



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:24 AM GMT

PDB ID : 3AL6
Title : Crystal structure of Human TYW5
Authors : Kato, M.; Araiso, Y.; Ishitani, R.; Nureki, O.
Deposited on : 2010-07-26
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

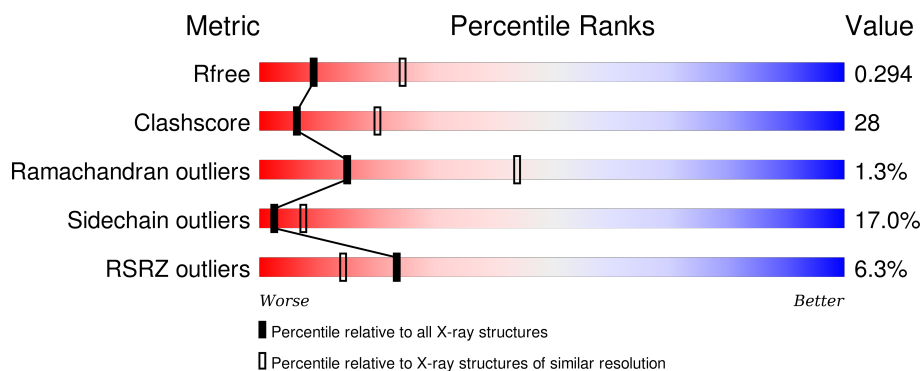
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	338	<div> <div>7%</div> <div>50% 32% 7% 12%</div> </div>
1	B	338	<div> <div>%</div> <div>55% 31% 5% 9%</div> </div>
1	C	338	<div> <div>15%</div> <div>39% 34% 7% 19%</div> </div>
1	D	338	<div> <div></div> <div>46% 38% 7% 9%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9037 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
1	A	299	Total	C	N	O	S	0	0	0
			2223	1435	377	405	6			
1	B	308	Total	C	N	O	S	0	0	0
			2442	1583	410	442	7			
1	C	273	Total	C	N	O	S	0	0	0
			1917	1230	316	365	6			
1	D	308	Total	C	N	O	S	0	0	0
			2431	1577	409	438	7			

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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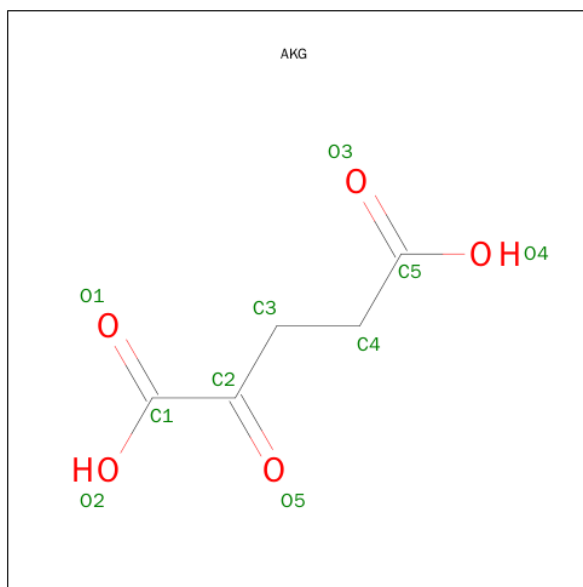
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	PHE	-	EXPRESSION TAG	UNP A2RUC4
C	-4	GLN	-	EXPRESSION TAG	UNP A2RUC4
C	-3	GLY	-	EXPRESSION TAG	UNP A2RUC4
C	-2	PRO	-	EXPRESSION TAG	UNP A2RUC4
C	-1	LEU	-	EXPRESSION TAG	UNP A2RUC4
C	0	HIS	-	EXPRESSION 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 NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ni 1 1	0	0
2	A	1	Total Ni 1 1	0	0
2	D	1	Total Ni 1 1	0	0
2	C	1	Total Ni 1 1	0	0

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C₅H₆O₅).



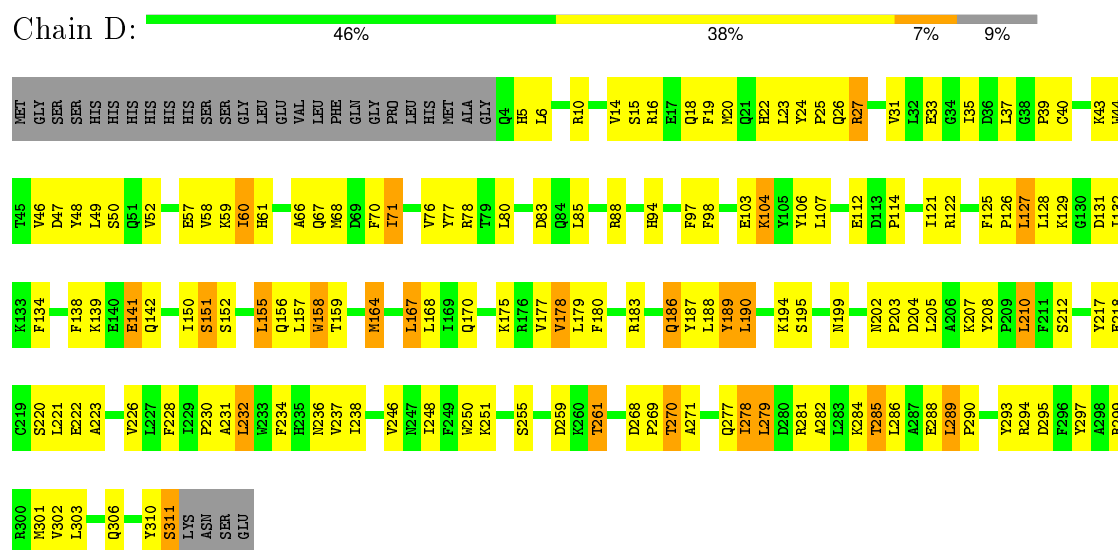
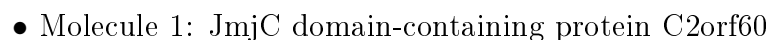
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

- Chain A:
-
- 7% 50% 32% 7% 12%
- MET GLY SER SER HIS HIS HIS HIS SER SER GLY GLU VAL LEU PRE GLN GLY LEU HIS MET ALA GLN HIS V8 P9 R10 L11 E12 G13 V14 S15 R16 E17 Q18 F19 H22 L23 Y24 P25 Q26 R27 L30 L32 W44 D47 Y48 L49 V52

- Chain B:
-

- 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	165.87Å 165.87Å 105.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.02 – 2.80 49.02 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.02-2.80) 99.6 (49.02-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6 _289)	Depositor
R, R_{free}	0.240 , 0.295 0.239 , 0.294	Depositor DCC
R_{free} test set	1841 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	77.5	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 68.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 36905 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9037	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NI, AKG

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	0.40	0/2280	0.59	1/3119 (0.0%)
1	B	0.54	0/2509	0.72	1/3411 (0.0%)
1	C	0.42	0/1962	0.61	0/2692
1	D	0.57	0/2498	0.72	0/3399
All	All	0.49	0/9249	0.67	2/12621 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	30	LEU	CA-CB-CG	5.23	127.34	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2223	0	2001	118	0
1	B	2442	0	2334	109	0
1	C	1917	0	1588	152	0
1	D	2431	0	2320	136	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	B	10	0	4	0	0
3	D	10	0	4	0	0
All	All	9037	0	8251	478	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 28.

All (478) 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:27:ARG:HH11	1:B:27:ARG:HG3	1.13	1.09
1:C:186:GLN:H	1:C:186:GLN:HE21	1.15	0.91
1:A:14:VAL:HA	1:A:18:GLN:HE22	1.35	0.91
1:B:60:ILE:HD11	1:B:85:LEU:HB2	1.55	0.88
1:A:14:VAL:HA	1:A:18:GLN:NE2	1.90	0.86
1:B:27:ARG:NH1	1:B:27:ARG:HG3	1.88	0.85
1:B:156:GLN:HG3	1:B:238:ILE:HG12	1.58	0.85
1:A:8:VAL:HG13	1:A:219:CYS:HB3	1.56	0.85
1:C:8:VAL:HG13	1:C:219:CYS:HB3	1.59	0.85
1:C:44:TRP:CZ2	1:C:131:ASP:HB2	2.12	0.82
1:A:156:GLN:HG2	1:A:238:ILE:HG12	1.61	0.82
1:C:186:GLN:H	1:C:186:GLN:NE2	1.77	0.82
1:C:286:LEU:HD13	1:C:294:ARG:HG3	1.63	0.81
1:B:291:GLU:HA	1:B:294:ARG:HG2	1.61	0.80
1:D:204:ASP:OD2	1:D:207:LYS:HE2	1.82	0.80
1:C:128:LEU:H	1:C:128:LEU:HD23	1.45	0.80
1:A:48:TYR:CE1	1:A:52:VAL:HG21	2.18	0.79
1:A:67:GLN:HE21	1:A:198:LEU:HB3	1.47	0.79
1:D:164:MET:CE	1:D:251:LYS:HA	2.14	0.77
1:A:122:ARG:HG2	1:A:129:LYS:HE3	1.66	0.77
1:B:6:LEU:HD23	1:B:6:LEU:N	2.01	0.76
1:A:5:HIS:CD2	1:A:216:ARG:HH21	2.03	0.76
1:C:32:LEU:HB2	1:C:35:ILE:HD11	1.67	0.75
1:D:94:HIS:HE1	1:D:103:GLU:O	1.68	0.75
1:D:295:ASP:O	1:D:299:ARG:HG3	1.87	0.74
1:C:44:TRP:CD1	1:C:48:TYR:CE1	2.76	0.74
1:C:282:ALA:H	1:D:278:ILE:HD11	1.52	0.74
1:A:48:TYR:O	1:A:52:VAL:HG23	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:SER:HB3	1:C:148:PHE:H	1.53	0.73
1:D:167:LEU:HD22	1:D:250:TRP:CZ3	2.23	0.72
1:C:266:ASN:HD22	1:C:266:ASN:H	1.36	0.72
1:A:231:ALA:O	1:A:232:LEU:HB2	1.87	0.72
1:C:16:ARG:O	1:C:20:MET:HE2	1.91	0.71
1:D:286:LEU:CD1	1:D:294:ARG:HG3	2.20	0.71
1:C:8:VAL:HG23	1:C:30:LEU:HA	1.72	0.71
1:C:286:LEU:HD13	1:C:294:ARG:CG	2.21	0.70
1:A:152:SER:HB3	1:A:153:PRO:HD2	1.73	0.70
1:D:164:MET:HE1	1:D:251:LYS:HA	1.72	0.70
1:C:278:ILE:CG2	1:D:282:ALA:HB2	2.21	0.69
1:B:109:SER:HB3	1:B:148:PHE:H	1.57	0.69
1:D:302:VAL:O	1:D:306:GLN:HG3	1.93	0.69
1:B:73:LYS:HE2	1:B:75:PHE:O	1.93	0.69
1:D:50:SER:HB3	1:D:83:ASP:HB2	1.73	0.69
1:A:24:TYR:HB3	1:A:25:PRO:HD3	1.75	0.68
1:A:306:GLN:O	1:A:310:TYR:HB2	1.94	0.68
1:A:287:ALA:HA	1:A:294:ARG:HD2	1.75	0.68
1:C:30:LEU:O	1:C:30:LEU:HD12	1.93	0.68
1:B:170:GLN:OE1	1:B:175:LYS:HD2	1.94	0.68
1:C:128:LEU:HA	1:C:131:ASP:OD2	1.94	0.68
1:C:172:THR:HB	1:C:244:VAL:H	1.59	0.68
1:B:16:ARG:CZ	1:B:20:MET:HE1	2.24	0.68
1:A:8:VAL:CG1	1:A:219:CYS:HB3	2.22	0.68
1:C:299:ARG:NH1	1:D:183:ARG:HG2	2.09	0.68
1:B:76:VAL:HG23	1:B:76:VAL:O	1.94	0.68
1:B:295:ASP:O	1:B:299:ARG:HG3	1.94	0.67
1:B:27:ARG:HH11	1:B:27:ARG:CG	1.99	0.67
1:C:282:ALA:N	1:D:278:ILE:HD11	2.09	0.67
1:D:27:ARG:HH11	1:D:27:ARG:HG3	1.58	0.67
1:C:282:ALA:HB2	1:D:278:ILE:HD11	1.77	0.66
1:B:129:LYS:HD3	1:B:129:LYS:O	1.95	0.66
1:D:156:GLN:HG3	1:D:238:ILE:CG1	2.25	0.66
1:B:85:LEU:HD21	1:B:107:LEU:HB2	1.78	0.66
1:C:121:ILE:HD12	1:C:148:PHE:CE1	2.31	0.66
1:D:59:LYS:HE3	1:D:77:TYR:CD1	2.31	0.66
1:A:107:LEU:HD12	1:A:108:ARG:N	2.10	0.65
1:A:15:SER:H	1:A:18:GLN:HE21	1.44	0.65
1:C:189:TYR:HH	1:C:209:PRO:HD2	1.62	0.65
1:C:186:GLN:N	1:C:186:GLN:HE21	1.92	0.64
1:D:122:ARG:HA	1:D:129:LYS:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:LEU:HD13	1:D:294:ARG:HG3	1.78	0.64
1:C:186:GLN:HB3	1:D:303:LEU:HD21	1.78	0.64
1:A:196:GLU:O	1:A:198:LEU:HD22	1.97	0.64
1:C:281:ARG:O	1:C:285:THR:HG23	1.98	0.64
1:A:107:LEU:HD12	1:A:108:ARG:H	1.64	0.63
1:A:150:ILE:HG12	1:A:244:VAL:HB	1.80	0.63
1:C:14:VAL:HA	1:C:18:GLN:OE1	1.99	0.63
1:D:61:HIS:HB2	1:D:106:TYR:HB3	1.78	0.63
1:D:27:ARG:HG3	1:D:27:ARG:NH1	2.13	0.63
1:D:112:GLU:O	1:D:114:PRO:HD3	1.99	0.63
1:C:160:HIS:CE1	1:C:235:HIS:HE2	2.17	0.62
1:A:176:ARG:HH11	1:A:176:ARG:HG2	1.64	0.62
1:B:85:LEU:CD2	1:B:107:LEU:HB2	2.29	0.62
1:C:160:HIS:CE1	1:C:235:HIS:NE2	2.67	0.62
1:C:44:TRP:CZ2	1:C:128:LEU:O	2.53	0.62
1:D:170:GLN:OE1	1:D:175:LYS:HD2	2.00	0.62
1:A:252:HIS:HD2	1:B:293:TYR:CE2	2.17	0.62
1:D:16:ARG:O	1:D:20:MET:HG3	1.99	0.62
1:D:231:ALA:O	1:D:232:LEU:HB2	1.98	0.62
1:D:5:HIS:CE1	1:D:218:GLU:OE1	2.52	0.62
1:C:24:TYR:OH	1:C:165:ASP:OD2	2.14	0.61
1:D:107:LEU:HD23	1:D:150:ILE:HD12	1.82	0.61
1:A:10:ARG:O	1:A:11:LEU:HD23	2.00	0.61
1:C:160:HIS:NE2	1:C:235:HIS:NE2	2.48	0.61
1:A:295:ASP:O	1:A:299:ARG:HG3	2.01	0.61
1:D:210:LEU:HD13	1:D:210:LEU:N	2.14	0.61
1:B:15:SER:H	1:B:18:GLN:HG3	1.65	0.61
1:D:106:TYR:CZ	1:D:157:LEU:HD11	2.35	0.60
1:B:39:PRO:HB2	1:B:43:LYS:HD2	1.83	0.60
1:B:61:HIS:HB2	1:B:106:TYR:HB3	1.82	0.60
1:A:134:PHE:CG	1:A:248:ILE:HD11	2.35	0.60
1:A:180:PHE:HB2	1:A:234:PHE:HB2	1.84	0.60
1:D:159:THR:OG1	1:D:236:ASN:HB2	2.01	0.60
1:A:278:ILE:HG12	1:B:282:ALA:HB2	1.81	0.60
1:B:55:LYS:HG2	1:B:83:ASP:OD1	2.00	0.60
1:C:44:TRP:HZ2	1:C:131:ASP:HB2	1.62	0.60
1:A:122:ARG:HA	1:A:129:LYS:HG3	1.82	0.60
1:D:199:ASN:ND2	1:D:202:ASN:HB3	2.17	0.60
1:A:170:GLN:OE1	1:A:170:GLN:HA	2.01	0.60
1:A:67:GLN:HE22	1:A:199:ASN:HB3	1.66	0.59
1:D:27:ARG:CG	1:D:27:ARG:HH11	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:SER:O	1:A:277:GLN:HG3	2.03	0.59
1:C:295:ASP:O	1:C:299:ARG:HG3	2.02	0.59
1:C:44:TRP:CD1	1:C:48:TYR:HE1	2.20	0.59
1:D:10:ARG:HG2	1:D:31:VAL:HG22	1.83	0.59
1:D:66:ALA:HA	1:D:104:LYS:HD2	1.86	0.58
1:A:85:LEU:HD21	1:A:107:LEU:HB2	1.84	0.58
1:A:205:LEU:HD13	1:A:209:PRO:HA	1.86	0.58
1:C:205:LEU:C	1:C:205:LEU:HD23	2.23	0.58
1:B:60:ILE:HD11	1:B:85:LEU:CB	2.31	0.58
1:D:290:PRO:HG2	1:D:293:TYR:HD2	1.68	0.58
1:C:210:LEU:C	1:C:212:SER:H	2.07	0.58
1:B:286:LEU:HD21	1:B:294:ARG:HB2	1.86	0.58
1:D:80:LEU:HD21	1:D:88:ARG:HD3	1.85	0.58
1:D:58:VAL:HG23	1:D:60:ILE:HD12	1.85	0.57
1:A:278:ILE:HD11	1:B:282:ALA:H	1.69	0.57
1:B:158:TRP:HE1	1:B:194:LYS:HZ2	1.52	0.57
1:C:199:ASN:O	1:C:203:PRO:HA	2.04	0.57
1:A:253:LEU:HD22	1:B:290:PRO:HG2	1.85	0.57
1:C:285:THR:OG1	1:C:286:LEU:N	2.37	0.57
1:D:164:MET:HE2	1:D:251:LYS:HA	1.86	0.57
1:D:156:GLN:HG3	1:D:238:ILE:HG13	1.86	0.57
1:B:53:GLY:HA2	1:B:128:LEU:HD11	1.86	0.57
1:C:47:ASP:O	1:C:50:SER:HB2	2.05	0.57
1:B:27:ARG:HD2	1:B:27:ARG:N	2.20	0.56
1:D:199:ASN:HD21	1:D:202:ASN:HB3	1.69	0.56
1:C:282:ALA:HB2	1:D:278:ILE:CD1	2.35	0.56
1:C:24:TYR:HB3	1:C:25:PRO:HD3	1.85	0.56
1:C:278:ILE:HD12	1:D:285:THR:HG21	1.87	0.56
1:D:80:LEU:HD21	1:D:88:ARG:CD	2.35	0.56
1:C:144:PHE:CB	1:C:250:TRP:HA	2.36	0.56
1:B:158:TRP:HE1	1:B:194:LYS:NZ	2.03	0.56
1:C:278:ILE:HG22	1:D:282:ALA:HB2	1.86	0.56
1:D:5:HIS:NE2	1:D:218:GLU:OE1	2.38	0.56
1:A:205:LEU:HD21	1:A:212:SER:OG	2.05	0.56
1:C:231:ALA:O	1:C:232:LEU:HB2	2.06	0.56
1:C:205:LEU:HD23	1:C:205:LEU:O	2.05	0.56
1:C:163:VAL:HG21	1:C:267:LYS:O	2.06	0.56
1:C:44:TRP:HH2	1:C:132:ILE:HG22	1.71	0.55
1:D:18:GLN:O	1:D:22:HIS:HB3	2.06	0.55
1:B:5:HIS:C	1:B:6:LEU:HD23	2.24	0.55
1:C:168:LEU:HG	1:C:168:LEU:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:MET:SD	1:C:137:PHE:O	2.65	0.55
1:A:24:TYR:CE2	1:A:250:TRP:HZ2	2.24	0.55
1:D:285:THR:O	1:D:288:GLU:HG2	2.07	0.55
1:C:302:VAL:O	1:C:306:GLN:HG3	2.07	0.55
1:A:23:LEU:HD22	1:A:30:LEU:HD21	1.88	0.55
1:A:252:HIS:HD2	1:B:293:TYR:HE2	1.54	0.55
1:D:85:LEU:CD2	1:D:107:LEU:HB2	2.36	0.55
1:C:149:ARG:HG3	1:C:247:ASN:HD21	1.71	0.54
1:D:70:PHE:O	1:D:71:ILE:CB	2.55	0.54
1:A:106:TYR:HB2	1:A:155:LEU:CD1	2.38	0.54
1:A:278:ILE:HD11	1:B:282:ALA:N	2.22	0.54
1:B:70:PHE:CE2	1:B:194:LYS:HB3	2.42	0.54
1:C:43:LYS:O	1:C:45:THR:HG23	2.07	0.54
1:C:278:ILE:CD1	1:D:285:THR:HG21	2.37	0.54
1:C:249:PHE:C	1:C:250:TRP:HE3	2.11	0.54
1:C:252:HIS:C	1:C:252:HIS:CD2	2.80	0.54
1:A:14:VAL:HG11	1:A:32:LEU:HD22	1.89	0.53
1:C:172:THR:HG22	1:C:173:GLY:N	2.23	0.53
1:B:60:ILE:CD1	1:B:85:LEU:HB2	2.33	0.53
1:A:44:TRP:HZ2	1:A:128:LEU:O	1.92	0.53
1:C:8:VAL:CG1	1:C:219:CYS:HB3	2.35	0.53
1:A:61:HIS:HB2	1:A:106:TYR:HB3	1.91	0.53
1:C:138:PHE:CZ	1:C:248:ILE:HG21	2.43	0.53
1:B:170:GLN:HG2	1:B:221:LEU:HB3	1.90	0.53
1:A:303:LEU:HD21	1:B:186:GLN:HA	1.89	0.53
1:A:19:PHE:HA	1:A:23:LEU:HD12	1.90	0.53
1:B:231:ALA:O	1:B:232:LEU:HB2	2.08	0.53
1:A:60:ILE:HG22	1:A:61:HIS:O	2.09	0.53
1:B:161:TYR:CE2	1:B:193:THR:HA	2.44	0.53
1:C:306:GLN:O	1:C:310:TYR:HB2	2.08	0.53
1:C:109:SER:HB2	1:C:148:PHE:HB2	1.90	0.52
1:D:15:SER:O	1:D:16:ARG:C	2.48	0.52
1:A:253:LEU:CD2	1:B:290:PRO:HG2	2.39	0.52
1:C:289:LEU:HD11	1:D:271:ALA:CB	2.39	0.52
1:A:89:ALA:HA	1:A:152:SER:OG	2.10	0.52
1:C:41:THR:HA	1:C:171:VAL:HG12	1.91	0.52
1:B:164:MET:CE	1:B:251:LYS:HA	2.39	0.52
1:A:221:LEU:HD11	1:A:227:LEU:HB2	1.92	0.52
1:A:177:VAL:HA	1:A:236:ASN:O	2.10	0.52
1:D:129:LYS:O	1:D:129:LYS:HD3	2.09	0.52
1:C:135:PRO:HB2	1:C:137:PHE:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ARG:HG2	1:B:20:MET:HE2	1.91	0.52
1:A:77:TYR:N	1:A:77:TYR:CD2	2.77	0.52
1:C:282:ALA:HB2	1:D:278:ILE:CG1	2.40	0.52
1:C:266:ASN:HD22	1:C:266:ASN:N	2.00	0.52
1:C:197:VAL:HG13	1:C:208:TYR:CD2	2.45	0.52
1:C:266:ASN:ND2	1:C:266:ASN:H	2.05	0.51
1:C:166:ASN:HA	1:C:250:TRP:CZ3	2.45	0.51
1:D:23:LEU:C	1:D:25:PRO:HD2	2.31	0.51
1:C:164:MET:HE1	1:C:251:LYS:HA	1.91	0.51
1:C:44:TRP:HA	1:C:48:TYR:CD1	2.46	0.51
1:A:286:LEU:HD23	1:B:275:ALA:CB	2.40	0.51
1:C:278:ILE:HG21	1:D:282:ALA:HB2	1.91	0.51
1:D:286:LEU:HD11	1:D:294:ARG:HA	1.93	0.51
1:A:178:VAL:HG21	1:A:216:ARG:HD2	1.93	0.51
1:C:32:LEU:HB2	1:C:35:ILE:CD1	2.39	0.51
1:D:70:PHE:HB2	1:D:158:TRP:CE3	2.46	0.51
1:C:41:THR:HA	1:C:171:VAL:CG1	2.41	0.51
1:A:69:ASP:H	1:A:74:ASN:CG	2.13	0.51
1:B:294:ARG:HG3	1:B:295:ASP:N	2.24	0.51
1:D:94:HIS:CE1	1:D:103:GLU:O	2.58	0.51
1:C:282:ALA:CB	1:D:278:ILE:HD11	2.41	0.51
1:C:148:PHE:O	1:C:149:ARG:HD3	2.11	0.51
1:B:153:PRO:HB3	1:B:241:GLU:HA	1.93	0.51
1:A:52:VAL:HB	1:A:128:LEU:HD21	1.93	0.50
1:B:73:LYS:HG3	1:B:73:LYS:O	2.10	0.50
1:A:165:ASP:OD2	1:A:252:HIS:HB2	2.10	0.50
1:C:8:VAL:CG2	1:C:30:LEU:HA	2.40	0.50
1:B:109:SER:HB2	1:B:148:PHE:HB2	1.93	0.50
1:C:197:VAL:HA	1:C:208:TYR:CE2	2.47	0.50
1:A:27:ARG:NH2	1:A:165:ASP:OD1	2.45	0.50
1:A:176:ARG:NH2	1:A:238:ILE:HD12	2.27	0.50
1:B:69:ASP:O	1:B:73:LYS:HA	2.11	0.50
1:A:167:LEU:O	1:A:247:ASN:HA	2.11	0.50
1:B:49:LEU:HD11	1:B:244:VAL:HG21	1.93	0.50
1:C:282:ALA:N	1:D:278:ILE:CD1	2.74	0.50
1:A:289:LEU:HD12	1:A:289:LEU:N	2.27	0.50
1:D:179:LEU:HA	1:D:234:PHE:O	2.12	0.50
1:D:178:VAL:HA	1:D:217:TYR:O	2.12	0.50
1:C:46:VAL:HG22	1:C:47:ASP:N	2.26	0.50
1:D:78:ARG:HG3	1:D:98:PHE:CD1	2.47	0.50
1:C:136:GLU:O	1:C:136:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:LEU:HD22	1:D:107:LEU:HB2	1.94	0.50
1:C:188:LEU:CD2	1:C:234:PHE:CD1	2.95	0.50
1:C:188:LEU:HD22	1:C:234:PHE:CD1	2.46	0.50
1:A:176:ARG:NH1	1:A:176:ARG:HG2	2.27	0.50
1:A:311:SER:N	1:B:295:ASP:OD1	2.45	0.50
1:A:60:ILE:HG22	1:A:61:HIS:N	2.27	0.50
1:C:227:LEU:HD12	1:C:228:PHE:N	2.26	0.50
1:A:310:TYR:O	1:A:311:SER:C	2.50	0.50
1:D:180:PHE:HB2	1:D:234:PHE:HB2	1.92	0.50
1:D:106:TYR:OH	1:D:157:LEU:HD11	2.12	0.49
1:C:21:GLN:O	1:C:25:PRO:HG2	2.12	0.49
1:B:259:ASP:OD1	1:B:259:ASP:C	2.51	0.49
1:A:91:GLU:O	1:A:93:LYS:N	2.45	0.49
1:A:31:VAL:O	1:A:32:LEU:HD23	2.12	0.49
1:C:188:LEU:HD22	1:C:234:PHE:CE1	2.47	0.49
1:D:167:LEU:HD22	1:D:250:TRP:HZ3	1.73	0.49
1:D:134:PHE:CD1	1:D:248:ILE:HD11	2.48	0.49
1:C:282:ALA:HB2	1:D:278:ILE:HG12	1.95	0.49
1:B:69:ASP:CG	1:B:198:LEU:HD11	2.33	0.49
1:C:25:PRO:O	1:C:27:ARG:HG2	2.13	0.49
1:B:302:VAL:O	1:B:306:GLN:HG3	2.12	0.49
1:C:237:VAL:CG2	1:C:237:VAL:O	2.60	0.49
1:A:5:HIS:CD2	1:A:216:ARG:NH2	2.79	0.49
1:D:60:ILE:HG12	1:D:85:LEU:HD13	1.95	0.49
1:A:302:VAL:HB	1:B:302:VAL:HB	1.95	0.49
1:C:44:TRP:HD1	1:C:48:TYR:CE1	2.27	0.48
1:A:147:VAL:HB	1:A:247:ASN:OD1	2.14	0.48
1:D:203:PRO:HG2	1:D:205:LEU:HD21	1.95	0.48
1:B:15:SER:OG	1:B:18:GLN:CG	2.61	0.48
1:B:153:PRO:HG3	1:B:242:PHE:N	2.28	0.48
1:B:281:ARG:O	1:B:285:THR:HG23	2.12	0.48
1:D:189:TYR:CD2	1:D:208:TYR:HD1	2.31	0.48
1:D:190:LEU:HD21	1:D:234:PHE:CZ	2.48	0.48
1:B:120:ASP:OD1	1:B:122:ARG:HB3	2.13	0.48
1:D:297:TYR:O	1:D:301:MET:HG3	2.12	0.48
1:A:205:LEU:HD13	1:A:205:LEU:O	2.14	0.48
1:B:60:ILE:HD11	1:B:85:LEU:HD13	1.95	0.48
1:A:295:ASP:OD2	1:A:299:ARG:HD2	2.14	0.48
1:A:282:ALA:HB2	1:B:278:ILE:CG2	2.44	0.48
1:C:205:LEU:C	1:C:205:LEU:CD2	2.82	0.48
1:D:24:TYR:N	1:D:25:PRO:CD	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:GLU:C	1:C:289:LEU:HD12	2.34	0.48
1:B:30:LEU:HD11	1:B:32:LEU:HD21	1.95	0.48
1:B:76:VAL:O	1:B:76:VAL:CG2	2.61	0.48
1:A:27:ARG:HH12	1:A:252:HIS:CD2	2.32	0.48
1:A:205:LEU:CD1	1:A:209:PRO:HA	2.44	0.48
1:A:289:LEU:N	1:A:289:LEU:CD1	2.77	0.48
1:C:179:LEU:HA	1:C:234:PHE:O	2.13	0.48
1:A:164:MET:HE3	1:A:251:LYS:HA	1.96	0.48
1:B:286:LEU:CD2	1:B:294:ARG:HB2	2.44	0.48
1:A:178:VAL:HG13	1:A:236:ASN:HB3	1.95	0.48
1:A:286:LEU:CD1	1:A:294:ARG:HA	2.44	0.48
1:C:295:ASP:OD1	1:C:299:ARG:NH1	2.47	0.48
1:C:299:ARG:O	1:C:303:LEU:HD23	2.13	0.48
1:A:124:GLN:C	1:A:126:PRO:HD3	2.35	0.48
1:C:189:TYR:OH	1:C:210:LEU:N	2.40	0.47
1:D:139:LYS:HB2	1:D:142:GLN:HG3	1.96	0.47
1:B:19:PHE:HA	1:B:23:LEU:HB2	1.96	0.47
1:B:15:SER:OG	1:B:18:GLN:HG2	2.14	0.47
1:C:283:LEU:O	1:C:287:ALA:HB2	2.15	0.47
1:D:281:ARG:O	1:D:284:LYS:N	2.47	0.47
1:B:189:TYR:O	1:B:196:GLU:HG3	2.15	0.47
1:C:125:PHE:HD1	1:C:128:LEU:HD21	1.78	0.47
1:D:104:LYS:HB3	1:D:152:SER:HB2	1.96	0.47
1:C:230:PRO:O	1:C:233:TRP:HB2	2.15	0.47
1:D:14:VAL:HG12	1:D:15:SER:N	2.28	0.47
1:D:14:VAL:CG1	1:D:15:SER:N	2.78	0.47
1:C:44:TRP:HZ2	1:C:128:LEU:O	1.97	0.47
1:A:134:PHE:CD1	1:A:248:ILE:HD11	2.50	0.47
1:B:180:PHE:HB2	1:B:234:PHE:HB2	1.97	0.47
1:B:16:ARG:O	1:B:20:MET:HB2	2.14	0.47
1:D:70:PHE:HB2	1:D:158:TRP:CZ3	2.50	0.47
1:A:298:ALA:O	1:A:301:MET:HB2	2.15	0.47
1:C:168:LEU:HA	1:C:247:ASN:HB3	1.96	0.46
1:C:135:PRO:HB3	1:C:137:PHE:CE2	2.50	0.46
1:D:106:TYR:HD1	1:D:151:SER:HB2	1.79	0.46
1:B:55:LYS:HA	1:B:83:ASP:OD1	2.16	0.46
1:C:142:GLN:O	1:C:250:TRP:HB2	2.15	0.46
1:D:259:ASP:OD1	1:D:259:ASP:C	2.54	0.46
1:B:139:LYS:O	1:B:142:GLN:HG3	2.14	0.46
1:D:22:HIS:O	1:D:25:PRO:HD2	2.15	0.46
1:D:52:VAL:HG13	1:D:127:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:PRO:HG3	1:B:242:PHE:H	1.81	0.46
1:A:111:GLY:HA2	1:A:124:GLN:OE1	2.15	0.46
1:C:91:GLU:O	1:C:92:GLU:C	2.54	0.46
1:B:60:ILE:HD13	1:B:80:LEU:HD12	1.98	0.46
1:D:281:ARG:O	1:D:285:THR:HG23	2.15	0.46
1:C:171:VAL:HG12	1:C:171:VAL:O	2.16	0.46
1:D:278:ILE:CG1	1:D:279:LEU:N	2.78	0.46
1:C:147:VAL:HG12	1:C:148:PHE:O	2.15	0.46
1:C:189:TYR:CE1	1:C:208:TYR:HB3	2.51	0.46
1:C:138:PHE:HZ	1:C:248:ILE:HG21	1.81	0.46
1:B:35:ILE:HG22	1:B:37:LEU:HD13	1.97	0.46
1:A:67:GLN:HE21	1:A:198:LEU:CB	2.25	0.46
1:D:22:HIS:C	1:D:25:PRO:HD2	2.36	0.46
1:C:232:LEU:HD21	1:D:293:TYR:CD1	2.51	0.45
1:A:15:SER:O	1:A:16:ARG:C	2.53	0.45
1:D:167:LEU:HD12	1:D:226:VAL:CG1	2.46	0.45
1:D:189:TYR:CE2	1:D:208:TYR:HD1	2.34	0.45
1:B:107:LEU:HD12	1:B:108:ARG:N	2.32	0.45
1:C:24:TYR:HB3	1:C:25:PRO:CD	2.45	0.45
1:A:31:VAL:C	1:A:32:LEU:HD23	2.36	0.45
1:B:109:SER:CB	1:B:148:PHE:H	2.26	0.45
1:B:30:LEU:HD11	1:B:32:LEU:CD2	2.47	0.45
1:A:205:LEU:HD22	1:A:205:LEU:HA	1.85	0.45
1:D:88:ARG:HH21	1:D:97:PHE:HA	1.80	0.45
1:D:306:GLN:HA	1:D:310:TYR:CD2	2.51	0.45
1:A:27:ARG:HG3	1:B:292:GLU:OE2	2.16	0.45
1:B:286:LEU:C	1:B:286:LEU:HD23	2.36	0.45
1:D:310:TYR:O	1:D:311:SER:C	2.55	0.45
1:B:121:ILE:HG22	1:B:129:LYS:HG2	1.97	0.45
1:C:279:LEU:O	1:C:279:LEU:HG	2.15	0.45
1:C:140:GLU:HG2	1:C:141:GLU:N	2.31	0.45
1:C:166:ASN:O	1:C:166:ASN:CG	2.55	0.45
1:D:270:THR:O	1:D:271:ALA:C	2.56	0.45
1:D:186:GLN:HG2	1:D:187:TYR:CD1	2.52	0.45
1:D:68:MET:HE2	1:D:158:TRP:CZ3	2.51	0.45
1:D:39:PRO:HB2	1:D:43:LYS:HG3	1.99	0.45
1:D:295:ASP:OD1	1:D:299:ARG:NH1	2.50	0.44
1:D:259:ASP:OD1	1:D:261:THR:HB	2.17	0.44
1:C:169:ILE:HA	1:C:226:VAL:HG22	1.98	0.44
1:B:247:ASN:C	1:B:247:ASN:ND2	2.71	0.44
1:B:27:ARG:NH2	1:B:165:ASP:OD2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:TRP:HE1	1:B:194:LYS:CE	2.31	0.44
1:D:48:TYR:CZ	1:D:52:VAL:HG21	2.53	0.44
1:B:295:ASP:OD2	1:B:299:ARG:NH1	2.46	0.44
1:A:199:ASN:O	1:A:199:ASN:CG	2.55	0.44
1:A:179:LEU:HA	1:A:234:PHE:O	2.17	0.44
1:D:10:ARG:NH2	1:D:33:GLU:OE1	2.49	0.44
1:C:87:GLN:O	1:C:91:GLU:HG3	2.18	0.44
1:A:242:PHE:CG	1:A:243:GLY:N	2.85	0.44
1:C:19:PHE:HA	1:C:23:LEU:HB2	1.99	0.44
1:D:40:CYS:HB3	1:D:131:ASP:O	2.18	0.44
1:A:8:VAL:CG2	1:A:31:VAL:HG12	2.48	0.44
1:D:67:GLN:HE21	1:D:156:GLN:HE22	1.65	0.44
1:D:37:LEU:O	1:D:132:ILE:HA	2.17	0.44
1:C:170:GLN:NE2	1:C:221:LEU:HB3	2.33	0.44
1:D:60:ILE:CD1	1:D:85:LEU:HD13	2.47	0.44
1:B:68:MET:HB3	1:B:68:MET:HE2	1.89	0.44
1:A:189:TYR:OH	1:A:210:LEU:HB2	2.17	0.44
1:A:293:TYR:OH	1:B:252:HIS:CD2	2.71	0.44
1:A:18:GLN:HA	1:A:22:HIS:HD2	1.83	0.44
1:C:24:TYR:N	1:C:25:PRO:HD2	2.33	0.44
1:A:156:GLN:HG2	1:A:238:ILE:CG1	2.42	0.43
1:C:246:VAL:O	1:C:247:ASN:HB3	2.18	0.43
1:A:290:PRO:O	1:A:291:GLU:C	2.57	0.43
1:D:68:MET:HE2	1:D:158:TRP:HZ3	1.82	0.43
1:C:172:THR:HB	1:C:244:VAL:N	2.29	0.43
1:A:186:GLN:H	1:A:186:GLN:HG2	1.68	0.43
1:C:227:LEU:HD12	1:C:228:PHE:H	1.82	0.43
1:D:58:VAL:HG23	1:D:60:ILE:CD1	2.46	0.43
1:A:293:TYR:OH	1:B:252:HIS:HD2	2.01	0.43
1:A:141:GLU:HG2	1:A:141:GLU:H	1.56	0.43
1:A:257:CYS:O	1:A:269:PRO:HB3	2.19	0.43
1:C:190:LEU:HA	1:C:195:SER:HA	2.00	0.43
1:C:20:MET:HE1	1:C:137:PHE:HD1	1.84	0.43
1:B:161:TYR:HE2	1:B:193:THR:HA	1.84	0.43
1:C:217:TYR:CD2	1:C:217:TYR:N	2.87	0.43
1:A:268:ASP:OD2	1:B:300:ARG:NH1	2.51	0.43
1:D:88:ARG:NH2	1:D:97:PHE:HA	2.34	0.43
1:A:125:PHE:N	1:A:126:PRO:HD3	2.33	0.43
1:B:17:GLU:N	1:B:17:GLU:CD	2.72	0.43
1:C:135:PRO:CB	1:C:137:PHE:CE2	3.02	0.42
1:D:170:GLN:OE1	1:D:170:GLN:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:TYR:N	1:A:77:TYR:HD2	2.16	0.42
1:C:170:GLN:NE2	1:C:221:LEU:CB	2.83	0.42
1:B:124:GLN:C	1:B:126:PRO:HD3	2.40	0.42
1:A:167:LEU:HD22	1:A:250:TRP:CZ3	2.54	0.42
1:D:188:LEU:O	1:D:189:TYR:HB2	2.19	0.42
1:B:60:ILE:CD1	1:B:85:LEU:HD13	2.49	0.42
1:C:44:TRP:CE2	1:C:131:ASP:HB2	2.51	0.42
1:D:60:ILE:HD11	1:D:85:LEU:HD13	2.01	0.42
1:D:141:GLU:H	1:D:141:GLU:HG3	1.62	0.42
1:A:32:LEU:HD12	1:A:137:PHE:HE2	1.85	0.42
1:C:8:VAL:HA	1:C:9:PRO:HD2	1.64	0.42
1:A:24:TYR:HE2	1:A:250:TRP:HZ2	1.64	0.42
1:D:85:LEU:HD21	1:D:107:LEU:HB2	2.00	0.42
1:B:94:HIS:CD2	1:B:101:GLU:O	2.73	0.42
1:C:20:MET:H	1:C:20:MET:HE2	1.83	0.42
1:A:10:ARG:NH2	1:A:225:ASP:OD1	2.53	0.42
1:D:222:GLU:O	1:D:223:ALA:C	2.57	0.42
1:C:189:TYR:OH	1:C:209:PRO:HD2	2.18	0.42
1:C:28:LYS:HB3	1:C:29:PRO:HD2	2.02	0.42
1:A:217:TYR:N	1:A:217:TYR:CD2	2.88	0.42
1:C:19:PHE:HD2	1:C:20:MET:HE1	1.85	0.42
1:B:16:ARG:CG	1:B:20:MET:HE2	2.50	0.42
1:D:121:ILE:HG22	1:D:129:LYS:HG2	2.02	0.42
1:B:190:LEU:HA	1:B:194:LYS:O	2.19	0.42
1:D:52:VAL:HG12	1:D:128:LEU:HG	2.02	0.42
1:B:205:LEU:HA	1:B:205:LEU:HD23	1.62	0.42
1:A:259:ASP:HB3	1:A:262:ASP:HB2	2.02	0.42
1:A:291:GLU:HA	1:A:294:ARG:NH1	2.34	0.41
1:B:54:GLY:O	1:B:83:ASP:OD1	2.37	0.41
1:D:125:PHE:N	1:D:126:PRO:HD3	2.35	0.41
1:B:128:LEU:O	1:B:129:LYS:C	2.57	0.41
1:C:164:MET:CE	1:C:251:LYS:HA	2.50	0.41
1:D:289:LEU:HD12	1:D:289:LEU:HA	1.72	0.41
1:C:164:MET:CE	1:C:258:TYR:CE1	3.03	0.41
1:C:283:LEU:HA	1:C:283:LEU:HD23	1.88	0.41
1:C:246:VAL:O	1:C:247:ASN:CB	2.68	0.41
1:D:40:CYS:HB2	1:D:44:TRP:CE2	2.55	0.41
1:D:155:LEU:HD23	1:D:155:LEU:HA	1.73	0.41
1:C:218:GLU:O	1:C:219:CYS:HB3	2.21	0.41
1:D:190:LEU:HA	1:D:194:LYS:O	2.20	0.41
1:C:120:ASP:HA	1:C:146:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:PHE:O	1:B:83:ASP:C	2.59	0.41
1:B:158:TRP:HE1	1:B:194:LYS:HE3	1.85	0.41
1:A:280:ASP:OD2	1:B:304:HIS:HE1	2.04	0.41
1:A:67:GLN:HE22	1:A:199:ASN:CB	2.32	0.41
1:B:70:PHE:CD1	1:B:70:PHE:C	2.93	0.41
1:B:229:ILE:HG21	1:B:229:ILE:HD13	1.84	0.41
1:B:62:VAL:HG21	1:B:98:PHE:CD2	2.56	0.41
1:A:177:VAL:CG2	1:A:179:LEU:HD11	2.51	0.41
1:C:148:PHE:O	1:C:149:ARG:CD	2.68	0.41
1:C:254:PRO:HB3	1:C:256:GLU:OE1	2.20	0.41
1:C:256:GLU:CD	1:C:256:GLU:H	2.23	0.41
1:D:268:ASP:HA	1:D:269:PRO:HD3	1.92	0.41
1:D:281:ARG:O	1:D:282:ALA:C	2.59	0.41
1:D:156:GLN:HG3	1:D:238:ILE:HG12	1.99	0.41
1:B:133:LYS:O	1:B:134:PHE:C	2.59	0.41
1:C:10:ARG:C	1:C:11:LEU:HD23	2.41	0.41
1:B:279:LEU:C	1:B:279:LEU:HD13	2.42	0.41
1:C:161:TYR:CE2	1:C:193:THR:HA	2.55	0.41
1:C:154:GLY:O	1:C:155:LEU:CB	2.67	0.41
1:C:30:LEU:C	1:C:30:LEU:HD12	2.41	0.40
1:C:19:PHE:CD2	1:C:20:MET:HE1	2.55	0.40
1:C:210:LEU:C	1:C:212:SER:N	2.72	0.40
1:A:252:HIS:CD2	1:B:293:TYR:HE2	2.35	0.40
1:C:284:LYS:O	1:C:287:ALA:HB3	2.21	0.40
1:D:138:PHE:N	1:D:138:PHE:CD1	2.89	0.40
1:A:67:GLN:NE2	1:A:198:LEU:HB3	2.26	0.40
1:A:286:LEU:HD23	1:B:275:ALA:HB3	2.03	0.40
1:D:66:ALA:CA	1:D:104:LYS:HD2	2.50	0.40
1:C:289:LEU:HD11	1:D:271:ALA:HB3	2.03	0.40
1:D:186:GLN:HE21	1:D:186:GLN:HB3	1.76	0.40
1:C:178:VAL:HA	1:C:217:TYR:O	2.21	0.40
1:D:278:ILE:O	1:D:281:ARG:HB2	2.21	0.40
1:D:5:HIS:ND1	1:D:5:HIS:O	2.54	0.40
1:D:290:PRO:HG2	1:D:293:TYR:CD2	2.53	0.40
1:D:19:PHE:HA	1:D:23:LEU:HD12	2.02	0.40
1:B:164:MET:HE3	1:B:164:MET:HA	2.04	0.40
1:A:110:LEU:HA	1:A:119:ALA:HB2	2.03	0.40
1:B:69:ASP:OD1	1:B:198:LEU:HD11	2.21	0.40
1:C:189:TYR:HH	1:C:210:LEU:HD12	1.86	0.40
1:D:228:PHE:CE2	1:D:230:PRO:HG3	2.56	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	291/338 (86%)	264 (91%)	26 (9%)	1 (0%)	46	79
1	B	306/338 (90%)	278 (91%)	27 (9%)	1 (0%)	46	79
1	C	257/338 (76%)	211 (82%)	35 (14%)	11 (4%)	3	10
1	D	306/338 (90%)	279 (91%)	25 (8%)	2 (1%)	26	62
All	All	1160/1352 (86%)	1032 (89%)	113 (10%)	15 (1%)	15	44

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	71	ILE
1	C	34	GLY
1	C	246	VAL
1	A	158	TRP
1	B	157	LEU
1	C	19	PHE
1	C	167	LEU
1	C	211	PHE
1	D	158	TRP
1	C	159	THR
1	C	247	ASN
1	C	271	ALA
1	C	278	ILE
1	C	265	GLY
1	C	269	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	210/300 (70%)	171 (81%)	39 (19%)	2	6
1	B	252/300 (84%)	213 (84%)	39 (16%)	3	10
1	C	163/300 (54%)	132 (81%)	31 (19%)	2	5
1	D	250/300 (83%)	210 (84%)	40 (16%)	3	9
All	All	875/1200 (73%)	726 (83%)	149 (17%)	2	7

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	12	GLU
1	A	14	VAL
1	A	27	ARG
1	A	30	LEU
1	A	31	VAL
1	A	47	ASP
1	A	52	VAL
1	A	76	VAL
1	A	85	LEU
1	A	86	VAL
1	A	117	ASP
1	A	155	LEU
1	A	156	GLN
1	A	157	LEU
1	A	167	LEU
1	A	168	LEU
1	A	178	VAL
1	A	186	GLN
1	A	190	LEU
1	A	199	ASN
1	A	205	LEU
1	A	208	TYR
1	A	212	SER
1	A	217	TYR
1	A	219	CYS
1	A	232	LEU
1	A	236	ASN
1	A	237	VAL
1	A	244	VAL
1	A	246	VAL

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Mol	Chain	Res	Type
1	A	255	SER
1	A	261	THR
1	A	266	ASN
1	A	278	ILE
1	A	279	LEU
1	A	286	LEU
1	A	302	VAL
1	A	303	LEU
1	B	17	GLU
1	B	18	GLN
1	B	26	GLN
1	B	27	ARG
1	B	30	LEU
1	B	31	VAL
1	B	37	LEU
1	B	46	VAL
1	B	47	ASP
1	B	60	ILE
1	B	84	GLN
1	B	88	ARG
1	B	121	ILE
1	B	127	LEU
1	B	142	GLN
1	B	155	LEU
1	B	157	LEU
1	B	164	MET
1	B	167	LEU
1	B	178	VAL
1	B	186	GLN
1	B	188	LEU
1	B	195	SER
1	B	216	ARG
1	B	220	SER
1	B	221	LEU
1	B	232	LEU
1	B	237	VAL
1	B	246	VAL
1	B	247	ASN
1	B	256	GLU
1	B	274	ARG
1	B	280	ASP
1	B	283	LEU

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Mol	Chain	Res	Type
1	B	285	THR
1	B	289	LEU
1	B	300	ARG
1	B	302	VAL
1	B	307	ASP
1	C	8	VAL
1	C	20	MET
1	C	31	VAL
1	C	35	ILE
1	C	41	THR
1	C	46	VAL
1	C	65	VAL
1	C	83	ASP
1	C	128	LEU
1	C	131	ASP
1	C	132	ILE
1	C	134	PHE
1	C	140	GLU
1	C	151	SER
1	C	152	SER
1	C	178	VAL
1	C	179	LEU
1	C	186	GLN
1	C	205	LEU
1	C	210	LEU
1	C	217	TYR
1	C	232	LEU
1	C	237	VAL
1	C	261	THR
1	C	266	ASN
1	C	268	ASP
1	C	270	THR
1	C	280	ASP
1	C	285	THR
1	C	286	LEU
1	C	302	VAL
1	D	6	LEU
1	D	26	GLN
1	D	27	ARG
1	D	35	ILE
1	D	46	VAL
1	D	47	ASP

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Mol	Chain	Res	Type
1	D	49	LEU
1	D	57	GLU
1	D	60	ILE
1	D	76	VAL
1	D	104	LYS
1	D	127	LEU
1	D	141	GLU
1	D	151	SER
1	D	155	LEU
1	D	164	MET
1	D	167	LEU
1	D	168	LEU
1	D	177	VAL
1	D	178	VAL
1	D	186	GLN
1	D	189	TYR
1	D	190	LEU
1	D	195	SER
1	D	210	LEU
1	D	212	SER
1	D	220	SER
1	D	221	LEU
1	D	232	LEU
1	D	237	VAL
1	D	246	VAL
1	D	255	SER
1	D	261	THR
1	D	270	THR
1	D	277	GLN
1	D	278	ILE
1	D	279	LEU
1	D	285	THR
1	D	289	LEU
1	D	311	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	18	GLN
1	A	22	HIS
1	A	26	GLN

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Mol	Chain	Res	Type
1	A	67	GLN
1	A	186	GLN
1	A	236	ASN
1	A	252	HIS
1	A	304	HIS
1	A	306	GLN
1	B	26	GLN
1	B	67	GLN
1	B	202	ASN
1	B	252	HIS
1	B	304	HIS
1	C	170	GLN
1	C	186	GLN
1	C	247	ASN
1	C	266	ASN
1	C	306	GLN
1	D	61	HIS
1	D	94	HIS
1	D	156	GLN
1	D	186	GLN
1	D	202	ASN
1	D	236	ASN
1	D	252	HIS
1	D	277	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AKG	B	501	2	3,9,9	1.84	1 (33%)	4,11,11	2.12	2 (50%)
3	AKG	D	501	2	3,9,9	0.14	0	4,11,11	3.09	3 (75%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AKG	B	501	2	-	0/3/9/9	0/0/0/0
3	AKG	D	501	2	-	0/3/9/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	AKG	C3-C2	3.02	1.55	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	AKG	C3-C2-C1	-3.95	112.04	121.51
3	D	501	AKG	C4-C3-C2	-3.49	104.15	112.98
3	D	501	AKG	C3-C4-C5	-3.02	107.22	112.75
3	B	501	AKG	C3-C2-C1	-2.63	115.20	121.51
3	B	501	AKG	C3-C4-C5	-2.60	107.98	112.75

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

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	299/338 (88%)	0.25	23 (7%) 16 8	60, 102, 149, 179	0
1	B	308/338 (91%)	-0.04	2 (0%) 90 86	49, 72, 99, 121	0
1	C	273/338 (80%)	0.82	50 (18%) 2 1	63, 119, 199, 214	0
1	D	308/338 (91%)	-0.05	0 100 100	44, 68, 101, 115	0
All	All	1188/1352 (87%)	0.23	75 (6%) 23 14	44, 85, 167, 214	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	58	VAL	9.1
1	C	105	TYR	7.0
1	C	248	ILE	6.3
1	C	239	SER	6.3
1	A	99	VAL	6.0
1	C	244	VAL	5.2
1	A	95	LYS	5.0
1	C	171	VAL	4.9
1	A	94	HIS	4.2
1	C	90	ALA	4.2
1	C	272	ALA	4.2
1	C	153	PRO	4.1
1	C	104	LYS	4.0
1	C	203	PRO	4.0
1	C	193	THR	3.9
1	A	200	ILE	3.8
1	C	86	VAL	3.8
1	A	96	GLU	3.7
1	A	74	ASN	3.6
1	C	208	TYR	3.6
1	C	103	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	102	ASP	3.5
1	C	201	ASP	3.4
1	C	150	ILE	3.4
1	C	311	SER	3.4
1	A	201	ASP	3.3
1	C	183	ARG	3.3
1	C	65	VAL	3.3
1	C	51	GLN	3.2
1	C	87	GLN	3.2
1	C	206	ALA	3.2
1	C	238	ILE	3.2
1	A	156	GLN	3.1
1	A	106	TYR	3.1
1	C	265	GLY	3.1
1	A	82	PHE	3.0
1	C	221	LEU	3.0
1	C	271	ALA	2.8
1	C	131	ASP	2.8
1	C	82	PHE	2.7
1	C	45	THR	2.7
1	C	188	LEU	2.6
1	A	238	ILE	2.6
1	C	44	TRP	2.6
1	A	100	SER	2.6
1	A	62	VAL	2.5
1	A	93	LYS	2.5
1	C	148	PHE	2.5
1	C	237	VAL	2.5
1	B	111	GLY	2.4
1	C	79	THR	2.4
1	C	202	ASN	2.4
1	C	270	THR	2.4
1	C	207	LYS	2.4
1	A	5	HIS	2.3
1	C	127	LEU	2.3
1	A	190	LEU	2.3
1	C	49	LEU	2.3
1	C	214	ALA	2.3
1	C	64	ALA	2.3
1	C	163	VAL	2.3
1	A	49	LEU	2.3
1	A	203	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	123	LYS	2.2
1	A	103	GLU	2.2
1	C	120	ASP	2.2
1	C	196	GLU	2.2
1	C	240	GLU	2.1
1	A	61	HIS	2.1
1	A	104	LYS	2.1
1	A	157	LEU	2.1
1	A	141	GLU	2.1
1	B	241	GLU	2.0
1	C	61	HIS	2.0
1	C	137	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	NI	A	401	1/1	0.94	0.27	1.63	101,101,101,101	0
2	NI	B	401	1/1	0.96	0.21	0.51	105,105,105,105	0
3	AKG	B	501	10/10	0.96	0.21	0.42	53,62,69,71	0
3	AKG	D	501	10/10	0.96	0.19	-0.21	49,60,68,69	0
2	NI	D	401	1/1	0.98	0.17	-0.49	68,68,68,68	0
2	NI	C	401	1/1	0.68	0.23	-	177,177,177,177	0

6.5 Other polymers [i](#)

There are no such residues in this entry.