Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2024 – 07:10 PM EST

PDB ID	:	3AL5
Title	:	Crystal structure of Human TYW5
Authors	:	Kato, M.; Araiso, Y.; Ishitani, R.; Nureki, O.
Deposited on	:	2010-07-26
Resolution	:	2.50 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 (i) 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 (1)) were used in the production of this report:

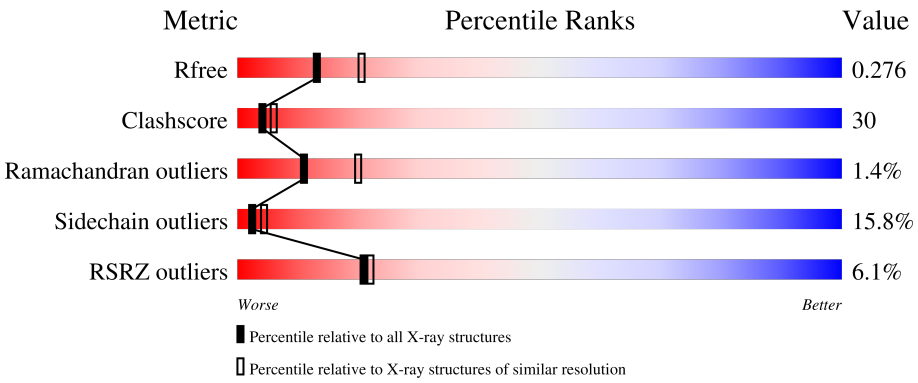
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	338	10%, 49%, 34%, 7%, 11%
1	B	338	54%, 33%, 5%, 8%
1	C	338	12%, 46%, 31%, 7%, 16%
1	D	338	47%, 36%, 8%, 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9288 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 JmjC domain-containing protein C2orf60.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	302	2237	1434	381	416	6	0	0	0
			Total	C	N	O	S			
1	B	311	2497	1615	420	454	8	0	0	0
			Total	C	N	O	S			
1	C	284	2056	1316	346	388	6	0	0	0
			Total	C	N	O	S			
1	D	308	2496	1614	418	457	7	0	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP A2RUC4
A	-21	GLY	-	expression tag	UNP A2RUC4
A	-20	SER	-	expression tag	UNP A2RUC4
A	-19	SER	-	expression tag	UNP A2RUC4
A	-18	HIS	-	expression tag	UNP A2RUC4
A	-17	HIS	-	expression tag	UNP A2RUC4
A	-16	HIS	-	expression tag	UNP A2RUC4
A	-15	HIS	-	expression tag	UNP A2RUC4
A	-14	HIS	-	expression tag	UNP A2RUC4
A	-13	HIS	-	expression tag	UNP A2RUC4
A	-12	SER	-	expression tag	UNP A2RUC4
A	-11	SER	-	expression tag	UNP A2RUC4
A	-10	GLY	-	expression tag	UNP A2RUC4
A	-9	LEU	-	expression tag	UNP A2RUC4
A	-8	GLU	-	expression tag	UNP A2RUC4
A	-7	VAL	-	expression tag	UNP A2RUC4
A	-6	LEU	-	expression tag	UNP A2RUC4
A	-5	PHE	-	expression tag	UNP A2RUC4
A	-4	GLN	-	expression tag	UNP A2RUC4
A	-3	GLY	-	expression tag	UNP A2RUC4
A	-2	PRO	-	expression tag	UNP A2RUC4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	LEU	-	expression tag	UNP A2RUC4
A	0	HIS	-	expression tag	UNP A2RUC4
B	-22	MET	-	expression tag	UNP A2RUC4
B	-21	GLY	-	expression tag	UNP A2RUC4
B	-20	SER	-	expression tag	UNP A2RUC4
B	-19	SER	-	expression tag	UNP A2RUC4
B	-18	HIS	-	expression tag	UNP A2RUC4
B	-17	HIS	-	expression tag	UNP A2RUC4
B	-16	HIS	-	expression tag	UNP A2RUC4
B	-15	HIS	-	expression tag	UNP A2RUC4
B	-14	HIS	-	expression tag	UNP A2RUC4
B	-13	HIS	-	expression tag	UNP A2RUC4
B	-12	SER	-	expression tag	UNP A2RUC4
B	-11	SER	-	expression tag	UNP A2RUC4
B	-10	GLY	-	expression tag	UNP A2RUC4
B	-9	LEU	-	expression tag	UNP A2RUC4
B	-8	GLU	-	expression tag	UNP A2RUC4
B	-7	VAL	-	expression tag	UNP A2RUC4
B	-6	LEU	-	expression tag	UNP A2RUC4
B	-5	PHE	-	expression tag	UNP A2RUC4
B	-4	GLN	-	expression tag	UNP A2RUC4
B	-3	GLY	-	expression tag	UNP A2RUC4
B	-2	PRO	-	expression tag	UNP A2RUC4
B	-1	LEU	-	expression tag	UNP A2RUC4
B	0	HIS	-	expression tag	UNP A2RUC4
C	-22	MET	-	expression tag	UNP A2RUC4
C	-21	GLY	-	expression tag	UNP A2RUC4
C	-20	SER	-	expression tag	UNP A2RUC4
C	-19	SER	-	expression tag	UNP A2RUC4
C	-18	HIS	-	expression tag	UNP A2RUC4
C	-17	HIS	-	expression tag	UNP A2RUC4
C	-16	HIS	-	expression tag	UNP A2RUC4
C	-15	HIS	-	expression tag	UNP A2RUC4
C	-14	HIS	-	expression tag	UNP A2RUC4
C	-13	HIS	-	expression tag	UNP A2RUC4
C	-12	SER	-	expression tag	UNP A2RUC4
C	-11	SER	-	expression tag	UNP A2RUC4
C	-10	GLY	-	expression tag	UNP A2RUC4
C	-9	LEU	-	expression tag	UNP A2RUC4
C	-8	GLU	-	expression tag	UNP A2RUC4
C	-7	VAL	-	expression tag	UNP A2RUC4
C	-6	LEU	-	expression tag	UNP A2RUC4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	PHE	-	expression tag	UNP A2RUC4
C	-4	GLN	-	expression tag	UNP A2RUC4
C	-3	GLY	-	expression tag	UNP A2RUC4
C	-2	PRO	-	expression tag	UNP A2RUC4
C	-1	LEU	-	expression tag	UNP A2RUC4
C	0	HIS	-	expression tag	UNP A2RUC4
D	-22	MET	-	expression tag	UNP A2RUC4
D	-21	GLY	-	expression tag	UNP A2RUC4
D	-20	SER	-	expression tag	UNP A2RUC4
D	-19	SER	-	expression tag	UNP A2RUC4
D	-18	HIS	-	expression tag	UNP A2RUC4
D	-17	HIS	-	expression tag	UNP A2RUC4
D	-16	HIS	-	expression tag	UNP A2RUC4
D	-15	HIS	-	expression tag	UNP A2RUC4
D	-14	HIS	-	expression tag	UNP A2RUC4
D	-13	HIS	-	expression tag	UNP A2RUC4
D	-12	SER	-	expression tag	UNP A2RUC4
D	-11	SER	-	expression tag	UNP A2RUC4
D	-10	GLY	-	expression tag	UNP A2RUC4
D	-9	LEU	-	expression tag	UNP A2RUC4
D	-8	GLU	-	expression tag	UNP A2RUC4
D	-7	VAL	-	expression tag	UNP A2RUC4
D	-6	LEU	-	expression tag	UNP A2RUC4
D	-5	PHE	-	expression tag	UNP A2RUC4
D	-4	GLN	-	expression tag	UNP A2RUC4
D	-3	GLY	-	expression tag	UNP A2RUC4
D	-2	PRO	-	expression tag	UNP A2RUC4
D	-1	LEU	-	expression tag	UNP A2RUC4
D	0	HIS	-	expression tag	UNP A2RUC4

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

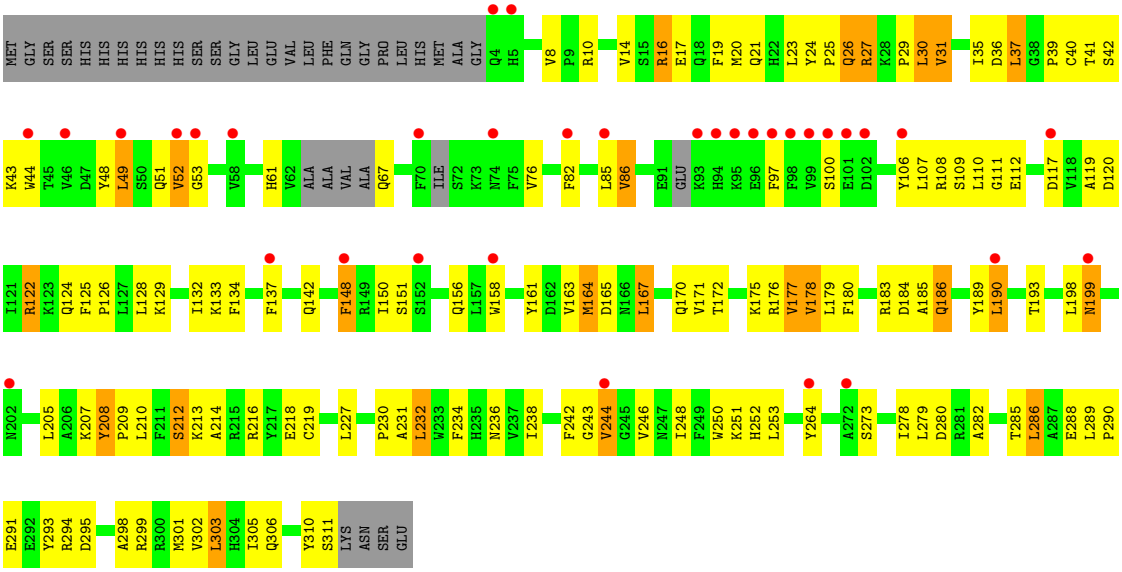
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	B	1	1	1	0	0
			Total	Mg		
2	D	1	1	1	0	0

3 Residue-property plots (i)

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

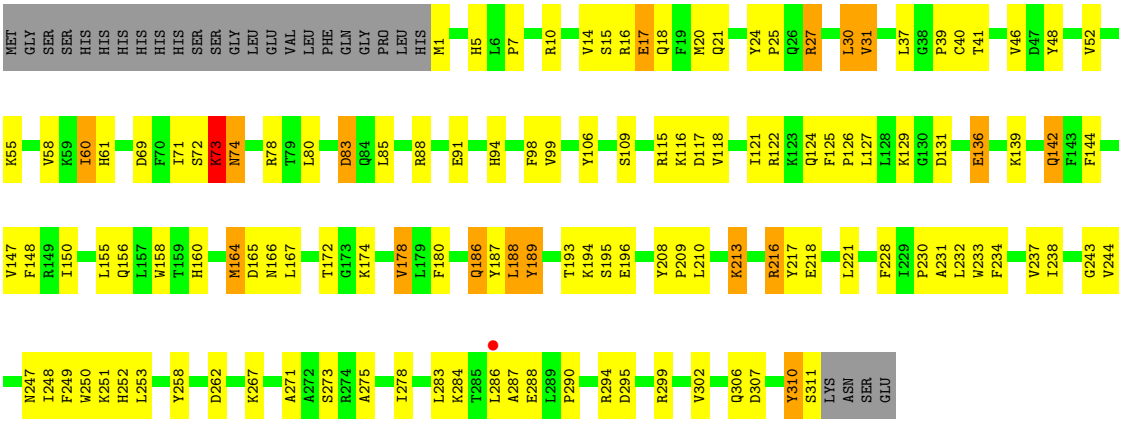
• Molecule 1: JmjC domain-containing protein C2orf60

Chain A: 10% 49% 34% 7% 11%



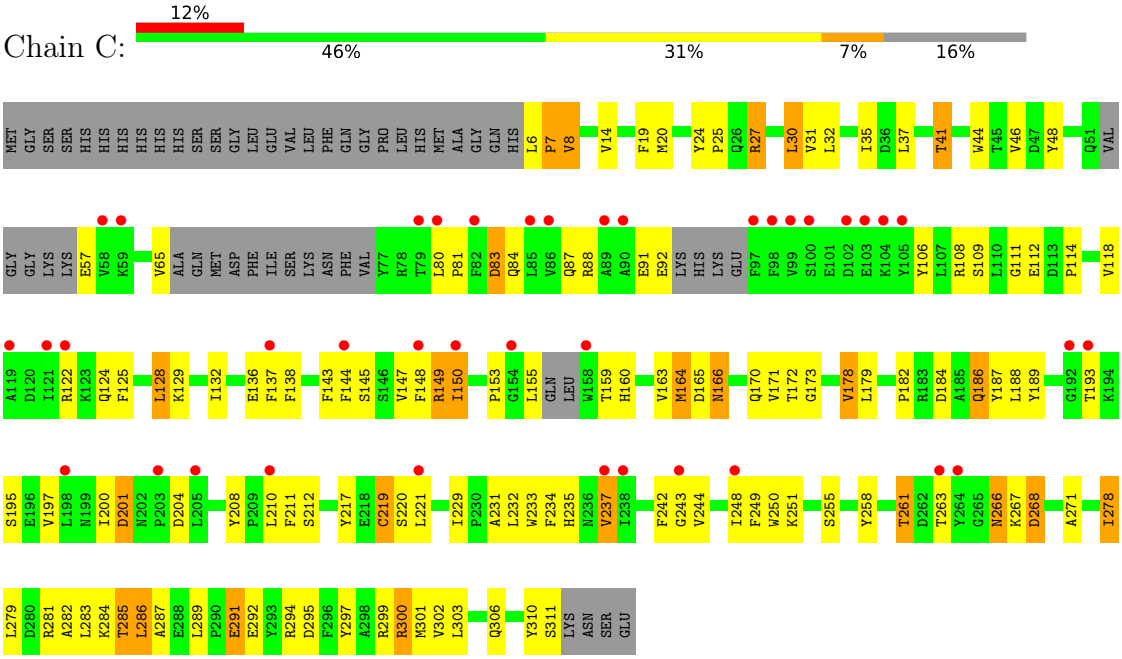
• Molecule 1: JmjC domain-containing protein C2orf60

Chain B: 54% 33% 5% 8%



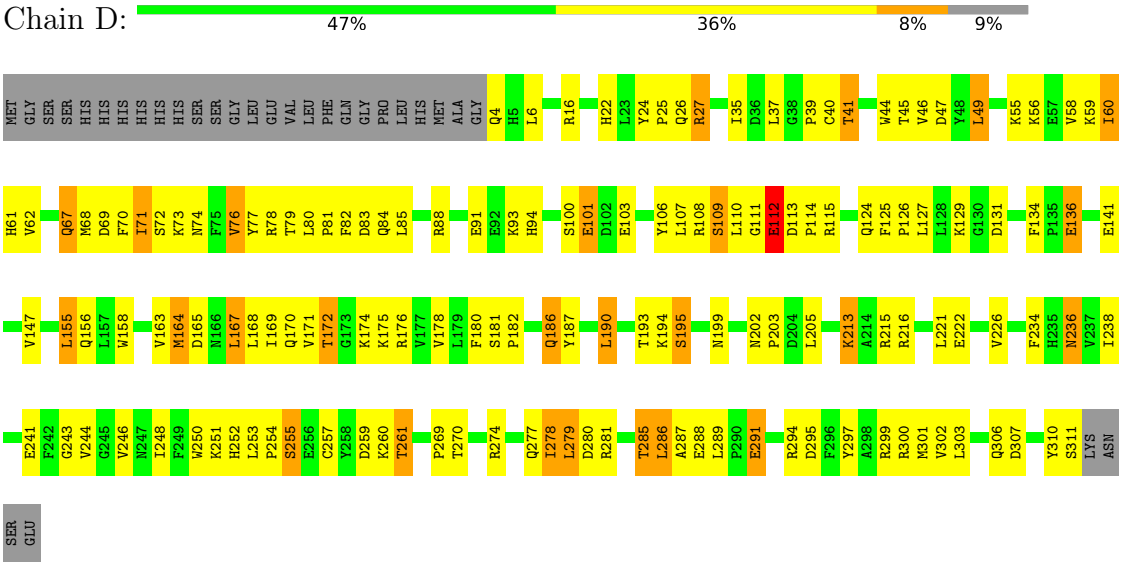
• Molecule 1: JmjC domain-containing protein C2orf60

Chain C:



• Molecule 1: JmjC domain-containing protein C2orf60

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	164.94Å 164.94Å 105.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 44.33 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.50) 97.7 (44.33-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.6_289	Depositor
R, R_{free}	0.220 , 0.281 0.216 , 0.276	Depositor DCC
R_{free} test set	2462 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	49.9	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 67.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9288	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.38	0/2292	0.56	0/3132
1	B	0.47	0/2564	0.66	0/3477
1	C	0.40	0/2105	0.56	0/2881
1	D	0.53	0/2563	0.67	0/3475
All	All	0.45	0/9524	0.62	0/12965

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	B	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	B	288	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2237	0	1993	137	0
1	B	2497	0	2420	120	0
1	C	2056	0	1778	161	0
1	D	2496	0	2426	149	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
All	All	9288	0	8617	534	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 30.

All (534) 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:C:172:THR:HB	1:C:244:VAL:H	1.12	1.08
1:A:122:ARG:HG3	1:A:122:ARG:HH11	1.18	1.06
1:C:149:ARG:HG3	1:C:149:ARG:HH11	1.23	0.99
1:C:41:THR:HA	1:C:171:VAL:HG13	1.43	0.98
1:D:164:MET:HE1	1:D:251:LYS:HA	1.50	0.93
1:C:109:SER:HB2	1:C:148:PHE:HB2	1.50	0.92
1:C:282:ALA:H	1:D:278:ILE:HD11	1.34	0.92
1:D:71:ILE:HG23	1:D:72:SER:H	1.33	0.91
1:D:67:GLN:HE21	1:D:156:GLN:HE22	1.19	0.91
1:D:67:GLN:HE21	1:D:156:GLN:NE2	1.72	0.88
1:A:8:VAL:HG13	1:A:219:CYS:HB3	1.56	0.87
1:C:44:TRP:CZ2	1:C:128:LEU:HB2	2.10	0.86
1:D:16:ARG:HE	1:D:136:GLU:HB2	1.40	0.85
1:C:166:ASN:HB3	1:C:249:PHE:CD1	2.16	0.81
1:A:122:ARG:HH11	1:A:122:ARG:CG	1.91	0.80
1:C:149:ARG:HG3	1:C:149:ARG:NH1	1.95	0.80
1:C:172:THR:HB	1:C:244:VAL:N	1.94	0.80
1:D:172:THR:HG22	1:D:243:GLY:HA2	1.65	0.79
1:C:128:LEU:HD23	1:C:128:LEU:H	1.46	0.79
1:D:164:MET:CE	1:D:251:LYS:HA	2.13	0.79
1:B:186:GLN:H	1:B:186:GLN:HE21	1.30	0.79
1:D:167:LEU:HD22	1:D:250:TRP:CZ3	2.18	0.79
1:D:174:LYS:HB2	1:D:241:GLU:HG3	1.63	0.78
1:A:231:ALA:O	1:A:232:LEU:HB2	1.83	0.78
1:D:44:TRP:HB3	1:D:49:LEU:HD21	1.66	0.78
1:A:170:GLN:OE1	1:A:175:LYS:HE2	1.85	0.77
1:C:210:LEU:C	1:C:212:SER:H	1.87	0.77
1:B:189:TYR:O	1:B:196:GLU:HG3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ALA:N	1:D:278:ILE:HD11	2.02	0.75
1:B:109:SER:HB3	1:B:148:PHE:H	1.50	0.75
1:B:164:MET:HE1	1:B:251:LYS:HA	1.69	0.75
1:B:139:LYS:O	1:B:142:GLN:HG2	1.86	0.74
1:B:189:TYR:HE1	1:B:210:LEU:HB2	1.53	0.74
1:C:108:ARG:HG2	1:C:149:ARG:HE	1.53	0.74
1:D:278:ILE:HG13	1:D:279:LEU:N	2.03	0.74
1:B:164:MET:CE	1:B:251:LYS:HA	2.17	0.73
1:A:49:LEU:HD21	1:A:244:VAL:HG11	1.70	0.73
1:C:8:VAL:CG1	1:C:219:CYS:HB3	2.18	0.73
1:A:24:TYR:HB3	1:A:25:PRO:HD3	1.71	0.72
1:D:274:ARG:O	1:D:278:ILE:HG23	1.90	0.72
1:B:16:ARG:HG3	1:B:20:MET:HE2	1.72	0.71
1:B:186:GLN:H	1:B:186:GLN:NE2	1.87	0.71
1:D:94:HIS:HE1	1:D:103:GLU:O	1.73	0.70
1:D:187:TYR:CE1	1:D:213:LYS:HG3	2.26	0.70
1:D:190:LEU:HD21	1:D:234:PHE:CZ	2.26	0.70
1:A:189:TYR:HH	1:A:210:LEU:HD12	1.55	0.70
1:C:186:GLN:H	1:C:186:GLN:NE2	1.89	0.70
1:B:147:VAL:HB	1:B:247:ASN:ND2	2.07	0.69
1:B:156:GLN:HG3	1:B:238:ILE:HG12	1.74	0.69
1:A:8:VAL:CG1	1:A:219:CYS:HB3	2.22	0.69
1:D:70:PHE:CD1	1:D:71:ILE:N	2.60	0.69
1:B:283:LEU:O	1:B:287:ALA:HB2	1.93	0.69
1:C:24:TYR:HB3	1:C:25:PRO:HD3	1.73	0.69
1:B:172:THR:HG22	1:B:243:GLY:HA2	1.75	0.68
1:B:74:ASN:C	1:B:74:ASN:HD22	1.95	0.68
1:C:266:ASN:H	1:C:266:ASN:HD22	1.42	0.68
1:A:122:ARG:HG3	1:A:122:ARG:NH1	1.98	0.68
1:C:164:MET:HE1	1:C:251:LYS:HA	1.76	0.67
1:D:35:ILE:HG22	1:D:37:LEU:HD12	1.74	0.67
1:A:106:TYR:HE2	1:A:108:ARG:HB2	1.59	0.67
1:A:164:MET:CE	1:A:251:LYS:HA	2.24	0.67
1:B:16:ARG:HG3	1:B:20:MET:CE	2.24	0.67
1:A:189:TYR:OH	1:A:210:LEU:HD12	1.94	0.67
1:D:58:VAL:HG23	1:D:60:ILE:HD12	1.77	0.67
1:B:27:ARG:HH11	1:B:27:ARG:HG3	1.60	0.67
1:D:71:ILE:HG23	1:D:72:SER:N	2.09	0.66
1:D:169:ILE:HG12	1:D:226:VAL:HG22	1.78	0.66
1:D:203:PRO:HG2	1:D:205:LEU:HD21	1.76	0.66
1:C:8:VAL:HG23	1:C:30:LEU:HA	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:THR:HG22	1:C:243:GLY:HA2	1.78	0.65
1:C:186:GLN:H	1:C:186:GLN:HE21	1.42	0.65
1:D:129:LYS:O	1:D:129:LYS:HD3	1.96	0.65
1:B:48:TYR:CZ	1:B:52:VAL:HG21	2.31	0.65
1:C:302:VAL:O	1:C:306:GLN:HG3	1.96	0.65
1:C:8:VAL:HG13	1:C:219:CYS:HB3	1.78	0.65
1:D:172:THR:O	1:D:243:GLY:HA3	1.97	0.65
1:A:122:ARG:HA	1:A:129:LYS:HG3	1.79	0.64
1:A:85:LEU:HD21	1:A:107:LEU:HB2	1.79	0.64
1:C:109:SER:HB3	1:C:148:PHE:H	1.62	0.64
1:D:61:HIS:HB2	1:D:106:TYR:HB3	1.79	0.64
1:A:48:TYR:O	1:A:52:VAL:HG23	1.98	0.64
1:B:27:ARG:HG3	1:B:27:ARG:NH1	2.13	0.64
1:C:281:ARG:O	1:C:285:THR:HG23	1.98	0.64
1:C:160:HIS:NE2	1:C:235:HIS:NE2	2.45	0.63
1:C:186:GLN:HB3	1:D:303:LEU:HD21	1.79	0.63
1:D:167:LEU:HD22	1:D:250:TRP:HZ3	1.62	0.63
1:C:186:GLN:HE21	1:C:186:GLN:N	1.97	0.63
1:A:27:ARG:HH22	1:A:165:ASP:CG	2.02	0.63
1:A:289:LEU:HD11	1:B:271:ALA:HB3	1.81	0.62
1:B:147:VAL:HB	1:B:247:ASN:HD21	1.62	0.62
1:C:125:PHE:CG	1:C:148:PHE:HE1	2.17	0.62
1:C:282:ALA:HB2	1:D:278:ILE:CG1	2.30	0.61
1:D:164:MET:HE3	1:D:164:MET:HA	1.82	0.61
1:D:285:THR:O	1:D:288:GLU:HG2	2.00	0.61
1:A:177:VAL:HG13	1:A:219:CYS:SG	2.41	0.61
1:C:8:VAL:CG2	1:C:30:LEU:HA	2.32	0.60
1:C:163:VAL:HG21	1:C:267:LYS:O	2.01	0.60
1:D:164:MET:HE2	1:D:250:TRP:O	2.01	0.60
1:A:67:GLN:HA	1:A:156:GLN:HB2	1.83	0.60
1:B:5:HIS:CD2	1:B:216:ARG:HE	2.20	0.60
1:B:189:TYR:CE1	1:B:210:LEU:HB2	2.35	0.60
1:C:20:MET:HE3	1:C:137:PHE:HA	1.83	0.60
1:A:301:MET:CE	1:B:275:ALA:HB1	2.32	0.60
1:C:184:ASP:O	1:C:188:LEU:HD13	2.02	0.60
1:A:286:LEU:HD13	1:A:294:ARG:HA	1.83	0.60
1:C:311:SER:HB2	1:D:291:GLU:CD	2.22	0.60
1:C:44:TRP:HZ2	1:C:128:LEU:O	1.83	0.59
1:C:210:LEU:C	1:C:212:SER:N	2.55	0.59
1:A:122:ARG:HG2	1:A:129:LYS:HE3	1.82	0.59
1:C:111:GLY:HA2	1:C:124:GLN:NE2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ARG:NH2	1:A:238:ILE:HD12	2.17	0.59
1:C:108:ARG:HG2	1:C:149:ARG:NE	2.15	0.59
1:D:186:GLN:H	1:D:186:GLN:HE21	1.50	0.59
1:B:306:GLN:HG2	1:B:310:TYR:CE1	2.37	0.59
1:A:190:LEU:HD21	1:A:234:PHE:CE2	2.38	0.59
1:B:15:SER:OG	1:B:18:GLN:HG2	2.02	0.59
1:D:125:PHE:N	1:D:126:PRO:HD3	2.16	0.59
1:D:295:ASP:OD1	1:D:299:ARG:NH1	2.36	0.59
1:A:134:PHE:CD1	1:A:248:ILE:HD11	2.38	0.59
1:C:284:LYS:O	1:C:287:ALA:HB3	2.02	0.59
1:A:170:GLN:OE1	1:A:175:LYS:CE	2.50	0.59
1:D:291:GLU:HG2	1:D:294:ARG:HH12	1.67	0.58
1:C:44:TRP:CD1	1:C:48:TYR:CE1	2.91	0.58
1:A:205:LEU:HD13	1:A:209:PRO:HA	1.86	0.58
1:B:27:ARG:HH11	1:B:27:ARG:CG	2.16	0.58
1:B:40:CYS:HB3	1:B:131:ASP:O	2.04	0.58
1:D:259:ASP:OD1	1:D:261:THR:HB	2.03	0.58
1:A:164:MET:HE1	1:A:251:LYS:HA	1.86	0.58
1:A:190:LEU:HD21	1:A:234:PHE:HE2	1.68	0.58
1:C:292:GLU:OE1	1:D:27:ARG:NH1	2.37	0.58
1:B:129:LYS:O	1:B:129:LYS:HD3	2.04	0.58
1:B:164:MET:HA	1:B:164:MET:HE3	1.86	0.58
1:A:183:ARG:C	1:A:185:ALA:H	2.06	0.58
1:A:302:VAL:HA	1:A:305:ILE:HD12	1.85	0.58
1:A:207:LYS:HB2	1:A:208:TYR:CE2	2.39	0.58
1:C:282:ALA:H	1:D:278:ILE:CD1	2.12	0.58
1:C:164:MET:HE2	1:C:250:TRP:O	2.04	0.57
1:B:156:GLN:NE2	1:B:238:ILE:HD11	2.18	0.57
1:D:108:ARG:HG2	1:D:147:VAL:HG11	1.85	0.57
1:D:110:LEU:O	1:D:124:GLN:NE2	2.37	0.57
1:C:170:GLN:NE2	1:C:221:LEU:HB2	2.19	0.57
1:D:70:PHE:O	1:D:71:ILE:C	2.43	0.57
1:C:283:LEU:O	1:C:287:ALA:HB2	2.04	0.57
1:C:282:ALA:HB2	1:D:278:ILE:HD11	1.87	0.57
1:C:153:PRO:HG3	1:C:242:PHE:N	2.19	0.57
1:A:49:LEU:CD2	1:A:244:VAL:HG11	2.33	0.57
1:B:262:ASP:HB2	1:B:267:LYS:HB2	1.86	0.57
1:A:24:TYR:HE2	1:A:250:TRP:HZ2	1.53	0.57
1:C:44:TRP:HD1	1:C:48:TYR:CE1	2.23	0.57
1:C:164:MET:HE2	1:C:164:MET:HA	1.86	0.57
1:A:282:ALA:HB2	1:B:278:ILE:CG2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:LYS:HG3	1:B:83:ASP:OD1	2.05	0.56
1:B:16:ARG:NE	1:B:20:MET:HE2	2.20	0.56
1:D:111:GLY:HA2	1:D:124:GLN:HE22	1.70	0.56
1:A:125:PHE:N	1:A:126:PRO:HD3	2.20	0.56
1:C:189:TYR:OH	1:C:210:LEU:HB2	2.04	0.56
1:D:91:GLU:OE2	1:D:94:HIS:HD2	1.88	0.56
1:B:17:GLU:H	1:B:17:GLU:CD	2.09	0.56
1:D:190:LEU:HD21	1:D:234:PHE:CE2	2.40	0.56
1:B:10:ARG:HG2	1:B:31:VAL:HG13	1.86	0.56
1:D:69:ASP:H	1:D:74:ASN:ND2	2.03	0.56
1:A:289:LEU:HD11	1:B:271:ALA:CB	2.35	0.56
1:A:293:TYR:OH	1:B:252:HIS:HD2	1.89	0.56
1:A:285:THR:O	1:A:288:GLU:HG2	2.06	0.56
1:B:125:PHE:N	1:B:126:PRO:HD3	2.21	0.56
1:C:170:GLN:HE22	1:C:221:LEU:HB2	1.70	0.56
1:C:311:SER:HB2	1:D:291:GLU:OE2	2.05	0.56
1:C:251:LYS:HB3	1:C:258:TYR:CE2	2.40	0.56
1:A:10:ARG:HG2	1:A:31:VAL:CG1	2.36	0.55
1:C:41:THR:HA	1:C:171:VAL:CG1	2.26	0.55
1:C:83:ASP:N	1:C:83:ASP:OD2	2.39	0.55
1:A:86:VAL:HG13	1:A:150:ILE:CD1	2.35	0.55
1:D:35:ILE:HG22	1:D:37:LEU:CD1	2.37	0.55
1:D:163:VAL:HG11	1:D:269:PRO:HD3	1.88	0.55
1:D:278:ILE:O	1:D:281:ARG:HB2	2.07	0.55
1:A:178:VAL:C	1:A:179:LEU:HD12	2.27	0.55
1:A:264:TYR:CD1	1:A:264:TYR:O	2.60	0.55
1:C:44:TRP:HD1	1:C:48:TYR:CD1	2.25	0.55
1:D:16:ARG:NE	1:D:136:GLU:HB2	2.18	0.55
1:D:286:LEU:HD13	1:D:294:ARG:CG	2.36	0.55
1:C:299:ARG:O	1:C:303:LEU:HD23	2.07	0.55
1:D:60:ILE:CD1	1:D:85:LEU:HD13	2.37	0.55
1:C:166:ASN:HB3	1:C:249:PHE:CE1	2.42	0.54
1:D:155:LEU:HD22	1:D:156:GLN:N	2.21	0.54
1:B:295:ASP:OD2	1:B:299:ARG:NH1	2.40	0.54
1:C:282:ALA:N	1:D:278:ILE:CD1	2.69	0.54
1:C:286:LEU:HD12	1:C:301:MET:CE	2.38	0.54
1:C:166:ASN:HB3	1:C:249:PHE:HD1	1.67	0.54
1:B:5:HIS:CE1	1:B:218:GLU:HB3	2.42	0.54
1:B:74:ASN:C	1:B:74:ASN:ND2	2.61	0.54
1:C:271:ALA:HB3	1:D:289:LEU:HD11	1.88	0.54
1:A:24:TYR:CE2	1:A:250:TRP:HZ2	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:PHE:HD2	1:A:167:LEU:HD21	1.73	0.53
1:D:69:ASP:H	1:D:74:ASN:HD21	1.55	0.53
1:A:39:PRO:O	1:A:42:SER:HB3	2.08	0.53
1:D:303:LEU:HA	1:D:306:GLN:NE2	2.23	0.53
1:A:198:LEU:N	1:A:198:LEU:HD22	2.24	0.53
1:C:125:PHE:CD2	1:C:148:PHE:HE1	2.27	0.53
1:A:205:LEU:HD13	1:A:205:LEU:O	2.09	0.53
1:A:8:VAL:CG2	1:A:31:VAL:HG12	2.39	0.53
1:C:295:ASP:OD1	1:C:299:ARG:NH1	2.42	0.53
1:A:27:ARG:NH2	1:A:165:ASP:OD2	2.42	0.53
1:A:53:GLY:HA3	1:A:82:PHE:CE1	2.43	0.52
1:D:22:HIS:O	1:D:25:PRO:HD2	2.08	0.52
1:B:14:VAL:HG13	1:B:18:GLN:HG3	1.91	0.52
1:D:39:PRO:HD2	1:D:131:ASP:O	2.09	0.52
1:D:111:GLY:HA2	1:D:124:GLN:NE2	2.25	0.52
1:A:216:ARG:O	1:A:216:ARG:HG3	2.09	0.52
1:B:10:ARG:HG2	1:B:31:VAL:CG1	2.39	0.52
1:C:24:TYR:HE2	1:C:250:TRP:HZ2	1.57	0.52
1:C:295:ASP:O	1:C:299:ARG:HG3	2.08	0.52
1:C:32:LEU:HB2	1:C:35:ILE:HD11	1.91	0.52
1:C:166:ASN:HD21	1:C:229:ILE:HB	1.74	0.52
1:D:286:LEU:HD13	1:D:294:ARG:HG2	1.92	0.52
1:C:286:LEU:HD12	1:C:301:MET:HE1	1.90	0.52
1:D:35:ILE:O	1:D:37:LEU:HD13	2.10	0.52
1:D:67:GLN:NE2	1:D:156:GLN:HE22	1.98	0.52
1:B:118:VAL:HG21	1:B:144:PHE:O	2.10	0.51
1:C:19:PHE:CE2	1:C:137:PHE:HB3	2.46	0.51
1:D:71:ILE:CG2	1:D:72:SER:H	2.13	0.51
1:D:81:PRO:HD2	1:D:84:GLN:HB2	1.93	0.51
1:B:230:PRO:HB2	1:B:233:TRP:CD1	2.45	0.51
1:C:172:THR:HG22	1:C:173:GLY:N	2.26	0.51
1:C:20:MET:CE	1:C:137:PHE:HA	2.41	0.51
1:D:60:ILE:HD11	1:D:85:LEU:HD13	1.91	0.51
1:D:100:SER:O	1:D:103:GLU:HG2	2.10	0.51
1:D:164:MET:CE	1:D:164:MET:HA	2.40	0.51
1:D:299:ARG:O	1:D:303:LEU:HD23	2.11	0.51
1:A:30:LEU:O	1:A:227:LEU:HD12	2.11	0.51
1:B:48:TYR:CE1	1:B:52:VAL:HG21	2.46	0.51
1:B:72:SER:O	1:B:73:LYS:C	2.49	0.51
1:B:164:MET:HE2	1:B:250:TRP:C	2.31	0.51
1:C:109:SER:CB	1:C:148:PHE:H	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LEU:HD12	1:B:31:VAL:N	2.26	0.50
1:C:91:GLU:O	1:C:92:GLU:O	2.29	0.50
1:A:61:HIS:HB2	1:A:106:TYR:HB3	1.94	0.50
1:A:129:LYS:HD3	1:A:129:LYS:O	2.10	0.50
1:A:172:THR:O	1:A:243:GLY:HA3	2.11	0.50
1:C:44:TRP:CZ2	1:C:128:LEU:O	2.64	0.50
1:C:178:VAL:HG21	1:C:200:ILE:HD12	1.93	0.50
1:A:122:ARG:CG	1:A:122:ARG:NH1	2.62	0.50
1:A:161:TYR:CE2	1:A:193:THR:HA	2.45	0.50
1:C:122:ARG:CG	1:C:129:LYS:HE3	2.42	0.50
1:A:177:VAL:HA	1:A:236:ASN:O	2.11	0.50
1:A:291:GLU:CD	1:B:311:SER:HB2	2.32	0.50
1:B:122:ARG:HA	1:B:129:LYS:HG3	1.92	0.50
1:D:203:PRO:HG2	1:D:205:LEU:CD2	2.40	0.50
1:A:176:ARG:HH22	1:A:238:ILE:HD12	1.76	0.50
1:A:291:GLU:HG3	1:A:294:ARG:NH2	2.26	0.50
1:C:164:MET:HA	1:C:164:MET:CE	2.42	0.50
1:D:297:TYR:O	1:D:301:MET:HG3	2.12	0.50
1:A:306:GLN:HG2	1:A:310:TYR:CZ	2.47	0.50
1:C:310:TYR:O	1:C:311:SER:CB	2.59	0.50
1:D:180:PHE:CE1	1:D:216:ARG:HB3	2.47	0.50
1:C:189:TYR:CE1	1:C:210:LEU:HB2	2.47	0.50
1:A:180:PHE:HE1	1:A:216:ARG:HB3	1.77	0.49
1:B:16:ARG:CG	1:B:20:MET:HE2	2.42	0.49
1:C:201:ASP:OD2	1:C:201:ASP:N	2.42	0.49
1:D:44:TRP:HB3	1:D:49:LEU:CD2	2.38	0.49
1:D:60:ILE:HG12	1:D:85:LEU:HD13	1.93	0.49
1:D:178:VAL:HG22	1:D:236:ASN:HB3	1.93	0.49
1:B:58:VAL:HG23	1:B:60:ILE:HD12	1.93	0.49
1:B:158:TRP:NE1	1:B:194:LYS:HD2	2.27	0.49
1:B:164:MET:HE2	1:B:250:TRP:O	2.12	0.49
1:C:122:ARG:HG2	1:C:129:LYS:HE3	1.93	0.49
1:D:291:GLU:HG2	1:D:294:ARG:NH1	2.28	0.49
1:C:122:ARG:HG2	1:C:129:LYS:HG3	1.94	0.49
1:A:301:MET:HE1	1:B:275:ALA:HB1	1.93	0.49
1:B:231:ALA:O	1:B:232:LEU:HB2	2.12	0.49
1:C:164:MET:CE	1:C:251:LYS:HA	2.41	0.49
1:D:60:ILE:HD11	1:D:85:LEU:HB2	1.93	0.49
1:B:189:TYR:CD1	1:B:189:TYR:N	2.81	0.49
1:B:189:TYR:CD2	1:B:208:TYR:HD1	2.30	0.49
1:D:286:LEU:HD11	1:D:294:ARG:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ARG:NH2	1:A:165:ASP:OD1	2.45	0.49
1:A:172:THR:HG22	1:A:243:GLY:HA2	1.95	0.49
1:D:40:CYS:SG	1:D:41:THR:N	2.85	0.49
1:D:44:TRP:CE3	1:D:171:VAL:HG11	2.48	0.49
1:D:287:ALA:HA	1:D:294:ARG:HD2	1.95	0.49
1:C:286:LEU:HD22	1:C:294:ARG:HA	1.95	0.49
1:D:68:MET:O	1:D:158:TRP:HE3	1.96	0.49
1:B:116:LYS:HG3	1:B:117:ASP:OD2	2.13	0.48
1:C:172:THR:CG2	1:C:173:GLY:N	2.76	0.48
1:A:10:ARG:HG2	1:A:31:VAL:HG13	1.95	0.48
1:A:179:LEU:HA	1:A:234:PHE:O	2.12	0.48
1:B:69:ASP:OD2	1:B:71:ILE:N	2.46	0.48
1:A:40:CYS:SG	1:A:41:THR:N	2.87	0.48
1:B:69:ASP:H	1:B:74:ASN:HD21	1.62	0.48
1:D:81:PRO:HG2	1:D:84:GLN:HG3	1.96	0.48
1:C:148:PHE:O	1:C:149:ARG:HD3	2.14	0.48
1:B:60:ILE:HD13	1:B:80:LEU:HB2	1.95	0.48
1:B:189:TYR:N	1:B:189:TYR:HD1	2.12	0.48
1:C:118:VAL:HG12	1:C:263:THR:HA	1.95	0.48
1:D:55:LYS:HE2	1:D:83:ASP:OD2	2.13	0.48
1:B:69:ASP:H	1:B:74:ASN:ND2	2.11	0.48
1:C:129:LYS:O	1:C:129:LYS:HD3	2.14	0.48
1:B:287:ALA:O	1:B:294:ARG:HD2	2.13	0.48
1:C:189:TYR:CD2	1:C:208:TYR:HD1	2.32	0.48
1:B:295:ASP:O	1:B:299:ARG:HG3	2.14	0.47
1:C:282:ALA:CB	1:D:278:ILE:HD11	2.44	0.47
1:D:70:PHE:CG	1:D:71:ILE:N	2.82	0.47
1:D:303:LEU:HA	1:D:306:GLN:HE21	1.78	0.47
1:C:41:THR:CA	1:C:171:VAL:HG13	2.32	0.47
1:C:112:GLU:O	1:C:114:PRO:HD3	2.15	0.47
1:A:19:PHE:HA	1:A:23:LEU:HD12	1.96	0.47
1:C:125:PHE:CD2	1:C:148:PHE:CE1	3.02	0.47
1:C:282:ALA:HB2	1:D:278:ILE:CD1	2.44	0.47
1:B:160:HIS:HA	1:B:193:THR:O	2.14	0.47
1:A:282:ALA:HB2	1:B:278:ILE:HG21	1.94	0.47
1:A:306:GLN:O	1:A:310:TYR:HB2	2.15	0.47
1:D:113:ASP:OD1	1:D:115:ARG:HG2	2.13	0.47
1:A:86:VAL:HG13	1:A:150:ILE:HD13	1.96	0.47
1:A:120:ASP:OD1	1:A:122:ARG:NH1	2.47	0.47
1:A:16:ARG:O	1:A:20:MET:HG2	2.14	0.47
1:A:67:GLN:HE22	1:A:199:ASN:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ASP:OD1	1:A:299:ARG:NH1	2.47	0.47
1:C:210:LEU:O	1:C:212:SER:N	2.47	0.47
1:D:62:VAL:HB	1:D:76:VAL:HG12	1.95	0.47
1:D:108:ARG:HG2	1:D:147:VAL:CG1	2.45	0.47
1:D:163:VAL:O	1:D:163:VAL:HG12	2.14	0.47
1:B:262:ASP:HB2	1:B:267:LYS:HD2	1.97	0.47
1:C:149:ARG:HH11	1:C:149:ARG:CG	2.06	0.47
1:A:170:GLN:NE2	1:A:172:THR:O	2.47	0.47
1:A:285:THR:OG1	1:A:286:LEU:N	2.48	0.47
1:B:39:PRO:O	1:B:40:CYS:C	2.54	0.47
1:C:27:ARG:HH21	1:C:165:ASP:CG	2.18	0.47
1:C:57:GLU:HA	1:C:81:PRO:HA	1.97	0.47
1:A:17:GLU:HG2	1:A:21:GLN:HE21	1.80	0.47
1:C:27:ARG:NH2	1:C:165:ASP:OD1	2.44	0.47
1:B:5:HIS:CD2	1:B:216:ARG:NE	2.82	0.46
1:B:188:LEU:HD12	1:B:188:LEU:HA	1.77	0.46
1:D:70:PHE:HB3	1:D:158:TRP:CE3	2.50	0.46
1:A:306:GLN:HG2	1:A:310:TYR:CE1	2.50	0.46
1:C:25:PRO:C	1:C:27:ARG:N	2.68	0.46
1:B:306:GLN:O	1:B:310:TYR:HB2	2.16	0.46
1:D:253:LEU:HB3	1:D:254:PRO:HD2	1.97	0.46
1:A:82:PHE:O	1:A:86:VAL:HG23	2.16	0.46
1:A:129:LYS:HD3	1:A:129:LYS:C	2.36	0.46
1:A:165:ASP:OD2	1:A:252:HIS:HB2	2.16	0.46
1:A:29:PRO:O	1:A:30:LEU:HD13	2.15	0.46
1:A:180:PHE:CE1	1:A:216:ARG:HB3	2.50	0.46
1:B:91:GLU:OE2	1:B:94:HIS:ND1	2.41	0.46
1:D:193:THR:OG1	1:D:194:LYS:HE2	2.16	0.46
1:D:251:LYS:HD3	1:D:255:SER:OG	2.16	0.46
1:A:110:LEU:HA	1:A:119:ALA:HB2	1.98	0.46
1:D:129:LYS:HE2	1:D:134:PHE:CZ	2.51	0.46
1:B:174:LYS:HA	1:B:221:LEU:O	2.14	0.46
1:B:180:PHE:HB2	1:B:234:PHE:HB2	1.97	0.46
1:D:85:LEU:HD22	1:D:107:LEU:HB2	1.97	0.46
1:D:253:LEU:HB3	1:D:254:PRO:CD	2.46	0.46
1:C:197:VAL:HG22	1:C:208:TYR:CD2	2.51	0.46
1:D:101:GLU:H	1:D:101:GLU:HG2	1.40	0.46
1:D:254:PRO:HD2	1:D:257:CYS:SG	2.56	0.46
1:A:41:THR:HA	1:A:171:VAL:HG13	1.98	0.46
1:A:109:SER:OG	1:A:148:PHE:HB2	2.16	0.46
1:A:8:VAL:HG22	1:A:31:VAL:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:SER:O	1:B:73:LYS:O	2.34	0.45
1:B:166:ASN:HB2	1:B:249:PHE:CD1	2.51	0.45
1:C:166:ASN:HA	1:C:248:ILE:O	2.16	0.45
1:C:266:ASN:ND2	1:C:267:LYS:N	2.64	0.45
1:B:16:ARG:HD2	1:B:136:GLU:HG3	1.98	0.45
1:C:44:TRP:HZ2	1:C:128:LEU:HB2	1.74	0.45
1:D:27:ARG:NH1	1:D:27:ARG:HG3	2.31	0.45
1:D:170:GLN:OE1	1:D:175:LYS:HD2	2.16	0.45
1:C:159:THR:HG22	1:C:234:PHE:HB3	1.99	0.45
1:D:55:LYS:HD3	1:D:83:ASP:OD1	2.17	0.45
1:D:91:GLU:HG3	1:D:94:HIS:CD2	2.52	0.45
1:A:216:ARG:NH2	1:A:218:GLU:OE1	2.49	0.45
1:B:121:ILE:CD1	1:B:148:PHE:CD1	3.00	0.45
1:D:156:GLN:HG3	1:D:238:ILE:HG12	1.98	0.45
1:C:306:GLN:HA	1:C:310:TYR:CD2	2.52	0.45
1:A:310:TYR:O	1:A:311:SER:C	2.55	0.45
1:C:172:THR:CG2	1:C:243:GLY:HA2	2.46	0.45
1:C:179:LEU:HB2	1:C:217:TYR:HB2	1.98	0.45
1:A:177:VAL:HG22	1:A:179:LEU:HD11	1.99	0.45
1:B:208:TYR:N	1:B:209:PRO:HD3	2.32	0.45
1:C:164:MET:HE1	1:C:258:TYR:CZ	2.52	0.45
1:D:4:GLN:HB2	1:D:215:ARG:HA	1.99	0.45
1:D:70:PHE:CE2	1:D:195:SER:O	2.70	0.45
1:C:279:LEU:O	1:C:279:LEU:HG	2.17	0.45
1:C:187:TYR:HB3	1:C:210:LEU:O	2.17	0.44
1:C:297:TYR:O	1:C:300:ARG:HB3	2.16	0.44
1:D:39:PRO:O	1:D:40:CYS:C	2.55	0.44
1:D:80:LEU:HG	1:D:81:PRO:HD2	1.99	0.44
1:A:35:ILE:HG22	1:A:36:ASP:N	2.33	0.44
1:A:44:TRP:HZ2	1:A:128:LEU:O	1.99	0.44
1:A:207:LYS:HB2	1:A:208:TYR:CD2	2.51	0.44
1:A:290:PRO:HG2	1:B:253:LEU:HD21	1.98	0.44
1:A:293:TYR:OH	1:B:252:HIS:CD2	2.70	0.44
1:D:24:TYR:N	1:D:25:PRO:CD	2.80	0.44
1:D:94:HIS:CE1	1:D:103:GLU:O	2.63	0.44
1:A:107:LEU:HD12	1:A:108:ARG:N	2.31	0.44
1:C:138:PHE:HE2	1:C:143:PHE:HB2	1.82	0.44
1:B:60:ILE:CD1	1:B:85:LEU:HD13	2.48	0.44
1:C:188:LEU:CD2	1:C:234:PHE:CD1	3.00	0.44
1:C:188:LEU:HD22	1:C:234:PHE:CE1	2.53	0.44
1:A:43:LYS:O	1:A:48:TYR:CD1	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ALA:O	1:A:301:MET:HB2	2.18	0.44
1:B:109:SER:HB3	1:B:148:PHE:N	2.24	0.44
1:A:24:TYR:OH	1:A:165:ASP:OD2	2.21	0.44
1:C:268:ASP:OD2	1:C:268:ASP:N	2.50	0.44
1:D:93:LYS:HA	1:D:101:GLU:O	2.17	0.44
1:A:161:TYR:CZ	1:A:193:THR:HG22	2.53	0.44
1:A:205:LEU:HD21	1:A:212:SER:OG	2.17	0.44
1:B:142:GLN:HE21	1:B:142:GLN:HB3	1.56	0.44
1:C:57:GLU:HA	1:C:80:LEU:O	2.17	0.44
1:C:148:PHE:C	1:C:149:ARG:HD3	2.37	0.44
1:A:85:LEU:CD2	1:A:107:LEU:HD22	2.48	0.44
1:B:253:LEU:HB2	1:B:258:TYR:CE2	2.53	0.44
1:C:283:LEU:HA	1:C:283:LEU:HD23	1.75	0.44
1:A:289:LEU:CD1	1:A:289:LEU:N	2.81	0.43
1:B:5:HIS:HE1	1:B:218:GLU:HB3	1.82	0.43
1:B:61:HIS:HB2	1:B:106:TYR:HB3	1.99	0.43
1:C:32:LEU:CD1	1:C:35:ILE:HD11	2.48	0.43
1:D:60:ILE:CG1	1:D:85:LEU:HD13	2.48	0.43
1:C:106:TYR:HA	1:C:150:ILE:O	2.18	0.43
1:A:10:ARG:HG2	1:A:31:VAL:HG11	2.00	0.43
1:D:302:VAL:O	1:D:306:GLN:HG3	2.18	0.43
1:A:26:GLN:HE21	1:A:26:GLN:HB2	1.58	0.43
1:B:109:SER:HB2	1:B:148:PHE:HB2	2.01	0.43
1:B:284:LYS:O	1:B:287:ALA:HB3	2.18	0.43
1:C:189:TYR:CZ	1:C:210:LEU:HB2	2.53	0.43
1:D:45:THR:O	1:D:49:LEU:HD22	2.17	0.43
1:B:15:SER:H	1:B:18:GLN:CG	2.31	0.43
1:B:24:TYR:HB3	1:B:25:PRO:HD3	2.01	0.43
1:B:121:ILE:HD12	1:B:148:PHE:CD1	2.54	0.43
1:B:187:TYR:CE2	1:B:213:LYS:HB2	2.53	0.43
1:C:261:THR:OG1	1:C:267:LYS:HD3	2.19	0.43
1:B:60:ILE:HD11	1:B:85:LEU:HB2	2.00	0.43
1:A:199:ASN:O	1:A:199:ASN:CG	2.56	0.43
1:B:228:PHE:CE2	1:B:230:PRO:HG3	2.54	0.43
1:C:128:LEU:H	1:C:128:LEU:CD2	2.25	0.43
1:C:153:PRO:HG3	1:C:242:PHE:CA	2.48	0.43
1:B:150:ILE:HG12	1:B:244:VAL:HG13	2.00	0.43
1:C:149:ARG:NH1	1:C:149:ARG:CG	2.69	0.43
1:B:121:ILE:CD1	1:B:148:PHE:HD1	2.32	0.43
1:C:84:GLN:O	1:C:88:ARG:HG3	2.19	0.43
1:C:237:VAL:O	1:C:237:VAL:CG2	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:LYS:HE3	1:D:77:TYR:HB3	2.00	0.43
1:D:113:ASP:HA	1:D:114:PRO:HD3	1.83	0.43
1:D:168:LEU:HD21	1:D:175:LYS:HD3	2.01	0.43
1:D:286:LEU:HD13	1:D:294:ARG:HG3	2.00	0.43
1:A:39:PRO:O	1:A:40:CYS:C	2.57	0.42
1:C:24:TYR:CE2	1:C:250:TRP:HZ2	2.37	0.42
1:C:179:LEU:HA	1:C:234:PHE:O	2.19	0.42
1:C:266:ASN:ND2	1:C:267:LYS:H	2.17	0.42
1:C:164:MET:CE	1:C:258:TYR:CE1	3.02	0.42
1:C:310:TYR:O	1:D:295:ASP:OD1	2.37	0.42
1:A:303:LEU:HD21	1:B:186:GLN:HA	2.01	0.42
1:B:27:ARG:NH2	1:B:165:ASP:OD1	2.52	0.42
1:C:147:VAL:HG12	1:C:148:PHE:N	2.34	0.42
1:D:111:GLY:CA	1:D:124:GLN:HE22	2.31	0.42
1:D:286:LEU:CD1	1:D:294:ARG:HG2	2.48	0.42
1:A:189:TYR:HH	1:A:209:PRO:HD2	1.85	0.42
1:C:109:SER:HB3	1:C:147:VAL:HG13	2.01	0.42
1:C:125:PHE:CG	1:C:148:PHE:CE1	3.02	0.42
1:C:165:ASP:OD1	1:C:231:ALA:N	2.46	0.42
1:A:39:PRO:HB2	1:A:43:LYS:CE	2.50	0.42
1:A:253:LEU:HD21	1:B:290:PRO:HG2	2.02	0.42
1:B:124:GLN:C	1:B:126:PRO:HD3	2.40	0.42
1:C:144:PHE:CD2	1:C:145:SER:HB2	2.54	0.42
1:C:166:ASN:ND2	1:C:229:ILE:HB	2.35	0.42
1:C:266:ASN:HD22	1:C:267:LYS:H	1.68	0.42
1:D:112:GLU:O	1:D:114:PRO:HD3	2.19	0.42
1:D:176:ARG:HH21	1:D:238:ILE:HD12	1.85	0.42
1:D:203:PRO:CG	1:D:205:LEU:HD21	2.49	0.42
1:A:198:LEU:N	1:A:198:LEU:CD2	2.83	0.42
1:A:302:VAL:HB	1:B:302:VAL:HG13	2.02	0.42
1:C:282:ALA:HB2	1:D:278:ILE:HG13	2.02	0.42
1:A:289:LEU:N	1:A:289:LEU:HD12	2.35	0.42
1:B:147:VAL:HG12	1:B:148:PHE:O	2.20	0.42
1:B:253:LEU:HB2	1:B:258:TYR:CZ	2.54	0.42
1:C:188:LEU:HD22	1:C:234:PHE:CD1	2.55	0.42
1:D:180:PHE:HB2	1:D:234:PHE:HB2	2.01	0.42
1:B:129:LYS:HD3	1:B:129:LYS:C	2.40	0.42
1:D:70:PHE:HE2	1:D:195:SER:O	2.02	0.42
1:D:129:LYS:HD3	1:D:129:LYS:C	2.40	0.42
1:D:190:LEU:HD21	1:D:234:PHE:HZ	1.83	0.42
1:A:27:ARG:NH2	1:A:165:ASP:CG	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ARG:HD2	1:B:98:PHE:CE1	2.55	0.42
1:B:217:TYR:CD2	1:B:217:TYR:N	2.87	0.42
1:C:24:TYR:HB3	1:C:25:PRO:CD	2.47	0.42
1:C:197:VAL:HG22	1:C:208:TYR:CG	2.54	0.42
1:C:278:ILE:CD1	1:D:285:THR:HG21	2.50	0.42
1:A:125:PHE:N	1:A:126:PRO:CD	2.83	0.41
1:C:6:LEU:HB3	1:C:7:PRO:CD	2.50	0.41
1:C:182:PRO:HD3	1:C:233:TRP:CE2	2.54	0.41
1:B:20:MET:HB2	1:B:20:MET:HE3	1.85	0.41
1:B:231:ALA:O	1:B:232:LEU:CB	2.68	0.41
1:C:271:ALA:HB3	1:D:289:LEU:CD1	2.49	0.41
1:D:134:PHE:CD1	1:D:248:ILE:HD11	2.56	0.41
1:A:37:LEU:HD12	1:A:37:LEU:HA	1.78	0.41
1:A:242:PHE:CG	1:A:243:GLY:N	2.88	0.41
1:B:213:LYS:HE3	1:B:213:LYS:HB3	1.81	0.41
1:D:165:ASP:OD2	1:D:252:HIS:HB2	2.21	0.41
1:A:205:LEU:CD1	1:A:209:PRO:HA	2.50	0.41
1:A:212:SER:C	1:A:214:ALA:H	2.23	0.41
1:B:166:ASN:HA	1:B:248:ILE:O	2.20	0.41
1:C:25:PRO:O	1:C:27:ARG:HB2	2.21	0.41
1:A:111:GLY:HA2	1:A:124:GLN:NE2	2.36	0.41
1:A:186:GLN:HE21	1:A:186:GLN:HB3	1.66	0.41
1:C:189:TYR:CD1	1:C:189:TYR:N	2.88	0.41
1:D:67:GLN:OE1	1:D:199:ASN:HB2	2.20	0.41
1:A:189:TYR:OH	1:A:209:PRO:HD2	2.20	0.41
1:A:295:ASP:OD1	1:B:310:TYR:O	2.38	0.41
1:C:268:ASP:OD1	1:D:300:ARG:NH1	2.44	0.41
1:A:37:LEU:O	1:A:132:ILE:HA	2.20	0.41
1:A:49:LEU:HD12	1:A:49:LEU:HA	1.76	0.41
1:B:178:VAL:HA	1:B:217:TYR:O	2.21	0.41
1:C:170:GLN:NE2	1:C:221:LEU:CB	2.83	0.41
1:C:291:GLU:OE1	1:D:311:SER:C	2.59	0.41
1:D:136:GLU:H	1:D:136:GLU:HG2	1.56	0.41
1:D:156:GLN:HG3	1:D:238:ILE:CG1	2.50	0.41
1:C:8:VAL:HG13	1:C:219:CYS:CB	2.50	0.41
1:D:82:PHE:CD1	1:D:82:PHE:C	2.93	0.41
1:A:97:PHE:CB	1:A:100:SER:O	2.69	0.40
1:C:255:SER:HA	1:C:258:TYR:HD2	1.85	0.40
1:D:58:VAL:O	1:D:79:THR:HA	2.21	0.40
1:A:24:TYR:HE2	1:A:250:TRP:CZ2	2.36	0.40
1:B:16:ARG:CG	1:B:20:MET:CE	2.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:LEU:O	1:C:132:ILE:HA	2.21	0.40
1:C:291:GLU:O	1:C:292:GLU:C	2.59	0.40
1:A:183:ARG:C	1:A:185:ALA:N	2.74	0.40
1:A:230:PRO:O	1:A:231:ALA:C	2.59	0.40
1:B:5:HIS:CE1	1:B:218:GLU:CB	3.04	0.40
1:B:60:ILE:CD1	1:B:80:LEU:HB2	2.52	0.40
1:C:155:LEU:HD13	1:C:155:LEU:C	2.42	0.40
1:C:159:THR:CG2	1:C:234:PHE:HB3	2.51	0.40
1:D:27:ARG:HH11	1:D:27:ARG:CG	2.34	0.40
1:A:167:LEU:HD22	1:A:250:TRP:CZ3	2.56	0.40
1:A:190:LEU:HD12	1:A:190:LEU:HA	1.73	0.40
1:D:77:TYR:O	1:D:78:ARG:HD3	2.21	0.40
1:D:181:SER:HA	1:D:182:PRO:HD3	1.97	0.40
1:D:190:LEU:HD12	1:D:195:SER:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	294/338 (87%)	258 (88%)	31 (10%)	5 (2%)	9 16
1	B	309/338 (91%)	289 (94%)	18 (6%)	2 (1%)	25 43
1	C	274/338 (81%)	242 (88%)	27 (10%)	5 (2%)	8 14
1	D	306/338 (90%)	285 (93%)	16 (5%)	5 (2%)	9 17
All	All	1183/1352 (88%)	1074 (91%)	92 (8%)	17 (1%)	11 20

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	73	LYS

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Mol	Chain	Res	Type
1	D	310	TYR
1	A	158	TRP
1	C	204	ASP
1	C	211	PHE
1	A	51	GLN
1	A	184	ASP
1	C	291	GLU
1	D	71	ILE
1	D	291	GLU
1	A	112	GLU
1	C	278	ILE
1	A	213	LYS
1	C	7	PRO
1	D	109	SER
1	D	112	GLU
1	B	99	VAL

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	210/300 (70%)	174 (83%)	36 (17%)	2 3
1	B	262/300 (87%)	228 (87%)	34 (13%)	4 7
1	C	184/300 (61%)	152 (83%)	32 (17%)	2 3
1	D	266/300 (89%)	222 (84%)	44 (16%)	2 4
All	All	922/1200 (77%)	776 (84%)	146 (16%)	2 4

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	16	ARG
1	A	26	GLN
1	A	27	ARG
1	A	30	LEU

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Mol	Chain	Res	Type
1	A	31	VAL
1	A	37	LEU
1	A	49	LEU
1	A	52	VAL
1	A	76	VAL
1	A	86	VAL
1	A	117	ASP
1	A	122	ARG
1	A	133	LYS
1	A	142	GLN
1	A	148	PHE
1	A	151	SER
1	A	163	VAL
1	A	164	MET
1	A	167	LEU
1	A	177	VAL
1	A	178	VAL
1	A	186	GLN
1	A	190	LEU
1	A	199	ASN
1	A	208	TYR
1	A	212	SER
1	A	232	LEU
1	A	244	VAL
1	A	246	VAL
1	A	273	SER
1	A	278	ILE
1	A	279	LEU
1	A	280	ASP
1	A	286	LEU
1	A	303	LEU
1	B	1	MET
1	B	7	PRO
1	B	17	GLU
1	B	21	GLN
1	B	27	ARG
1	B	30	LEU
1	B	31	VAL
1	B	37	LEU
1	B	41	THR
1	B	46	VAL
1	B	60	ILE

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Mol	Chain	Res	Type
1	B	73	LYS
1	B	74	ASN
1	B	83	ASP
1	B	88	ARG
1	B	115	ARG
1	B	127	LEU
1	B	136	GLU
1	B	142	GLN
1	B	155	LEU
1	B	164	MET
1	B	167	LEU
1	B	178	VAL
1	B	186	GLN
1	B	188	LEU
1	B	189	TYR
1	B	195	SER
1	B	213	LYS
1	B	216	ARG
1	B	237	VAL
1	B	273	SER
1	B	286	LEU
1	B	307	ASP
1	B	310	TYR
1	C	8	VAL
1	C	14	VAL
1	C	27	ARG
1	C	30	LEU
1	C	31	VAL
1	C	41	THR
1	C	46	VAL
1	C	65	VAL
1	C	83	ASP
1	C	87	GLN
1	C	128	LEU
1	C	136	GLU
1	C	149	ARG
1	C	150	ILE
1	C	164	MET
1	C	166	ASN
1	C	178	VAL
1	C	186	GLN
1	C	193	THR

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Mol	Chain	Res	Type
1	C	195	SER
1	C	201	ASP
1	C	219	CYS
1	C	220	SER
1	C	232	LEU
1	C	237	VAL
1	C	261	THR
1	C	266	ASN
1	C	268	ASP
1	C	285	THR
1	C	286	LEU
1	C	289	LEU
1	C	300	ARG
1	D	6	LEU
1	D	26	GLN
1	D	27	ARG
1	D	41	THR
1	D	46	VAL
1	D	47	ASP
1	D	49	LEU
1	D	56	LYS
1	D	60	ILE
1	D	67	GLN
1	D	73	LYS
1	D	76	VAL
1	D	88	ARG
1	D	101	GLU
1	D	109	SER
1	D	112	GLU
1	D	127	LEU
1	D	136	GLU
1	D	141	GLU
1	D	155	LEU
1	D	164	MET
1	D	167	LEU
1	D	172	THR
1	D	186	GLN
1	D	190	LEU
1	D	195	SER
1	D	202	ASN
1	D	213	LYS
1	D	221	LEU

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Mol	Chain	Res	Type
1	D	222	GLU
1	D	236	ASN
1	D	244	VAL
1	D	246	VAL
1	D	255	SER
1	D	260	LYS
1	D	261	THR
1	D	270	THR
1	D	277	GLN
1	D	278	ILE
1	D	279	LEU
1	D	280	ASP
1	D	285	THR
1	D	286	LEU
1	D	307	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	21	GLN
1	A	26	GLN
1	A	67	GLN
1	A	186	GLN
1	A	199	ASN
1	A	236	ASN
1	A	252	HIS
1	A	306	GLN
1	B	26	GLN
1	B	74	ASN
1	B	142	GLN
1	B	186	GLN
1	B	247	ASN
1	B	252	HIS
1	B	306	GLN
1	C	166	ASN
1	C	186	GLN
1	C	247	ASN
1	C	266	ASN
1	C	306	GLN
1	D	26	GLN
1	D	94	HIS

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Mol	Chain	Res	Type
1	D	156	GLN
1	D	186	GLN
1	D	202	ASN
1	D	236	ASN
1	D	252	HIS
1	D	277	GLN
1	D	306	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	302/338 (89%)	0.52	34 (11%) 5 4	45, 94, 143, 169	0
1	B	311/338 (92%)	-0.04	1 (0%) 94 94	34, 61, 88, 112	0
1	C	284/338 (84%)	0.70	39 (13%) 3 2	51, 97, 141, 161	0
1	D	308/338 (91%)	-0.03	0 100 100	31, 57, 89, 108	0
All	All	1205/1352 (89%)	0.28	74 (6%) 21 22	31, 75, 132, 169	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	PHE	8.7
1	C	119	ALA	8.5
1	C	103	GLU	7.4
1	A	99	VAL	7.2
1	C	90	ALA	7.2
1	A	82	PHE	7.0
1	C	86	VAL	6.5
1	C	99	VAL	5.6
1	C	105	TYR	5.1
1	A	94	HIS	5.1
1	A	5	HIS	5.1
1	A	58	VAL	4.9
1	C	85	LEU	4.5
1	A	95	LYS	4.4
1	C	158	TRP	4.4
1	C	104	LYS	4.3
1	A	49	LEU	4.0
1	A	93	LYS	4.0
1	C	198	LEU	4.0
1	A	4	GLN	3.9
1	C	58	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	98	PHE	3.9
1	A	46	VAL	3.8
1	A	190	LEU	3.7
1	C	193	THR	3.6
1	C	238	ILE	3.6
1	C	79	THR	3.4
1	A	53	GLY	3.4
1	C	97	PHE	3.4
1	C	248	ILE	3.3
1	A	106	TYR	3.3
1	C	89	ALA	3.2
1	C	98	PHE	3.2
1	C	237	VAL	3.1
1	A	202	ASN	3.1
1	C	154	GLY	3.1
1	C	192	GLY	3.0
1	A	148	PHE	2.9
1	C	122	ARG	2.9
1	C	121	ILE	2.9
1	C	137	PHE	2.8
1	A	102	ASP	2.8
1	C	59	LYS	2.7
1	A	52	VAL	2.6
1	A	272	ALA	2.6
1	C	150	ILE	2.6
1	A	152	SER	2.5
1	C	102	ASP	2.5
1	A	199	ASN	2.5
1	C	263	THR	2.5
1	C	221	LEU	2.5
1	C	205	LEU	2.4
1	B	286	LEU	2.4
1	C	210	LEU	2.4
1	A	96	GLU	2.4
1	C	100	SER	2.4
1	A	117	ASP	2.4
1	A	137	PHE	2.3
1	A	264	TYR	2.3
1	C	264	TYR	2.3
1	C	80	LEU	2.3
1	C	148	PHE	2.2
1	C	243	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	85	LEU	2.1
1	A	158	TRP	2.1
1	A	101	GLU	2.1
1	C	203	PRO	2.1
1	C	144	PHE	2.1
1	A	74	ASN	2.0
1	A	100	SER	2.0
1	A	97	PHE	2.0
1	A	244	VAL	2.0
1	C	82	PHE	2.0
1	A	44	TRP	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	MG	B	401	1/1	0.90	0.12	67,67,67,67	0
2	MG	D	401	1/1	0.96	0.19	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.