PRO:HG2	1:E:314:GLN:HG3	1.99	0.45
1:A:88:ILE:O	1:A:88:ILE:HG13	2.16	0.44
1:D:137:ARG:HE	1:D:180:ASN:ND2	1.97	0.44
1:C:337:LEU:HD22	1:C:363:PRO:HB2	2.00	0.44
1:E:9:ILE:CD1	1:E:76:LEU:HD12	2.47	0.44
1:E:129:VAL:HB	1:E:130:PRO:HD3	1.98	0.44
1:E:174:GLY:HA2	1:E:194:ILE:HD11	2.00	0.44
1:E:294:TYR:OH	1:E:296:VAL:HB	2.16	0.44
1:F:29:ARG:HG3	1:F:29:ARG:HH11	1.81	0.44
1:E:299:MET:HB2	1:E:300:PRO:HD3	1.99	0.44
1:G:104:ALA:HA	1:G:107:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:VAL:HG22	1:G:193:THR:HG23	1.98	0.44
1:D:195:LEU:HA	1:D:216:LEU:O	2.18	0.44
1:D:264:ASP:OD1	1:D:266:ALA:HB3	2.18	0.44
1:C:223:ILE:O	1:C:227:VAL:HG23	2.18	0.44
1:C:330:LEU:HD12	1:C:330:LEU:N	2.33	0.44
1:E:76:LEU:O	1:E:77:PRO:C	2.60	0.44
1:F:149:LYS:HB3	1:F:150:PRO:HD3	2.00	0.44
1:C:72:VAL:O	1:C:92:TYR:HB2	2.18	0.43
1:E:205:LEU:HD23	1:E:205:LEU:HA	1.87	0.43
1:F:71:LYS:HE3	1:F:73:LYS:O	2.17	0.43
1:G:95:LEU:HD12	1:G:341:ASN:HD22	1.83	0.43
1:A:223:ILE:O	1:A:227:VAL:HG23	2.18	0.43
1:C:170:VAL:HG11	1:C:226:SER:HB3	2.00	0.43
1:F:77:PRO:HA	1:F:80:TYR:CE2	2.53	0.43
1:G:91:THR:HA	1:G:115:TYR:CE2	2.53	0.43
1:D:125:LEU:O	1:D:129:VAL:HG23	2.18	0.43
1:E:298:ASN:HD22	1:E:301:GLY:HA3	1.83	0.43
1:G:11:THR:O	1:G:12:LEU:HB2	2.18	0.43
1:C:322:LEU:HD21	1:C:330:LEU:HD11	2.00	0.43
1:D:134:VAL:HG23	1:D:300:PRO:HG3	2.01	0.43
1:E:142:VAL:HG21	1:E:299:MET:HE2	2.00	0.43
1:G:49:GLU:HA	1:G:52:ARG:NH1	2.34	0.43
1:A:28:ARG:HH12	1:G:224:LYS:NZ	2.16	0.43
1:E:110:VAL:HG22	1:E:111:THR:N	2.34	0.43
1:E:342:THR:HA	1:E:346:ARG:O	2.19	0.43
1:D:95:LEU:CD1	1:D:341:ASN:HD22	2.31	0.43
1:D:340:LEU:HG	1:D:348:THR:OG1	2.17	0.43
1:C:49:GLU:HA	1:C:52:ARG:NH1	2.34	0.43
1:D:194:ILE:HD13	1:D:205:LEU:CD1	2.48	0.43
1:E:105:MET:CE	1:E:112:GLY:HA3	2.49	0.43
1:E:199:HIS:HD2	2:E:424:HOH:O	2.01	0.43
1:F:88:ILE:HG13	1:F:88:ILE:O	2.19	0.43
1:A:249:THR:OG1	1:A:251:ASP:HB2	2.18	0.43
1:A:16:VAL:HG11	1:A:45:LEU:HD12	2.00	0.43
1:A:222:ASN:HD22	1:A:222:ASN:HA	1.60	0.43
1:E:17:ALA:HB2	1:E:71:LYS:C	2.44	0.43
1:E:37:ARG:NH2	2:E:403:HOH:O	2.52	0.43
1:E:50:TYR:O	1:E:53:ALA:HB3	2.19	0.43
1:E:99:ARG:HD2	1:E:356:PHE:CD1	2.54	0.43
1:F:195:LEU:HG	1:F:216:LEU:HB2	2.01	0.43
1:C:350:PRO:HD3	1:C:360:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:ASN:ND2	1:E:301:GLY:CA	2.82	0.43
1:E:361:THR:O	1:E:362:PRO:C	2.62	0.43
1:F:363:PRO:O	1:F:367:LEU:HB2	2.19	0.42
1:G:99:ARG:HB2	1:G:356:PHE:CE1	2.54	0.42
1:A:129:VAL:HB	1:A:130:PRO:HD3	2.01	0.42
1:E:250:ARG:HG2	1:E:250:ARG:HH11	1.84	0.42
1:F:1:MET:N	1:F:31:HIS:CD2	2.87	0.42
1:G:106:LEU:HD23	1:G:106:LEU:HA	1.84	0.42
1:G:122:ASP:OD2	1:G:124:THR:HG23	2.19	0.42
1:A:308:THR:O	1:A:312:THR:HG23	2.19	0.42
1:D:23:VAL:HG22	1:D:33:VAL:HG11	2.01	0.42
1:G:88:ILE:C	1:G:88:ILE:HD12	2.45	0.42
1:F:301:GLY:O	1:F:304:PRO:HD3	2.19	0.42
1:A:177:VAL:HG23	2:A:398:HOH:O	2.18	0.42
1:C:84:ARG:HG2	1:C:84:ARG:HH11	1.84	0.42
1:C:170:VAL:HG22	1:C:193:THR:HG23	2.00	0.42
1:F:34:LEU:HD11	2:F:375:HOH:O	2.18	0.42
1:F:142:VAL:HG11	1:F:294:TYR:CE2	2.54	0.42
1:A:35:VAL:CG2	1:A:55:ALA:HB1	2.50	0.42
1:E:9:ILE:HD11	1:E:79:GLU:CD	2.44	0.42
1:F:349:HIS:HA	1:F:350:PRO:HD2	1.82	0.42
1:C:204:TYR:CE2	1:C:208:VAL:HG11	2.55	0.42
1:E:250:ARG:HG2	1:E:250:ARG:NH1	2.34	0.42
1:F:130:PRO:CG	1:F:314:GLN:HG3	2.49	0.42
1:D:163:GLY:O	1:G:216:LEU:HA	2.19	0.42
1:D:206:ASP:O	1:D:210:GLY:O	2.37	0.42
1:E:145:GLN:O	1:E:148:GLU:HB2	2.19	0.42
1:C:124:THR:HG21	1:F:200:LYS:HZ3	1.82	0.42
1:D:47:ASP:HB3	1:D:57:LEU:CD1	2.48	0.42
1:D:238:LEU:CB	1:D:266:ALA:HB1	2.49	0.42
1:E:130:PRO:CG	1:E:314:GLN:HG3	2.50	0.42
1:E:356:PHE:O	1:E:357:GLY:C	2.63	0.42
1:D:142:VAL:HG11	1:D:294:TYR:CE2	2.55	0.42
1:D:316:LEU:HB3	1:D:317:PRO:HD3	2.00	0.42
1:F:237:VAL:HB	1:F:238:LEU:H	1.51	0.42
1:G:209:PHE:O	1:G:212:ARG:HD3	2.20	0.42
1:A:9:ILE:HG13	1:A:76:LEU:HD12	2.02	0.41
1:C:38:GLY:HA2	1:C:41:GLU:HG3	2.02	0.41
1:F:350:PRO:HD3	1:F:360:TYR:CE1	2.55	0.41
1:A:92:TYR:CD1	1:A:115:TYR:HB2	2.55	0.41
1:A:173:GLY:O	1:A:178:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:MET:HE2	1:D:302:ALA:HB3	2.01	0.41
1:D:288:VAL:O	1:D:289:ASP:HB2	2.20	0.41
1:D:77:PRO:HD2	2:D:390:HOH:O	2.19	0.41
1:E:172:LEU:HD23	1:E:195:LEU:HD13	2.01	0.41
1:E:320:LEU:HD12	1:E:320:LEU:HA	1.87	0.41
1:G:3:ILE:HD11	1:G:323:ALA:CB	2.47	0.41
1:G:95:LEU:C	1:G:97:ALA:N	2.78	0.41
1:G:114:ALA:N	1:G:339:GLY:O	2.48	0.41
1:G:136:GLY:O	1:G:140:PRO:HD2	2.19	0.41
1:A:68:MET:CA	1:A:88:ILE:HG23	2.50	0.41
1:C:7:LYS:HG3	1:C:39:ALA:HA	2.03	0.41
1:E:1:MET:N	1:E:31:HIS:HD2	2.19	0.41
1:E:29:ARG:HG3	1:E:29:ARG:NH1	2.31	0.41
1:F:56:GLU:OE1	2:F:375:HOH:O	2.21	0.41
1:F:119:GLN:O	1:F:335:ALA:HA	2.21	0.41
1:G:288:VAL:HB	1:G:293:HIS:CE1	2.56	0.41
1:A:138:MET:SD	1:D:157:LEU:HD13	2.60	0.41
1:A:227:VAL:O	1:A:256:MET:HG2	2.20	0.41
1:A:349:HIS:HA	1:A:350:PRO:HD2	1.86	0.41
1:E:1:MET:HG3	1:E:67:GLU:OE1	2.21	0.41
1:E:75:PRO:HA	1:E:79:GLU:OE1	2.21	0.41
1:G:17:ALA:HB2	1:G:71:LYS:C	2.45	0.41
1:G:72:VAL:O	1:G:92:TYR:HB2	2.21	0.41
1:A:1:MET:HG2	1:A:2:VAL:N	2.35	0.41
1:C:172:LEU:O	1:C:237:VAL:HG22	2.20	0.41
1:C:250:ARG:HH11	1:C:250:ARG:HG2	1.85	0.41
1:D:79:GLU:C	1:D:81:GLY:N	2.77	0.41
1:E:122:ASP:CG	1:E:124:THR:HG23	2.46	0.41
1:E:343:HIS:O	1:E:344:LYS:HB2	2.20	0.41
1:A:122:ASP:CG	1:A:124:THR:HG23	2.46	0.41
1:A:299:MET:C	1:A:301:GLY:N	2.76	0.41
1:C:237:VAL:HB	1:C:238:LEU:H	1.49	0.41
1:D:62:GLU:HB2	2:D:414:HOH:O	2.19	0.41
1:E:129:VAL:N	1:E:130:PRO:CD	2.84	0.41
1:E:348:THR:HA	1:E:361:THR:O	2.19	0.41
1:G:325:LYS:O	1:G:328:ASP:HB2	2.21	0.41
1:G:367:LEU:HD12	1:G:367:LEU:HA	1.84	0.41
1:A:76:LEU:O	1:A:77:PRO:C	2.63	0.41
1:A:142:VAL:HG21	1:A:299:MET:CE	2.50	0.41
1:A:224:LYS:NZ	1:E:28:ARG:NH1	2.68	0.41
1:A:315:THR:O	1:A:319:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:LEU:HD12	1:C:341:ASN:HB3	2.03	0.41
1:C:140:PRO:HG3	1:C:184:ILE:HB	2.03	0.41
1:D:337:LEU:CD2	1:D:363:PRO:HB2	2.51	0.41
1:E:61:GLU:HG3	1:E:82:PHE:HE2	1.86	0.41
1:E:161:VAL:O	1:E:162:PRO:C	2.64	0.41
1:F:26:LEU:CD1	1:F:320:LEU:HD12	2.51	0.41
1:F:129:VAL:N	1:F:130:PRO:CD	2.84	0.41
1:A:130:PRO:HG3	1:A:314:GLN:HG3	2.02	0.41
1:C:69:VAL:HG23	1:C:87:LEU:HD11	2.03	0.41
1:D:68:MET:HG3	1:D:88:ILE:HG13	2.03	0.41
1:E:78:GLU:HB3	2:E:387:HOH:O	2.20	0.41
1:G:249:THR:C	1:G:251:ASP:N	2.79	0.41
1:A:3:ILE:HD12	1:A:26:LEU:HG	2.02	0.40
1:A:256:MET:HE3	1:A:291:VAL:HG21	2.03	0.40
1:C:91:THR:HA	1:C:115:TYR:CE2	2.56	0.40
1:C:145:GLN:O	1:C:148:GLU:HB2	2.21	0.40
1:E:88:ILE:O	1:E:88:ILE:HG13	2.21	0.40
1:E:95:LEU:O	1:E:356:PHE:HE2	2.04	0.40
1:F:134:VAL:HG21	1:F:300:PRO:HB3	2.04	0.40
1:D:204:TYR:O	1:D:208:VAL:HG13	2.21	0.40
1:A:60:ARG:CG	1:A:60:ARG:HH11	2.34	0.40
1:C:361:THR:O	1:C:362:PRO:C	2.65	0.40
1:D:367:LEU:HD12	1:D:367:LEU:HA	1.88	0.40
1:E:165:ALA:HB2	1:F:216:LEU:HD21	2.03	0.40
1:F:199:HIS:O	1:F:203:GLN:HG3	2.21	0.40
1:F:232:LEU:HD13	1:F:261:VAL:HG22	2.03	0.40
1:A:193:THR:HG22	2:A:377:HOH:O	2.20	0.40
1:C:113:ILE:HA	1:C:339:GLY:O	2.22	0.40
1:D:224:LYS:HE2	1:D:224:LYS:HB2	1.88	0.40
1:E:120:LEU:HD12	1:E:124:THR:OG1	2.21	0.40
1:F:186:LEU:HG	1:F:213:VAL:CG2	2.52	0.40
1:G:84:ARG:O	1:G:110:VAL:HA	2.22	0.40
1:F:2:VAL:HG22	1:F:32:THR:HG23	2.04	0.40
1:F:256:MET:CE	1:F:291:VAL:HG11	2.51	0.40
1:F:303:VAL:O	1:F:303:VAL:HG23	2.22	0.40
1:F:362:PRO:HA	1:F:363:PRO:HD2	1.87	0.40
1:G:219:THR:O	1:G:223:ILE:HG13	2.22	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	337/369 (91%)	308 (91%)	26 (8%)	3 (1%)	14	33
1	C	337/369 (91%)	319 (95%)	15 (4%)	3 (1%)	14	33
1	D	337/369 (91%)	317 (94%)	17 (5%)	3 (1%)	14	33
1	E	337/369 (91%)	310 (92%)	22 (6%)	5 (2%)	8	20
1	F	337/369 (91%)	317 (94%)	17 (5%)	3 (1%)	14	33
1	G	337/369 (91%)	324 (96%)	10 (3%)	3 (1%)	14	33
All	All	2022/2214 (91%)	1895 (94%)	107 (5%)	20 (1%)	12	30

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	VAL
1	A	297	ALA
1	C	297	ALA
1	D	297	ALA
1	E	297	ALA
1	F	297	ALA
1	G	297	ALA
1	A	298	ASN
1	D	298	ASN
1	E	237	VAL
1	F	237	VAL
1	G	237	VAL
1	C	237	VAL
1	D	237	VAL
1	G	218	ALA
1	E	298	ASN
1	F	211	GLY
1	E	80	TYR
1	C	211	GLY
1	E	211	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	259/282 (92%)	242 (93%)	17 (7%)	15	35
1	C	259/282 (92%)	243 (94%)	16 (6%)	16	38
1	D	259/282 (92%)	243 (94%)	16 (6%)	16	38
1	E	259/282 (92%)	245 (95%)	14 (5%)	20	43
1	F	259/282 (92%)	242 (93%)	17 (7%)	15	35
1	G	259/282 (92%)	243 (94%)	16 (6%)	16	38
All	All	1554/1692 (92%)	1458 (94%)	96 (6%)	16	38

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	32	THR
1	A	34	LEU
1	A	60	ARG
1	A	88	ILE
1	A	103	GLU
1	A	111	THR
1	A	134	VAL
1	A	161	VAL
1	A	186	LEU
1	A	208	VAL
1	A	237	VAL
1	A	253	LEU
1	A	261	VAL
1	A	320	LEU
1	A	337	LEU
1	A	367	LEU
1	C	26	LEU
1	C	32	THR
1	C	34	LEU
1	C	60	ARG
1	C	88	ILE

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Mol	Chain	Res	Type
1	C	111	THR
1	C	134	VAL
1	C	186	LEU
1	C	193	THR
1	C	208	VAL
1	C	237	VAL
1	C	253	LEU
1	C	261	VAL
1	C	320	LEU
1	C	337	LEU
1	C	367	LEU
1	D	26	LEU
1	D	32	THR
1	D	34	LEU
1	D	60	ARG
1	D	88	ILE
1	D	111	THR
1	D	134	VAL
1	D	186	LEU
1	D	193	THR
1	D	208	VAL
1	D	222	ASN
1	D	237	VAL
1	D	261	VAL
1	D	320	LEU
1	D	337	LEU
1	D	367	LEU
1	E	32	THR
1	E	34	LEU
1	E	60	ARG
1	E	77	PRO
1	E	88	ILE
1	E	111	THR
1	E	134	VAL
1	E	186	LEU
1	E	193	THR
1	E	208	VAL
1	E	237	VAL
1	E	261	VAL
1	E	320	LEU
1	E	337	LEU
1	F	32	THR

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Mol	Chain	Res	Type
1	F	34	LEU
1	F	60	ARG
1	F	88	ILE
1	F	111	THR
1	F	124	THR
1	F	134	VAL
1	F	186	LEU
1	F	193	THR
1	F	208	VAL
1	F	237	VAL
1	F	253	LEU
1	F	257	LYS
1	F	261	VAL
1	F	320	LEU
1	F	337	LEU
1	F	367	LEU
1	G	26	LEU
1	G	32	THR
1	G	34	LEU
1	G	60	ARG
1	G	88	ILE
1	G	111	THR
1	G	134	VAL
1	G	186	LEU
1	G	193	THR
1	G	208	VAL
1	G	237	VAL
1	G	253	LEU
1	G	261	VAL
1	G	320	LEU
1	G	337	LEU
1	G	367	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	31	HIS
1	A	94	HIS
1	A	145	GLN
1	A	180	ASN
1	A	191	GLN

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Mol	Chain	Res	Type
1	A	222	ASN
1	A	298	ASN
1	A	341	ASN
1	A	343	HIS
1	C	14	ASN
1	C	31	HIS
1	C	141	GLN
1	C	180	ASN
1	C	191	GLN
1	C	199	HIS
1	C	222	ASN
1	C	228	GLN
1	C	298	ASN
1	C	341	ASN
1	C	343	HIS
1	D	14	ASN
1	D	141	GLN
1	D	180	ASN
1	D	191	GLN
1	D	222	ASN
1	D	293	HIS
1	D	341	ASN
1	D	343	HIS
1	E	14	ASN
1	E	31	HIS
1	E	141	GLN
1	E	145	GLN
1	E	180	ASN
1	E	191	GLN
1	E	199	HIS
1	E	222	ASN
1	E	298	ASN
1	E	314	GLN
1	E	341	ASN
1	E	343	HIS
1	F	14	ASN
1	F	31	HIS
1	F	141	GLN
1	F	145	GLN
1	F	180	ASN
1	F	191	GLN
1	F	199	HIS

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Mol	Chain	Res	Type
1	F	222	ASN
1	F	343	HIS
1	G	31	HIS
1	G	141	GLN
1	G	145	GLN
1	G	180	ASN
1	G	199	HIS
1	G	222	ASN
1	G	293	HIS
1	G	343	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](#)

There are no ligands in this entry.

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	343/369 (92%)	0.15	19 (5%) 30 27	13, 35, 61, 72	0
1	C	343/369 (92%)	-0.16	15 (4%) 39 36	11, 26, 58, 70	0
1	D	343/369 (92%)	-0.08	16 (4%) 36 33	15, 28, 59, 69	0
1	E	343/369 (92%)	0.05	16 (4%) 36 33	13, 34, 60, 72	0
1	F	343/369 (92%)	-0.07	15 (4%) 39 36	11, 28, 60, 74	0
1	G	343/369 (92%)	-0.05	9 (2%) 57 54	14, 32, 59, 72	0
All	All	2058/2214 (92%)	-0.02	90 (4%) 39 36	11, 31, 60, 74	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	238	LEU	5.1
1	G	369	GLY	4.6
1	A	287	VAL	4.4
1	F	294	TYR	4.3
1	C	297	ALA	4.1
1	E	369	GLY	4.1
1	C	289	ASP	4.0
1	C	252	MET	3.8
1	F	247	LEU	3.7
1	C	266	ALA	3.5
1	F	369	GLY	3.5
1	F	297	ALA	3.4
1	F	238	LEU	3.4
1	E	67	GLU	3.4
1	F	210	GLY	3.4
1	C	294	TYR	3.3
1	C	287	VAL	3.3
1	C	247	LEU	3.3
1	D	354	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	289	ASP	3.2
1	G	247	LEU	3.2
1	E	288	VAL	3.2
1	F	287	VAL	3.2
1	A	250	ARG	3.1
1	D	288	VAL	3.1
1	D	107	ARG	3.1
1	E	85	GLU	3.0
1	F	266	ALA	3.0
1	D	287	VAL	2.9
1	A	288	VAL	2.9
1	C	288	VAL	2.9
1	A	369	GLY	2.8
1	F	289	ASP	2.8
1	F	293	HIS	2.8
1	C	253	LEU	2.7
1	A	238	LEU	2.7
1	A	345	GLY	2.7
1	D	103	GLU	2.6
1	D	255	LEU	2.6
1	F	248	VAL	2.6
1	C	246	LYS	2.5
1	F	368	ARG	2.5
1	G	246	LYS	2.5
1	A	294	TYR	2.5
1	A	247	LEU	2.5
1	C	238	LEU	2.5
1	E	361	THR	2.5
1	C	250	ARG	2.5
1	F	255	LEU	2.5
1	E	250	ARG	2.4
1	A	210	GLY	2.4
1	A	295	GLY	2.4
1	A	346	ARG	2.4
1	C	251	ASP	2.4
1	D	297	ALA	2.4
1	E	86	GLY	2.4
1	E	297	ALA	2.4
1	E	210	GLY	2.3
1	D	99	ARG	2.3
1	E	296	VAL	2.3
1	F	288	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	296	VAL	2.3
1	D	210	GLY	2.3
1	G	107	ARG	2.3
1	A	289	ASP	2.3
1	C	295	GLY	2.3
1	A	253	LEU	2.2
1	E	295	GLY	2.2
1	F	295	GLY	2.2
1	G	287	VAL	2.2
1	A	266	ALA	2.2
1	D	246	LYS	2.2
1	A	251	ASP	2.2
1	D	294	TYR	2.1
1	D	266	ALA	2.1
1	G	359	PRO	2.1
1	D	355	ALA	2.1
1	E	246	LYS	2.1
1	G	288	VAL	2.1
1	E	298	ASN	2.1
1	A	293	HIS	2.1
1	C	296	VAL	2.1
1	A	355	ALA	2.0
1	D	251	ASP	2.0
1	E	103	GLU	2.0
1	G	289	ASP	2.0
1	A	105	MET	2.0
1	A	248	VAL	2.0
1	E	80	TYR	2.0
1	E	360	TYR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.