Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 09:27 PM EDT

PDB ID	:	6XF9
Title	:	Crystal structure of KSHV ORF68
Authors	:	Didychuk, A.L.; Gates, S.N.; Martin, A.; Glaunsinger, B.
Deposited on	:	2020-06-15
Resolution	:	2.22 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:

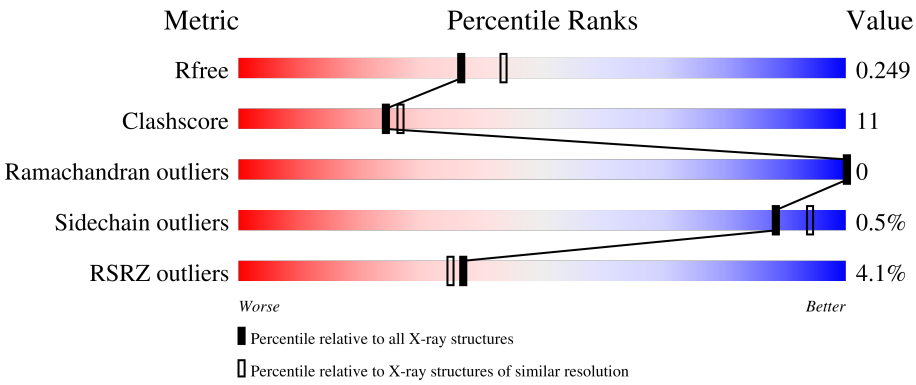
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	467	3% 72% 19% 9%
1	B	467	4% 74% 17% 9%
1	C	467	3% 72% 19% 9%
1	D	467	4% 77% 14% 9%
1	E	467	5% 72% 18% • 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16391 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 Packaging protein UL32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	425	3284	2106	555	594	29	0	1	0
1	B	424	3262	2093	554	587	28	0	1	0
1	C	424	3277	2104	555	589	29	0	1	0
1	D	426	3283	2106	556	592	29	0	1	0
1	E	425	3267	2095	550	593	29	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	3	3	3	0	0
2	B	3	3	3	0	0
2	C	3	3	3	0	0
2	D	3	3	3	0	0
2	E	3	3	3	0	0

- Molecule 3 is water.

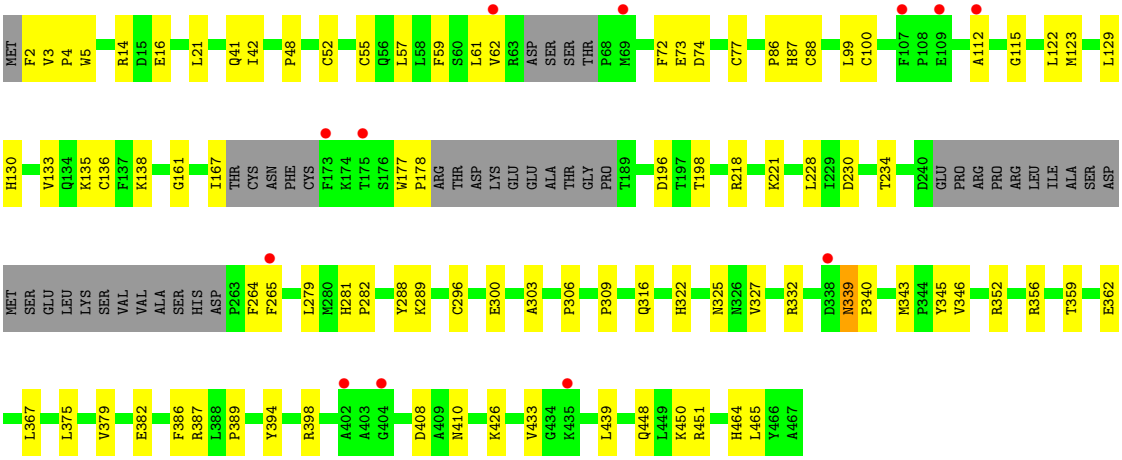
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	B	1	1	1	0	0
3	D	2	2	2	0	0

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.

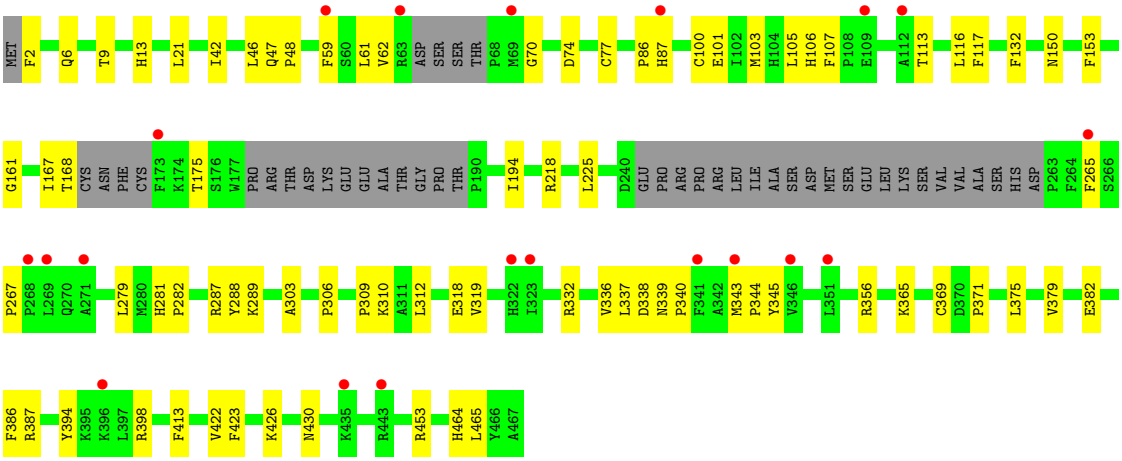
• Molecule 1: Packaging protein UL32

Chain A:



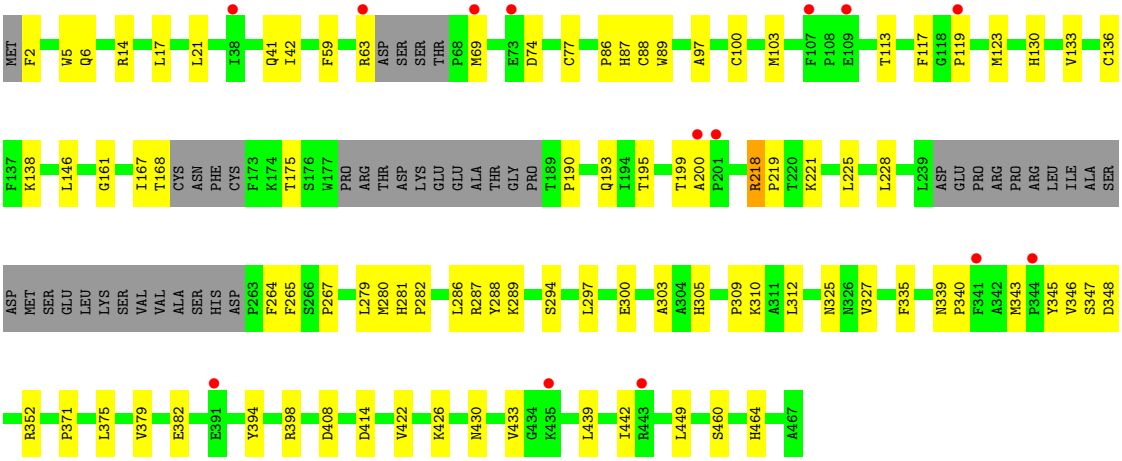
• Molecule 1: Packaging protein UL32

Chain B:



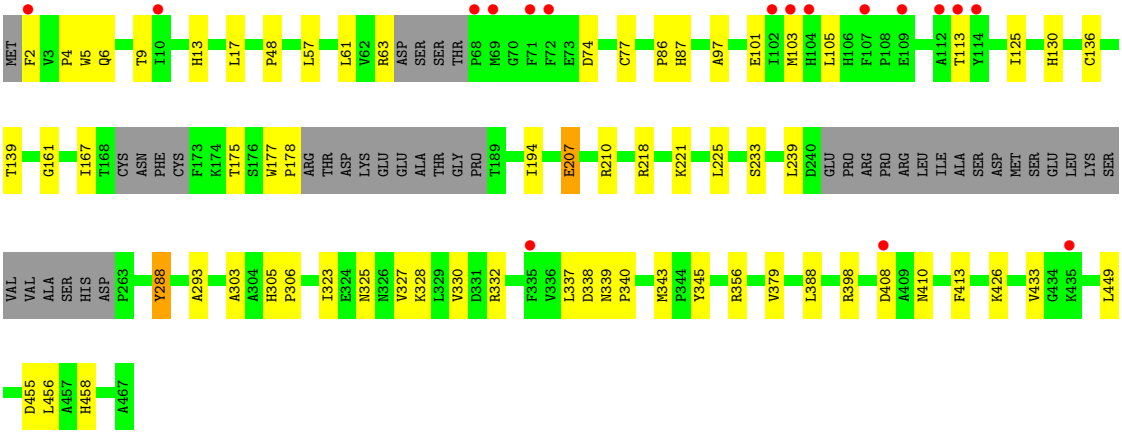
• Molecule 1: Packaging protein UL32

Chain C:



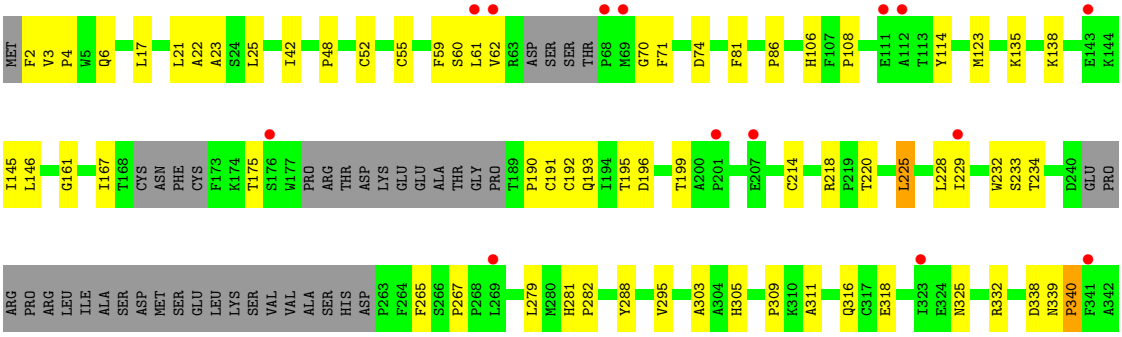
- Molecule 1: Packaging protein UL32

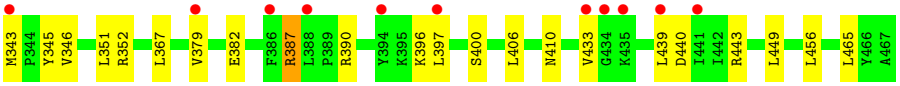
Chain D:



- Molecule 1: Packaging protein UL32

Chain E:




M343
P344
Y345
V346
L351
R352
L367
V379
E382
F386
R387
L388
P389
R390
Y394
K395
K396
L397
S400
L406
N410
V433
G434
K435
L439
D440
I441
I442
R443
L449
L456
L465
Y466
A467

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	134.99Å 224.04Å 192.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.54 – 2.22 49.54 – 2.23	Depositor EDS
% Data completeness (in resolution range)	63.4 (49.54-2.22) 65.1 (49.54-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.222 , 0.248 0.224 , 0.249	Depositor DCC
R_{free} test set	2000 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å^2)	55.7	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.010 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.013 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16391	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: ZN

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	0.72	3/3367 (0.1%)	0.76	4/4578 (0.1%)
1	B	0.68	2/3344 (0.1%)	0.72	2/4547 (0.0%)
1	C	0.68	3/3357 (0.1%)	0.72	1/4564 (0.0%)
1	D	0.66	3/3366 (0.1%)	0.70	2/4578 (0.0%)
1	E	0.68	2/3345 (0.1%)	0.72	1/4549 (0.0%)
All	All	0.68	13/16779 (0.1%)	0.72	10/22816 (0.0%)

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	A	0	1
1	E	0	1
All	All	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	340	PRO	N-CD	15.97	1.70	1.47
1	A	100	CYS	CB-SG	-7.78	1.69	1.82
1	E	288	TYR	CE1-CZ	-7.64	1.28	1.38
1	D	288	TYR	CE1-CZ	-7.16	1.29	1.38
1	C	288	TYR	CE2-CZ	-6.89	1.29	1.38
1	A	288	TYR	CE1-CZ	-6.74	1.29	1.38
1	A	99	LEU	C-N	6.11	1.48	1.34
1	B	288	TYR	CE1-CZ	-6.11	1.30	1.38
1	B	288	TYR	CE2-CZ	-5.99	1.30	1.38
1	C	288	TYR	CE1-CZ	-5.88	1.30	1.38
1	D	288	TYR	CE2-CZ	-5.37	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	288	TYR	CZ-OH	-5.04	1.29	1.37
1	D	288	TYR	CZ-OH	-5.03	1.29	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	103	MET	CB-CG-SD	-6.98	91.46	112.40
1	A	450	LYS	CA-CB-CG	-6.68	98.70	113.40
1	D	87[A]	HIS	CB-CA-C	-6.36	97.68	110.40
1	D	87[B]	HIS	CB-CA-C	-6.36	97.68	110.40
1	A	100	CYS	CA-CB-SG	6.13	125.04	114.00
1	C	200	ALA	N-CA-C	-5.90	95.06	111.00
1	A	122	LEU	CA-CB-CG	5.75	128.52	115.30
1	A	450	LYS	CB-CG-CD	5.74	126.52	111.60
1	E	225	LEU	CB-CG-CD2	-5.31	101.98	111.00
1	B	46	LEU	C-N-CA	-5.02	109.14	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	61	LEU	Mainchain
1	E	61	LEU	Mainchain

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	3284	0	3258	65	0
1	B	3262	0	3233	77	0
1	C	3277	0	3252	95	0
1	D	3283	0	3256	60	0
1	E	3267	0	3234	89	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3	0	0	0	0
3	B	1	0	0	0	0
3	D	2	0	0	0	0
All	All	16391	0	16233	359	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 11.

All (359) 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:E:340:PRO:N	1:E:340:PRO:CD	1.70	1.45
1:B:161:GLY:HA3	1:B:167:ILE:CD1	1.54	1.36
1:B:87[B]:HIS:CD2	1:B:132:PHE:HB3	1.63	1.32
1:E:379:VAL:HG13	1:E:410:ASN:ND2	1.65	1.10
1:D:161:GLY:HA3	1:D:167:ILE:HD13	1.34	1.09
1:D:175:THR:HG22	1:E:439:LEU:HD22	1.33	1.07
1:B:161:GLY:HA3	1:B:167:ILE:HD11	1.04	1.03
1:D:161:GLY:HA3	1:D:167:ILE:CD1	1.89	1.03
1:B:161:GLY:CA	1:B:167:ILE:CD1	2.40	0.99
1:C:339:ASN:OD1	1:C:340:PRO:HD2	1.65	0.97
1:B:87[B]:HIS:HD2	1:B:132:PHE:HB3	0.81	0.97
1:A:439:LEU:HD22	1:E:175:THR:HG21	1.49	0.94
1:B:87[B]:HIS:HD2	1:B:132:PHE:CB	1.78	0.94
1:E:70:GLY:C	1:E:106:HIS:CE1	2.42	0.93
1:A:167:ILE:HG12	1:A:433:VAL:HG22	1.47	0.93
1:B:161:GLY:HA3	1:B:167:ILE:HD13	1.48	0.91
1:B:161:GLY:CA	1:B:167:ILE:HD11	1.98	0.91
1:D:139:THR:OG1	1:D:408:ASP:OD1	1.90	0.89
1:E:339:ASN:OD1	1:E:340:PRO:HD2	1.72	0.89
1:B:161:GLY:CA	1:B:167:ILE:HD13	2.04	0.87
1:A:339:ASN:OD1	1:A:340:PRO:HD2	1.74	0.87
1:D:175:THR:CG2	1:E:439:LEU:HD22	2.05	0.86
1:D:63:ARG:HD3	1:E:338:ASP:OD2	1.77	0.85
1:A:41:GLN:HB3	1:A:123:MET:HE1	1.59	0.84
1:B:87[B]:HIS:CD2	1:B:132:PHE:CB	2.58	0.83
1:D:175:THR:HG22	1:E:439:LEU:CD2	2.09	0.82
1:D:175:THR:CG2	1:E:439:LEU:CD2	2.58	0.82
1:E:234:THR:HG21	1:E:265:PHE:O	1.79	0.82
1:E:309:PRO:HG2	1:E:382:GLU:HB3	1.63	0.81
1:E:193:GLN:OE1	1:E:199:THR:HG21	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:GLN:OE1	1:C:199:THR:HG23	1.83	0.79
1:B:74:ASP:OD1	1:B:398:ARG:NH2	2.15	0.78
1:B:289:LYS:NZ	1:B:464:HIS:O	2.15	0.78
1:E:21:LEU:HB3	1:E:265:PHE:CE2	2.20	0.77
1:C:87[A]:HIS:HE1	1:C:133:VAL:CG2	1.98	0.77
1:C:287:ARG:NH1	1:C:430:ASN:HB3	1.99	0.76
1:B:287:ARG:NH2	1:B:430:ASN:HB3	2.00	0.76
1:E:339:ASN:OD1	1:E:340:PRO:CD	2.34	0.76
1:D:194:ILE:CD1	1:D:413:PHE:CE2	2.70	0.75
1:A:161:GLY:HA3	1:A:167:ILE:CD1	2.16	0.75
1:C:310:LYS:HZ2	1:C:382:GLU:HG3	1.51	0.75
1:A:346:VAL:O	1:A:352:ARG:NH2	2.20	0.74
1:C:63:ARG:HG3	1:C:63:ARG:HH11	1.52	0.74
1:D:194:ILE:HD11	1:D:413:PHE:CD2	2.22	0.74
1:E:346:VAL:HG11	1:E:351:LEU:HD22	1.68	0.74
1:D:86:PRO:HG2	1:D:303:ALA:HB2	1.69	0.73
1:E:379:VAL:CG1	1:E:410:ASN:ND2	2.50	0.73
1:C:14:ARG:HD2	1:C:264:PHE:CD2	2.24	0.73
1:D:161:GLY:CA	1:D:167:ILE:HD13	2.15	0.73
1:E:190:PRO:HB2	1:E:195:THR:HG23	1.71	0.72
1:B:21:LEU:CB	1:B:265:PHE:CE1	2.73	0.72
1:B:59:PHE:CD2	1:C:335:PHE:CG	2.76	0.72
1:E:70:GLY:HA3	1:E:106:HIS:HE1	1.55	0.71
1:D:175:THR:HG21	1:E:439:LEU:HD21	1.73	0.71
1:B:86:PRO:HG2	1:B:303:ALA:HB2	1.71	0.71
1:E:21:LEU:HB3	1:E:265:PHE:CD2	2.25	0.71
1:C:193:GLN:OE1	1:C:199:THR:CG2	2.38	0.71
1:C:375:LEU:O	1:C:379:VAL:HG23	1.91	0.70
1:D:339:ASN:OD1	1:D:340:PRO:HD2	1.91	0.70
1:B:287:ARG:HH21	1:B:430:ASN:HB3	1.53	0.70
1:C:287:ARG:NH1	1:C:430:ASN:OD1	2.24	0.70
1:A:14:ARG:HB2	1:A:264:PHE:CE2	2.27	0.69
1:E:21:LEU:CB	1:E:265:PHE:CD2	2.75	0.69
1:B:59:PHE:HB2	1:C:335:PHE:CZ	2.28	0.69
1:E:218:ARG:HB2	1:E:387:ARG:HD3	1.73	0.69
1:A:161:GLY:HA3	1:A:167:ILE:HD13	1.74	0.69
1:C:394:TYR:CE2	1:C:398:ARG:HD2	2.28	0.68
1:C:87[A]:HIS:HE1	1:C:133:VAL:HG22	1.59	0.68
1:C:339:ASN:OD1	1:C:340:PRO:CD	2.39	0.68
1:C:218:ARG:HH21	1:C:219:PRO:HD3	1.59	0.67
1:C:287:ARG:NH1	1:C:430:ASN:CG	2.47	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:LEU:CB	1:E:265:PHE:CE2	2.77	0.67
1:A:177:TRP:CD2	1:A:178:PRO:HD2	2.29	0.67
1:B:21:LEU:HB2	1:B:265:PHE:CE1	2.29	0.67
1:E:167:ILE:HG13	1:E:433:VAL:HG22	1.77	0.67
1:E:346:VAL:O	1:E:352:ARG:NH2	2.28	0.67
1:E:70:GLY:O	1:E:106:HIS:CE1	2.48	0.66
1:A:309:PRO:HG2	1:A:382:GLU:HB3	1.79	0.65
1:C:346:VAL:O	1:C:352:ARG:NH2	2.30	0.64
1:A:343:MET:O	1:A:352:ARG:NH1	2.23	0.64
1:C:310:LYS:NZ	1:C:382:GLU:HG3	2.12	0.64
1:D:103:MET:HB3	1:D:113:THR:HG23	1.80	0.64
1:B:21:LEU:HB2	1:B:265:PHE:CD1	2.34	0.63
1:B:21:LEU:HB3	1:B:265:PHE:CE1	2.33	0.63
1:D:339:ASN:OD1	1:D:340:PRO:CD	2.47	0.63
1:A:177:TRP:CG	1:A:178:PRO:HD2	2.34	0.63
1:E:2:PHE:HB3	1:E:74:ASP:OD1	1.99	0.63
1:E:346:VAL:HG11	1:E:351:LEU:CD2	2.29	0.63
1:B:318:GLU:OE2	1:B:345:TYR:CE2	2.52	0.62
1:B:74:ASP:OD2	1:B:106:HIS:NE2	2.33	0.62
1:A:57:LEU:HD11	1:A:112:ALA:HB1	1.82	0.61
1:C:167:ILE:HG22	1:C:168:THR:H	1.65	0.61
1:C:287:ARG:NH1	1:C:430:ASN:CB	2.61	0.61
1:A:289:LYS:NZ	1:A:464:HIS:O	2.34	0.61
1:D:177:TRP:CD2	1:D:178:PRO:HD2	2.36	0.61
1:E:70:GLY:CA	1:E:106:HIS:HE1	2.12	0.60
1:B:59:PHE:CZ	1:C:335:PHE:HA	2.37	0.60
1:B:318:GLU:OE2	1:B:345:TYR:HE2	1.85	0.59
1:A:59:PHE:HA	1:A:62:VAL:HG22	1.83	0.59
1:D:194:ILE:CD1	1:D:413:PHE:CD2	2.85	0.59
1:C:87[A]:HIS:CD2	1:C:282:PRO:HG3	2.38	0.59
1:A:228:LEU:HD11	1:A:300:GLU:HB3	1.85	0.58
1:A:465:LEU:HD21	1:E:48:PRO:HB2	1.85	0.58
1:B:21:LEU:CB	1:B:265:PHE:CD1	2.86	0.58
1:C:63:ARG:NE	1:D:338:ASP:OD2	2.36	0.58
1:D:161:GLY:HA3	1:D:167:ILE:HD11	1.82	0.58
1:E:21:LEU:HB2	1:E:265:PHE:CD2	2.38	0.58
1:D:175:THR:HG21	1:E:439:LEU:CD2	2.26	0.58
1:D:77:CYS:SG	1:D:398:ARG:HG2	2.44	0.58
1:E:108:PRO:O	1:E:114:TYR:OH	2.07	0.58
1:E:379:VAL:HG13	1:E:410:ASN:HD22	1.60	0.58
1:C:87[A]:HIS:HE1	1:C:133:VAL:HG23	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:PHE:HB3	1:A:74:ASP:OD1	2.03	0.57
1:E:346:VAL:CG1	1:E:351:LEU:HD22	2.34	0.57
1:B:59:PHE:CD2	1:C:335:PHE:CD1	2.92	0.57
1:D:177:TRP:CG	1:D:178:PRO:HD2	2.39	0.57
1:A:74:ASP:OD1	1:A:398:ARG:NH2	2.38	0.57
1:B:343:MET:N	1:B:344:PRO:HD3	2.19	0.57
1:D:194:ILE:HD12	1:D:413:PHE:CE2	2.39	0.57
1:E:23:ALA:HB1	1:E:123:MET:CE	2.34	0.57
1:E:225:LEU:HD12	1:E:305:HIS:HD2	1.70	0.57
1:A:230:ASP:O	1:A:234:THR:HG23	2.04	0.56
1:B:6:GLN:HB2	1:B:9:THR:OG1	2.06	0.56
1:B:287:ARG:HH21	1:B:430:ASN:CB	2.18	0.56
1:D:175:THR:CG2	1:E:439:LEU:HD21	2.30	0.56
1:E:191:CYS:SG	1:E:195:THR:HG21	2.45	0.56
1:C:77:CYS:SG	1:C:398:ARG:HG2	2.46	0.55
1:C:86:PRO:HG2	1:C:303:ALA:HB2	1.87	0.55
1:B:281:HIS:CG	1:B:282:PRO:HD2	2.41	0.55
1:A:281:HIS:CG	1:A:282:PRO:HD2	2.41	0.55
1:B:59:PHE:CE2	1:C:335:PHE:CB	2.90	0.55
1:C:289:LYS:NZ	1:C:464:HIS:O	2.37	0.55
1:E:86:PRO:HG2	1:E:303:ALA:HB2	1.89	0.55
1:C:69:MET:HG3	1:C:69:MET:O	2.06	0.55
1:D:167:ILE:HG13	1:D:433:VAL:HG22	1.89	0.55
1:C:63:ARG:HG3	1:C:63:ARG:NH1	2.20	0.54
1:E:4:PRO:HB2	1:E:81:PHE:CD2	2.43	0.54
1:A:4:PRO:O	1:A:221:LYS:NZ	2.39	0.54
1:C:21:LEU:CB	1:C:265:PHE:CE1	2.90	0.54
1:E:70:GLY:CA	1:E:106:HIS:CE1	2.89	0.54
1:C:167:ILE:HG13	1:C:433:VAL:HG22	1.90	0.54
1:C:63:ARG:HH11	1:C:63:ARG:CG	2.19	0.54
1:C:265:PHE:HE2	1:C:267:PRO:HB3	1.73	0.54
1:C:225:LEU:HD23	1:C:228:LEU:HD23	1.89	0.54
1:D:103:MET:CB	1:D:113:THR:HG23	2.38	0.54
1:C:371:PRO:HB2	1:C:422:VAL:HG22	1.90	0.53
1:E:42:ILE:CD1	1:E:279:LEU:HD13	2.37	0.53
1:C:2:PHE:HB3	1:C:74:ASP:OD1	2.08	0.53
1:A:59:PHE:HE2	1:B:338:ASP:OD2	1.92	0.53
1:A:73:GLU:OE1	1:A:398:ARG:NH1	2.42	0.53
1:E:325:ASN:O	1:E:332:ARG:NH2	2.42	0.53
1:B:59:PHE:CE2	1:C:335:PHE:HA	2.44	0.53
1:E:316:GLN:HB2	1:E:367:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ILE:HG12	1:A:433:VAL:CG2	2.30	0.53
1:B:101:GLU:O	1:B:105:LEU:HD13	2.08	0.53
1:D:48:PRO:HB2	1:E:465:LEU:HD21	1.91	0.53
1:D:103:MET:HE2	1:D:113:THR:HA	1.90	0.53
1:A:218:ARG:O	1:A:387:ARG:NH1	2.43	0.52
1:B:70:GLY:O	1:B:74:ASP:OD2	2.27	0.52
1:E:281:HIS:ND1	1:E:282:PRO:HD2	2.23	0.52
1:A:59:PHE:O	1:A:62:VAL:HG22	2.09	0.52
1:C:309:PRO:HG2	1:C:382:GLU:HB3	1.90	0.52
1:E:343:MET:HG2	1:E:345:TYR:OH	2.09	0.52
1:C:281:HIS:CG	1:C:282:PRO:HD2	2.45	0.52
1:C:286:LEU:HA	1:C:294:SER:OG	2.10	0.52
1:D:2:PHE:HB3	1:D:74:ASP:OD1	2.10	0.52
1:C:21:LEU:HB2	1:C:265:PHE:CE1	2.45	0.51
1:C:42:ILE:CD1	1:C:279:LEU:HD13	2.39	0.51
1:B:318:GLU:OE2	1:B:345:TYR:OH	2.20	0.51
1:C:41:GLN:NE2	1:C:123:MET:HG3	2.26	0.51
1:C:167:ILE:HG22	1:C:168:THR:N	2.25	0.51
1:C:63:ARG:NH1	1:C:63:ARG:CG	2.73	0.51
1:E:225:LEU:HD12	1:E:305:HIS:CD2	2.46	0.51
1:A:352:ARG:O	1:A:356:ARG:HG3	2.11	0.50
1:B:168:THR:HG23	1:B:168:THR:O	2.12	0.50
1:A:3:VAL:HG21	1:A:389:PRO:HG3	1.92	0.49
1:B:194:ILE:HD11	1:B:413:PHE:CD2	2.47	0.49
1:E:339:ASN:OD1	1:E:340:PRO:N	2.46	0.49
1:A:21:LEU:HB2	1:A:265:PHE:CD1	2.47	0.49
1:C:14:ARG:HD2	1:C:264:PHE:CE2	2.47	0.49
1:A:167:ILE:CG1	1:A:433:VAL:HG22	2.33	0.49
1:A:306:PRO:HG3	1:A:386:PHE:CG	2.46	0.49
1:B:309:PRO:HG2	1:B:382:GLU:HB3	1.95	0.49
1:C:343:MET:HG2	1:C:345:TYR:OH	2.13	0.49
1:C:218:ARG:NH2	1:C:219:PRO:HD3	2.25	0.49
1:E:440:ASP:OD1	1:E:443:ARG:NH1	2.46	0.49
1:D:218:ARG:HD3	1:D:388:LEU:O	2.13	0.49
1:B:306:PRO:HG3	1:B:386:PHE:CD1	2.48	0.49
1:E:70:GLY:O	1:E:106:HIS:NE2	2.45	0.49
1:D:6:GLN:HB2	1:D:9:THR:OG1	2.13	0.48
1:A:21:LEU:HB2	1:A:265:PHE:CE1	2.48	0.48
1:E:449:LEU:HD13	1:E:456:LEU:HD12	1.95	0.48
1:E:397:LEU:HD11	1:E:406:LEU:HD22	1.95	0.48
1:B:59:PHE:CE2	1:C:335:PHE:HB3	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:ALA:HB1	1:E:123:MET:HE3	1.96	0.48
1:E:196:ASP:OD2	1:E:199:THR:HG23	2.14	0.48
1:D:57:LEU:O	1:D:61:LEU:HG	2.14	0.48
1:D:328:LYS:HG3	1:D:330:VAL:HG22	1.95	0.48
1:B:194:ILE:O	1:B:453:ARG:NH2	2.47	0.48
1:A:316:GLN:HB2	1:A:367:LEU:HD22	1.96	0.47
1:A:281:HIS:CD2	1:A:282:PRO:HD2	2.49	0.47
1:A:306:PRO:HG3	1:A:386:PHE:CD1	2.49	0.47
1:C:167:ILE:CG1	1:C:433:VAL:HG22	2.44	0.47
1:E:59:PHE:HA	1:E:62:VAL:HG22	1.95	0.47
1:C:88:CYS:HB2	1:C:300:GLU:OE2	2.15	0.47
1:B:310:LYS:NZ	1:B:382:GLU:HG3	2.30	0.47
1:D:225:LEU:HD23	1:D:225:LEU:HA	1.72	0.47
1:A:87[A]:HIS:HE1	1:A:133:VAL:CG2	2.28	0.47
1:C:225:LEU:HD12	1:C:305:HIS:HD2	1.79	0.47
1:A:343:MET:HG2	1:A:345:TYR:OH	2.14	0.47
1:E:25:LEU:HD11	1:E:265:PHE:HZ	1.80	0.47
1:E:146:LEU:HA	1:E:146:LEU:HD23	1.72	0.47
1:B:375:LEU:O	1:B:379:VAL:HG23	2.15	0.47
1:B:218:ARG:HB2	1:B:387:ARG:HD2	1.97	0.47
1:E:167:ILE:CG1	1:E:433:VAL:HG22	2.44	0.47
1:E:214:CYS:O	1:E:390:ARG:NH2	2.47	0.47
1:C:408:ASP:OD1	1:C:408:ASP:N	2.48	0.46
1:C:21:LEU:HB3	1:C:265:PHE:CE1	2.51	0.46
1:C:87[A]:HIS:CE1	1:C:133:VAL:CG2	2.90	0.46
1:A:325:ASN:O	1:A:332:ARG:NH2	2.48	0.46
1:A:379:VAL:HG13	1:A:410:ASN:ND2	2.30	0.46
1:D:455:ASP:O	1:D:456:LEU:HD23	2.16	0.46
1:A:281:HIS:CE1	1:A:282:PRO:HD2	2.50	0.46
1:C:14:ARG:NH1	1:C:264:PHE:HA	2.31	0.46
1:C:175:THR:HG22	1:D:458:HIS:HE1	1.80	0.46
1:B:338:ASP:O	1:B:339:ASN:C	2.53	0.46
1:C:89:TRP:HD1	1:C:280:MET:HB2	1.81	0.46
1:C:119:PRO:HA	1:C:123:MET:CE	2.46	0.46
1:C:218:ARG:N	1:C:218:ARG:HD2	2.25	0.46
1:E:229:ILE:O	1:E:233:SER:OG	2.29	0.46
1:B:175:THR:HG21	1:C:460:SER:HB3	1.98	0.46
1:C:100:CYS:HG	1:C:117:PHE:HE2	1.64	0.46
1:D:86:PRO:CG	1:D:303:ALA:HB2	2.44	0.46
1:E:17:LEU:HD23	1:E:17:LEU:HA	1.74	0.46
1:C:21:LEU:HB2	1:C:265:PHE:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:CD1	1:A:300:GLU:HB3	2.46	0.45
1:C:6:GLN:HG2	1:C:221:LYS:HD2	1.97	0.45
1:A:129:LEU:HA	1:A:133:VAL:HB	1.98	0.45
1:B:13:HIS:CD2	1:B:100:CYS:HB3	2.51	0.45
1:D:449:LEU:HD23	1:D:449:LEU:HA	1.75	0.45
1:E:228:LEU:HD12	1:E:232:TRP:CD1	2.52	0.45
1:A:325:ASN:HB2	1:A:327:VAL:HG23	1.97	0.45
1:C:347:SER:OG	1:C:348:ASP:N	2.50	0.45
1:D:130:HIS:CE1	1:D:136:CYS:HB2	2.51	0.45
1:B:42:ILE:CD1	1:B:279:LEU:HD13	2.47	0.45
1:E:3:VAL:HA	1:E:4:PRO:HD3	1.75	0.45
1:A:135:LYS:HD3	1:A:138:LYS:HD2	1.97	0.45
1:A:448:GLN:OE1	1:A:451:ARG:NH1	2.48	0.45
1:B:77:CYS:SG	1:B:398:ARG:HG2	2.57	0.45
1:B:87[A]:HIS:CD2	1:B:423:PHE:HZ	2.35	0.45
1:B:340:PRO:HA	1:B:356:ARG:HH22	1.82	0.45
1:C:87[A]:HIS:CE1	1:C:133:VAL:HG23	2.49	0.45
1:B:59:PHE:CE2	1:C:335:PHE:CG	3.05	0.45
1:D:323:ILE:HG23	1:D:325:ASN:OD1	2.17	0.45
1:E:265:PHE:HE1	1:E:267:PRO:HB3	1.81	0.45
1:E:318:GLU:OE2	1:E:345:TYR:HE2	2.00	0.45
1:C:325:ASN:HB2	1:C:327:VAL:HG23	1.99	0.44
1:D:288:TYR:CE2	1:D:293:ALA:HB2	2.52	0.44
1:C:426:LYS:HA	1:C:426:LYS:HD2	1.83	0.44
1:B:394:TYR:O	1:B:398:ARG:HG3	2.18	0.44
1:D:167:ILE:CG1	1:D:433:VAL:HG22	2.47	0.44
1:D:379:VAL:HG13	1:D:410:ASN:ND2	2.32	0.44
1:E:318:GLU:OE2	1:E:345:TYR:CE2	2.70	0.44
1:A:21:LEU:CB	1:A:265:PHE:CE1	3.00	0.44
1:B:225:LEU:HD23	1:B:225:LEU:HA	1.69	0.44
1:C:190:PRO:HB3	1:C:195:THR:O	2.18	0.44
1:E:25:LEU:HD11	1:E:265:PHE:CZ	2.52	0.44
1:C:218:ARG:HD2	1:C:218:ARG:HA	1.53	0.44
1:E:52:CYS:HB3	1:E:55:CYS:HB2	2.00	0.44
1:C:312:LEU:HA	1:C:312:LEU:HD23	1.81	0.44
1:D:103:MET:HB3	1:D:113:THR:CG2	2.47	0.44
1:D:305:HIS:HA	1:D:306:PRO:HD3	1.87	0.44
1:A:3:VAL:HG22	1:A:394:TYR:CZ	2.53	0.44
1:A:72:PHE:N	1:A:72:PHE:CD1	2.83	0.44
1:B:21:LEU:HB3	1:B:265:PHE:CD1	2.53	0.44
1:B:107:PHE:O	1:B:113:THR:OG1	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:MET:CE	1:B:356:ARG:HG3	2.48	0.43
1:E:22:ALA:N	1:E:265:PHE:HE2	2.16	0.43
1:E:145:ILE:HD13	1:E:145:ILE:HA	1.80	0.43
1:D:17:LEU:HD11	1:D:97:ALA:HB2	1.99	0.43
1:E:311:ALA:HB2	1:E:346:VAL:HG22	2.00	0.43
1:A:87[A]:HIS:HE1	1:A:133:VAL:HG23	1.82	0.43
1:A:359:THR:OG1	1:A:362:GLU:HG3	2.19	0.43
1:B:2:PHE:HB3	1:B:74:ASP:OD1	2.18	0.43
1:D:101:GLU:O	1:D:105:LEU:HD13	2.18	0.43
1:D:327:VAL:HG12	1:D:332:ARG:HG3	2.00	0.43
1:C:130:HIS:CE1	1:C:136:CYS:HB2	2.53	0.43
1:D:343:MET:HG2	1:D:345:TYR:OH	2.18	0.43
1:A:196:ASP:OD1	1:A:198:THR:HB	2.18	0.43
1:B:306:PRO:HG3	1:B:386:PHE:CG	2.54	0.43
1:B:161:GLY:HA2	1:B:167:ILE:HD13	1.93	0.43
1:D:13:HIS:HE1	1:D:101:GLU:OE1	2.01	0.43
1:D:207:GLU:OE2	1:D:210:ARG:NH2	2.46	0.43
1:C:59:PHE:HE2	1:D:338:ASP:OD2	2.02	0.42
1:D:4:PRO:O	1:D:221:LYS:NZ	2.51	0.42
1:B:59:PHE:CE2	1:C:335:PHE:CA	3.02	0.42
1:C:87[A]:HIS:CE1	1:C:133:VAL:HG22	2.45	0.42
1:C:218:ARG:NH2	1:C:219:PRO:CD	2.83	0.42
1:C:449:LEU:HA	1:C:449:LEU:HD23	1.76	0.42
1:E:396:LYS:NZ	1:E:400:SER:HB2	2.34	0.42
1:A:77:CYS:SG	1:A:398:ARG:HG2	2.60	0.42
1:C:439:LEU:HD23	1:C:442:ILE:HD12	2.01	0.42
1:A:343:MET:C	1:A:352:ARG:HH12	2.14	0.42
1:A:375:LEU:O	1:A:379:VAL:HG23	2.20	0.42
1:B:365:LYS:HA	1:B:369:CYS:HB2	2.01	0.42
1:C:17:LEU:HD11	1:C:97:ALA:HB2	2.01	0.42
1:C:343:MET:HA	1:C:345:TYR:CE1	2.55	0.42
1:A:296:CYS:O	1:A:300:GLU:HG2	2.20	0.42
1:C:21:LEU:CB	1:C:265:PHE:CD1	3.02	0.42
1:C:103:MET:HB3	1:C:113:THR:HG23	2.00	0.42
1:E:192:CYS:H	1:E:195:THR:CG2	2.32	0.42
1:D:426:LYS:HA	1:D:426:LYS:HD2	1.79	0.42
1:C:218:ARG:HA	1:C:219:PRO:HD3	1.37	0.42
1:E:135:LYS:HD3	1:E:138:LYS:HD2	2.02	0.42
1:E:397:LEU:CD1	1:E:406:LEU:HD22	2.50	0.42
1:A:16:GLU:OE2	1:A:115:GLY:N	2.53	0.42
1:A:88:CYS:HB2	1:A:300:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:VAL:HG12	1:B:337:LEU:HD23	2.02	0.42
1:E:225:LEU:HA	1:E:225:LEU:HD23	1.87	0.42
1:A:42:ILE:CD1	1:A:279:LEU:HD13	2.49	0.41
1:C:161:GLY:HA3	1:C:167:ILE:HD13	2.02	0.41
1:B:116:LEU:HD23	1:B:117:PHE:CZ	2.55	0.41
1:B:312:LEU:HA	1:B:312:LEU:HD23	1.81	0.41
1:E:449:LEU:HD23	1:E:449:LEU:HA	1.87	0.41
1:C:63:ARG:CD	1:D:338:ASP:OD2	2.69	0.41
1:E:281:HIS:CG	1:E:282:PRO:HD2	2.55	0.41
1:B:371:PRO:HB2	1:B:422:VAL:HG22	2.02	0.41
1:C:193:GLN:OE1	1:C:199:THR:HG21	2.18	0.41
1:D:233:SER:HB3	1:D:239:LEU:HD12	2.01	0.41
1:A:86:PRO:HG2	1:A:303:ALA:HB2	2.02	0.41
1:A:426:LYS:HA	1:A:426:LYS:HD2	1.91	0.41
1:B:265:PHE:HE2	1:B:267:PRO:HB3	1.85	0.41
1:E:220:THR:HG22	1:E:387:ARG:HH12	1.85	0.41
1:E:281:HIS:CD2	1:E:295:VAL:HG13	2.55	0.41
1:B:426:LYS:HA	1:B:426:LYS:HD2	1.85	0.41
1:C:146:LEU:HA	1:C:146:LEU:HD23	1.71	0.41
1:E:3:VAL:O	1:E:6:GLN:HG3	2.20	0.41
1:E:161:GLY:HA3	1:E:167:ILE:HD13	2.02	0.41
1:B:61:LEU:HB3	1:B:107:PHE:CE2	2.56	0.41
1:C:218:ARG:HH21	1:C:218:ARG:HA	1.86	0.41
1:E:71:PHE:N	1:E:106:HIS:CE1	2.88	0.41
1:A:408:ASP:OD1	1:A:408:ASP:N	2.54	0.41
1:B:62:VAL:O	1:B:62:VAL:HG23	2.20	0.41
1:B:150:ASN:O	1:B:153:PHE:HB3	2.21	0.41
1:B:319:VAL:O	1:B:332:ARG:HD3	2.20	0.41
1:C:161:GLY:HA3	1:C:167:ILE:CD1	2.51	0.41
1:D:325:ASN:O	1:D:332:ARG:NH2	2.53	0.41
1:E:192:CYS:H	1:E:195:THR:HG22	1.86	0.41
1:E:193:GLN:OE1	1:E:199:THR:CG2	2.49	0.41
1:D:125:ILE:HD12	1:D:125:ILE:HA	1.86	0.40
1:E:265:PHE:CE1	1:E:267:PRO:HB3	2.55	0.40
1:A:48:PRO:HB2	1:B:465:LEU:HD21	2.03	0.40
1:C:138:LYS:NZ	1:C:414:ASP:OD2	2.40	0.40
1:A:52:CYS:HB3	1:A:55:CYS:HB2	2.04	0.40
1:B:47:GLN:HA	1:B:48:PRO:HD3	1.94	0.40
1:A:130:HIS:CE1	1:A:136:CYS:HB2	2.57	0.40
1:B:318:GLU:OE2	1:B:345:TYR:CZ	2.74	0.40
1:C:297:LEU:HD12	1:C:297:LEU:HA	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:LEU:HD22	1:D:356:ARG:HG2	2.03	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	416/467 (89%)	409 (98%)	7 (2%)	0	100	100
1	B	415/467 (89%)	407 (98%)	8 (2%)	0	100	100
1	C	415/467 (89%)	403 (97%)	12 (3%)	0	100	100
1	D	417/467 (89%)	411 (99%)	6 (1%)	0	100	100
1	E	415/467 (89%)	408 (98%)	7 (2%)	0	100	100
All	All	2078/2335 (89%)	2038 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	361/407 (89%)	358 (99%)	3 (1%)	81	89
1	B	356/407 (88%)	356 (100%)	0	100	100
1	C	359/407 (88%)	357 (99%)	2 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	360/407 (88%)	358 (99%)	2 (1%)	86	92
1	E	358/407 (88%)	356 (99%)	2 (1%)	86	92
All	All	1794/2035 (88%)	1785 (100%)	9 (0%)	88	94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	TRP
1	A	322	HIS
1	A	339	ASN
1	C	5	TRP
1	C	218	ARG
1	D	5	TRP
1	D	207	GLU
1	E	60	SER
1	E	387	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 15 ligands modelled in this entry, 15 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	425/467 (91%)	0.18	12 (2%)	53	51	35, 55, 87, 141	0
1	B	424/467 (90%)	0.26	20 (4%)	31	29	32, 58, 95, 144	0
1	C	424/467 (90%)	0.18	14 (3%)	46	44	36, 59, 97, 155	0
1	D	426/467 (91%)	0.25	17 (3%)	38	36	32, 58, 92, 163	0
1	E	425/467 (91%)	0.39	25 (5%)	22	21	42, 65, 108, 165	0
All	All	2124/2335 (90%)	0.25	88 (4%)	37	35	32, 59, 98, 165	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	69	MET	8.8
1	C	201	PRO	5.7
1	C	200	ALA	5.6
1	D	112	ALA	5.4
1	E	69	MET	5.2
1	D	113	THR	4.8
1	B	112	ALA	4.8
1	C	69	MET	4.4
1	D	114	TYR	4.2
1	D	107	PHE	4.2
1	E	434	GLY	4.0
1	E	269	LEU	4.0
1	E	201	PRO	3.9
1	A	265	PHE	3.8
1	B	87[A]	HIS	3.8
1	B	346	VAL	3.8
1	B	69	MET	3.8
1	E	435	LYS	3.6
1	D	103	MET	3.4
1	E	441	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	394	TYR	3.4
1	C	107	PHE	3.3
1	B	63	ARG	3.2
1	D	68	PRO	3.2
1	E	343	MET	3.2
1	A	69	MET	3.1
1	D	109	GLU	3.1
1	A	112	ALA	3.0
1	D	10	ILE	3.0
1	B	269	LEU	3.0
1	B	265	PHE	3.0
1	D	71	PHE	2.9
1	B	109	GLU	2.9
1	E	388	LEU	2.9
1	D	104	HIS	2.9
1	D	408	ASP	2.9
1	B	396	LYS	2.9
1	E	61	LEU	2.8
1	A	173	PHE	2.7
1	E	207	GLU	2.7
1	B	173	PHE	2.7
1	E	386	PHE	2.7
1	A	109	GLU	2.7
1	B	322	HIS	2.7
1	D	72	PHE	2.6
1	B	59	PHE	2.6
1	B	341	PHE	2.6
1	E	112	ALA	2.6
1	E	439	LEU	2.6
1	A	62	VAL	2.6
1	A	107	PHE	2.6
1	B	435	LYS	2.5
1	D	435	LYS	2.5
1	B	323	ILE	2.5
1	C	38	ILE	2.5
1	A	402	ALA	2.4
1	E	62	VAL	2.4
1	C	435	LYS	2.3
1	E	341	PHE	2.3
1	B	351	LEU	2.3
1	E	143	GLU	2.3
1	E	176	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	102	ILE	2.3
1	E	68	PRO	2.3
1	B	271	ALA	2.3
1	A	404	GLY	2.3
1	A	175	THR	2.2
1	C	119	PRO	2.2
1	C	344	PRO	2.2
1	E	397	LEU	2.2
1	E	323	ILE	2.2
1	C	391	GLU	2.2
1	C	341	PHE	2.2
1	E	111	GLU	2.1
1	E	229	ILE	2.1
1	A	338	ASP	2.1
1	D	335	PHE	2.1
1	C	109	GLU	2.1
1	C	63	ARG	2.1
1	C	443	ARG	2.1
1	E	379	VAL	2.1
1	E	433	VAL	2.1
1	B	268	PRO	2.1
1	C	73	GLU	2.0
1	B	443	ARG	2.0
1	D	2	PHE	2.0
1	B	343	MET	2.0
1	A	435	LYS	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	ZN	A	501	1/1	0.97	0.14	49,49,49,49	0
2	ZN	D	503	1/1	0.97	0.14	50,50,50,50	0
2	ZN	E	503	1/1	0.97	0.13	54,54,54,54	0
2	ZN	B	501	1/1	0.98	0.14	48,48,48,48	0
2	ZN	A	502	1/1	0.98	0.15	42,42,42,42	0
2	ZN	E	501	1/1	0.98	0.13	50,50,50,50	0
2	ZN	E	502	1/1	0.98	0.11	51,51,51,51	0
2	ZN	A	503	1/1	0.98	0.14	45,45,45,45	0
2	ZN	B	502	1/1	0.99	0.17	46,46,46,46	0
2	ZN	B	503	1/1	0.99	0.14	47,47,47,47	0
2	ZN	C	501	1/1	0.99	0.14	46,46,46,46	0
2	ZN	C	502	1/1	0.99	0.13	46,46,46,46	0
2	ZN	D	501	1/1	1.00	0.15	50,50,50,50	0
2	ZN	D	502	1/1	1.00	0.15	47,47,47,47	0
2	ZN	C	503	1/1	1.00	0.15	49,49,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.