



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:50 AM UTC

PDB ID : 3K1G / pdb_00003k1g
Title : Crystal structure of Dipeptide Epimerase from *Enterococcus faecalis* V583 complexed with Mg and dipeptide L-Ser-L-Tyr
Authors : Fedorov, A.A.; Fedorov, E.V.; Imker, H.J.; Sakai, A.; Gerlt, J.A.; Almo, S.C.
Deposited on : 2009-09-27
Resolution : 2.00 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

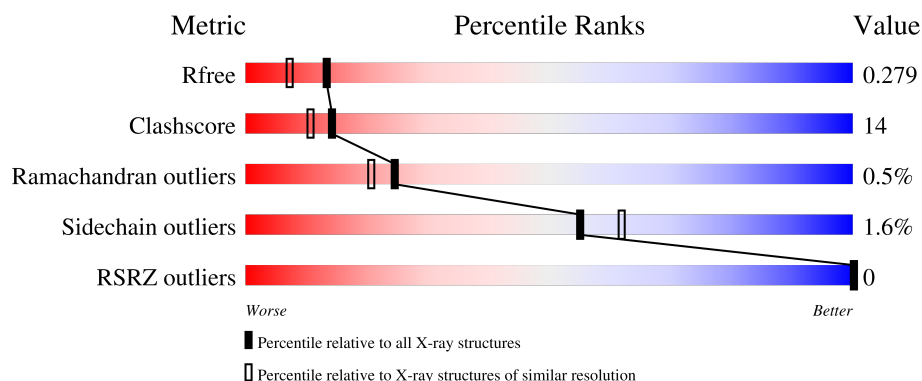
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

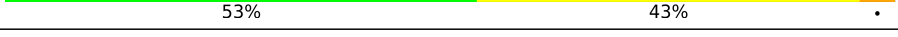
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	354	
1	B	354	
1	C	354	
1	D	354	
1	E	354	

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Mol	Chain	Length	Quality of chain
1	F	354	 58% 40% •
1	G	354	 74% 25% •
1	H	354	 82% 17% •

2 Entry composition

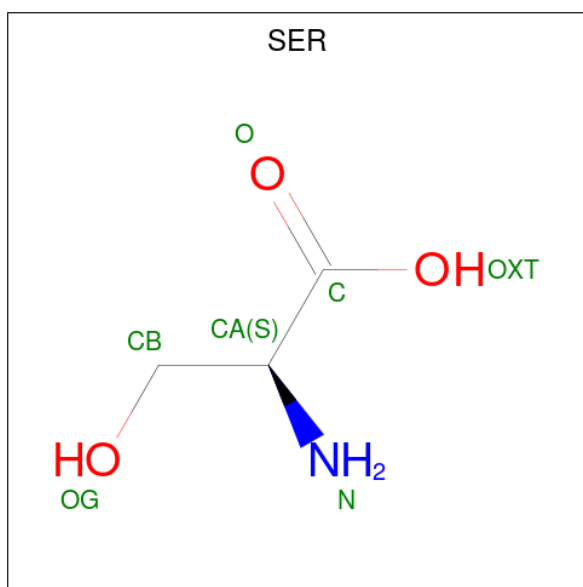
There are 6 unique types of molecules in this entry. The entry contains 21863 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dipeptide Epimerase.

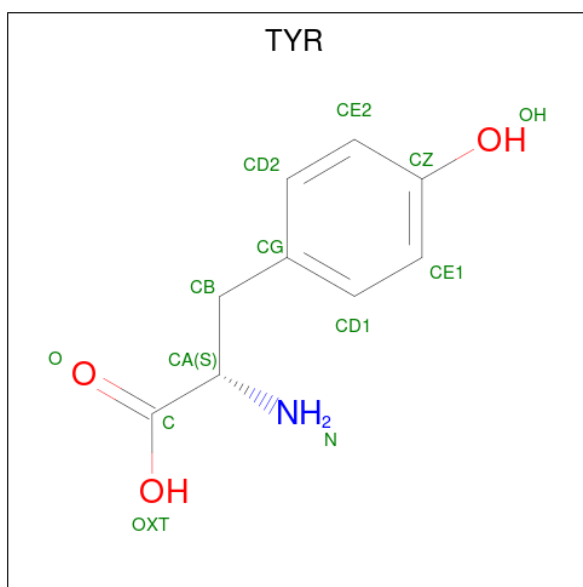
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2649	1680	437	518	14			
1	B	353	Total	C	N	O	S	0	0	0
			2638	1674	434	516	14			
1	C	354	Total	C	N	O	S	0	0	0
			2649	1680	437	518	14			
1	D	354	Total	C	N	O	S	0	0	0
			2649	1680	437	518	14			
1	E	354	Total	C	N	O	S	0	0	0
			2649	1680	437	518	14			
1	F	354	Total	C	N	O	S	0	0	0
			2649	1680	437	518	14			
1	G	354	Total	C	N	O	S	0	0	0
			2649	1680	437	518	14			
1	H	353	Total	C	N	O	S	0	0	0
			2638	1674	434	516	14			

- Molecule 2 is SERINE (CCD ID: SER) (formula: $\text{C}_3\text{H}_7\text{NO}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			6	3	1	2		
2	B	1	Total	C	N	O	0	0
			6	3	1	2		
2	C	1	Total	C	N	O	0	0
			6	3	1	2		
2	D	1	Total	C	N	O	0	0
			6	3	1	2		
2	E	1	Total	C	N	O	0	0
			6	3	1	2		
2	F	1	Total	C	N	O	0	0
			6	3	1	2		
2	G	1	Total	C	N	O	0	0
			6	3	1	2		
2	H	1	Total	C	N	O	0	0
			6	3	1	2		

- Molecule 3 is TYROSINE (CCD ID: TYR) (formula: C₉H₁₁NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	9	1	3		
3	B	1	Total	C	N	O	0	0
			13	9	1	3		
3	C	1	Total	C	N	O	0	0
			13	9	1	3		
3	D	1	Total	C	N	O	0	0
			13	9	1	3		
3	E	1	Total	C	N	O	0	0
			13	9	1	3		
3	F	1	Total	C	N	O	0	0
			13	9	1	3		
3	G	1	Total	C	N	O	0	0
			13	9	1	3		
3	H	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total 1	Mg 1	0	0
5	F	1	Total 1	Mg 1	0	0
5	G	1	Total 1	Mg 1	0	0
5	H	1	Total 1	Mg 1	0	0

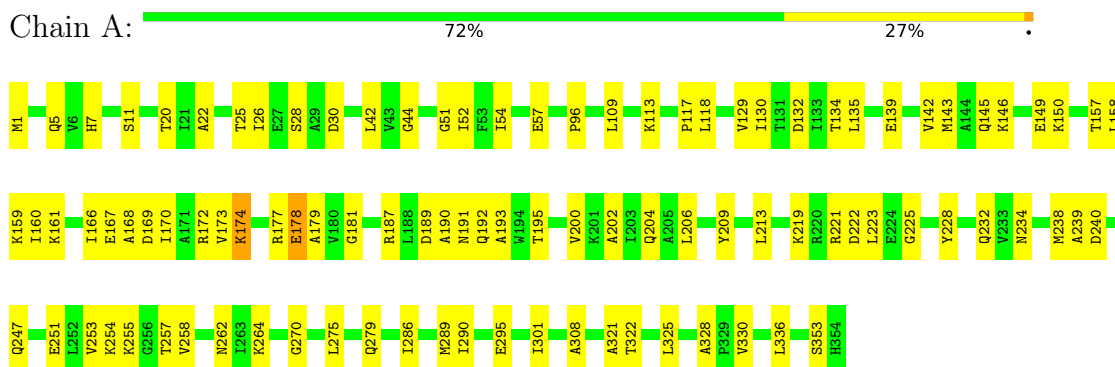
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	70	Total 70	O 70	0	0
6	B	93	Total 93	O 93	0	0
6	C	47	Total 47	O 47	0	0
6	D	26	Total 26	O 26	0	0
6	E	56	Total 56	O 56	0	0
6	F	27	Total 27	O 27	0	0
6	G	74	Total 74	O 74	0	0
6	H	92	Total 92	O 92	0	0

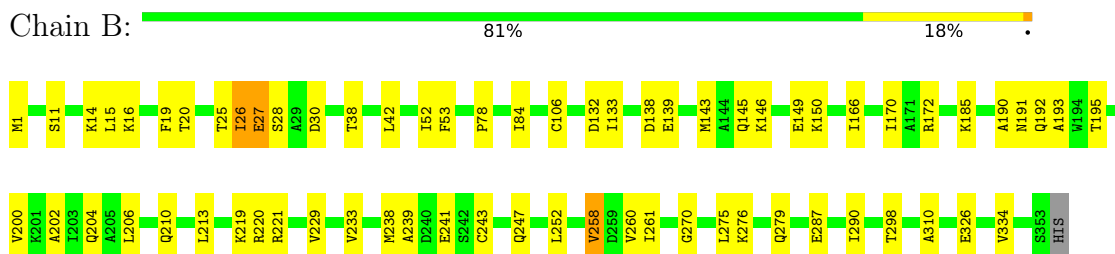
3 Residue-property plots

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

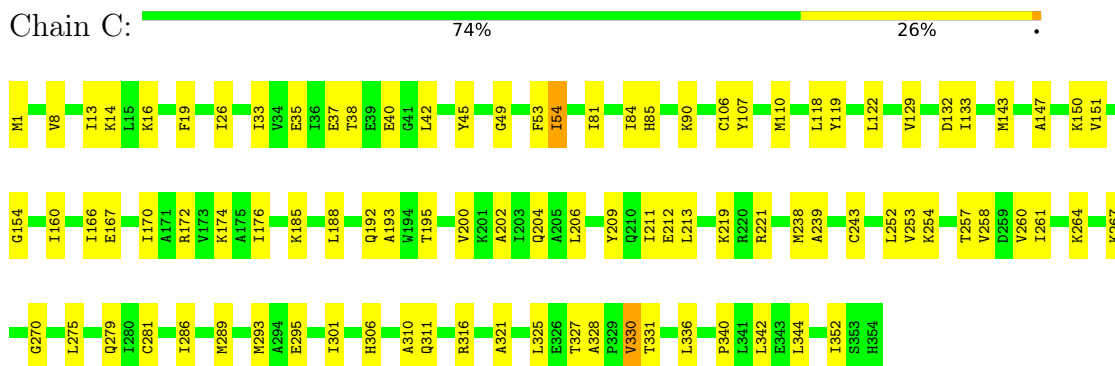
• Molecule 1: Dipeptide Epimerase



• Molecule 1: Dipeptide Epimerase

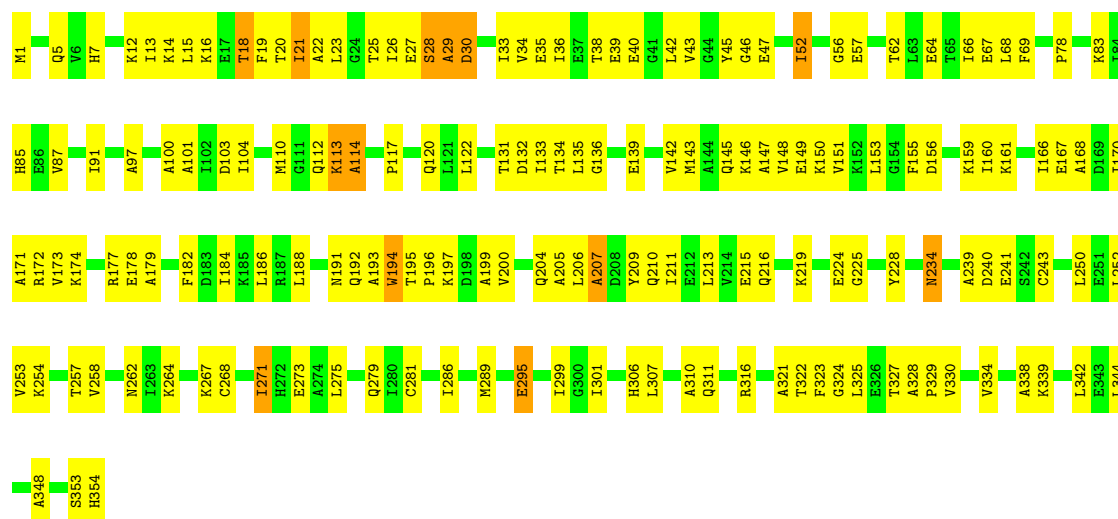


• Molecule 1: Dipeptide Epimerase



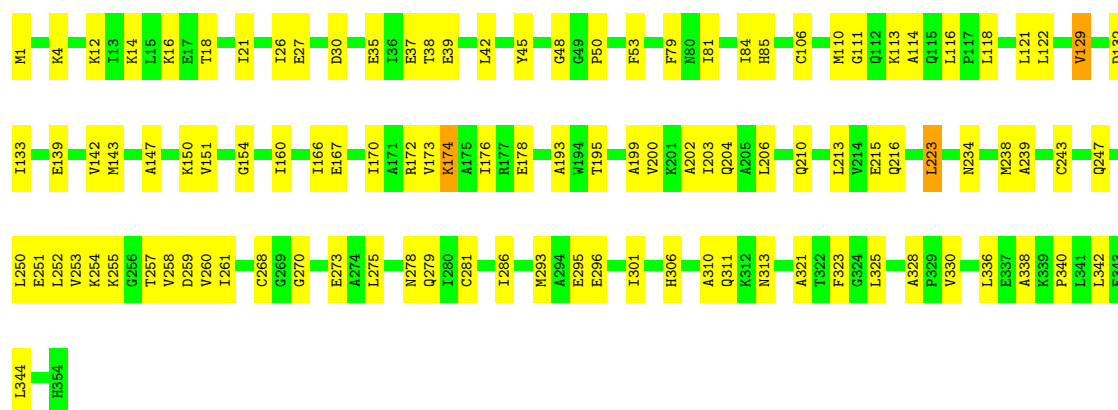
• Molecule 1: Dipeptide Epimerase

Chain D:  53% 43%



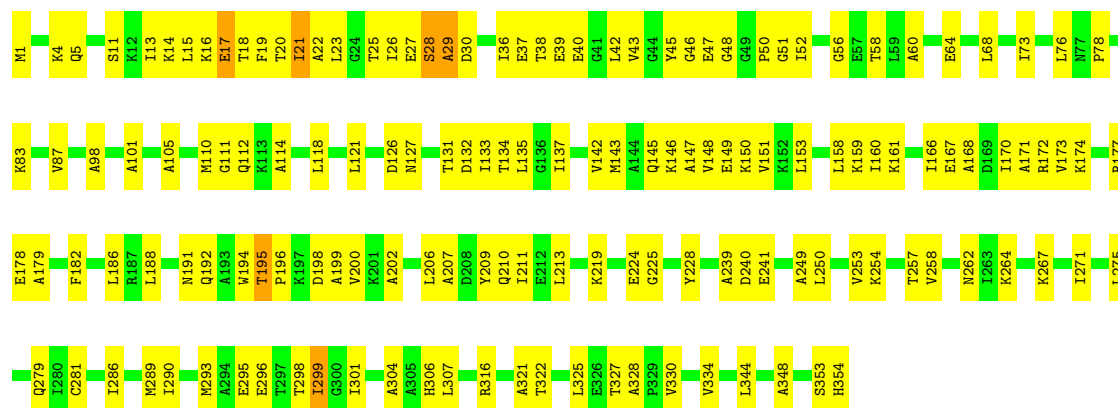
• Molecule 1: Dipeptide Epimerase

Chain E:  70% 29%

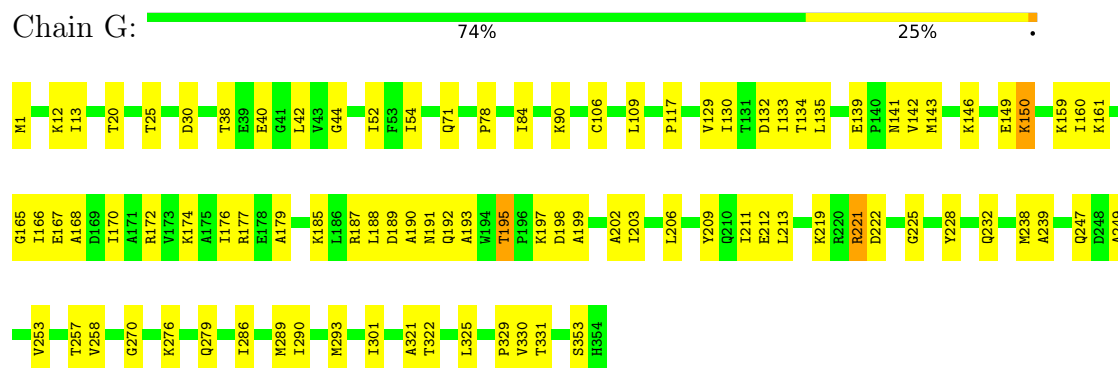


• Molecule 1: Dipeptide Epimerase

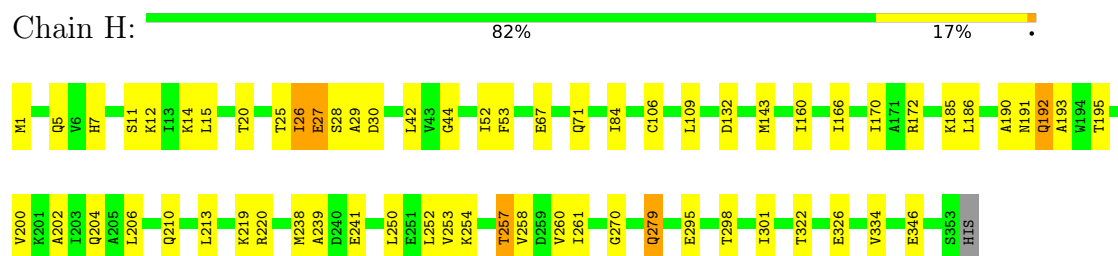
Chain F:  58% 40%



- Molecule 1: Dipeptide Epimerase



- Molecule 1: Dipeptide Epimerase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	163.66Å 163.66Å 318.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.73 – 2.00 24.73 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.73-2.00) 99.9 (24.73-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.282 0.244 , 0.279	Depositor DCC
R_{free} test set	10773 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 27.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.487 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21863	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GOL

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	0.43	0/2679	0.90	9/3620 (0.2%)
1	B	0.45	0/2667	0.93	6/3605 (0.2%)
1	C	0.37	0/2679	0.90	8/3620 (0.2%)
1	D	0.34	0/2679	0.89	9/3620 (0.2%)
1	E	0.38	0/2679	0.90	5/3620 (0.1%)
1	F	0.35	0/2679	0.86	2/3620 (0.1%)
1	G	0.42	0/2679	0.87	5/3620 (0.1%)
1	H	0.47	0/2667	0.93	6/3605 (0.2%)
All	All	0.40	0/21408	0.90	50/28930 (0.2%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	193	ALA	N-CA-C	8.03	120.94	111.71
1	F	257	THR	N-CA-C	7.65	119.62	111.28
1	E	257	THR	N-CA-C	7.27	119.29	111.36
1	D	114	ALA	N-CA-C	-7.06	105.85	114.75
1	A	270	GLY	N-CA-C	7.02	119.17	112.08
1	D	193	ALA	N-CA-C	6.99	118.98	111.36
1	G	270	GLY	N-CA-C	6.97	119.12	112.08
1	H	270	GLY	N-CA-C	6.90	120.13	111.85
1	A	193	ALA	N-CA-C	6.86	119.60	111.71
1	C	193	ALA	N-CA-C	6.74	119.63	111.82
1	H	193	ALA	N-CA-C	6.69	120.70	112.54
1	A	257	THR	N-CA-C	6.58	118.53	111.36
1	D	257	THR	N-CA-C	6.54	118.49	111.36
1	H	257	THR	N-CA-C	6.46	118.33	111.28
1	H	195	THR	N-CA-C	-6.38	101.01	110.20
1	F	195	THR	N-CA-C	-6.34	100.88	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	195	THR	N-CA-C	-6.22	101.06	110.39
1	C	257	THR	N-CA-C	6.10	118.00	111.36
1	B	310	ALA	N-CA-C	6.04	117.86	111.28
1	C	270	GLY	N-CA-C	6.00	118.20	111.85
1	G	257	THR	N-CA-C	5.94	117.83	111.36
1	C	49	GLY	CA-C-N	5.82	126.28	119.99
1	C	49	GLY	C-N-CA	5.82	126.28	119.99
1	E	193	ALA	N-CA-C	5.77	119.58	112.54
1	B	52	ILE	N-CA-C	5.76	117.19	110.62
1	A	52	ILE	N-CA-C	5.74	117.17	110.62
1	E	270	GLY	N-CA-C	5.73	117.92	111.85
1	B	270	GLY	N-CA-C	5.72	119.03	111.70
1	C	195	THR	N-CA-C	-5.61	101.98	110.39
1	D	194	TRP	N-CA-C	5.59	119.09	110.42
1	G	193	ALA	N-CA-C	5.59	118.14	111.71
1	A	234	ASN	N-CA-C	-5.58	106.48	113.28
1	D	271	ILE	N-CA-C	5.57	116.30	110.62
1	E	311	GLN	N-CA-C	5.49	117.67	108.73
1	A	195	THR	N-CA-C	-5.40	103.13	110.36
1	G	52	ILE	N-CA-C	5.32	116.69	110.62
1	A	54	ILE	N-CA-C	-5.32	106.48	111.48
1	D	52	ILE	N-CA-C	5.31	116.68	110.62
1	H	52	ILE	N-CA-C	5.28	116.64	110.62
1	B	195	THR	N-CA-C	-5.25	102.51	110.39
1	C	311	GLN	N-CA-C	5.25	117.28	108.73
1	B	258	VAL	N-CA-C	5.24	114.93	108.53
1	D	234	ASN	N-CA-C	-5.23	106.75	113.23
1	G	117	PRO	N-CA-C	-5.18	103.06	111.14
1	D	311	GLN	N-CA-C	5.14	117.11	108.73
1	A	118	LEU	N-CA-C	5.12	117.53	111.33
1	A	117	PRO	N-CA-C	-5.10	103.28	111.38
1	C	54	ILE	N-CA-C	-5.09	107.60	111.62
1	E	195	THR	N-CA-C	-5.09	102.76	110.39
1	H	192	GLN	N-CA-C	5.01	119.25	113.38

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	2649	0	2733	72	0
1	B	2638	0	2726	45	0
1	C	2649	0	2733	63	0
1	D	2649	0	2733	147	0
1	E	2649	0	2733	70	0
1	F	2649	0	2733	122	0
1	G	2649	0	2733	69	0
1	H	2638	0	2726	43	0
2	A	6	0	4	0	0
2	B	6	0	4	0	0
2	C	6	0	4	0	0
2	D	6	0	4	1	0
2	E	6	0	4	0	0
2	F	6	0	4	2	0
2	G	6	0	4	0	0
2	H	6	0	4	0	0
3	A	13	0	9	0	0
3	B	13	0	9	0	0
3	C	13	0	9	1	0
3	D	13	0	9	0	0
3	E	13	0	9	2	0
3	F	13	0	9	1	0
3	G	13	0	9	0	0
3	H	13	0	9	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
4	E	6	0	8	0	0
4	F	6	0	8	0	0
4	G	6	0	8	0	0
4	H	6	0	8	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	70	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	93	0	0	1	0
6	C	47	0	0	2	0
6	D	26	0	0	2	0
6	E	56	0	0	2	0
6	F	27	0	0	0	0
6	G	74	0	0	2	0
6	H	92	0	0	3	0
All	All	21863	0	22018	617	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 14.

All (617) 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:G:1:MET:HE2	1:G:38:THR:HG21	1.31	1.12
1:B:1:MET:HE2	1:B:38:THR:HG21	1.45	0.98
1:E:328:ALA:HB2	1:E:336:LEU:HD11	1.44	0.97
1:C:328:ALA:HB2	1:C:336:LEU:HD11	1.48	0.95
1:C:1:MET:HE2	1:C:38:THR:HG21	1.50	0.91
1:A:330:VAL:HG22	1:A:353:SER:O	1.72	0.89
1:G:276:LYS:HG2	1:H:279:GLN:HG3	1.56	0.87
1:G:330:VAL:HG22	1:G:353:SER:O	1.78	0.84
1:G:139:GLU:HB2	1:G:142:VAL:HG23	1.58	0.83
1:D:20:THR:HA	1:D:25:THR:HG22	1.61	0.83
1:A:139:GLU:HB2	1:A:142:VAL:HG23	1.60	0.83
1:D:1:MET:HE2	1:D:38:THR:HG21	1.60	0.82
1:F:1:MET:HE2	1:F:38:THR:HG21	1.59	0.82
1:H:1:MET:HE1	1:H:42:LEU:HD12	1.64	0.79
1:H:15:LEU:HD11	1:H:26:ILE:HD12	1.64	0.79
1:F:264:LYS:HB2	1:F:267:LYS:HD3	1.65	0.78
1:C:279:GLN:OE1	1:D:279:GLN:HG3	1.83	0.78
1:D:133:ILE:HD13	1:D:150:LYS:HD2	1.65	0.78
1:A:167:GLU:HG2	1:A:168:ALA:H	1.48	0.78
1:F:20:THR:HA	1:F:25:THR:HG22	1.64	0.78
1:F:21:ILE:HG23	1:F:23:LEU:H	1.49	0.76
1:E:275:LEU:O	1:E:279:GLN:HG2	1.86	0.76
1:B:15:LEU:HD11	1:B:26:ILE:HD12	1.66	0.76
1:G:71:GLN:HG2	6:G:420:HOH:O	1.89	0.73
1:H:1:MET:CE	1:H:42:LEU:HD12	2.19	0.72
1:F:135:LEU:HD11	1:F:158:LEU:HD22	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:26:ILE:HD11	1:H:28:SER:O	1.89	0.72
1:A:26:ILE:HD11	1:A:28:SER:O	1.90	0.72
1:A:239:ALA:HB2	1:A:258:VAL:HG11	1.72	0.72
1:G:195:THR:HG23	1:G:198:ASP:HB2	1.72	0.71
1:A:1:MET:HE1	1:A:113:LYS:HB2	1.70	0.71
1:D:143:MET:SD	1:D:172:ARG:HD3	2.30	0.71
1:D:21:ILE:HD11	1:D:161:LYS:HE3	1.72	0.71
1:F:133:ILE:HD13	1:F:150:LYS:HD2	1.72	0.71
1:F:78:PRO:O	1:F:110:MET:HE2	1.91	0.70
1:D:170:ILE:HG12	1:D:206:LEU:HD11	1.73	0.70
1:A:279:GLN:HG3	1:B:279:GLN:OE1	1.92	0.70
1:C:1:MET:HE3	1:C:42:LEU:HD12	1.73	0.70
1:F:1:MET:HG3	1:F:40:GLU:OE1	1.92	0.70
1:D:1:MET:HG3	1:D:40:GLU:OE1	1.92	0.69
1:D:45:TYR:CE2	1:D:353:SER:HA	2.27	0.69
1:B:26:ILE:HD11	1:B:28:SER:O	1.92	0.69
1:D:67:GLU:HB3	6:D:361:HOH:O	1.90	0.69
1:F:45:TYR:CE2	1:F:353:SER:HA	2.27	0.69
1:D:64:GLU:O	1:D:68:LEU:HG	1.91	0.69
1:F:21:ILE:HD11	1:F:161:LYS:HE3	1.73	0.69
1:F:250:LEU:O	1:F:253:VAL:HG22	1.94	0.68
1:D:1:MET:HE3	1:D:42:LEU:HD12	1.76	0.68
1:D:78:PRO:O	1:D:110:MET:HE2	1.94	0.67
1:C:253:VAL:HG12	1:C:286:ILE:HD12	1.76	0.67
1:D:306:HIS:ND1	1:D:344:LEU:HD13	2.09	0.67
1:A:221:ARG:HH11	1:E:247:GLN:HB2	1.60	0.67
1:G:276:LYS:HG2	1:H:279:GLN:CG	2.24	0.67
1:F:306:HIS:ND1	1:F:344:LEU:HD13	2.10	0.66
1:G:13:ILE:HD11	1:G:329:PRO:HB3	1.76	0.66
1:F:146:LYS:O	1:F:150:LYS:HG2	1.95	0.66
1:A:20:THR:HG23	1:A:25:THR:HG22	1.77	0.66
1:G:1:MET:CE	1:G:38:THR:HG21	2.19	0.66
1:B:247:GLN:HG3	6:B:410:HOH:O	1.95	0.66
1:H:238:MET:HE2	1:H:260:VAL:HG11	1.76	0.66
1:G:238:MET:SD	1:G:289:MET:HE2	2.36	0.65
1:D:112:GLN:HA	1:D:348:ALA:HB1	1.78	0.65
1:F:174:LYS:O	1:F:178:GLU:HG3	1.97	0.65
1:A:251:GLU:OE1	1:A:255:LYS:HE2	1.97	0.64
1:D:146:LYS:O	1:D:150:LYS:HG2	1.97	0.64
1:D:18:THR:HG22	1:D:27:GLU:HG2	1.77	0.64
1:G:1:MET:HE3	1:G:42:LEU:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:168:ALA:O	1:G:172:ARG:HG3	1.98	0.64
1:D:136:GLY:O	1:D:143:MET:HE3	1.96	0.64
1:F:330:VAL:HG22	1:F:353:SER:O	1.97	0.64
1:A:1:MET:CE	1:A:42:LEU:HD12	2.28	0.64
1:F:143:MET:SD	1:F:172:ARG:HD3	2.38	0.64
1:A:213:LEU:HD12	1:A:213:LEU:C	2.23	0.64
1:A:254:LYS:HD2	6:A:415:HOH:O	1.96	0.64
1:F:170:ILE:HG12	1:F:206:LEU:HD11	1.80	0.64
1:B:202:ALA:O	1:B:206:LEU:HD13	1.97	0.63
1:A:325:LEU:HB2	1:A:336:LEU:HD23	1.79	0.63
1:D:264:LYS:HB2	1:D:267:LYS:HD3	1.79	0.63
1:D:206:LEU:HA	1:D:209:TYR:HD2	1.62	0.63
1:F:147:ALA:O	1:F:151:VAL:HG23	1.98	0.63
1:G:192:GLN:HB3	1:G:219:LYS:HA	1.80	0.63
1:H:202:ALA:O	1:H:206:LEU:HD13	1.98	0.63
1:D:264:LYS:HD2	1:D:267:LYS:HD3	1.81	0.63
1:F:64:GLU:O	1:F:68:LEU:HG	1.99	0.62
1:A:253:VAL:HG12	1:A:286:ILE:HD12	1.80	0.62
1:C:107:TYR:HA	1:C:110:MET:HE3	1.82	0.62
1:A:228:TYR:O	1:A:232:GLN:HG2	1.99	0.62
1:D:240:ASP:HB3	1:D:241:GLU:OE1	2.00	0.62
1:G:166:ILE:O	1:G:170:ILE:HG13	1.98	0.62
1:C:202:ALA:O	1:C:206:LEU:HD13	2.00	0.62
1:F:240:ASP:HB3	1:F:241:GLU:OE1	2.00	0.61
1:F:159:LYS:HZ3	1:F:161:LYS:HE2	1.65	0.61
1:A:139:GLU:HB2	1:A:142:VAL:CG2	2.30	0.61
1:B:143:MET:SD	1:B:172:ARG:HD3	2.40	0.61
1:F:275:LEU:O	1:F:279:GLN:HG2	2.00	0.61
1:H:298:THR:HG23	1:H:334:VAL:O	2.01	0.61
1:F:5:GLN:HB3	1:F:37:GLU:CD	2.25	0.61
1:F:196:PRO:O	1:F:200:VAL:HG23	2.00	0.61
1:A:174:LYS:O	1:A:178:GLU:HG2	2.01	0.61
1:E:26:ILE:HD12	1:E:27:GLU:H	1.66	0.61
1:B:1:MET:HE1	1:B:42:LEU:HD12	1.82	0.61
1:F:174:LYS:HE2	1:F:209:TYR:CE2	2.36	0.60
1:D:174:LYS:HG2	1:D:209:TYR:CE2	2.35	0.60
1:G:174:LYS:HE2	1:G:209:TYR:CE2	2.36	0.60
1:D:149:GLU:O	1:D:153:LEU:HD13	2.01	0.60
1:D:113:LYS:O	1:D:113:LYS:HG3	2.01	0.60
1:D:134:THR:HG1	2:D:355:SER:N	1.98	0.60
1:D:253:VAL:HG12	1:D:286:ILE:HD12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:VAL:HG22	1:F:179:ALA:O	2.02	0.60
1:G:146:LYS:O	1:G:149:GLU:HB2	2.02	0.60
1:D:173:VAL:HG11	1:D:206:LEU:HD23	1.83	0.60
1:F:21:ILE:HD11	1:F:161:LYS:CE	2.32	0.60
1:E:173:VAL:HG11	1:E:206:LEU:HD23	1.84	0.59
1:G:139:GLU:HB2	1:G:142:VAL:CG2	2.32	0.59
1:B:26:ILE:HD13	1:B:28:SER:H	1.68	0.59
1:E:253:VAL:HG12	1:E:286:ILE:HD12	1.83	0.59
1:D:142:VAL:O	1:D:145:GLN:HB2	2.02	0.59
1:F:1:MET:HE3	1:F:42:LEU:HD12	1.85	0.59
1:G:170:ILE:HG22	1:G:174:LYS:HE3	1.84	0.59
1:G:228:TYR:O	1:G:232:GLN:HG2	2.03	0.59
1:A:247:GLN:HG3	6:A:416:HOH:O	2.01	0.59
1:D:21:ILE:CG2	1:D:23:LEU:H	2.16	0.59
1:D:330:VAL:HG22	1:D:353:SER:O	2.02	0.59
1:F:18:THR:HG22	1:F:27:GLU:HG2	1.83	0.59
1:F:134:THR:HG1	2:F:355:SER:N	2.01	0.59
1:G:150:LYS:H	1:G:150:LYS:HD2	1.68	0.58
1:E:1:MET:HE1	1:E:113:LYS:HB2	1.85	0.58
1:G:247:GLN:HG3	6:G:410:HOH:O	2.03	0.58
1:G:253:VAL:HG12	1:G:286:ILE:HD12	1.85	0.58
1:C:185:LYS:HE2	1:C:212:GLU:HG3	1.86	0.58
1:E:254:LYS:HD2	6:E:377:HOH:O	2.04	0.58
1:H:71:GLN:HG3	6:H:417:HOH:O	2.04	0.58
1:F:173:VAL:HG11	1:F:206:LEU:HD23	1.85	0.58
1:F:249:ALA:O	1:F:253:VAL:HG13	2.04	0.58
1:C:37:GLU:HA	1:C:42:LEU:O	2.05	0.57
1:D:83:LYS:O	1:D:87:VAL:HG23	2.03	0.57
1:F:145:GLN:HA	1:F:145:GLN:OE1	2.03	0.57
1:G:202:ALA:O	1:G:206:LEU:HD13	2.04	0.57
1:D:156:ASP:HA	1:D:184:ILE:HD12	1.87	0.57
1:B:238:MET:HE2	1:B:260:VAL:HG11	1.87	0.57
1:H:238:MET:HE2	1:H:260:VAL:CG1	2.34	0.57
1:A:168:ALA:O	1:A:172:ARG:HG3	2.05	0.57
1:G:20:THR:HG23	1:G:25:THR:HG22	1.87	0.57
1:H:200:VAL:O	1:H:204:GLN:HG3	2.05	0.56
1:D:15:LEU:HG	1:D:27:GLU:O	2.06	0.56
1:D:174:LYS:HE2	1:D:209:TYR:HE2	1.71	0.56
1:H:170:ILE:HG12	1:H:206:LEU:HD11	1.87	0.56
1:A:145:GLN:O	1:A:149:GLU:HG3	2.05	0.56
1:E:202:ALA:O	1:E:206:LEU:HD13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:ILE:HD11	1:F:161:LYS:CD	2.36	0.56
1:F:250:LEU:HG	1:F:254:LYS:HE3	1.87	0.56
1:F:301:ILE:HD11	1:F:321:ALA:HB3	1.87	0.56
1:A:181:GLY:HA3	6:A:383:HOH:O	2.06	0.56
1:C:221:ARG:HG3	1:G:247:GLN:OE1	2.05	0.56
1:D:34:VAL:HG21	1:D:101:ALA:HB1	1.88	0.56
1:F:112:GLN:HA	1:F:348:ALA:HB1	1.88	0.56
1:F:281:CYS:HB3	1:F:286:ILE:O	2.06	0.56
1:E:1:MET:HE2	1:E:38:THR:HG21	1.87	0.56
1:C:185:LYS:HE2	1:C:212:GLU:CD	2.31	0.56
1:F:137:ILE:HG12	1:F:161:LYS:O	2.06	0.56
1:B:238:MET:HE2	1:B:260:VAL:CG1	2.36	0.56
1:C:160:ILE:HB	1:C:188:LEU:HD23	1.87	0.56
1:G:170:ILE:CG2	1:G:174:LYS:HE3	2.36	0.56
1:C:133:ILE:HD13	1:C:150:LYS:HG3	1.88	0.55
1:F:206:LEU:HA	1:F:209:TYR:HD2	1.71	0.55
1:A:166:ILE:HG22	1:A:202:ALA:HB2	1.88	0.55
1:C:129:VAL:HG13	1:C:342:LEU:HB2	1.87	0.55
1:D:38:THR:C	1:D:40:GLU:H	2.14	0.55
1:F:47:GLU:HG2	1:F:48:GLY:N	2.21	0.55
1:G:221:ARG:HH21	1:G:221:ARG:HB3	1.71	0.55
1:G:239:ALA:HB2	1:G:258:VAL:HG11	1.88	0.55
1:F:83:LYS:O	1:F:87:VAL:HG23	2.07	0.55
1:H:143:MET:SD	1:H:172:ARG:HD3	2.46	0.55
1:C:166:ILE:O	1:C:170:ILE:HG13	2.07	0.55
1:F:166:ILE:O	1:F:170:ILE:HG13	2.07	0.55
1:A:202:ALA:O	1:A:206:LEU:HD13	2.06	0.55
1:F:177:ARG:NH1	1:F:182:PHE:HA	2.22	0.55
1:F:174:LYS:HG2	1:F:209:TYR:CZ	2.42	0.55
1:C:16:LYS:HE3	1:C:325:LEU:O	2.06	0.54
1:B:26:ILE:HD13	1:B:27:GLU:N	2.22	0.54
1:B:239:ALA:HB2	1:B:258:VAL:HG11	1.88	0.54
1:D:170:ILE:CG2	1:D:174:LYS:HE3	2.37	0.54
1:F:46:GLY:C	1:F:299:ILE:HG21	2.31	0.54
1:B:200:VAL:O	1:B:204:GLN:HG3	2.07	0.54
1:C:13:ILE:HD13	1:C:327:THR:O	2.07	0.54
1:D:173:VAL:HG11	1:D:211:ILE:HD11	1.89	0.54
1:B:19:PHE:HB3	1:B:26:ILE:HG22	1.90	0.54
1:D:196:PRO:O	1:D:200:VAL:HG23	2.07	0.54
1:E:239:ALA:HB2	1:E:258:VAL:HG11	1.89	0.54
1:E:37:GLU:HA	1:E:42:LEU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:210:GLN:O	1:H:210:GLN:HG2	2.07	0.54
1:D:275:LEU:O	1:D:279:GLN:HG2	2.08	0.54
1:B:16:LYS:NZ	1:B:16:LYS:HB3	2.22	0.54
1:D:139:GLU:HB2	1:D:142:VAL:HG23	1.89	0.54
1:D:239:ALA:HB2	1:D:258:VAL:HG11	1.90	0.54
1:D:281:CYS:HB3	1:D:286:ILE:O	2.08	0.54
1:F:174:LYS:HE2	1:F:209:TYR:HE2	1.72	0.54
1:B:166:ILE:O	1:B:170:ILE:HG13	2.08	0.54
1:D:323:PHE:CD2	1:D:338:ALA:HA	2.43	0.54
1:F:14:LYS:HA	1:F:28:SER:HA	1.90	0.53
1:F:173:VAL:HG22	1:F:188:LEU:HD21	1.90	0.53
1:A:206:LEU:HA	1:A:209:TYR:HD2	1.73	0.53
1:D:155:PHE:HZ	1:D:323:PHE:HE2	1.56	0.53
1:D:210:GLN:HG2	1:D:210:GLN:O	2.08	0.53
1:A:1:MET:HE1	1:A:42:LEU:HD12	1.89	0.53
1:E:147:ALA:O	1:E:151:VAL:HG23	2.08	0.53
1:D:14:LYS:HA	1:D:28:SER:HA	1.89	0.53
1:E:114:ALA:HB1	1:E:116:LEU:HD12	1.91	0.53
1:H:20:THR:OG1	1:H:25:THR:HG22	2.08	0.53
1:A:173:VAL:HG11	1:A:206:LEU:HD23	1.91	0.53
1:B:210:GLN:O	1:B:210:GLN:HG2	2.09	0.53
1:D:46:GLY:C	1:D:299:ILE:HG21	2.34	0.53
1:H:220:ARG:HG3	1:H:241:GLU:O	2.09	0.53
1:C:336:LEU:N	1:C:336:LEU:HD12	2.25	0.52
1:D:174:LYS:HG2	1:D:209:TYR:CZ	2.43	0.52
1:E:251:GLU:OE2	1:E:255:LYS:HE2	2.08	0.52
1:G:150:LYS:HD2	1:G:150:LYS:N	2.24	0.52
1:H:26:ILE:HD13	1:H:28:SER:H	1.75	0.52
1:A:1:MET:HE2	1:A:42:LEU:HD12	1.91	0.52
1:F:213:LEU:HD12	1:F:213:LEU:C	2.35	0.52
1:D:166:ILE:O	1:D:170:ILE:HG13	2.09	0.52
1:E:154:GLY:O	1:E:340:PRO:HG3	2.10	0.52
1:C:38:THR:OG1	1:C:40:GLU:HG2	2.10	0.52
1:D:243:CYS:HB2	1:D:252:LEU:HD11	1.92	0.52
1:F:18:THR:CG2	1:F:27:GLU:HG2	2.40	0.52
1:A:26:ILE:HD12	6:A:366:HOH:O	2.08	0.52
1:G:12:LYS:HG2	1:G:30:ASP:OD1	2.10	0.52
1:D:250:LEU:O	1:D:254:LYS:HG3	2.09	0.52
1:C:254:LYS:HD2	6:C:391:HOH:O	2.09	0.51
1:D:147:ALA:O	1:D:151:VAL:HG23	2.10	0.51
1:G:225:GLY:O	1:G:228:TYR:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:LYS:N	1:C:150:LYS:HD2	2.25	0.51
1:D:250:LEU:HG	1:D:254:LYS:HE3	1.91	0.51
1:E:18:THR:HG22	1:E:27:GLU:HB3	1.92	0.51
1:C:213:LEU:C	1:C:213:LEU:HD12	2.36	0.51
1:E:143:MET:SD	1:E:172:ARG:HD3	2.50	0.51
1:A:159:LYS:HA	1:A:187:ARG:HG3	1.91	0.51
1:D:174:LYS:HE2	1:D:209:TYR:CE2	2.45	0.51
1:G:159:LYS:HA	1:G:187:ARG:HG3	1.92	0.51
1:D:173:VAL:HG21	1:D:206:LEU:HD21	1.93	0.51
1:E:170:ILE:HG22	1:E:174:LYS:HE2	1.92	0.51
1:F:135:LEU:HD12	1:F:135:LEU:N	2.26	0.51
1:F:239:ALA:HB2	1:F:258:VAL:HG11	1.92	0.51
1:D:117:PRO:HG2	1:D:120:GLN:HG2	1.93	0.51
1:E:268:CYS:HB2	1:E:273:GLU:CG	2.41	0.51
1:F:173:VAL:HG11	1:F:211:ILE:HD11	1.93	0.51
1:H:192:GLN:HB3	1:H:219:LYS:HA	1.92	0.51
1:D:322:THR:HA	1:D:325:LEU:HG	1.94	0.50
1:F:301:ILE:CG2	1:F:334:VAL:HG11	2.40	0.50
1:G:211:ILE:N	1:G:211:ILE:HD12	2.26	0.50
1:E:111:GLY:HA2	1:E:121:LEU:HD11	1.93	0.50
1:G:213:LEU:C	1:G:213:LEU:HD12	2.36	0.50
1:D:16:LYS:HE3	1:D:325:LEU:O	2.11	0.50
1:D:177:ARG:CZ	1:D:186:LEU:HD12	2.42	0.50
1:G:185:LYS:HE2	1:G:212:GLU:CG	2.42	0.50
1:C:174:LYS:HG2	1:C:209:TYR:CZ	2.46	0.50
1:F:160:ILE:HB	1:F:188:LEU:HD23	1.93	0.50
1:A:290:ILE:HG23	1:A:290:ILE:O	2.11	0.50
1:E:200:VAL:O	1:E:204:GLN:HG3	2.12	0.50
1:A:166:ILE:O	1:A:170:ILE:HG13	2.12	0.50
1:B:213:LEU:C	1:B:213:LEU:HD12	2.37	0.50
1:C:295:GLU:CD	3:C:356:TYR:HH	2.20	0.50
1:D:18:THR:CG2	1:D:27:GLU:HG2	2.41	0.50
1:D:21:ILE:HG22	1:D:23:LEU:H	1.77	0.50
1:D:192:GLN:HB3	1:D:219:LYS:HA	1.93	0.50
1:E:133:ILE:HD13	1:E:150:LYS:HD2	1.92	0.50
1:G:1:MET:HG2	1:G:40:GLU:OE2	2.12	0.50
1:C:167:GLU:CD	1:C:167:GLU:H	2.19	0.50
1:F:22:ALA:HB3	1:F:191:ASN:HB2	1.93	0.50
1:E:1:MET:CE	1:E:113:LYS:HB2	2.42	0.50
1:D:213:LEU:HD12	1:D:213:LEU:C	2.36	0.49
1:C:174:LYS:HE2	1:C:209:TYR:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:ILE:HG12	1:E:206:LEU:HD11	1.94	0.49
1:F:322:THR:HA	1:F:325:LEU:HG	1.94	0.49
1:D:47:GLU:H	1:D:101:ALA:HA	1.76	0.49
1:H:239:ALA:HB2	1:H:258:VAL:HG11	1.94	0.49
1:F:293:MET:O	1:F:296:GLU:HG2	2.12	0.49
1:G:161:LYS:HD3	1:G:189:ASP:HB3	1.94	0.49
1:D:177:ARG:NH1	1:D:182:PHE:HA	2.28	0.49
1:E:122:LEU:C	1:E:310:ALA:HB1	2.37	0.49
1:F:26:ILE:CD1	1:F:295:GLU:HG3	2.42	0.49
1:A:167:GLU:HG2	1:A:168:ALA:N	2.23	0.49
1:D:34:VAL:HG12	1:D:35:GLU:N	2.28	0.49
1:H:160:ILE:HD11	1:H:186:LEU:HD22	1.94	0.49
1:D:13:ILE:HD11	1:D:329:PRO:HD3	1.95	0.49
1:F:1:MET:HE3	1:F:42:LEU:CD1	2.43	0.49
1:D:155:PHE:HZ	1:D:323:PHE:CE2	2.30	0.49
1:E:279:GLN:HG3	1:F:279:GLN:HG3	1.95	0.49
1:G:290:ILE:HG23	1:G:290:ILE:O	2.13	0.49
1:C:133:ILE:HD13	1:C:150:LYS:CG	2.42	0.49
1:C:160:ILE:HD13	1:C:176:ILE:HD12	1.95	0.49
1:D:206:LEU:HD12	1:D:206:LEU:N	2.27	0.49
1:E:1:MET:HE3	1:E:42:LEU:HD12	1.94	0.49
1:A:192:GLN:HB3	1:A:219:LYS:HA	1.95	0.49
1:D:204:GLN:O	1:D:207:ALA:HB2	2.12	0.49
1:F:11:SER:O	1:F:30:ASP:HA	2.13	0.48
1:D:5:GLN:HG2	1:D:7:HIS:CE1	2.47	0.48
1:E:301:ILE:HD11	1:E:321:ALA:HB3	1.95	0.48
1:G:132:ASP:OD1	1:G:132:ASP:C	2.56	0.48
1:G:301:ILE:HG13	1:G:322:THR:HG23	1.94	0.48
1:C:143:MET:SD	1:C:172:ARG:HD3	2.52	0.48
1:C:239:ALA:HB2	1:C:258:VAL:HG11	1.95	0.48
1:C:330:VAL:HG13	1:C:331:THR:N	2.27	0.48
1:D:34:VAL:CG2	1:D:101:ALA:HB1	2.43	0.48
1:D:322:THR:HA	1:D:325:LEU:CD1	2.43	0.48
1:G:301:ILE:HD11	1:G:321:ALA:HB3	1.94	0.48
1:B:192:GLN:HB3	1:B:219:LYS:HA	1.94	0.48
1:E:12:LYS:HG2	1:E:30:ASP:OD1	2.13	0.48
1:E:84:ILE:HD13	1:E:106:CYS:SG	2.53	0.48
1:F:327:THR:OG1	1:F:328:ALA:N	2.47	0.48
1:G:330:VAL:HG22	1:G:331:THR:H	1.79	0.48
1:C:1:MET:HG2	1:C:40:GLU:OE2	2.14	0.48
1:C:132:ASP:C	1:C:132:ASP:OD1	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:26:ILE:HD13	1:H:27:GLU:N	2.29	0.48
1:E:167:GLU:H	1:E:167:GLU:CD	2.22	0.48
1:H:190:ALA:O	1:H:191:ASN:C	2.57	0.48
1:A:11:SER:O	1:A:30:ASP:HA	2.14	0.48
1:C:35:GLU:HG2	1:C:45:TYR:CE1	2.49	0.48
1:C:264:LYS:HB2	1:C:267:LYS:HE2	1.95	0.48
1:D:301:ILE:CG2	1:D:334:VAL:HG11	2.44	0.48
1:D:174:LYS:O	1:D:178:GLU:HG3	2.14	0.47
1:E:295:GLU:CD	3:E:356:TYR:HH	2.21	0.47
1:A:221:ARG:NH1	1:E:247:GLN:HB2	2.26	0.47
1:D:299:ILE:HD12	1:D:299:ILE:H	1.78	0.47
1:D:323:PHE:CD1	1:D:323:PHE:N	2.81	0.47
1:F:131:THR:OG1	1:F:132:ASP:N	2.47	0.47
1:F:48:GLY:O	1:F:50:PRO:HD3	2.14	0.47
1:D:323:PHE:HD1	1:D:323:PHE:H	1.61	0.47
1:E:306:HIS:HA	1:E:344:LEU:HD11	1.96	0.47
1:G:133:ILE:HG21	1:G:150:LYS:HG2	1.96	0.47
1:H:26:ILE:HD13	1:H:26:ILE:C	2.39	0.47
1:A:275:LEU:O	1:A:279:GLN:HG2	2.15	0.47
1:E:259:ASP:O	1:E:286:ILE:HG23	2.14	0.47
1:F:52:ILE:O	1:F:56:GLY:HA2	2.15	0.47
1:F:146:LYS:O	1:F:149:GLU:HB3	2.14	0.47
1:B:170:ILE:HG12	1:B:206:LEU:HD11	1.96	0.47
1:D:69:PHE:HE1	1:D:91:ILE:HB	1.79	0.47
1:D:112:GLN:C	1:D:114:ALA:H	2.22	0.47
1:D:323:PHE:N	1:D:323:PHE:HD1	2.13	0.47
1:F:210:GLN:O	1:F:210:GLN:HG2	2.13	0.47
1:G:206:LEU:HA	1:G:209:TYR:HD2	1.78	0.47
1:A:206:LEU:N	1:A:206:LEU:HD12	2.28	0.47
1:B:145:GLN:O	1:B:149:GLU:HG3	2.14	0.47
1:C:185:LYS:HE2	1:C:212:GLU:CG	2.45	0.47
1:D:250:LEU:O	1:D:253:VAL:HG22	2.14	0.47
1:D:327:THR:OG1	1:D:328:ALA:N	2.47	0.47
1:D:100:ALA:O	1:D:104:ILE:HG13	2.14	0.47
1:E:210:GLN:O	1:E:210:GLN:HG2	2.15	0.47
1:F:73:ILE:HA	1:F:76:LEU:HD12	1.96	0.47
1:F:177:ARG:CZ	1:F:186:LEU:HD12	2.45	0.47
1:C:84:ILE:HD13	1:C:106:CYS:SG	2.55	0.47
1:F:28:SER:O	1:F:29:ALA:HB2	2.15	0.47
1:A:132:ASP:C	1:A:132:ASP:OD1	2.57	0.46
1:F:206:LEU:O	1:F:209:TYR:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:THR:HG22	1:G:135:LEU:N	2.30	0.46
1:G:143:MET:HB3	1:G:176:ILE:HD11	1.97	0.46
1:C:19:PHE:HB3	1:C:26:ILE:HG23	1.97	0.46
1:D:339:LYS:NZ	1:D:342:LEU:HD23	2.30	0.46
1:C:200:VAL:O	1:C:204:GLN:HG3	2.14	0.46
1:D:306:HIS:CE1	1:D:344:LEU:HD13	2.49	0.46
1:A:290:ILE:HG21	1:A:308:ALA:HB2	1.98	0.46
1:D:159:LYS:HE2	1:D:215:GLU:OE1	2.16	0.46
1:F:177:ARG:HD2	1:F:182:PHE:CD1	2.50	0.46
1:A:146:LYS:O	1:A:150:LYS:HG2	2.14	0.46
1:B:14:LYS:HB2	1:B:326:GLU:HG3	1.96	0.46
1:B:220:ARG:HG3	1:B:241:GLU:O	2.16	0.46
1:B:275:LEU:O	1:B:279:GLN:HG3	2.16	0.46
1:D:243:CYS:HB2	1:D:252:LEU:CD1	2.45	0.46
1:F:45:TYR:HE2	1:F:353:SER:HA	1.78	0.46
1:F:192:GLN:HB3	1:F:219:LYS:HA	1.96	0.46
1:A:222:ASP:OD2	1:A:225:GLY:HA3	2.15	0.46
1:D:52:ILE:O	1:D:56:GLY:HA2	2.16	0.46
1:E:132:ASP:C	1:E:132:ASP:OD1	2.58	0.46
1:F:225:GLY:O	1:F:228:TYR:HB3	2.16	0.46
1:D:13:ILE:HG23	1:D:327:THR:HG22	1.98	0.46
1:E:238:MET:HE2	1:E:260:VAL:HG11	1.97	0.46
1:E:268:CYS:HB2	1:E:273:GLU:HG2	1.98	0.46
1:A:301:ILE:HG13	1:A:322:THR:HG23	1.98	0.46
1:D:146:LYS:O	1:D:149:GLU:HB3	2.15	0.46
1:F:167:GLU:CD	1:F:167:GLU:H	2.23	0.46
1:G:276:LYS:HA	1:H:279:GLN:HG2	1.98	0.46
1:C:289:MET:HB2	1:C:316:ARG:HB2	1.97	0.46
1:D:132:ASP:OD1	1:D:132:ASP:C	2.59	0.46
1:F:170:ILE:CG2	1:F:174:LYS:HE3	2.45	0.46
1:D:13:ILE:CD1	1:D:329:PRO:HD3	2.46	0.46
1:D:271:ILE:HG23	1:D:307:LEU:HD13	1.98	0.46
1:G:174:LYS:HG2	1:G:209:TYR:CZ	2.51	0.46
1:H:14:LYS:HB2	1:H:326:GLU:HG3	1.97	0.46
1:C:122:LEU:C	1:C:310:ALA:HB1	2.41	0.45
1:D:19:PHE:HZ	1:D:134:THR:CG2	2.29	0.45
1:D:64:GLU:OE1	1:F:58:THR:HB	2.16	0.45
1:F:142:VAL:O	1:F:145:GLN:HB2	2.16	0.45
1:H:253:VAL:HG23	1:H:254:LYS:N	2.31	0.45
1:D:33:ILE:CD1	1:D:329:PRO:HB2	2.46	0.45
1:F:4:LYS:HD2	1:F:39:GLU:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:206:LEU:HD12	1:G:206:LEU:N	2.31	0.45
1:A:5:GLN:HG2	1:A:7:HIS:CE1	2.52	0.45
1:D:197:LYS:HD3	1:E:234:ASN:O	2.17	0.45
1:A:134:THR:HG22	1:A:135:LEU:N	2.31	0.45
1:A:301:ILE:HD11	1:A:321:ALA:HB3	1.98	0.45
1:E:48:GLY:O	1:E:50:PRO:HD3	2.16	0.45
1:G:279:GLN:OE1	1:H:279:GLN:NE2	2.49	0.45
1:A:322:THR:HA	1:A:325:LEU:HG	1.99	0.45
1:C:301:ILE:HD11	1:C:321:ALA:HB3	1.99	0.45
1:D:225:GLY:O	1:D:228:TYR:HB3	2.17	0.45
1:E:261:ILE:HD12	1:E:281:CYS:SG	2.57	0.45
1:F:195:THR:OG1	1:F:198:ASP:HB2	2.17	0.45
1:H:5:GLN:HG3	1:H:7:HIS:CE1	2.52	0.45
1:D:301:ILE:HD11	1:D:321:ALA:HB3	1.99	0.45
1:G:177:ARG:C	1:G:179:ALA:H	2.25	0.45
1:C:253:VAL:HG12	1:C:286:ILE:CD1	2.45	0.45
1:H:26:ILE:HD13	1:H:28:SER:N	2.32	0.45
1:B:26:ILE:HD13	1:B:28:SER:N	2.32	0.44
1:E:160:ILE:HD13	1:E:176:ILE:HD12	1.98	0.44
1:E:213:LEU:C	1:E:213:LEU:HD12	2.42	0.44
1:E:278:ASN:OD1	1:E:313:ASN:HB3	2.17	0.44
1:E:336:LEU:N	1:E:336:LEU:HD12	2.32	0.44
1:B:20:THR:OG1	1:B:25:THR:HG22	2.17	0.44
1:D:167:GLU:CD	1:D:167:GLU:H	2.25	0.44
1:E:79:PHE:CD1	1:E:110:MET:HG2	2.52	0.44
1:H:44:GLY:HA3	1:H:109:LEU:HG	1.99	0.44
1:H:84:ILE:HD13	1:H:106:CYS:SG	2.58	0.44
1:D:38:THR:C	1:D:40:GLU:N	2.76	0.44
1:D:131:THR:OG1	1:D:132:ASP:N	2.49	0.44
1:F:19:PHE:HZ	1:F:134:THR:CG2	2.31	0.44
2:F:355:SER:O	3:F:356:TYR:HB2	2.18	0.44
1:G:44:GLY:HA3	1:G:109:LEU:HG	1.98	0.44
1:C:221:ARG:NH2	1:C:221:ARG:HB3	2.32	0.44
1:D:21:ILE:HD11	1:D:161:LYS:HG3	2.00	0.44
1:E:250:LEU:HA	1:E:253:VAL:HG22	1.99	0.44
1:F:36:ILE:O	1:F:43:VAL:HA	2.18	0.44
1:F:289:MET:HB2	1:F:316:ARG:HB2	2.00	0.44
1:A:161:LYS:HD3	1:A:189:ASP:HB3	1.99	0.44
1:B:19:PHE:HB3	1:B:26:ILE:CG2	2.47	0.44
1:D:22:ALA:HB3	1:D:191:ASN:HB2	1.99	0.44
1:D:46:GLY:O	1:D:299:ILE:HG21	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:ILE:HD12	1:F:105:ALA:HB3	2.00	0.44
1:F:38:THR:OG1	1:F:42:LEU:HB2	2.17	0.44
1:F:98:ALA:O	1:F:101:ALA:HB3	2.17	0.44
1:D:46:GLY:O	1:D:47:GLU:HB2	2.18	0.44
1:F:271:ILE:HG23	1:F:307:LEU:HD13	2.00	0.44
1:A:279:GLN:NE2	1:B:276:LYS:HG2	2.33	0.44
1:B:132:ASP:OD1	1:B:132:ASP:C	2.61	0.44
1:B:220:ARG:HH11	1:B:221:ARG:HD2	1.83	0.44
1:E:35:GLU:HG2	1:E:45:TYR:CE1	2.53	0.44
1:F:13:ILE:HD13	1:F:327:THR:O	2.18	0.44
1:F:111:GLY:HA2	1:F:121:LEU:HD11	1.99	0.44
1:B:84:ILE:HD13	1:B:106:CYS:SG	2.57	0.44
1:D:299:ILE:HD12	1:D:299:ILE:N	2.33	0.44
1:E:81:ILE:HG13	1:E:85:HIS:HD2	1.81	0.44
1:B:190:ALA:O	1:B:191:ASN:C	2.61	0.43
1:E:323:PHE:CD1	1:E:338:ALA:HA	2.53	0.43
1:G:1:MET:HB3	1:G:78:PRO:HD2	2.00	0.43
1:G:84:ILE:HD13	1:G:106:CYS:SG	2.58	0.43
1:A:129:VAL:HG22	1:A:130:ILE:N	2.33	0.43
1:F:174:LYS:HG2	1:F:209:TYR:CE2	2.53	0.43
1:C:118:LEU:HB3	1:C:306:HIS:ND1	2.33	0.43
1:B:260:VAL:HG12	1:B:261:ILE:N	2.32	0.43
1:D:20:THR:CA	1:D:25:THR:HG22	2.41	0.43
1:D:353:SER:O	1:D:354:HIS:C	2.61	0.43
1:E:199:ALA:O	1:E:203:ILE:HG13	2.19	0.43
1:H:260:VAL:HG12	1:H:261:ILE:N	2.33	0.43
1:A:238:MET:SD	1:A:289:MET:HE2	2.59	0.43
1:C:238:MET:HE2	1:C:260:VAL:HG11	1.99	0.43
1:D:21:ILE:HG23	1:D:22:ALA:N	2.34	0.43
1:F:149:GLU:O	1:F:153:LEU:HD13	2.19	0.43
1:F:177:ARG:NH2	1:F:186:LEU:HD12	2.33	0.43
1:F:290:ILE:HG12	1:F:304:ALA:HB1	2.00	0.43
1:B:11:SER:O	1:B:30:ASP:HA	2.19	0.43
1:D:170:ILE:HG22	1:D:174:LYS:HE3	2.01	0.43
1:F:15:LEU:HG	1:F:27:GLU:O	2.18	0.43
1:F:46:GLY:O	1:F:47:GLU:HB2	2.19	0.43
1:F:194:TRP:CE3	1:F:199:ALA:HA	2.52	0.43
1:H:301:ILE:HG13	1:H:322:THR:HG23	2.01	0.43
1:A:336:LEU:HD12	6:A:397:HOH:O	2.17	0.43
1:C:238:MET:SD	1:C:289:MET:HE2	2.58	0.43
1:D:159:LYS:NZ	1:D:161:LYS:HE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:VAL:O	1:D:204:GLN:HG3	2.17	0.43
1:E:243:CYS:HB2	1:E:252:LEU:HD11	2.00	0.43
1:H:166:ILE:O	1:H:170:ILE:HG13	2.19	0.43
1:A:251:GLU:CD	1:A:255:LYS:HE2	2.43	0.43
1:B:146:LYS:O	1:B:150:LYS:HG2	2.19	0.43
1:C:330:VAL:CG1	1:C:352:ILE:HG23	2.49	0.43
1:D:173:VAL:HG21	1:D:206:LEU:CD2	2.48	0.43
1:F:51:GLY:HA2	1:F:295:GLU:OE2	2.19	0.43
1:G:322:THR:HA	1:G:325:LEU:HG	1.99	0.43
1:B:26:ILE:HD13	1:B:26:ILE:C	2.43	0.43
1:E:21:ILE:HD13	3:E:356:TYR:CD1	2.53	0.43
1:H:29:ALA:HA	1:H:295:GLU:HA	2.01	0.43
1:H:346:GLU:HG2	6:H:428:HOH:O	2.19	0.43
1:A:328:ALA:HB2	1:A:336:LEU:HD11	2.00	0.42
1:C:8:VAL:HA	1:C:33:ILE:O	2.19	0.42
1:D:13:ILE:CD1	1:D:327:THR:HG23	2.49	0.42
1:D:64:GLU:OE1	1:F:60:ALA:HB3	2.19	0.42
1:E:251:GLU:CD	1:E:255:LYS:HE2	2.44	0.42
1:E:174:LYS:O	1:E:178:GLU:HG2	2.19	0.42
1:A:51:GLY:HA2	1:A:295:GLU:OE2	2.20	0.42
1:A:157:THR:O	1:A:158:LEU:HD23	2.19	0.42
1:C:154:GLY:O	1:C:340:PRO:HG3	2.20	0.42
1:F:170:ILE:O	1:F:174:LYS:HG3	2.19	0.42
1:H:12:LYS:HB2	6:H:425:HOH:O	2.17	0.42
1:C:275:LEU:O	1:C:279:GLN:HG3	2.19	0.42
1:F:47:GLU:O	1:F:101:ALA:HA	2.19	0.42
1:A:143:MET:HE2	1:A:160:ILE:HG23	2.00	0.42
1:A:169:ASP:O	1:A:172:ARG:HB2	2.19	0.42
1:D:62:THR:O	1:D:66:ILE:HG13	2.20	0.42
1:A:44:GLY:HA3	1:A:109:LEU:HG	2.02	0.42
1:A:178:GLU:HG2	1:A:178:GLU:H	1.50	0.42
1:C:81:ILE:HG13	1:C:85:HIS:HD2	1.83	0.42
1:D:26:ILE:HD13	1:D:295:GLU:HG3	2.01	0.42
1:E:215:GLU:O	1:E:216:GLN:C	2.63	0.42
1:C:281:CYS:HB3	1:C:286:ILE:O	2.20	0.42
1:G:185:LYS:HE2	1:G:212:GLU:HG3	2.02	0.42
1:G:190:ALA:O	1:G:191:ASN:C	2.62	0.42
1:H:213:LEU:C	1:H:213:LEU:HD12	2.44	0.42
1:A:22:ALA:HB3	1:A:191:ASN:HB2	2.00	0.42
1:B:138:ASP:OD1	1:B:139:GLU:N	2.40	0.42
1:B:243:CYS:HB2	1:B:252:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:HIS:CD2	1:C:344:LEU:HD13	2.55	0.42
1:G:129:VAL:HG22	1:G:130:ILE:N	2.33	0.42
1:G:249:ALA:O	1:G:253:VAL:HG13	2.19	0.42
1:H:252:LEU:HD22	1:H:257:THR:HB	2.02	0.42
1:D:85:HIS:NE2	1:D:103:ASP:OD1	2.33	0.42
1:D:168:ALA:O	1:D:171:ALA:HB3	2.20	0.42
1:D:322:THR:C	1:D:324:GLY:N	2.78	0.42
1:H:250:LEU:O	1:H:253:VAL:HG22	2.19	0.42
1:A:325:LEU:HB2	1:A:336:LEU:CD2	2.48	0.41
1:D:177:ARG:NH2	1:D:186:LEU:HD12	2.35	0.41
1:E:4:LYS:HB2	1:E:39:GLU:HG2	2.02	0.41
1:E:166:ILE:O	1:E:170:ILE:HG13	2.20	0.41
1:G:143:MET:HE2	1:G:160:ILE:HG23	2.02	0.41
1:D:12:LYS:HG2	1:D:30:ASP:CG	2.44	0.41
1:D:21:ILE:HG23	1:D:23:LEU:H	1.84	0.41
1:F:168:ALA:O	1:F:171:ALA:HB3	2.20	0.41
1:G:222:ASP:OD2	1:G:225:GLY:HA3	2.20	0.41
1:A:200:VAL:O	1:A:204:GLN:HG3	2.20	0.41
1:C:147:ALA:O	1:C:151:VAL:HG23	2.20	0.41
1:E:1:MET:N	6:E:443:HOH:O	2.52	0.41
1:E:114:ALA:O	1:E:116:LEU:HG	2.20	0.41
1:D:113:LYS:O	1:D:113:LYS:CG	2.66	0.41
1:D:215:GLU:O	1:D:216:GLN:C	2.64	0.41
1:F:21:ILE:CG2	1:F:23:LEU:H	2.25	0.41
1:B:290:ILE:O	1:B:290:ILE:HG23	2.19	0.41
1:C:119:TYR:CD1	1:C:119:TYR:C	2.98	0.41
1:F:126:ASP:OD1	1:F:127:ASN:N	2.50	0.41
1:G:54:ILE:HG21	1:G:293:MET:HE1	2.02	0.41
1:G:199:ALA:O	1:G:203:ILE:HG13	2.20	0.41
1:B:229:VAL:O	1:B:233:VAL:HG22	2.21	0.41
1:D:122:LEU:C	1:D:310:ALA:HB1	2.46	0.41
1:D:148:VAL:HG22	1:D:179:ALA:O	2.21	0.41
1:F:5:GLN:H	1:F:37:GLU:HG3	1.85	0.41
1:A:262:ASN:C	1:A:262:ASN:OD1	2.64	0.41
1:B:260:VAL:HG13	1:B:287:GLU:O	2.21	0.41
1:C:211:ILE:N	1:C:211:ILE:HD12	2.36	0.41
1:C:336:LEU:HD12	1:C:336:LEU:H	1.83	0.41
1:D:234:ASN:O	1:G:197:LYS:HD3	2.20	0.41
1:D:262:ASN:HD22	1:D:289:MET:HE2	1.86	0.41
1:E:293:MET:O	1:E:296:GLU:HG2	2.21	0.41
1:H:132:ASP:OD1	1:H:132:ASP:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLU:OE1	1:A:96:PRO:HG2	2.20	0.41
1:A:225:GLY:O	1:A:228:TYR:HB3	2.21	0.41
1:B:1:MET:CG	1:B:78:PRO:HD2	2.50	0.41
1:C:35:GLU:HG3	6:C:445:HOH:O	2.20	0.41
1:D:38:THR:OG1	1:D:42:LEU:HB2	2.20	0.41
1:D:57:GLU:OE1	1:D:97:ALA:HB2	2.21	0.41
1:D:194:TRP:CE3	1:D:199:ALA:HA	2.56	0.41
1:D:264:LYS:HD2	1:D:267:LYS:CD	2.51	0.41
1:D:268:CYS:HB2	1:D:273:GLU:HB3	2.02	0.41
1:E:129:VAL:HG13	1:E:342:LEU:HB2	2.03	0.41
1:E:238:MET:HE2	1:E:260:VAL:CG1	2.51	0.41
1:F:1:MET:CE	1:F:38:THR:HG21	2.42	0.41
1:F:26:ILE:HD11	1:F:295:GLU:HG3	2.03	0.41
1:F:146:LYS:HA	1:F:149:GLU:HB3	2.03	0.41
1:F:206:LEU:N	1:F:206:LEU:HD12	2.36	0.41
1:G:160:ILE:HB	1:G:188:LEU:HD23	2.02	0.41
1:G:165:GLY:O	1:G:166:ILE:C	2.63	0.41
1:G:185:LYS:HE2	1:G:212:GLU:CD	2.46	0.41
1:C:243:CYS:HB2	1:C:252:LEU:HD11	2.03	0.41
1:D:316:ARG:HG3	6:D:373:HOH:O	2.21	0.41
1:E:16:LYS:HE3	1:E:325:LEU:O	2.20	0.41
1:A:177:ARG:C	1:A:179:ALA:H	2.29	0.40
1:D:13:ILE:HG12	1:D:327:THR:HG23	2.02	0.40
1:D:160:ILE:HB	1:D:188:LEU:HD23	2.03	0.40
1:E:250:LEU:O	1:E:253:VAL:HG22	2.21	0.40
1:F:16:LYS:C	1:F:17:GLU:HG3	2.46	0.40
1:F:21:ILE:HD11	1:F:161:LYS:HG3	2.02	0.40
1:F:38:THR:HG1	1:F:42:LEU:H	1.69	0.40
1:F:47:GLU:CG	1:F:48:GLY:N	2.83	0.40
1:A:173:VAL:HG21	1:A:206:LEU:HD21	2.03	0.40
1:B:133:ILE:HD13	1:B:150:LYS:HD2	2.03	0.40
1:B:298:THR:HG23	1:B:334:VAL:O	2.20	0.40
1:C:54:ILE:HG21	1:C:293:MET:HE1	2.03	0.40
1:D:205:ALA:C	1:D:207:ALA:H	2.29	0.40
1:D:322:THR:C	1:D:324:GLY:H	2.28	0.40
1:E:139:GLU:HB2	1:E:142:VAL:HG23	2.03	0.40
1:F:21:ILE:HG23	1:F:22:ALA:N	2.35	0.40
1:F:353:SER:O	1:F:354:HIS:C	2.64	0.40
1:G:170:ILE:HG23	1:G:206:LEU:HD11	2.03	0.40
1:H:11:SER:O	1:H:30:ASP:HA	2.21	0.40
1:A:190:ALA:O	1:A:191:ASN:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:GLN:HB3	1:C:219:LYS:HA	2.02	0.40
1:C:260:VAL:HG12	1:C:261:ILE:N	2.36	0.40
1:D:36:ILE:O	1:D:43:VAL:HA	2.21	0.40
1:E:223:LEU:HA	1:E:223:LEU:HD12	1.84	0.40
1:E:306:HIS:ND1	1:E:344:LEU:HD13	2.36	0.40
1:F:4:LYS:HB2	1:F:39:GLU:HA	2.03	0.40
1:F:4:LYS:HB2	1:F:39:GLU:N	2.36	0.40
1:F:112:GLN:C	1:F:114:ALA:H	2.30	0.40
1:A:240:ASP:OD1	1:A:264:LYS:NZ	2.55	0.40
1:D:151:VAL:HG13	1:D:184:ILE:HD11	2.03	0.40
1:D:206:LEU:N	1:D:206:LEU:CD1	2.84	0.40
1:F:262:ASN:ND2	1:F:289:MET:HE2	2.36	0.40
1:A:170:ILE:HG22	1:A:174:LYS:HE2	2.03	0.40
1:A:213:LEU:C	1:A:213:LEU:CD1	2.94	0.40
1:D:28:SER:O	1:D:29:ALA:HB2	2.22	0.40
1:F:202:ALA:O	1:F:206:LEU:HD13	2.22	0.40
1:G:167:GLU:CD	1:G:167:GLU:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	352/354 (99%)	328 (93%)	24 (7%)	0	100	100
1	B	351/354 (99%)	336 (96%)	15 (4%)	0	100	100
1	C	352/354 (99%)	333 (95%)	19 (5%)	0	100	100
1	D	352/354 (99%)	312 (89%)	34 (10%)	6 (2%)	7	3
1	E	352/354 (99%)	337 (96%)	14 (4%)	1 (0%)	36	35
1	F	352/354 (99%)	315 (90%)	31 (9%)	6 (2%)	7	3
1	G	352/354 (99%)	330 (94%)	22 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	351/354 (99%)	334 (95%)	17 (5%)	0	100	100
All	All	2814/2832 (99%)	2625 (93%)	176 (6%)	13 (0%)	24	21

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	29	ALA
1	F	29	ALA
1	F	118	LEU
1	D	28	SER
1	E	118	LEU
1	F	298	THR
1	D	39	GLU
1	D	113	LYS
1	F	28	SER
1	F	207	ALA
1	D	18	THR
1	D	207	ALA
1	F	299	ILE

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	278/278 (100%)	275 (99%)	3 (1%)	65	73
1	B	277/278 (100%)	273 (99%)	4 (1%)	59	66
1	C	278/278 (100%)	274 (99%)	4 (1%)	59	66
1	D	278/278 (100%)	273 (98%)	5 (2%)	51	58
1	E	278/278 (100%)	272 (98%)	6 (2%)	45	50
1	F	278/278 (100%)	275 (99%)	3 (1%)	65	73
1	G	278/278 (100%)	273 (98%)	5 (2%)	51	58
1	H	277/278 (100%)	271 (98%)	6 (2%)	45	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2222/2224 (100%)	2186 (98%)	36 (2%)	55 62

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	LYS
1	A	178	GLU
1	A	223	LEU
1	B	26	ILE
1	B	27	GLU
1	B	53	PHE
1	B	185	LYS
1	C	14	LYS
1	C	53	PHE
1	C	90	LYS
1	C	330	VAL
1	D	21	ILE
1	D	30	ASP
1	D	135	LEU
1	D	224	GLU
1	D	295	GLU
1	E	14	LYS
1	E	53	PHE
1	E	129	VAL
1	E	174	LYS
1	E	223	LEU
1	E	330	VAL
1	F	17	GLU
1	F	21	ILE
1	F	224	GLU
1	G	90	LYS
1	G	141	ASN
1	G	150	LYS
1	G	195	THR
1	G	221	ARG
1	H	26	ILE
1	H	27	GLU
1	H	53	PHE
1	H	67	GLU
1	H	185	LYS
1	H	279	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	354	HIS
1	B	234	ASN
1	C	247	GLN
1	C	262	ASN
1	D	112	GLN
1	D	204	GLN
1	E	7	HIS
1	E	262	ASN
1	F	204	GLN
1	F	247	GLN
1	G	5	GLN
1	G	7	HIS
1	H	210	GLN
1	H	234	ASN
1	H	279	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 32 ligands modelled in this entry, 8 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	F	357	-	5,5,5	0.34	0	5,5,5	0.28	0
4	GOL	B	357	-	5,5,5	0.22	0	5,5,5	0.29	0
4	GOL	G	357	-	5,5,5	0.26	0	5,5,5	0.27	0
2	SER	E	355	3	4,5,6	0.53	0	1,5,7	0.69	0
3	TYR	H	356	5,2	12,13,13	0.77	0	13,17,17	0.20	0
4	GOL	D	357	-	5,5,5	0.27	0	5,5,5	0.30	0
2	SER	H	355	3	4,5,6	0.55	0	1,5,7	0.66	0
2	SER	A	355	3	4,5,6	0.67	0	1,5,7	0.52	0
4	GOL	C	357	-	5,5,5	0.23	0	5,5,5	0.33	0
3	TYR	A	356	5,2	12,13,13	0.69	0	13,17,17	0.23	0
3	TYR	D	356	5,2	12,13,13	0.71	0	13,17,17	0.19	0
4	GOL	H	357	-	5,5,5	0.29	0	5,5,5	0.29	0
2	SER	B	355	3	4,5,6	0.60	0	1,5,7	0.75	0
2	SER	G	355	3	4,5,6	0.69	0	1,5,7	0.40	0
3	TYR	C	356	5,2	12,13,13	0.66	0	13,17,17	0.26	0
4	GOL	E	357	-	5,5,5	0.35	0	5,5,5	0.33	0
3	TYR	E	356	5,2	12,13,13	0.66	0	13,17,17	0.28	0
3	TYR	G	356	5,2	12,13,13	0.69	0	13,17,17	0.29	0
3	TYR	B	356	5,2	12,13,13	0.82	0	13,17,17	0.20	0
2	SER	F	355	3	4,5,6	0.58	0	1,5,7	0.71	0
2	SER	D	355	3	4,5,6	0.57	0	1,5,7	0.81	0
3	TYR	F	356	5,2	12,13,13	0.69	0	13,17,17	0.20	0
4	GOL	A	357	-	5,5,5	0.27	0	5,5,5	0.26	0
2	SER	C	355	3	4,5,6	0.51	0	1,5,7	0.68	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
4	GOL	F	357	-	-	0/4/4/4	-
4	GOL	B	357	-	-	4/4/4/4	-
4	GOL	G	357	-	-	4/4/4/4	-
2	SER	E	355	3	-	0/2/4/6	-
3	TYR	H	356	5,2	-	2/8/8/8	0/1/1/1
4	GOL	D	357	-	-	0/4/4/4	-
2	SER	H	355	3	-	0/2/4/6	-
2	SER	A	355	3	-	0/2/4/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	357	-	-	2/4/4/4	-
3	TYR	A	356	5,2	-	2/8/8/8	0/1/1/1
3	TYR	D	356	5,2	-	2/8/8/8	0/1/1/1
4	GOL	H	357	-	-	3/4/4/4	-
2	SER	B	355	3	-	0/2/4/6	-
2	SER	G	355	3	-	0/2/4/6	-
3	TYR	C	356	5,2	-	3/8/8/8	0/1/1/1
4	GOL	E	357	-	-	2/4/4/4	-
3	TYR	E	356	5,2	-	3/8/8/8	0/1/1/1
3	TYR	G	356	5,2	-	2/8/8/8	0/1/1/1
3	TYR	B	356	5,2	-	2/8/8/8	0/1/1/1
2	SER	F	355	3	-	0/2/4/6	-
2	SER	D	355	3	-	0/2/4/6	-
3	TYR	F	356	5,2	-	2/8/8/8	0/1/1/1
4	GOL	A	357	-	-	2/4/4/4	-
2	SER	C	355	3	-	0/2/4/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	357	GOL	O1-C1-C2-O2
4	B	357	GOL	O1-C1-C2-C3
4	C	357	GOL	O1-C1-C2-O2
4	C	357	GOL	O1-C1-C2-C3
4	G	357	GOL	O1-C1-C2-C3
4	G	357	GOL	C1-C2-C3-O3
4	H	357	GOL	O2-C2-C3-O3
4	A	357	GOL	O1-C1-C2-C3
4	B	357	GOL	C1-C2-C3-O3
4	E	357	GOL	C1-C2-C3-O3
4	H	357	GOL	C1-C2-C3-O3
4	G	357	GOL	O1-C1-C2-O2
4	G	357	GOL	O2-C2-C3-O3
4	A	357	GOL	O1-C1-C2-O2
4	E	357	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	D	356	TYR	CA-CB-CG-CD2
3	D	356	TYR	CA-CB-CG-CD1
4	B	357	GOL	O2-C2-C3-O3
3	B	356	TYR	CA-CB-CG-CD2
3	F	356	TYR	CA-CB-CG-CD1
3	F	356	TYR	CA-CB-CG-CD2
3	B	356	TYR	CA-CB-CG-CD1
3	A	356	TYR	CA-CB-CG-CD2
3	A	356	TYR	CA-CB-CG-CD1
3	H	356	TYR	CA-CB-CG-CD2
3	H	356	TYR	CA-CB-CG-CD1
3	G	356	TYR	CA-CB-CG-CD2
3	G	356	TYR	CA-CB-CG-CD1
4	H	357	GOL	O1-C1-C2-C3
3	C	356	TYR	CA-CB-CG-CD2
3	E	356	TYR	CA-CB-CG-CD2
3	C	356	TYR	CA-CB-CG-CD1
3	E	356	TYR	CA-CB-CG-CD1
3	E	356	TYR	OXT-C-CA-CB
3	C	356	TYR	OXT-C-CA-CB

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	356	TYR	1	0
3	E	356	TYR	2	0
2	F	355	SER	2	0
2	D	355	SER	1	0
3	F	356	TYR	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	354/354 (100%)	-1.26	0 100 100	20, 36, 57, 66	0
1	B	353/354 (99%)	-1.36	0 100 100	18, 30, 50, 61	0
1	C	354/354 (100%)	-1.24	0 100 100	25, 40, 54, 62	0
1	D	354/354 (100%)	-0.95	0 100 100	33, 54, 73, 82	0
1	E	354/354 (100%)	-1.26	0 100 100	26, 39, 53, 62	0
1	F	354/354 (100%)	-0.96	0 100 100	32, 54, 73, 81	0
1	G	354/354 (100%)	-1.26	0 100 100	22, 36, 57, 66	0
1	H	353/354 (99%)	-1.36	0 100 100	17, 30, 50, 59	0
All	All	2830/2832 (99%)	-1.21	0 100 100	17, 39, 65, 82	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SER	D	355	6/7	0.98	0.05	47,48,49,49	0
2	SER	F	355	6/7	0.98	0.04	51,52,52,53	0
2	SER	G	355	6/7	0.98	0.05	42,43,44,44	0
3	TYR	D	356	13/13	0.98	0.05	46,52,57,57	0
4	GOL	A	357	6/6	0.98	0.06	54,57,58,59	0
4	GOL	C	357	6/6	0.98	0.07	72,73,74,75	0
4	GOL	E	357	6/6	0.98	0.06	59,61,61,61	0
4	GOL	G	357	6/6	0.98	0.07	55,59,61,62	0
4	GOL	H	357	6/6	0.98	0.06	54,59,60,62	0
5	MG	D	358	1/1	0.98	0.05	42,42,42,42	0
3	TYR	C	356	13/13	0.99	0.04	37,40,45,45	0
2	SER	A	355	6/7	0.99	0.05	42,43,44,45	0
3	TYR	E	356	13/13	0.99	0.04	33,39,44,48	0
3	TYR	F	356	13/13	0.99	0.05	50,56,60,62	0
3	TYR	G	356	13/13	0.99	0.04	38,42,44,44	0
3	TYR	H	356	13/13	0.99	0.04	34,43,52,54	0
2	SER	E	355	6/7	0.99	0.03	32,35,35,35	0
4	GOL	B	357	6/6	0.99	0.06	55,59,60,60	0
2	SER	B	355	6/7	0.99	0.03	35,36,37,41	0
4	GOL	D	357	6/6	0.99	0.07	76,76,77,78	0
2	SER	C	355	6/7	0.99	0.03	34,35,36,37	0
4	GOL	F	357	6/6	0.99	0.06	72,73,74,74	0
2	SER	H	355	6/7	0.99	0.03	34,36,37,38	0
3	TYR	A	356	13/13	0.99	0.04	40,42,43,44	0
5	MG	A	358	1/1	0.99	0.03	34,34,34,34	0
5	MG	B	358	1/1	0.99	0.04	37,37,37,37	0
5	MG	C	358	1/1	0.99	0.03	33,33,33,33	0
3	TYR	B	356	13/13	0.99	0.04	35,39,47,49	0
5	MG	F	358	1/1	0.99	0.07	41,41,41,41	0
5	MG	H	358	1/1	0.99	0.07	32,32,32,32	0
5	MG	G	358	1/1	1.00	0.02	33,33,33,33	0
5	MG	E	358	1/1	1.00	0.04	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.