



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2023 – 12:26 PM EDT

PDB ID : 3P0J
Title : Leishmania major Tyrosyl-tRNA synthetase in complex with tyrosinol, triclinic crystal form 1
Authors : Larson, E.T.; Merritt, E.A.; Medical Structural Genomics of Pathogenic Protozoa (MSGPP)
Deposited on : 2010-09-28
Resolution : 2.89 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

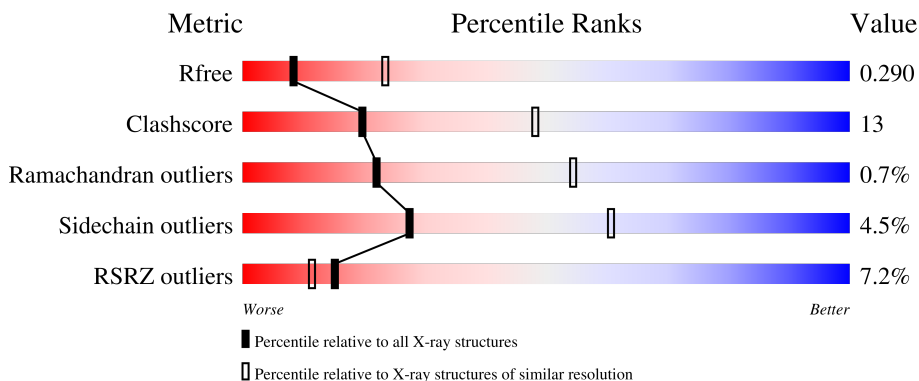
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	690	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 100%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">2% 71% 22% • 5%</p>
1	B	690	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 100%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">6% 62% 20% • 16%</p>
1	C	690	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 70%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 100%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">10% 70% 24% • •</p>
1	D	690	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 100%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">9% 71% 24% • •</p>

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 19700 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 Tyrosyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	657	Total 5067	C 3188	N 881	O 961	S 37	0	0	0
1	B	581	Total 4381	C 2763	N 746	O 837	S 35	0	0	0
1	C	663	Total 5106	C 3216	N 884	O 969	S 37	0	1	0
1	D	665	Total 5096	C 3206	N 885	O 967	S 38	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

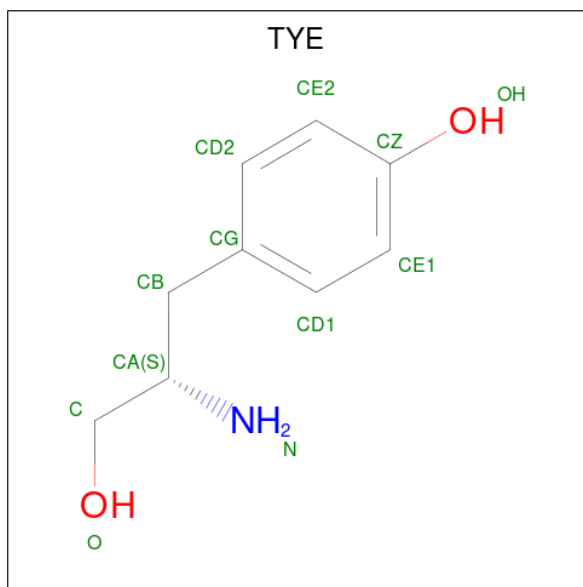
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q4QFJ7
A	-6	ALA	-	expression tag	UNP Q4QFJ7
A	-5	HIS	-	expression tag	UNP Q4QFJ7
A	-4	HIS	-	expression tag	UNP Q4QFJ7
A	-3	HIS	-	expression tag	UNP Q4QFJ7
A	-2	HIS	-	expression tag	UNP Q4QFJ7
A	-1	HIS	-	expression tag	UNP Q4QFJ7
A	0	HIS	-	expression tag	UNP Q4QFJ7
B	-7	MET	-	expression tag	UNP Q4QFJ7
B	-6	ALA	-	expression tag	UNP Q4QFJ7
B	-5	HIS	-	expression tag	UNP Q4QFJ7
B	-4	HIS	-	expression tag	UNP Q4QFJ7
B	-3	HIS	-	expression tag	UNP Q4QFJ7
B	-2	HIS	-	expression tag	UNP Q4QFJ7
B	-1	HIS	-	expression tag	UNP Q4QFJ7
B	0	HIS	-	expression tag	UNP Q4QFJ7
C	-7	MET	-	expression tag	UNP Q4QFJ7
C	-6	ALA	-	expression tag	UNP Q4QFJ7
C	-5	HIS	-	expression tag	UNP Q4QFJ7
C	-4	HIS	-	expression tag	UNP Q4QFJ7
C	-3	HIS	-	expression tag	UNP Q4QFJ7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP Q4QFJ7
C	-1	HIS	-	expression tag	UNP Q4QFJ7
C	0	HIS	-	expression tag	UNP Q4QFJ7
D	-7	MET	-	expression tag	UNP Q4QFJ7
D	-6	ALA	-	expression tag	UNP Q4QFJ7
D	-5	HIS	-	expression tag	UNP Q4QFJ7
D	-4	HIS	-	expression tag	UNP Q4QFJ7
D	-3	HIS	-	expression tag	UNP Q4QFJ7
D	-2	HIS	-	expression tag	UNP Q4QFJ7
D	-1	HIS	-	expression tag	UNP Q4QFJ7
D	0	HIS	-	expression tag	UNP Q4QFJ7

- Molecule 2 is 4-[(2S)-2-amino-3-hydroxypropyl]phenol (three-letter code: TYE) (formula: $C_9H_{13}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	12	9	1	2	0	0
2	B	1	12	9	1	2	0	0
2	C	1	12	9	1	2	0	0
2	D	1	12	9	1	2	0	0

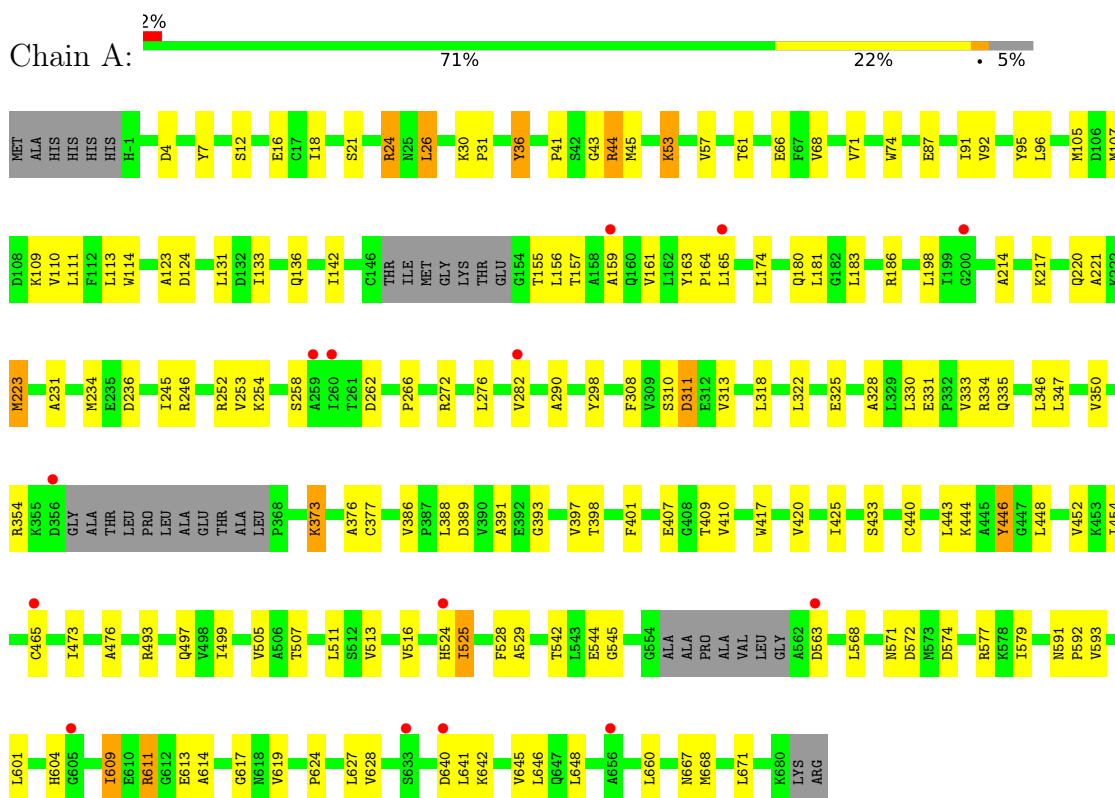
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	C	1	Total 1	Na 1	0	0

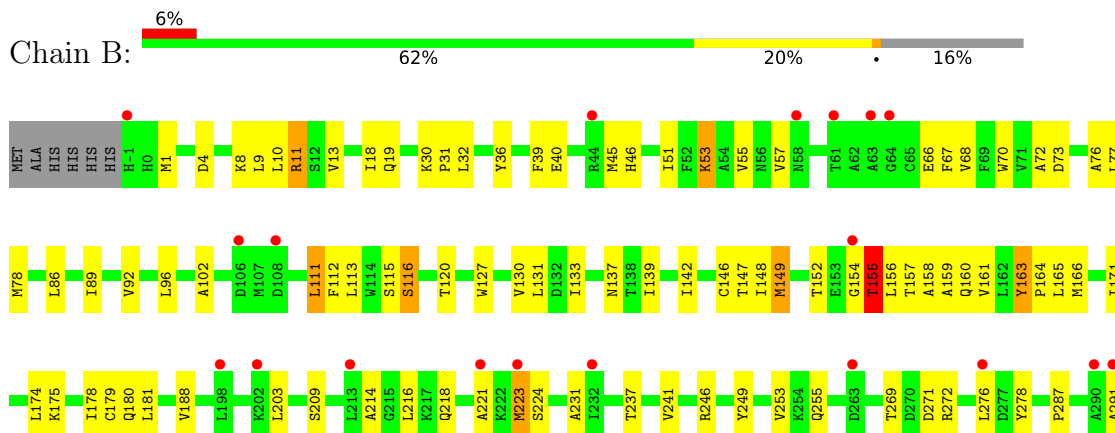
3 Residue-property plots

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: Tyrosyl-tRNA synthetase



• Molecule 1: Tyrosyl-tRNA synthetase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.52Å 111.93Å 141.04Å 74.47° 80.83° 77.13°	Depositor
Resolution (Å)	50.00 – 2.89 47.57 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-2.89) 98.1 (47.57-2.89)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.91Å)	Xtrriage
Refinement program	REFMAC refmac_5.5.0110	Depositor
R, R_{free}	0.244 , 0.293 0.239 , 0.290	Depositor DCC
R_{free} test set	3649 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	73.3	Xtrriage
Anisotropy	0.328	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 73.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.029 for h,h-k,h-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19700	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: TYE, NA

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	0.50	0/5153	0.63	0/6976
1	B	0.43	0/4456	0.59	0/6051
1	C	0.39	0/5194	0.53	0/7033
1	D	0.36	0/5182	0.51	0/7022
All	All	0.42	0/19985	0.57	0/27082

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	635	ALA	Peptide

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	5067	0	5063	105	0
1	B	4381	0	4268	124	0
1	C	5106	0	5119	142	0
1	D	5096	0	5076	136	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
2	C	12	0	12	1	0
2	D	12	0	12	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
All	All	19700	0	19574	499	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (499) 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:B:417:TRP:O	1:B:420:VAL:HG22	1.47	1.11
1:D:159:ALA:HB3	1:D:476:ALA:HB1	1.11	1.10
1:C:45:MET:HE2	1:C:99:VAL:CG1	1.80	1.10
1:C:45:MET:HE2	1:C:99:VAL:HG11	1.10	1.08
1:C:45:MET:CE	1:C:99:VAL:HG11	1.87	1.05
1:B:148:ILE:HD13	1:B:188:VAL:HG21	1.33	1.04
1:D:159:ALA:CB	1:D:476:ALA:HB1	1.87	1.04
1:D:159:ALA:HB3	1:D:476:ALA:CB	1.92	0.99
1:C:417:TRP:O	1:C:420:VAL:HG22	1.64	0.97
1:D:142:ILE:HD13	1:D:165:LEU:HD21	1.49	0.94
1:B:149:MET:HE3	1:B:163:TYR:CG	2.02	0.94
1:B:102:ALA:HB3	1:B:333:VAL:HG23	1.50	0.93
1:B:148:ILE:HD13	1:B:188:VAL:CG2	2.00	0.90
1:D:57:VAL:HG21	1:D:105:MET:HE1	1.52	0.90
1:A:330:LEU:O	1:A:333:VAL:HG12	1.72	0.90
1:A:159:ALA:HB3	1:A:476:ALA:HB1	1.54	0.89
1:A:440:CYS:SG	1:A:454:ILE:HD13	2.12	0.88
1:D:77:LEU:HD22	1:D:86:LEU:HD12	1.54	0.88
1:B:68:VAL:HG22	1:B:111:LEU:HD13	1.55	0.87
1:C:391:ALA:HB2	1:C:568:LEU:HD11	1.58	0.85
1:B:78:MET:SD	1:B:166:MET:HE1	2.16	0.85
1:D:45:MET:HE3	1:D:99:VAL:HG11	1.57	0.85
1:B:155:THR:OG1	1:B:482:SER:N	2.09	0.85
1:C:91:ILE:HG23	1:C:346:LEU:HD23	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:MET:CE	1:C:99:VAL:CG1	2.52	0.83
1:D:57:VAL:HG21	1:D:105:MET:CE	2.09	0.82
1:B:78:MET:SD	1:B:166:MET:CE	2.68	0.81
1:B:148:ILE:CD1	1:B:188:VAL:HG21	2.10	0.80
1:B:45:MET:HE2	1:B:96:LEU:HD22	1.64	0.80
1:D:142:ILE:CD1	1:D:165:LEU:HD21	2.10	0.80
1:B:149:MET:CE	1:B:163:TYR:HB3	2.12	0.79
1:B:417:TRP:O	1:B:420:VAL:CG2	2.29	0.79
1:D:40:GLU:HB2	1:D:76:ALA:HB2	1.65	0.78
1:A:386:VAL:HB	1:A:568:LEU:HD13	1.67	0.77
1:D:596:VAL:HG12	1:D:600:LEU:HD11	1.67	0.76
1:C:95:TYR:CE1	1:C:347:LEU:HD13	2.21	0.76
1:C:420:VAL:HG12	1:C:432:ILE:HD12	1.66	0.76
1:B:102:ALA:CB	1:B:333:VAL:HG23	2.15	0.76
1:C:223:MET:HG3	1:C:231:ALA:HB2	1.66	0.76
1:B:149:MET:HE3	1:B:163:TYR:HB3	1.66	0.74
1:D:45:MET:CE	1:D:99:VAL:HG11	2.16	0.74
1:D:438:VAL:HG11	1:D:668:MET:CE	2.18	0.74
1:A:391:ALA:HB2	1:A:568:LEU:HD11	1.70	0.73
1:C:159:ALA:HB3	1:C:476:ALA:HB1	1.70	0.73
1:A:159:ALA:CB	1:A:476:ALA:HB1	2.18	0.73
1:D:596:VAL:O	1:D:600:LEU:HD12	1.89	0.72
1:C:105:MET:HE3	1:C:110:VAL:HG11	1.71	0.72
1:C:51:ILE:HG21	1:C:329:LEU:HD13	1.71	0.72
1:A:18:ILE:HG22	1:A:18:ILE:O	1.90	0.71
1:D:18:ILE:HD13	1:D:207:ILE:HD12	1.71	0.71
1:B:149:MET:HE3	1:B:163:TYR:CB	2.19	0.71
1:A:66:GLU:OE2	1:B:66:GLU:OE2	2.10	0.70
1:A:131:LEU:HD22	1:A:499:ILE:HG21	1.73	0.70
1:C:516:VAL:HG13	1:C:537:ILE:HG21	1.74	0.69
1:D:163:TYR:HB3	1:D:164:PRO:HD3	1.74	0.69
1:D:51:ILE:HG21	1:D:282:VAL:HG13	1.75	0.69
1:C:660:LEU:HD22	1:C:668:MET:HE3	1.75	0.69
1:A:613:GLU:O	1:A:614:ALA:HB3	1.93	0.69
1:B:149:MET:CE	1:B:160:GLN:HB3	2.23	0.68
1:C:585:ALA:HB3	1:C:588:GLU:CD	2.13	0.68
1:D:46:HIS:NE2	1:D:48:ALA:HB3	2.08	0.68
1:A:133:ILE:HG22	1:A:165:LEU:HD22	1.75	0.68
1:C:611:ARG:NH2	1:C:635:ALA:O	2.25	0.68
1:D:346:LEU:O	1:D:350:VAL:HG13	1.94	0.68
1:A:542:THR:HG21	1:A:544:GLU:OE2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:542:THR:HG21	1:D:544:GLU:OE2	1.93	0.68
1:A:507:THR:HG22	1:A:511:LEU:HD12	1.76	0.68
1:B:116:SER:O	1:B:120:THR:HG23	1.94	0.68
1:B:307:ALA:HB1	1:B:313:VAL:HG13	1.75	0.68
1:A:542:THR:HG23	1:A:544:GLU:HG3	1.75	0.68
1:D:589:GLU:O	1:D:594:ILE:HD13	1.95	0.67
1:C:113:LEU:HD11	1:D:32:LEU:HD11	1.77	0.67
1:A:660:LEU:HD22	1:A:668:MET:CE	2.25	0.67
1:B:142:ILE:CD1	1:B:165:LEU:HD21	2.25	0.67
1:B:142:ILE:HD12	1:B:495:ALA:CB	2.25	0.66
1:B:149:MET:HE1	1:B:160:GLN:HB3	1.77	0.66
1:D:473:ILE:O	1:D:476:ALA:HB3	1.95	0.66
1:B:78:MET:HE1	1:B:163:TYR:HA	1.78	0.66
1:C:32:LEU:HD11	1:D:113:LEU:HD11	1.77	0.66
1:C:91:ILE:HG23	1:C:346:LEU:CD2	2.25	0.66
1:C:386:VAL:HB	1:C:568:LEU:HD13	1.77	0.66
1:D:157:THR:HG22	1:D:160:GLN:HG3	1.77	0.66
1:B:78:MET:HG2	1:B:473:ILE:HG23	1.78	0.66
1:C:397:VAL:HG21	1:C:542:THR:HA	1.78	0.66
1:D:464:ASN:HB2	1:D:510:MET:HE1	1.78	0.65
1:A:113:LEU:HD12	1:A:174:LEU:HD21	1.78	0.65
1:B:542:THR:HG21	1:B:544:GLU:OE2	1.96	0.65
1:C:440:CYS:SG	1:C:454:ILE:HD13	2.37	0.65
1:D:417:TRP:O	1:D:420:VAL:HG22	1.95	0.65
1:B:154:GLY:O	1:B:155:THR:HG22	1.97	0.65
1:D:347:LEU:HA	1:D:350:VAL:HG22	1.79	0.64
1:D:261:THR:HG23	1:D:264:GLY:H	1.63	0.64
1:D:438:VAL:HG11	1:D:668:MET:HE2	1.79	0.64
1:A:417:TRP:O	1:A:420:VAL:HG22	1.97	0.64
1:D:565:VAL:CG1	1:D:567:TYR:CZ	2.81	0.64
1:B:376:ALA:HB2	1:B:401:PHE:CZ	2.32	0.64
1:B:142:ILE:HD12	1:B:495:ALA:HB2	1.80	0.64
1:A:53:LYS:O	1:A:57:VAL:HG23	1.98	0.63
1:A:668:MET:HA	1:A:671:LEU:HD13	1.80	0.63
1:C:542:THR:HG23	1:C:544:GLU:HG3	1.80	0.63
1:C:601:LEU:HD23	1:C:601:LEU:C	2.19	0.63
1:D:221:ALA:HB2	1:D:268:ALA:N	2.13	0.62
1:D:347:LEU:HD12	1:D:350:VAL:CG2	2.29	0.62
1:A:660:LEU:HD22	1:A:668:MET:HE3	1.80	0.62
1:B:269:THR:HG22	1:B:271:ASP:H	1.63	0.62
1:A:611:ARG:NH1	1:A:617:GLY:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:GLN:NE2	1:D:271:ASP:O	2.30	0.62
1:D:95:TYR:CE1	1:D:347:LEU:HD13	2.35	0.62
1:A:113:LEU:HD12	1:A:174:LEU:CD2	2.29	0.62
1:A:245:ILE:HD12	1:A:322:LEU:HD23	1.81	0.62
1:C:613:GLU:O	1:C:614:ALA:HB3	1.99	0.62
1:D:180:GLN:NE2	1:D:208:LEU:O	2.33	0.61
1:D:565:VAL:HG12	1:D:567:TYR:CZ	2.36	0.61
1:C:376:ALA:HB2	1:C:401:PHE:CZ	2.34	0.61
1:D:159:ALA:CB	1:D:476:ALA:CB	2.66	0.61
1:C:223:MET:HG3	1:C:231:ALA:CB	2.30	0.61
1:A:113:LEU:HD11	1:B:32:LEU:HD11	1.83	0.61
1:C:111:LEU:HD11	1:D:111:LEU:HD21	1.82	0.61
1:A:214:ALA:HB2	1:A:272:ARG:HD3	1.82	0.61
1:D:45:MET:HE1	1:D:99:VAL:HB	1.83	0.61
1:B:112:PHE:O	1:B:113:LEU:HD23	2.00	0.60
1:C:131:LEU:HD22	1:C:499:ILE:HG21	1.83	0.60
1:C:236:ASP:O	1:C:334:ARG:NH1	2.33	0.60
1:C:516:VAL:HG23	1:C:516:VAL:O	2.02	0.60
1:B:127:TRP:O	1:B:130:VAL:HG22	2.02	0.60
1:C:142:ILE:HD13	1:C:165:LEU:HD21	1.83	0.60
1:B:78:MET:SD	1:B:166:MET:HE2	2.41	0.60
1:C:142:ILE:CD1	1:C:165:LEU:HD21	2.32	0.59
1:A:71:VAL:HG11	1:A:114:TRP:CZ3	2.37	0.59
1:A:308:PHE:HA	1:A:313:VAL:HG23	1.83	0.59
1:B:155:THR:HG1	1:B:482:SER:H	1.46	0.59
1:D:82:VAL:HG12	1:D:82:VAL:O	2.03	0.59
1:B:388:LEU:HD11	1:B:446:TYR:CZ	2.38	0.59
1:C:131:LEU:CD2	1:C:499:ILE:HG21	2.33	0.59
1:D:72:ALA:HB1	1:D:75:PHE:HB2	1.85	0.59
1:B:78:MET:CE	1:B:166:MET:CE	2.80	0.59
1:C:279:PHE:O	1:C:283:VAL:HG23	2.03	0.59
1:D:45:MET:HE2	1:D:96:LEU:HD23	1.85	0.59
1:C:261:THR:HG23	1:C:264:GLY:H	1.68	0.58
1:B:360:LEU:CB	1:B:361:PRO:CD	2.81	0.58
1:A:613:GLU:O	1:A:614:ALA:CB	2.51	0.58
1:D:10:LEU:HD23	1:D:27:ILE:HD11	1.86	0.58
1:D:171:ILE:HD12	1:D:192:ALA:HB2	1.85	0.58
1:B:214:ALA:HA	1:B:221:ALA:O	2.03	0.58
1:C:660:LEU:HD22	1:C:668:MET:CE	2.33	0.58
1:D:159:ALA:HB3	1:D:476:ALA:CA	2.33	0.58
1:C:142:ILE:HD12	1:C:495:ALA:CB	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:ASP:N	1:D:466:ASP:OD1	2.35	0.58
1:D:142:ILE:HD12	1:D:495:ALA:CB	2.33	0.58
1:A:398:THR:HG21	1:A:452:VAL:HG21	1.86	0.58
1:D:386:VAL:HB	1:D:568:LEU:HD12	1.86	0.57
1:B:51:ILE:O	1:B:55:VAL:HG23	2.04	0.57
1:D:154:GLY:O	1:D:155:THR:HG22	2.05	0.57
1:B:92:VAL:HG22	1:B:350:VAL:HG22	1.86	0.57
1:D:91:ILE:HG23	1:D:346:LEU:CD2	2.34	0.57
1:B:77:LEU:HD22	1:B:86:LEU:HD13	1.85	0.57
1:C:391:ALA:CB	1:C:568:LEU:HD11	2.33	0.57
1:D:393:GLY:O	1:D:397:VAL:HG23	2.04	0.57
1:C:18:ILE:CG2	1:C:18:ILE:O	2.52	0.57
1:D:18:ILE:O	1:D:18:ILE:HG22	2.03	0.57
1:A:667:ASN:O	1:A:671:LEU:CD1	2.53	0.57
1:C:45:MET:HE2	1:C:99:VAL:CB	2.32	0.57
1:A:440:CYS:SG	1:A:454:ILE:CD1	2.89	0.56
1:B:149:MET:CE	1:B:163:TYR:CG	2.84	0.56
1:C:351:LYS:HG2	1:C:354:ARG:CZ	2.35	0.56
1:C:95:TYR:CZ	1:C:347:LEU:HD13	2.40	0.56
1:B:142:ILE:HD13	1:B:165:LEU:HD21	1.86	0.56
1:B:155:THR:OG1	1:B:482:SER:CB	2.54	0.56
1:C:509:LEU:HD11	1:C:532:TYR:HE2	1.70	0.56
1:A:91:ILE:HG23	1:A:346:LEU:HD23	1.87	0.56
1:D:162:LEU:HG	1:D:166:MET:HE2	1.87	0.56
1:C:242:ALA:HA	1:C:323:ILE:HD13	1.88	0.56
1:A:393:GLY:O	1:A:397:VAL:HG23	2.06	0.56
1:B:159:ALA:HB3	1:B:476:ALA:HB1	1.88	0.56
1:C:417:TRP:O	1:C:420:VAL:CG2	2.49	0.56
1:B:76:ALA:HB3	1:B:89:ILE:HD13	1.88	0.56
1:B:142:ILE:HD11	1:B:165:LEU:HD21	1.87	0.56
1:C:51:ILE:O	1:C:55:VAL:HG23	2.07	0.56
1:A:105:MET:HB3	1:A:107:MET:HE2	1.87	0.55
1:B:149:MET:CE	1:B:163:TYR:CB	2.78	0.55
1:B:154:GLY:C	1:B:156:LEU:H	2.10	0.55
1:B:155:THR:C	1:B:157:THR:N	2.58	0.55
1:B:68:VAL:CG2	1:B:111:LEU:HD13	2.33	0.55
1:C:245:ILE:HD12	1:C:322:LEU:HD23	1.88	0.55
1:C:275:VAL:HG13	1:C:322:LEU:HD22	1.89	0.55
1:B:149:MET:HE1	1:B:163:TYR:HB3	1.89	0.55
1:B:18:ILE:CG2	1:B:18:ILE:O	2.55	0.55
1:D:398:THR:HG21	1:D:452:VAL:CG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLY:HA2	1:A:92:VAL:HG13	1.89	0.55
1:C:542:THR:HG21	1:C:544:GLU:OE2	2.07	0.54
1:D:263:ASP:OD2	1:D:265:ALA:HB2	2.07	0.54
1:C:138:THR:HG23	1:C:141:ARG:H	1.73	0.54
1:C:139:ILE:HD11	1:C:481:LEU:HD11	1.89	0.54
1:C:223:MET:HE2	1:C:231:ALA:HB1	1.88	0.54
1:C:378:MET:O	1:C:412:LEU:HD12	2.07	0.54
1:D:608:SER:HA	1:D:620:SER:HA	1.89	0.54
1:D:78:MET:HE2	1:D:163:TYR:HB2	1.89	0.54
1:B:139:ILE:CD1	1:B:498:VAL:HG21	2.37	0.54
1:D:93:GLY:HA2	1:D:96:LEU:HD12	1.89	0.53
1:A:440:CYS:HG	1:A:454:ILE:HD13	1.73	0.53
1:B:420:VAL:HG23	1:B:421:ALA:N	2.23	0.53
1:A:61:THR:HG22	1:A:109:LYS:HB2	1.89	0.53
1:B:13:VAL:HG12	1:B:180:GLN:NE2	2.24	0.53
1:C:18:ILE:O	1:C:18:ILE:HG22	2.08	0.53
1:A:524:HIS:O	1:A:525:ILE:C	2.46	0.53
1:B:149:MET:HE3	1:B:163:TYR:CD1	2.42	0.53
1:B:1:MET:CE	1:B:9:LEU:HD22	2.39	0.53
1:D:18:ILE:O	1:D:18:ILE:CG2	2.57	0.53
1:A:159:ALA:HA	1:A:161:VAL:HG12	1.90	0.53
1:A:221:ALA:HB1	1:A:266:PRO:HB2	1.91	0.53
1:B:376:ALA:HB2	1:B:401:PHE:CE1	2.44	0.53
1:C:159:ALA:CB	1:C:476:ALA:HB1	2.38	0.53
1:B:70:TRP:CZ3	1:B:174:LEU:HD21	2.44	0.52
1:D:146:CYS:SG	1:D:147:THR:N	2.82	0.52
1:B:133:ILE:O	1:B:137:ASN:ND2	2.42	0.52
1:C:456:THR:O	1:C:460:VAL:HG23	2.09	0.52
1:D:234:MET:HE3	1:D:330:LEU:HD22	1.91	0.52
1:C:74:TRP:CZ3	1:C:473:ILE:HD12	2.45	0.52
1:C:613:GLU:O	1:C:614:ALA:CB	2.57	0.52
1:D:135:ARG:HD3	1:D:420:VAL:O	2.09	0.52
1:A:74:TRP:HZ3	1:A:473:ILE:HD12	1.75	0.52
1:B:46:HIS:CD2	1:B:223:MET:HG2	2.45	0.52
1:B:32:LEU:HD22	1:B:66:GLU:HB2	1.92	0.52
1:B:255:GLN:HE22	1:B:272:ARG:HA	1.74	0.52
1:D:32:LEU:HD22	1:D:66:GLU:HB2	1.91	0.52
1:B:11:ARG:O	1:B:11:ARG:HD3	2.09	0.52
1:A:444:LYS:NZ	1:A:454:ILE:HD12	2.25	0.51
1:D:601:LEU:C	1:D:601:LEU:HD23	2.31	0.51
1:A:667:ASN:O	1:A:671:LEU:HD12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:LEU:O	1:B:645:VAL:HG23	2.11	0.51
1:C:74:TRP:HZ3	1:C:473:ILE:HD12	1.75	0.51
1:D:157:THR:HG22	1:D:160:GLN:CG	2.40	0.51
1:A:593:VAL:HG11	1:A:642:LYS:HG2	1.93	0.51
1:B:57:VAL:HG22	1:B:67:PHE:CE1	2.45	0.51
1:C:388:LEU:HD22	1:C:566:LEU:HB3	1.93	0.51
1:D:146:CYS:SG	1:D:153:GLU:HB2	2.50	0.51
1:C:337:PHE:CE1	1:C:343:ALA:HB1	2.45	0.51
1:C:337:PHE:CD1	1:C:343:ALA:HB1	2.46	0.51
1:C:601:LEU:HD23	1:C:602:ALA:N	2.26	0.51
1:A:36:TYR:HA	1:A:68:VAL:O	2.11	0.51
1:C:487:LEU:HD13	1:C:528:PHE:HB2	1.92	0.51
1:D:236:ASP:O	1:D:334:ARG:NH1	2.43	0.51
1:A:331:GLU:OE2	1:A:335:GLN:NE2	2.45	0.50
1:B:146:CYS:SG	1:B:147:THR:N	2.85	0.50
1:D:74:TRP:CD1	1:D:86:LEU:HD11	2.46	0.50
1:D:78:MET:SD	1:D:166:MET:HE3	2.52	0.50
1:A:641:LEU:O	1:A:645:VAL:HG23	2.12	0.50
1:C:146:CYS:SG	1:C:147:THR:N	2.84	0.50
1:C:283:VAL:HG11	1:C:325:GLU:HG2	1.94	0.50
1:D:353:TYR:O	1:D:354:ARG:C	2.50	0.50
1:B:73:ASP:OD2	1:B:116:SER:OG	2.30	0.50
1:A:105:MET:CE	1:A:110:VAL:HG21	2.42	0.50
1:C:159:ALA:HB3	1:C:476:ALA:CB	2.40	0.50
1:B:18:ILE:O	1:B:18:ILE:HG22	2.11	0.50
1:C:43:GLY:HA2	1:C:92:VAL:HG13	1.93	0.50
1:D:398:THR:HG21	1:D:452:VAL:HG21	1.93	0.50
1:A:579:ILE:HG21	1:A:646:LEU:HB2	1.94	0.50
1:A:660:LEU:HD22	1:A:668:MET:HE2	1.94	0.50
1:D:34:ARG:NH1	1:D:174:LEU:O	2.45	0.50
1:D:45:MET:HE1	1:D:99:VAL:CB	2.41	0.50
1:D:425:ILE:HG22	1:D:426:THR:H	1.77	0.50
1:A:619:VAL:HG13	1:A:619:VAL:O	2.12	0.50
1:C:18:ILE:HG21	1:C:193:ARG:HD2	1.94	0.50
1:C:466:ASP:OD1	1:C:466:ASP:N	2.43	0.50
1:D:18:ILE:HG23	1:D:19:GLN:HG2	1.94	0.50
1:B:516:VAL:HG13	1:B:537:ILE:HG21	1.94	0.49
1:C:511:LEU:O	1:C:512:SER:HB3	2.12	0.49
1:A:44:ARG:CZ	1:A:354:ARG:HD3	2.42	0.49
1:B:102:ALA:HB1	1:B:333:VAL:HA	1.95	0.49
1:D:78:MET:HE1	1:D:163:TYR:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ALA:HB1	1:A:298:TYR:O	2.13	0.49
1:A:516:VAL:O	1:A:516:VAL:HG23	2.13	0.49
1:D:142:ILE:CG2	1:D:161:VAL:HG22	2.43	0.49
1:D:347:LEU:HD12	1:D:350:VAL:HG22	1.94	0.49
1:D:384:LEU:HD23	1:D:675:GLU:OE1	2.12	0.49
1:B:163:TYR:HB3	1:B:164:PRO:HD3	1.94	0.49
1:B:181:LEU:N	1:B:181:LEU:HD12	2.28	0.49
1:A:57:VAL:HG11	1:A:105:MET:HE3	1.95	0.48
1:A:105:MET:CB	1:A:107:MET:HE2	2.43	0.48
1:C:362:LEU:HD12	1:C:362:LEU:O	2.13	0.48
1:C:392:GLU:OE2	1:C:652:ARG:NH2	2.47	0.48
1:A:350:VAL:HG12	1:A:354:ARG:NH2	2.29	0.48
1:D:609:ILE:HD12	1:D:636:LEU:HD11	1.96	0.48
1:B:13:VAL:CG1	1:B:180:GLN:NE2	2.76	0.48
1:D:388:LEU:HD11	1:D:446:TYR:CZ	2.47	0.48
1:A:563:ASP:OD2	1:A:577:ARG:NH1	2.35	0.48
1:B:414:LEU:HB2	1:B:456:THR:HG22	1.95	0.48
1:C:407:GLU:OE1	1:C:407:GLU:N	2.45	0.48
1:C:246:ARG:NH2	1:C:320:SER:OG	2.45	0.48
1:C:461:ILE:O	1:C:465:CYS:N	2.47	0.48
1:D:131:LEU:CD2	1:D:499:ILE:HG21	2.43	0.48
1:B:376:ALA:HB3	1:B:410:VAL:HG13	1.95	0.48
1:A:111:LEU:HD21	1:B:66:GLU:HG3	1.95	0.48
1:A:142:ILE:HD12	1:A:165:LEU:HD21	1.95	0.48
1:A:236:ASP:O	1:A:334:ARG:NH1	2.46	0.47
1:A:308:PHE:HA	1:A:313:VAL:CG2	2.44	0.47
1:C:273:ASN:HB3	1:C:276:LEU:HD12	1.95	0.47
1:D:625:GLU:O	1:D:628:VAL:HG22	2.14	0.47
1:A:660:LEU:CD2	1:A:668:MET:HE2	2.45	0.47
1:A:376:ALA:HB2	1:A:401:PHE:CZ	2.49	0.47
1:B:388:LEU:HD11	1:B:446:TYR:OH	2.14	0.47
1:C:86:LEU:HG	1:C:90:ARG:HE	1.80	0.47
1:C:346:LEU:O	1:C:350:VAL:HG23	2.15	0.47
1:C:249:TYR:CZ	1:C:251:PRO:HG3	2.50	0.47
1:C:392:GLU:OE1	1:C:599:HIS:NE2	2.41	0.47
1:A:133:ILE:HG22	1:A:165:LEU:CD2	2.43	0.47
1:B:377:CYS:HB2	1:B:513:VAL:HG21	1.97	0.47
1:D:592:PRO:O	1:D:596:VAL:HG23	2.15	0.47
1:A:388:LEU:HD11	1:A:446:TYR:CZ	2.49	0.47
1:B:171:ILE:HD13	1:B:179:CYS:SG	2.54	0.47
1:B:223:MET:SD	1:B:224:SER:N	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LYS:O	1:A:220:GLN:HG2	2.15	0.47
1:A:310:SER:O	1:A:311:ASP:CB	2.63	0.47
1:D:78:MET:SD	1:D:166:MET:CE	3.03	0.47
1:C:378:MET:HE3	1:C:412:LEU:HD13	1.97	0.47
1:B:223:MET:SD	1:B:223:MET:C	2.94	0.46
1:B:468:PHE:O	1:B:471:SER:HB3	2.15	0.46
1:C:45:MET:HG3	1:C:49:GLN:HB3	1.97	0.46
1:A:505:VAL:HG22	1:A:529:ALA:HA	1.97	0.46
1:C:133:ILE:HG22	1:C:165:LEU:HD22	1.97	0.46
1:C:18:ILE:HB	1:C:207:ILE:HB	1.97	0.46
1:D:74:TRP:HD1	1:D:86:LEU:HD11	1.80	0.46
1:B:142:ILE:HD12	1:B:495:ALA:HB1	1.97	0.46
1:D:438:VAL:HG11	1:D:668:MET:HE3	1.95	0.46
1:A:163:TYR:HB2	1:A:164:PRO:HD3	1.97	0.46
1:D:611:ARG:NH2	1:D:619:VAL:HG11	2.31	0.46
1:B:53:LYS:HE3	1:B:53:LYS:HA	1.96	0.46
1:C:273:ASN:CB	1:C:276:LEU:HD12	2.46	0.46
1:A:123:ALA:HB1	1:A:465:CYS:SG	2.56	0.46
1:B:181:LEU:O	1:B:209:SER:HA	2.15	0.46
1:C:142:ILE:CG2	1:C:161:VAL:HG23	2.47	0.46
1:D:139:ILE:HD11	1:D:481:LEU:HD11	1.98	0.46
1:D:139:ILE:HD13	1:D:492:VAL:HG21	1.97	0.46
1:D:623:THR:HG23	1:D:626:ALA:HB3	1.98	0.46
1:D:641:LEU:O	1:D:645:VAL:HG23	2.15	0.46
1:C:493:ARG:N	1:C:497:GLN:OE1	2.48	0.45
1:D:351:LYS:HA	1:D:354:ARG:HG2	1.98	0.45
1:A:609:ILE:HD12	1:A:640:ASP:HB3	1.98	0.45
1:B:158:ALA:C	1:B:160:GLN:H	2.19	0.45
1:D:71:VAL:HG11	1:D:114:TRP:CZ3	2.52	0.45
1:A:7:TYR:CD1	1:A:24:ARG:HG2	2.52	0.45
1:A:276:LEU:CD1	1:A:318:LEU:HD21	2.47	0.45
1:A:591:ASN:HB2	1:A:592:PRO:CD	2.46	0.45
1:B:425:ILE:HG22	1:B:426:THR:H	1.81	0.45
1:C:71:VAL:HG11	1:C:114:TRP:CZ3	2.51	0.45
1:D:45:MET:CE	1:D:99:VAL:CG1	2.90	0.45
1:C:604:HIS:HD1	1:C:604:HIS:C	2.19	0.45
1:B:39:PHE:O	1:B:72:ALA:HB3	2.16	0.45
1:B:130:VAL:HG23	1:B:131:LEU:N	2.31	0.45
1:D:347:LEU:O	1:D:350:VAL:HG22	2.16	0.45
1:B:253:VAL:HG11	1:B:271:ASP:HB3	1.99	0.45
1:C:516:VAL:HG13	1:C:537:ILE:CG2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:TYR:HB3	1:D:164:PRO:CD	2.46	0.45
1:A:234:MET:SD	1:A:330:LEU:HD21	2.57	0.45
1:C:163:TYR:HB2	1:C:164:PRO:HD3	1.97	0.45
1:D:15:GLU:OE1	1:D:211:HIS:ND1	2.44	0.45
1:C:41:PRO:HB3	1:C:92:VAL:HG12	1.99	0.45
1:D:671:LEU:O	1:D:674:ALA:HB3	2.16	0.45
1:A:253:VAL:HG12	1:A:254:LYS:O	2.17	0.44
1:B:127:TRP:HA	1:B:130:VAL:HG22	1.99	0.44
1:C:367:LEU:HD23	1:C:368:PRO:HD2	1.98	0.44
1:C:393:GLY:O	1:C:397:VAL:HG23	2.18	0.44
1:D:180:GLN:C	1:D:181:LEU:HD12	2.38	0.44
1:C:464:ASN:OD1	1:C:464:ASN:N	2.50	0.44
1:C:610:GLU:O	1:C:611:ARG:HG2	2.17	0.44
1:C:627:LEU:HD23	1:C:627:LEU:O	2.17	0.44
1:D:10:LEU:CD2	1:D:27:ILE:HD11	2.46	0.44
1:D:604:HIS:ND1	1:D:604:HIS:C	2.70	0.44
1:A:105:MET:HE3	1:A:110:VAL:HG21	2.00	0.44
1:A:183:LEU:O	1:A:186:ARG:HB2	2.18	0.44
1:A:624:PRO:O	1:A:628:VAL:HG23	2.17	0.44
1:A:181:LEU:HD12	1:A:181:LEU:N	2.32	0.44
1:B:223:MET:HB2	1:B:231:ALA:HB2	1.99	0.44
1:C:46:HIS:CE1	1:C:48:ALA:HB3	2.52	0.44
1:C:95:TYR:O	1:C:99:VAL:HG23	2.17	0.44
1:D:126:TYR:O	1:D:130:VAL:HG23	2.18	0.44
1:C:159:ALA:HB3	1:C:476:ALA:CA	2.48	0.44
1:C:232:ILE:HD13	1:C:244:LYS:HD2	2.00	0.44
1:C:245:ILE:HD12	1:C:322:LEU:CD2	2.48	0.44
1:C:307:ALA:HB1	1:C:313:VAL:HG13	2.00	0.44
1:D:46:HIS:CD2	1:D:48:ALA:HB3	2.52	0.44
1:C:279:PHE:HA	1:C:283:VAL:CG2	2.48	0.43
1:D:91:ILE:HG23	1:D:346:LEU:HD23	1.99	0.43
1:D:159:ALA:CB	1:D:476:ALA:CA	2.94	0.43
1:C:185:GLN:O	1:C:189:ASN:ND2	2.49	0.43
1:B:142:ILE:CD1	1:B:495:ALA:CB	2.96	0.43
1:D:142:ILE:HG21	1:D:161:VAL:HG22	2.00	0.43
1:B:39:PHE:N	1:B:39:PHE:CD2	2.86	0.43
1:B:397:VAL:HG21	1:B:542:THR:HA	2.00	0.43
1:C:185:GLN:NE2	2:C:701:TYE:H	2.33	0.43
1:D:138:THR:HG23	1:D:141:ARG:H	1.83	0.43
1:D:623:THR:HG23	1:D:626:ALA:CB	2.48	0.43
1:B:340:ASN:HD21	1:B:342:GLU:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:ALA:HB2	1:C:401:PHE:CE1	2.54	0.43
1:C:398:THR:HG21	1:C:452:VAL:HG21	2.01	0.43
1:D:156:LEU:O	1:D:156:LEU:HD23	2.19	0.43
1:A:105:MET:HE1	1:A:107:MET:HE1	2.00	0.43
1:C:195:TYR:HA	1:C:198:LEU:HD12	2.00	0.43
1:A:571:ASN:OD1	1:A:574:ASP:N	2.41	0.43
1:B:360:LEU:CB	1:B:361:PRO:HD2	2.48	0.43
1:D:646:LEU:C	1:D:646:LEU:HD23	2.39	0.43
1:A:604:HIS:NE2	1:A:648:LEU:HD22	2.34	0.43
1:C:165:LEU:CD1	1:C:499:ILE:HD11	2.48	0.43
1:C:344:HIS:CE1	1:C:348:GLU:HG3	2.54	0.43
1:C:434:ALA:O	1:C:438:VAL:HG23	2.19	0.43
1:D:346:LEU:O	1:D:349:ALA:HB3	2.19	0.43
1:D:607:LEU:O	1:D:621:TYR:N	2.40	0.43
1:B:165:LEU:HD12	1:B:499:ILE:HD11	2.01	0.43
1:C:18:ILE:HG22	1:C:207:ILE:H	1.84	0.43
1:C:46:HIS:ND1	1:C:48:ALA:HB3	2.34	0.43
1:C:601:LEU:HD12	1:C:607:LEU:HB3	2.01	0.42
1:D:376:ALA:HB2	1:D:401:PHE:CZ	2.53	0.42
1:A:223:MET:HB2	1:A:231:ALA:HB2	2.01	0.42
1:B:216:LEU:HD21	1:B:278:TYR:CZ	2.54	0.42
1:C:43:GLY:CA	1:C:92:VAL:HG13	2.49	0.42
1:D:653:SER:O	1:D:654:ALA:C	2.57	0.42
1:A:389:ASP:OD2	1:A:545:GLY:N	2.49	0.42
1:A:493:ARG:N	1:A:497:GLN:OE1	2.41	0.42
1:C:53:LYS:HE3	1:C:53:LYS:HA	2.02	0.42
1:C:111:LEU:HD12	1:C:111:LEU:N	2.34	0.42
1:C:242:ALA:HA	1:C:323:ILE:CD1	2.48	0.42
1:D:223:MET:HB2	1:D:231:ALA:HB2	2.01	0.42
1:B:154:GLY:O	1:B:156:LEU:N	2.46	0.42
1:B:431:ASP:OD1	1:B:670:VAL:HG12	2.19	0.42
1:C:409:THR:CG2	1:C:410:VAL:N	2.81	0.42
1:D:38:GLY:HA2	1:D:70:TRP:O	2.19	0.42
1:D:44:ARG:HG2	1:D:354:ARG:NH1	2.34	0.42
1:A:325:GLU:O	1:A:328:ALA:HB3	2.20	0.42
1:A:601:LEU:HD23	1:A:601:LEU:O	2.19	0.42
1:C:187:LYS:HE2	1:C:263:ASP:HA	2.02	0.42
1:D:291:ALA:O	1:D:297:THR:HG23	2.18	0.42
1:A:136:GLN:HB3	1:A:198:LEU:HD13	2.02	0.42
1:C:105:MET:HB3	1:C:105:MET:HE2	1.74	0.42
1:C:611:ARG:NH1	1:C:616:GLY:HA3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ARG:HG3	1:A:24:ARG:HH11	1.85	0.42
1:A:30:LYS:HA	1:A:31:PRO:HD3	1.90	0.42
1:D:44:ARG:HG2	1:D:354:ARG:CZ	2.50	0.42
1:B:1:MET:HE2	1:B:9:LEU:HD22	2.02	0.42
1:C:591:ASN:C	1:C:591:ASN:OD1	2.57	0.42
1:B:378:MET:O	1:B:412:LEU:HD12	2.20	0.42
1:B:448:LEU:HG	1:B:449:PRO:HD2	2.01	0.42
1:A:105:MET:CE	1:A:110:VAL:HG11	2.50	0.41
1:A:331:GLU:O	1:A:335:GLN:HG2	2.20	0.41
1:A:409:THR:HG22	1:A:410:VAL:N	2.35	0.41
1:B:78:MET:HB2	1:B:78:MET:HE3	1.67	0.41
1:C:579:ILE:O	1:C:582:ALA:HB3	2.20	0.41
1:D:44:ARG:HH21	1:D:354:ARG:HD3	1.84	0.41
1:D:659:LEU:HD22	1:D:663:GLU:HB3	2.02	0.41
1:A:111:LEU:HD11	1:B:111:LEU:HD21	2.03	0.41
1:A:444:LYS:HA	1:A:448:LEU:HB3	2.02	0.41
1:B:10:LEU:HD21	1:B:178:ILE:CD1	2.51	0.41
1:B:330:LEU:O	1:B:333:VAL:HG12	2.19	0.41
1:C:370:ALA:HB2	1:C:536:ARG:HD2	2.01	0.41
1:B:139:ILE:HD11	1:B:161:VAL:HG21	2.02	0.41
1:B:473:ILE:O	1:B:476:ALA:HB3	2.20	0.41
1:C:165:LEU:HD12	1:C:499:ILE:HD11	2.02	0.41
1:A:377:CYS:HB2	1:A:513:VAL:HG21	2.02	0.41
1:D:472:VAL:HG13	1:D:502:LEU:HB3	2.03	0.41
1:A:214:ALA:CB	1:A:272:ARG:HD3	2.48	0.41
1:B:292:THR:HG23	1:B:296:THR:O	2.21	0.41
1:C:283:VAL:O	1:C:286:ARG:HB2	2.21	0.41
1:A:95:TYR:CE1	1:A:347:LEU:HD13	2.55	0.41
1:B:218:GLN:HA	1:B:249:TYR:CD2	2.55	0.41
1:D:398:THR:HG23	1:D:410:VAL:HG11	2.03	0.41
1:A:443:LEU:HD23	1:A:448:LEU:HD22	2.02	0.41
1:B:291:ALA:O	1:B:297:THR:HG23	2.21	0.41
1:C:31:PRO:HA	1:D:122:HIS:CE1	2.56	0.41
1:C:34:ARG:NH1	1:C:174:LEU:O	2.54	0.41
1:C:161:VAL:O	1:C:161:VAL:HG22	2.20	0.41
1:C:245:ILE:HG22	1:C:319:LYS:HB3	2.02	0.41
1:C:343:ALA:HA	1:C:346:LEU:HD12	2.01	0.41
1:D:349:ALA:O	1:D:352:SER:OG	2.33	0.41
1:A:26:LEU:HD12	1:A:26:LEU:HA	1.96	0.41
1:A:45:MET:CE	1:A:96:LEU:HD22	2.51	0.41
1:B:45:MET:CE	1:B:96:LEU:HD22	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:GLU:HB3	1:B:332:PRO:HD3	2.02	0.41
1:B:414:LEU:N	1:B:414:LEU:HD23	2.36	0.41
1:B:480:LEU:O	1:B:484:VAL:HG23	2.21	0.41
1:B:516:VAL:HG23	1:B:516:VAL:O	2.21	0.41
1:C:291:ALA:O	1:C:297:THR:HG23	2.21	0.41
1:C:351:LYS:HA	1:C:354:ARG:NE	2.35	0.41
1:C:480:LEU:N	1:C:480:LEU:HD12	2.36	0.41
1:C:601:LEU:C	1:C:601:LEU:CD2	2.88	0.41
1:D:47:ILE:HG21	1:D:278:TYR:CE1	2.55	0.41
1:D:91:ILE:HG23	1:D:346:LEU:HD22	2.01	0.41
1:D:162:LEU:O	1:D:166:MET:HE2	2.21	0.41
1:A:161:VAL:O	1:A:161:VAL:HG22	2.21	0.40
1:B:30:LYS:HA	1:B:31:PRO:HD3	1.89	0.40
1:C:428:VAL:HG12	1:C:430:LYS:H	1.86	0.40
1:D:337:PHE:CE1	1:D:347:LEU:HB2	2.56	0.40
1:B:237:THR:O	1:B:241:VAL:HG23	2.21	0.40
1:D:156:LEU:O	1:D:156:LEU:CD2	2.70	0.40
1:A:373:LYS:HG2	1:A:407:GLU:HG2	2.04	0.40
1:B:331:GLU:O	1:B:335:GLN:HG3	2.22	0.40
1:D:45:MET:HE1	1:D:99:VAL:CG1	2.52	0.40
1:D:290:ALA:HB1	1:D:298:TYR:O	2.21	0.40
1:C:79:ASN:OD1	1:C:79:ASN:N	2.55	0.40
1:D:95:TYR:O	1:D:99:VAL:HG23	2.22	0.40
1:D:367:LEU:HD12	1:D:368:PRO:HD2	2.04	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	649/690 (94%)	607 (94%)	37 (6%)	5 (1%)	19 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	573/690 (83%)	529 (92%)	40 (7%)	4 (1%)	22	54
1	C	656/690 (95%)	622 (95%)	31 (5%)	3 (0%)	29	61
1	D	659/690 (96%)	624 (95%)	30 (5%)	5 (1%)	19	51
All	All	2537/2760 (92%)	2382 (94%)	138 (5%)	17 (1%)	22	54

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	ASP
1	A	525	ILE
1	D	31	PRO
1	D	425	ILE
1	A	262	ASP
1	A	425	ILE
1	B	425	ILE
1	C	425	ILE
1	C	451	SER
1	C	512	SER
1	B	155	THR
1	D	158	ALA
1	D	311	ASP
1	D	654	ALA
1	A	41	PRO
1	B	287	PRO
1	B	361	PRO

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	540/567 (95%)	512 (95%)	28 (5%)	23	55
1	B	453/567 (80%)	429 (95%)	24 (5%)	22	54
1	C	544/567 (96%)	521 (96%)	23 (4%)	30	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	539/567 (95%)	520 (96%)	19 (4%)	36 70
All	All	2076/2268 (92%)	1982 (96%)	94 (4%)	27 61

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	12	SER
1	A	16	GLU
1	A	21	SER
1	A	24	ARG
1	A	26	LEU
1	A	36	TYR
1	A	44	ARG
1	A	53	LYS
1	A	87	GLU
1	A	124	ASP
1	A	155	THR
1	A	156	LEU
1	A	157	THR
1	A	180	GLN
1	A	223	MET
1	A	246	ARG
1	A	252	ARG
1	A	258	SER
1	A	282	VAL
1	A	373	LYS
1	A	433	SER
1	A	446	TYR
1	A	528	PHE
1	A	572	ASP
1	A	609	ILE
1	A	611	ARG
1	A	627	LEU
1	B	4	ASP
1	B	8	LYS
1	B	11	ARG
1	B	19	GLN
1	B	36	TYR
1	B	40	GLU
1	B	53	LYS
1	B	111	LEU

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Mol	Chain	Res	Type
1	B	115	SER
1	B	116	SER
1	B	149	MET
1	B	152	THR
1	B	155	THR
1	B	163	TYR
1	B	175	LYS
1	B	203	LEU
1	B	223	MET
1	B	246	ARG
1	B	276	LEU
1	B	333	VAL
1	B	341	GLU
1	B	450	SER
1	B	510	MET
1	B	528	PHE
1	C	36	TYR
1	C	53	LYS
1	C	73	ASP
1	C	79	ASN
1	C	87	GLU
1	C	157	THR
1	C	175	LYS
1	C	222	LYS
1	C	223	MET
1	C	226	SER
1	C	246	ARG
1	C	283	VAL
1	C	342	GLU
1	C	451	SER
1	C	464	ASN
1	C	466	ASP
1	C	492	VAL
1	C	510	MET
1	C	518	SER
1	C	604	HIS
1	C	611	ARG
1	C	637	HIS
1	C	646	LEU
1	D	18	ILE
1	D	36	TYR
1	D	53	LYS

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Mol	Chain	Res	Type
1	D	115	SER
1	D	157	THR
1	D	160	GLN
1	D	161	VAL
1	D	201	ARG
1	D	223	MET
1	D	246	ARG
1	D	341	GLU
1	D	354	ARG
1	D	433	SER
1	D	450	SER
1	D	466	ASP
1	D	538	ASP
1	D	546	ARG
1	D	551	HIS
1	D	623	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	79	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TYE	C	701	-	12,12,12	0.99	1 (8%)	13,15,15	0.63	0
2	TYE	A	701	-	12,12,12	0.75	0	13,15,15	1.03	1 (7%)
2	TYE	B	701	-	12,12,12	0.87	0	13,15,15	0.53	0
2	TYE	D	701	-	12,12,12	0.99	1 (8%)	13,15,15	0.61	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
2	TYE	C	701	-	-	3/6/6/6	0/1/1/1
2	TYE	A	701	-	-	0/6/6/6	0/1/1/1
2	TYE	B	701	-	-	2/6/6/6	0/1/1/1
2	TYE	D	701	-	-	4/6/6/6	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	TYE	C-CA	3.10	1.57	1.52
2	D	701	TYE	C-CA	2.91	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	TYE	CB-CA-C	-2.20	108.22	112.21

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	701	TYE	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	D	701	TYE	N-CA-CB-CG
2	C	701	TYE	C-CA-CB-CG
2	D	701	TYE	C-CA-CB-CG
2	B	701	TYE	O-C-CA-CB
2	C	701	TYE	O-C-CA-CB
2	D	701	TYE	CA-CB-CG-CD2
2	D	701	TYE	CA-CB-CG-CD1
2	B	701	TYE	O-C-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	TYE	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

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	657/690 (95%)	0.08	14 (2%) 63 61	60, 60, 60, 60	0
1	B	581/690 (84%)	0.50	43 (7%) 14 11	60, 60, 60, 60	0
1	C	663/690 (96%)	0.49	67 (10%) 7 5	60, 60, 60, 60	0
1	D	665/690 (96%)	0.51	62 (9%) 8 6	60, 60, 60, 60	0
All	All	2566/2760 (92%)	0.39	186 (7%) 15 11	60, 60, 60, 60	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	661	ASN	10.7
1	D	43	GLY	7.5
1	D	635	ALA	7.4
1	C	260	ILE	7.2
1	C	267	VAL	7.2
1	C	91	ILE	6.8
1	C	82	VAL	6.7
1	C	253	VAL	6.2
1	C	-1	HIS	6.2
1	B	641	LEU	6.2
1	C	624	PRO	6.1
1	B	408	GLY	5.9
1	C	155	THR	5.7
1	D	374	PRO	5.6
1	C	313	VAL	5.5
1	D	291	ALA	5.5
1	A	260	ILE	5.5
1	B	386	VAL	5.3
1	D	465	CYS	5.2
1	D	237	THR	5.2
1	D	633	SER	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	223	MET	4.8
1	B	446	TYR	4.8
1	A	356	ASP	4.7
1	D	81	LYS	4.7
1	B	308	PHE	4.6
1	C	74	TRP	4.5
1	C	548	PRO	4.4
1	C	308	PHE	4.4
1	C	81	LYS	4.3
1	D	614	ALA	4.2
1	D	229	ASP	4.1
1	D	155	THR	4.1
1	D	216	LEU	4.1
1	B	295	GLY	4.1
1	C	154	GLY	4.0
1	C	661	ASN	4.0
1	D	550	LEU	4.0
1	D	337	PHE	3.9
1	D	234	MET	3.9
1	D	82	VAL	3.9
1	B	442	LEU	3.9
1	D	39	PHE	3.9
1	D	44	ARG	3.8
1	D	256	SER	3.7
1	C	275	VAL	3.7
1	D	333	VAL	3.7
1	C	325	GLU	3.7
1	C	377	CYS	3.7
1	C	362	LEU	3.6
1	D	293	ILE	3.6
1	C	585	ALA	3.5
1	D	51	ILE	3.5
1	C	103	ALA	3.5
1	D	641	LEU	3.5
1	D	607	LEU	3.4
1	A	465	CYS	3.4
1	C	261	THR	3.4
1	D	468	PHE	3.4
1	A	633	SER	3.4
1	C	76	ALA	3.4
1	A	200	GLY	3.4
1	C	346	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	648	LEU	3.4
1	D	585	ALA	3.3
1	C	222	LYS	3.3
1	A	259	ALA	3.3
1	B	434	ALA	3.3
1	C	83	GLY	3.3
1	A	563	ASP	3.2
1	B	310	SER	3.2
1	D	252	ARG	3.1
1	D	153	GLU	3.1
1	D	366	ALA	3.1
1	D	342	GLU	3.1
1	D	298	TYR	3.1
1	B	221	ALA	3.0
1	D	329	LEU	3.0
1	C	229	ASP	3.0
1	D	527	ALA	3.0
1	D	279	PHE	3.0
1	C	569	ASP	3.0
1	C	379	TRP	3.0
1	B	513	VAL	3.0
1	A	656	ALA	2.9
1	C	627	LEU	2.9
1	D	95	TYR	2.9
1	C	465	CYS	2.9
1	C	631	CYS	2.9
1	C	607	LEU	2.9
1	B	645	VAL	2.8
1	B	549	ALA	2.8
1	B	313	VAL	2.8
1	D	313	VAL	2.8
1	C	235	GLU	2.8
1	D	263	ASP	2.8
1	D	627	LEU	2.7
1	D	376	ALA	2.7
1	C	156	LEU	2.7
1	D	114	TRP	2.7
1	B	391	ALA	2.7
1	C	372	ALA	2.7
1	C	588	GLU	2.7
1	D	546	ARG	2.7
1	C	9	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	291	ALA	2.7
1	B	300	THR	2.6
1	B	108	ASP	2.6
1	C	513	VAL	2.6
1	C	568	LEU	2.6
1	C	302	GLU	2.6
1	C	401	PHE	2.6
1	D	304	LEU	2.6
1	B	198	LEU	2.6
1	D	163	TYR	2.6
1	B	61	THR	2.6
1	B	292	THR	2.6
1	D	260	ILE	2.6
1	A	605	GLY	2.5
1	C	528	PHE	2.5
1	C	382	ALA	2.5
1	C	259	ALA	2.4
1	B	213	LEU	2.4
1	C	339	SER	2.4
1	B	58	ASN	2.4
1	C	90	ARG	2.4
1	B	376	ALA	2.4
1	C	610	GLU	2.4
1	C	622	ASN	2.4
1	B	550	LEU	2.4
1	B	44	ARG	2.4
1	C	75	PHE	2.4
1	C	521	LEU	2.4
1	D	117	GLU	2.3
1	B	223	MET	2.3
1	C	245	ILE	2.3
1	C	337	PHE	2.3
1	B	-1	HIS	2.3
1	D	267	VAL	2.3
1	C	44	ARG	2.3
1	C	215	GLY	2.3
1	B	202	LYS	2.3
1	A	159	ALA	2.3
1	D	230	SER	2.2
1	A	640	ASP	2.2
1	C	353	TYR	2.2
1	B	106	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	339	SER	2.2
1	D	437	GLN	2.2
1	B	290	ALA	2.2
1	A	282	VAL	2.2
1	D	582	ALA	2.2
1	D	410	VAL	2.2
1	C	612	GLY	2.2
1	A	165	LEU	2.2
1	B	377	CYS	2.2
1	C	232	ILE	2.2
1	C	338	ALA	2.2
1	D	239	GLU	2.2
1	C	162	LEU	2.2
1	C	462	LEU	2.2
1	B	63	ALA	2.2
1	B	547	ILE	2.2
1	D	250	CYS	2.2
1	B	64	GLY	2.1
1	B	276	LEU	2.1
1	D	251	PRO	2.1
1	B	232	ILE	2.1
1	D	589	GLU	2.1
1	C	378	MET	2.1
1	A	524	HIS	2.1
1	C	584	SER	2.1
1	D	127	TRP	2.1
1	C	641	LEU	2.1
1	D	162	LEU	2.1
1	B	652	ARG	2.1
1	B	263	ASP	2.1
1	C	327	ASN	2.1
1	D	605	GLY	2.0
1	B	541	GLN	2.0
1	D	102	ALA	2.0
1	B	381	PRO	2.0
1	C	78	MET	2.0
1	B	378	MET	2.0
1	B	154	GLY	2.0
1	D	120	THR	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TYE	C	701	12/12	0.77	0.34	60,60,60,60	0
2	TYE	D	701	12/12	0.82	0.32	60,60,60,60	0
3	NA	C	711	1/1	0.83	0.42	119,119,119,119	0
3	NA	A	711	1/1	0.87	0.38	68,68,68,68	0
2	TYE	B	701	12/12	0.87	0.31	60,60,60,60	0
2	TYE	A	701	12/12	0.88	0.24	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.