Full wwPDB X-ray Structure Validation Report (i)

Mar 13, 2023 – 03:16 pm GMT

PDB ID	:	8CIA
Title	:	Crystal structure of the kelch domain of human KLHL20
Authors	:	Sweeney, M.N.; Bradshaw, W.J.; Chen, Z.; Bullock, A.N.
Deposited on	:	2023-02-09
Resolution	:	3.72 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 (i)) were used in the production of this report:

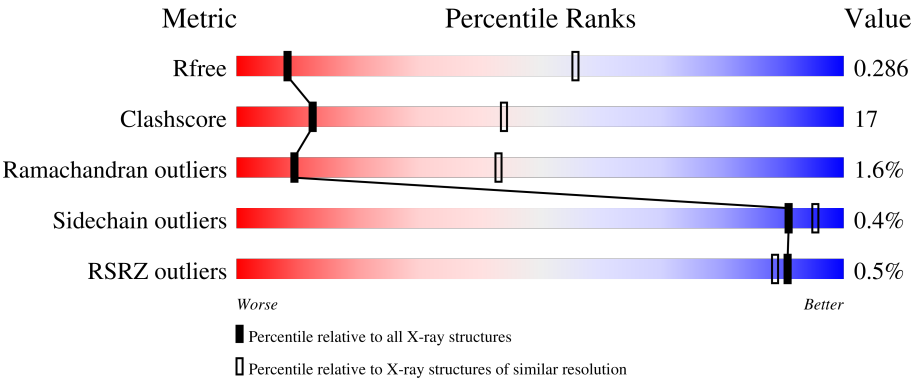
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 3.72 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	1089 (3.90-3.54)
Clashscore	141614	1012 (3.88-3.56)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)

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	307	53% 36% · 7%
1	C	307	65% 28% · 6%
1	D	307	% 57% 35% · 7%
2	B	307	% 64% 29% 7%
3	E	307	62% 31% · 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10843 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 Kelch-like protein 20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2164	1347	391	415	11			
1	C	288	Total	C	N	O	S	0	0	0
			2180	1357	394	418	11			
1	D	285	Total	C	N	O	S	0	0	0
			2164	1347	391	415	11			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	299	GLY	GLU	conflict	UNP Q9Y2M5
A	300	HIS	ARG	conflict	UNP Q9Y2M5
A	301	MET	PRO	conflict	UNP Q9Y2M5
A	302	SER	LEU	conflict	UNP Q9Y2M5
A	316	ALA	CYS	engineered mutation	UNP Q9Y2M5
A	327	ALA	CYS	engineered mutation	UNP Q9Y2M5
A	402	ALA	CYS	engineered mutation	UNP Q9Y2M5
A	426	ALA	CYS	engineered mutation	UNP Q9Y2M5
A	604	ALA	CYS	engineered mutation	UNP Q9Y2M5
C	299	GLY	GLU	conflict	UNP Q9Y2M5
C	300	HIS	ARG	conflict	UNP Q9Y2M5
C	301	MET	PRO	conflict	UNP Q9Y2M5
C	302	SER	LEU	conflict	UNP Q9Y2M5
C	316	ALA	CYS	engineered mutation	UNP Q9Y2M5
C	327	ALA	CYS	engineered mutation	UNP Q9Y2M5
C	402	ALA	CYS	engineered mutation	UNP Q9Y2M5
C	426	ALA	CYS	engineered mutation	UNP Q9Y2M5
C	604	ALA	CYS	engineered mutation	UNP Q9Y2M5
D	299	GLY	GLU	conflict	UNP Q9Y2M5
D	300	HIS	ARG	conflict	UNP Q9Y2M5
D	301	MET	PRO	conflict	UNP Q9Y2M5
D	302	SER	LEU	conflict	UNP Q9Y2M5
D	316	ALA	CYS	engineered mutation	UNP Q9Y2M5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	327	ALA	CYS	engineered mutation	UNP Q9Y2M5
D	402	ALA	CYS	engineered mutation	UNP Q9Y2M5
D	426	ALA	CYS	engineered mutation	UNP Q9Y2M5
D	604	ALA	CYS	engineered mutation	UNP Q9Y2M5

- Molecule 2 is a protein called Kelch like family member 20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	285	Total	C	N	O	S	0	0	0
			2164	1348	392	413	11			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	299	GLY	-	expression tag	UNP A0A673T7L2
B	300	HIS	-	expression tag	UNP A0A673T7L2
B	301	MET	-	expression tag	UNP A0A673T7L2
B	302	SER	-	expression tag	UNP A0A673T7L2
B	316	ALA	CYS	conflict	UNP A0A673T7L2
B	327	ALA	CYS	conflict	UNP A0A673T7L2
B	402	ALA	CYS	conflict	UNP A0A673T7L2
B	426	ALA	CYS	conflict	UNP A0A673T7L2
B	437	LYS	GLU	conflict	UNP A0A673T7L2
B	604	ALA	CYS	conflict	UNP A0A673T7L2

- Molecule 3 is a protein called Kelch like family member 20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	286	Total	C	N	O	S	0	0	0
			2171	1351	391	418	11			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	299	GLY	-	expression tag	UNP A0A452F0N4
E	300	HIS	-	expression tag	UNP A0A452F0N4
E	301	MET	-	expression tag	UNP A0A452F0N4
E	302	SER	-	expression tag	UNP A0A452F0N4
E	316	ALA	CYS	conflict	UNP A0A452F0N4
E	327	ALA	CYS	conflict	UNP A0A452F0N4
E	402	ALA	CYS	conflict	UNP A0A452F0N4
E	426	ALA	CYS	conflict	UNP A0A452F0N4

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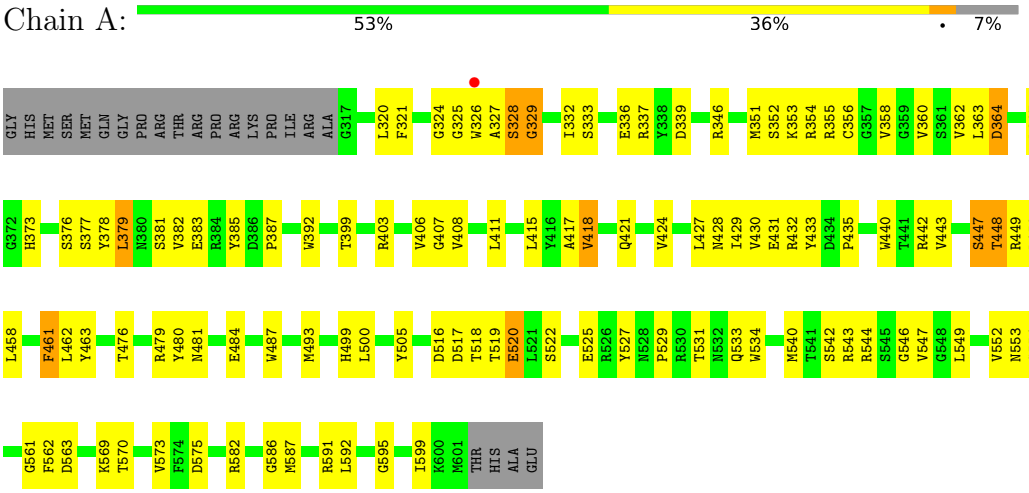
Chain	Residue	Modelled	Actual	Comment	Reference
E	483	GLU	GLN	conflict	UNP A0A452F0N4
E	604	ALA	CYS	conflict	UNP A0A452F0N4

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.

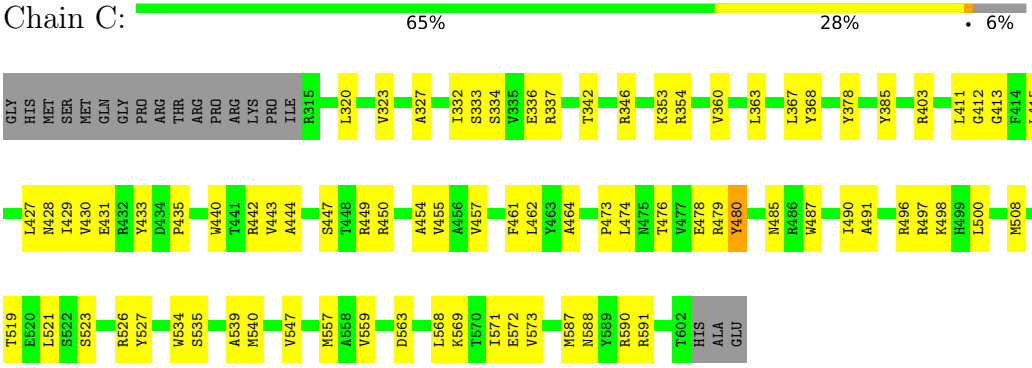
• Molecule 1: Kelch-like protein 20

Chain A:



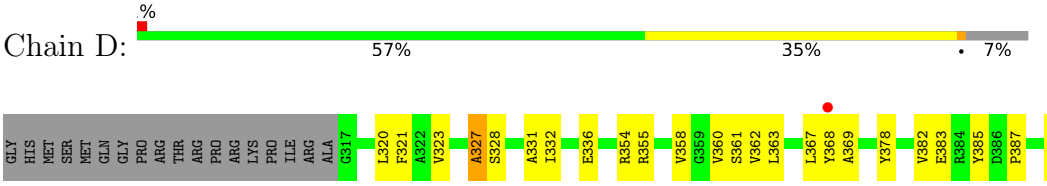
• Molecule 1: Kelch-like protein 20

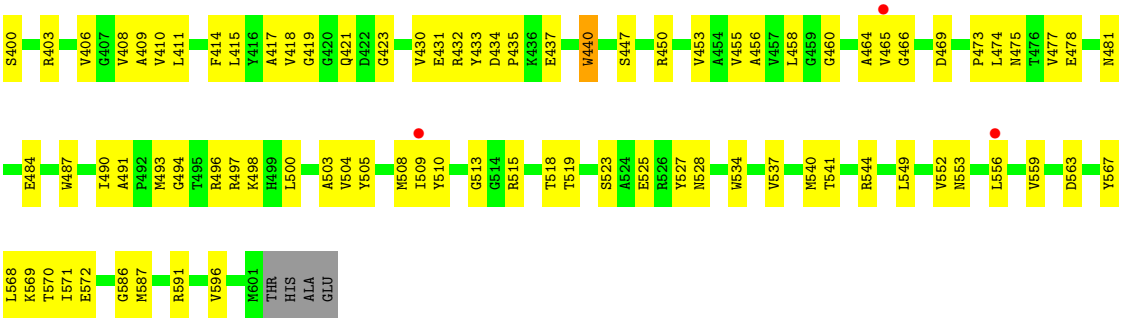
Chain C:



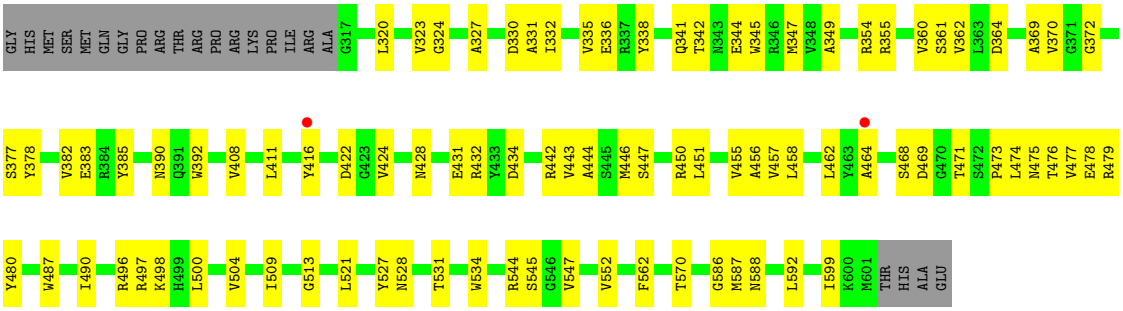
• Molecule 1: Kelch-like protein 20

Chain D:

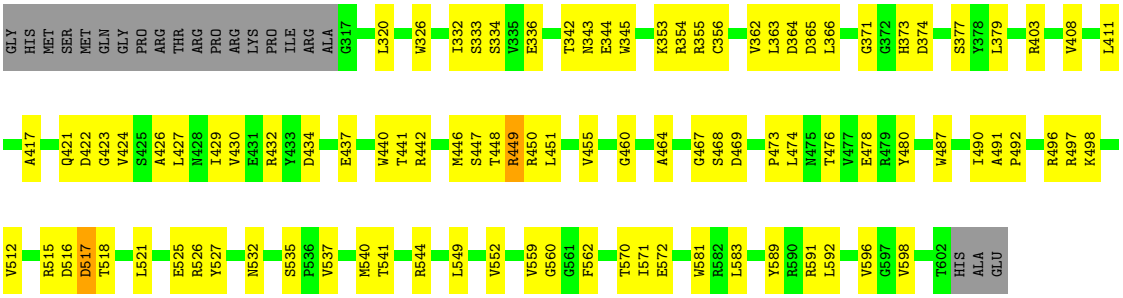




• Molecule 2: Kelch like family member 20



• Molecule 3: Kelch like family member 20



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.93Å 152.93Å 195.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	71.23 – 3.72 109.70 – 3.71	Depositor EDS
% Data completeness (in resolution range)	95.7 (71.23-3.72) 88.0 (109.70-3.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.73 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.226 , 0.287 0.226 , 0.286	Depositor DCC
R_{free} test set	1356 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	69.2	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 28.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	10843	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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

5.1 Standard geometry

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	0.32	0/2209	0.61	1/2999 (0.0%)
1	C	0.28	0/2225	0.60	0/3022
1	D	0.28	0/2209	0.56	0/2999
2	B	0.30	0/2209	0.59	0/2998
3	E	0.27	0/2216	0.57	0/3009
All	All	0.29	0/11068	0.59	1/15027 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	379	LEU	CA-CB-CG	5.28	127.45	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2164	0	2104	95	0
1	C	2180	0	2115	58	0
1	D	2164	0	2104	80	0
2	B	2164	0	2111	71	0
3	E	2171	0	2109	66	0
All	All	10843	0	10543	360	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 17.

All (360) 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)
3:E:473:PRO:HG3	3:E:498:LYS:HE2	1.58	0.84
3:E:320:LEU:HB2	3:E:552:VAL:HG21	1.59	0.83
1:C:479:ARG:HB3	1:C:490:ILE:HD11	1.59	0.82
1:A:324:GLY:HA3	1:A:591:ARG:HD2	1.59	0.81
2:B:362:VAL:HG21	2:B:599:ILE:HG22	1.66	0.78
1:A:544:ARG:HB3	1:A:547:VAL:HG11	1.65	0.77
3:E:559:VAL:HG23	3:E:571:ILE:HG22	1.67	0.77
1:A:424:VAL:HA	2:B:341:GLN:HG2	1.67	0.76
3:E:497:ARG:HH22	3:E:525:GLU:HG3	1.52	0.74
1:A:355:ARG:HE	1:A:371:GLY:HA2	1.53	0.74
1:D:497:ARG:NH2	1:D:523:SER:OG	2.21	0.74
3:E:342:THR:O	3:E:344:GLU:N	2.21	0.74
2:B:528:ASN:HB3	2:B:531:THR:HG22	1.71	0.73
3:E:422:ASP:O	3:E:424:VAL:N	2.22	0.73
1:C:557:MET:HG2	1:C:573:VAL:HG12	1.70	0.73
1:D:586:GLY:O	3:E:515:ARG:NH2	2.23	0.72
1:A:415:LEU:HB3	1:A:433:TYR:HB3	1.72	0.71
3:E:432:ARG:HB3	3:E:441:THR:HB	1.71	0.71
1:C:498:LYS:HB3	1:C:515:ARG:HB3	1.71	0.71
1:A:544:ARG:NH2	1:A:570:THR:OG1	2.22	0.71
1:C:490:ILE:HG22	1:C:491:ALA:H	1.54	0.70
3:E:353:LYS:HE3	3:E:374:ASP:HB2	1.74	0.70
1:A:353:LYS:HE3	1:A:379:LEU:HD11	1.74	0.70
1:D:559:VAL:HA	1:D:571:ILE:HG22	1.72	0.69
1:A:356:CYS:HB3	1:A:373:HIS:HB3	1.74	0.69
1:A:363:LEU:HD21	1:A:435:PRO:HG3	1.73	0.69
2:B:450:ARG:HH22	2:B:476:THR:HG23	1.58	0.68
1:C:367:LEU:HB3	1:C:385:TYR:HB3	1.76	0.68
1:C:457:VAL:HA	1:C:462:LEU:HA	1.74	0.68
1:A:362:VAL:HG21	1:A:599:ILE:HG12	1.76	0.67
2:B:320:LEU:HB2	2:B:552:VAL:HG11	1.75	0.67
3:E:427:LEU:HD13	3:E:429:ILE:HD12	1.78	0.66
3:E:474:LEU:HA	3:E:496:ARG:HH11	1.59	0.66
1:C:461:PHE:CD2	1:C:479:ARG:HA	2.31	0.66
1:A:549:LEU:HD11	1:A:556:LEU:HD21	1.78	0.66
2:B:479:ARG:HD2	2:B:490:ILE:HD11	1.79	0.66
1:A:326:TRP:HB2	1:A:592:LEU:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ASP:OD2	1:A:582:ARG:NH1	2.29	0.64
1:D:541:THR:HB	1:D:572:GLU:OE2	1.97	0.64
3:E:544:ARG:NH1	3:E:560:GLY:O	2.31	0.64
1:C:563:ASP:HB3	1:C:568:LEU:HD11	1.79	0.63
1:D:544:ARG:HH12	1:D:572:GLU:HG3	1.64	0.63
1:A:360:VAL:HG12	1:A:369:ALA:HA	1.79	0.63
3:E:450:ARG:NH2	3:E:476:THR:OG1	2.31	0.63
1:A:448:THR:OG1	1:A:450:ARG:NH1	2.32	0.62
1:C:516:ASP:OD1	1:C:517:ASP:N	2.32	0.62
1:D:408:VAL:HG12	1:D:417:ALA:HA	1.81	0.62
1:C:450:ARG:NH2	1:C:476:THR:OG1	2.33	0.62
2:B:323:VAL:HG21	2:B:360:VAL:HG11	1.81	0.62
2:B:330:ASP:HB3	2:B:354:ARG:HH12	1.62	0.62
2:B:544:ARG:NH1	2:B:570:THR:O	2.32	0.62
1:A:387:PRO:HG3	1:A:599:ILE:HD13	1.81	0.61
3:E:355:ARG:NH1	3:E:371:GLY:O	2.33	0.61
1:A:557:MET:HB3	1:A:573:VAL:HG22	1.83	0.61
2:B:447:SER:H	2:B:487:TRP:HE1	1.48	0.61
3:E:516:ASP:O	3:E:518:THR:N	2.33	0.61
3:E:490:ILE:HG13	3:E:491:ALA:H	1.67	0.60
2:B:562:PHE:HB2	2:B:592:LEU:HD13	1.84	0.60
1:A:433:TYR:CD1	1:A:440:TRP:HE3	2.20	0.59
1:A:433:TYR:HB2	1:A:440:TRP:CE3	2.36	0.59
1:D:367:LEU:HB3	1:D:385:TYR:HB3	1.83	0.59
3:E:421:GLN:HB2	3:E:451:LEU:HD12	1.83	0.59
1:A:370:VAL:HG21	1:A:408:VAL:HG11	1.85	0.59
2:B:509:ILE:HG23	2:B:527:TYR:HB3	1.84	0.59
3:E:455:VAL:HG12	3:E:464:ALA:HA	1.83	0.59
1:D:418:VAL:HG23	1:D:430:VAL:HG22	1.84	0.59
1:C:422:ASP:O	1:C:424:VAL:N	2.36	0.58
1:C:415:LEU:HB3	1:C:433:TYR:HB3	1.84	0.58
1:D:414:PHE:HD2	1:D:432:ARG:HD3	1.68	0.58
2:B:331:ALA:HB3	2:B:354:ARG:HB3	1.85	0.58
1:A:352:SER:HB2	1:A:383:GLU:OE2	2.03	0.58
1:A:370:VAL:HA	1:A:382:VAL:HG22	1.84	0.58
2:B:447:SER:OG	2:B:478:GLU:OE2	2.22	0.58
2:B:431:GLU:HB3	2:B:442:ARG:HD2	1.84	0.58
2:B:323:VAL:HG12	2:B:335:VAL:HG22	1.85	0.58
1:A:377:SER:O	1:A:379:LEU:N	2.35	0.57
1:A:549:LEU:HD21	1:A:556:LEU:HD11	1.87	0.57
3:E:512:VAL:HG22	3:E:549:LEU:HD22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:TYR:HE2	1:C:433:TYR:HE2	1.52	0.57
1:A:332:ILE:HD11	1:A:591:ARG:HD3	1.87	0.57
1:D:450:ARG:HB3	1:D:453:VAL:HB	1.87	0.57
3:E:476:THR:HA	3:E:492:PRO:HB3	1.85	0.57
1:A:325:GLY:HA3	1:A:355:ARG:O	2.05	0.56
1:C:454:ALA:HB3	1:C:500:LEU:HD12	1.87	0.56
1:D:497:ARG:NH1	1:D:513:GLY:O	2.38	0.56
3:E:572:GLU:HG2	3:E:583:LEU:HB3	1.86	0.56
1:A:411:LEU:HD13	1:A:457:VAL:HG11	1.88	0.56
1:D:469:ASP:HB3	1:D:474:LEU:HD11	1.86	0.56
3:E:541:THR:OG1	3:E:572:GLU:OE2	2.22	0.56
3:E:562:PHE:HB2	3:E:592:LEU:HD13	1.87	0.56
1:A:407:GLY:O	1:A:418:VAL:HG22	2.06	0.56
1:A:481:ASN:HB3	1:A:484:GLU:HG2	1.87	0.56
2:B:360:VAL:HG12	2:B:369:ALA:HA	1.88	0.56
1:C:497:ARG:HB2	1:C:500:LEU:HD23	1.88	0.56
3:E:540:MET:HA	3:E:581:TRP:CD1	2.41	0.56
1:A:505:TYR:HB2	1:A:556:LEU:HD12	1.88	0.56
1:A:421:GLN:OE1	2:B:342:THR:HG21	2.06	0.55
3:E:432:ARG:O	3:E:441:THR:N	2.39	0.55
2:B:336:GLU:OE2	2:B:587:MET:HB3	2.06	0.55
1:D:456:ALA:HB3	1:D:509:ILE:HD12	1.87	0.55
1:C:403:ARG:NH2	1:C:431:GLU:OE1	2.39	0.55
1:D:355:ARG:HB3	1:D:358:VAL:HB	1.88	0.55
2:B:432:ARG:HH22	2:B:434:ASP:HB2	1.72	0.55
1:C:569:LYS:HB3	1:C:590:ARG:HG2	1.88	0.55
1:A:337:ARG:HH21	1:A:346:ARG:HH22	1.54	0.55
3:E:411:LEU:HD11	3:E:460:GLY:HA2	1.89	0.54
3:E:544:ARG:NH2	3:E:570:THR:OG1	2.38	0.54
3:E:449:ARG:O	3:E:469:ASP:HA	2.08	0.54
1:A:333:SER:HB3	1:A:354:ARG:HA	1.89	0.54
1:D:549:LEU:HD21	1:D:556:LEU:HD11	1.90	0.54
3:E:373:HIS:ND1	3:E:377:SER:O	2.37	0.54
3:E:516:ASP:HB2	3:E:521:LEU:HD21	1.89	0.54
2:B:355:ARG:HD2	2:B:372:GLY:HA3	1.89	0.54
1:A:418:VAL:HA	1:A:430:VAL:HG22	1.89	0.54
1:D:368:TYR:HD2	1:D:415:LEU:HD22	1.71	0.54
1:A:355:ARG:HB3	1:A:358:VAL:HG22	1.89	0.54
2:B:474:LEU:HD12	2:B:476:THR:HG22	1.91	0.53
1:A:461:PHE:HB3	1:A:463:TYR:HE1	1.74	0.53
1:D:378:TYR:HE2	1:D:423:GLY:HA3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:447:SER:HB3	3:E:478:GLU:OE2	2.08	0.53
1:A:432:ARG:HG2	1:A:433:TYR:H	1.73	0.53
2:B:327:ALA:HB3	2:B:332:ILE:HD11	1.91	0.53
2:B:544:ARG:HB3	2:B:547:VAL:HG22	1.91	0.53
1:C:587:MET:O	1:D:515:ARG:NH2	2.42	0.53
1:D:518:THR:OG1	1:D:519:THR:N	2.40	0.53
1:A:587:MET:CE	1:A:591:ARG:HG3	2.37	0.53
1:A:339:ASP:OD1	1:A:339:ASP:N	2.36	0.53
2:B:361:SER:OG	2:B:362:VAL:N	2.40	0.53
1:D:505:TYR:HB3	1:D:510:TYR:CD1	2.43	0.53
1:C:363:LEU:HD13	1:C:415:LEU:HB2	1.90	0.53
2:B:443:VAL:HG22	2:B:444:ALA:H	1.74	0.52
3:E:526:ARG:HG2	3:E:537:VAL:HG13	1.89	0.52
1:A:320:LEU:HB2	1:A:552:VAL:HG21	1.91	0.52
2:B:330:ASP:HB3	2:B:354:ARG:NH1	2.24	0.52
3:E:497:ARG:HH12	3:E:525:GLU:HG3	1.73	0.52
1:A:356:CYS:N	1:A:373:HIS:O	2.41	0.52
1:A:337:ARG:HH21	1:A:346:ARG:NH2	2.07	0.52
2:B:370:VAL:HG13	2:B:382:VAL:HG11	1.90	0.52
3:E:497:ARG:NH2	3:E:525:GLU:HG3	2.23	0.52
1:C:480:TYR:HE1	1:C:485:ASN:HA	1.75	0.52
1:C:455:VAL:HG12	1:C:464:ALA:HA	1.91	0.52
1:D:327:ALA:HB2	1:D:332:ILE:HG22	1.92	0.52
1:D:331:ALA:O	1:D:354:ARG:HD3	2.09	0.52
1:D:434:ASP:OD1	1:D:434:ASP:N	2.43	0.52
1:C:462:LEU:HD12	1:C:462:LEU:O	2.09	0.52
2:B:468:SER:HB2	2:B:498:LYS:HG2	1.91	0.51
3:E:374:ASP:HB3	3:E:379:LEU:HD11	1.91	0.51
3:E:559:VAL:HG11	3:E:596:VAL:HG11	1.91	0.51
2:B:324:GLY:HA2	2:B:332:ILE:O	2.10	0.51
2:B:444:ALA:HB1	2:B:487:TRP:CZ3	2.45	0.51
1:C:526:ARG:O	1:C:535:SER:N	2.42	0.51
1:D:431:GLU:HB3	1:D:440:TRP:CD1	2.45	0.51
2:B:456:ALA:HB3	2:B:509:ILE:HD12	1.93	0.51
1:A:540:MET:HE1	1:A:558:ALA:HB3	1.93	0.51
1:D:447:SER:HB3	1:D:478:GLU:OE2	2.11	0.51
3:E:326:TRP:HB2	3:E:356:CYS:SG	2.50	0.51
1:C:480:TYR:CE1	1:C:485:ASN:HA	2.45	0.51
1:A:336:GLU:OE1	1:A:587:MET:HB2	2.11	0.50
2:B:336:GLU:HB3	2:B:347:MET:SD	2.51	0.50
1:D:320:LEU:HB2	1:D:552:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:416:TYR:CD1	2:B:432:ARG:HB3	2.46	0.50
2:B:355:ARG:NH2	2:B:383:GLU:HG2	2.27	0.50
1:D:409:ALA:O	1:D:415:LEU:HD12	2.11	0.50
1:D:563:ASP:HB3	1:D:568:LEU:HD11	1.93	0.50
1:A:431:GLU:HA	1:A:442:ARG:HA	1.93	0.50
3:E:365:ASP:O	3:E:366:LEU:HD23	2.10	0.50
2:B:331:ALA:O	2:B:354:ARG:NH1	2.44	0.50
3:E:434:ASP:HB3	3:E:437:GLU:HB2	1.94	0.50
1:D:433:TYR:HB2	1:D:440:TRP:CE2	2.46	0.50
1:A:499:HIS:NE2	2:B:344:GLU:OE2	2.37	0.50
1:D:475:ASN:O	1:D:493:MET:N	2.40	0.50
1:C:333:SER:HB3	1:C:354:ARG:HG2	1.93	0.49
1:A:326:TRP:CB	1:A:592:LEU:HB3	2.42	0.49
2:B:458:LEU:HD13	2:B:504:VAL:HG21	1.94	0.49
1:C:336:GLU:OE2	1:C:588:ASN:HB2	2.12	0.49
1:D:477:VAL:HG12	1:D:490:ILE:HB	1.94	0.49
1:A:543:ARG:O	1:A:563:ASP:HB3	2.13	0.49
1:A:569:LYS:NZ	1:C:519:THR:HA	2.28	0.49
2:B:336:GLU:OE1	2:B:588:ASN:HB2	2.11	0.49
1:D:328:SER:HA	1:D:567:TYR:CE2	2.47	0.49
3:E:473:PRO:HG2	3:E:517:ASP:HA	1.93	0.49
1:A:355:ARG:NH2	1:A:381:SER:OG	2.46	0.49
1:A:403:ARG:HH11	1:A:406:VAL:HG21	1.77	0.49
1:D:455:VAL:HG12	1:D:464:ALA:HA	1.95	0.49
1:A:403:ARG:NH1	1:A:418:VAL:O	2.45	0.49
1:A:327:ALA:O	1:A:329:GLY:N	2.47	0.48
1:A:518:THR:OG1	1:A:519:THR:N	2.45	0.48
2:B:447:SER:N	2:B:487:TRP:HE1	2.09	0.48
1:C:323:VAL:HG11	1:C:360:VAL:HG21	1.95	0.48
1:C:334:SER:OG	1:C:591:ARG:NH2	2.47	0.48
1:C:447:SER:OG	1:C:478:GLU:OE2	2.23	0.48
3:E:448:THR:HB	3:E:450:ARG:NH1	2.27	0.48
1:D:418:VAL:HG11	1:D:455:VAL:HG11	1.96	0.48
1:A:531:THR:OG1	1:A:533:GLN:HG2	2.12	0.48
1:C:497:ARG:CB	1:C:500:LEU:HD23	2.42	0.48
1:A:408:VAL:HG12	1:A:417:ALA:HA	1.95	0.48
1:A:447:SER:O	1:A:448:THR:OG1	2.28	0.48
1:A:480:TYR:HB2	1:A:487:TRP:CZ3	2.48	0.48
1:D:570:THR:HG22	3:E:518:THR:OG1	2.13	0.48
1:C:473:PRO:O	1:C:496:ARG:HD3	2.14	0.48
1:A:516:ASP:OD1	1:A:517:ASP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:LEU:HA	1:C:496:ARG:HH11	1.79	0.48
1:D:363:LEU:HD22	1:D:415:LEU:HB2	1.95	0.48
1:A:379:LEU:HD23	1:A:381:SER:H	1.78	0.47
2:B:462:LEU:HG	2:B:480:TYR:HB3	1.96	0.47
1:D:559:VAL:HG11	1:D:596:VAL:HG11	1.96	0.47
3:E:332:ILE:HG22	3:E:334:SER:H	1.78	0.47
1:D:491:ALA:HB3	1:D:527:TYR:HE2	1.78	0.47
2:B:355:ARG:HH22	2:B:383:GLU:HG2	1.80	0.47
1:D:403:ARG:HD2	1:D:406:VAL:HG21	1.97	0.47
1:D:323:VAL:HB	1:D:360:VAL:HG21	1.97	0.47
1:C:363:LEU:HD21	1:C:435:PRO:HG3	1.97	0.47
1:C:518:THR:OG1	1:C:519:THR:N	2.47	0.47
1:A:547:VAL:HG12	1:A:561:GLY:HA3	1.97	0.47
2:B:451:LEU:N	2:B:468:SER:O	2.25	0.47
1:D:456:ALA:HB1	1:D:504:VAL:HG13	1.97	0.47
1:D:481:ASN:N	1:D:481:ASN:OD1	2.48	0.47
3:E:446:MET:HE3	3:E:450:ARG:HH11	1.80	0.47
1:A:570:THR:HA	1:A:586:GLY:HA3	1.95	0.47
2:B:416:TYR:CE1	2:B:432:ARG:HB3	2.50	0.47
1:A:326:TRP:CE2	1:A:356:CYS:SG	3.08	0.47
1:C:516:ASP:HB2	1:C:521:LEU:HD21	1.96	0.47
3:E:498:LYS:H	3:E:515:ARG:H	1.62	0.47
1:A:399:THR:HA	1:A:440:TRP:NE1	2.30	0.46
1:D:385:TYR:HE1	1:D:387:PRO:HA	1.81	0.46
1:D:481:ASN:ND2	1:D:484:GLU:HB2	2.31	0.46
3:E:403:ARG:HD3	3:E:427:LEU:HD12	1.98	0.46
1:C:430:VAL:HG21	1:C:487:TRP:CZ2	2.51	0.46
3:E:480:TYR:HB2	3:E:487:TRP:CZ3	2.50	0.46
2:B:469:ASP:OD1	2:B:471:THR:OG1	2.34	0.46
2:B:527:TYR:HB2	2:B:534:TRP:CE2	2.51	0.46
3:E:408:VAL:HG12	3:E:417:ALA:HA	1.98	0.46
1:A:427:LEU:HD22	1:A:429:ILE:HG23	1.98	0.46
1:C:411:LEU:O	1:C:413:GLY:N	2.49	0.46
1:D:411:LEU:HD11	1:D:460:GLY:HA2	1.96	0.46
1:A:458:LEU:HD23	1:A:529:PRO:HG3	1.97	0.46
1:D:382:VAL:HG21	1:D:440:TRP:HH2	1.81	0.45
3:E:432:ARG:HE	3:E:441:THR:HG21	1.81	0.45
2:B:450:ARG:NH2	2:B:476:THR:HG23	2.30	0.45
2:B:497:ARG:HB2	2:B:500:LEU:HD22	1.98	0.45
3:E:490:ILE:HG13	3:E:491:ALA:N	2.30	0.45
2:B:422:ASP:HB3	2:B:424:VAL:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:527:TYR:HB2	1:C:534:TRP:CE3	2.52	0.45
1:D:508:MET:HE1	1:D:528:ASN:HB2	1.99	0.45
3:E:336:GLU:OE2	3:E:591:ARG:NH2	2.47	0.45
1:A:552:VAL:O	1:A:554:GLY:N	2.49	0.45
3:E:426:ALA:HB2	3:E:451:LEU:HD22	1.99	0.45
1:A:385:TYR:HB2	1:A:392:TRP:CD2	2.51	0.45
1:A:520:GLU:O	1:A:543:ARG:HD3	2.17	0.45
2:B:455:VAL:HG12	2:B:464:ALA:HA	1.98	0.45
1:D:363:LEU:HD21	1:D:435:PRO:HD3	1.97	0.45
1:D:367:LEU:HD12	1:D:367:LEU:HA	1.82	0.45
1:D:450:ARG:HD2	1:D:466:GLY:O	2.17	0.44
1:A:326:TRP:HZ3	2:B:347:MET:HB2	1.83	0.44
1:D:503:ALA:HB3	1:D:549:LEU:HD23	1.99	0.44
3:E:430:VAL:O	3:E:442:ARG:NH1	2.49	0.44
3:E:446:MET:HE3	3:E:450:ARG:NH1	2.32	0.44
2:B:349:ALA:HB2	2:B:390:ASN:HD21	1.82	0.44
1:C:428:ASN:HB3	1:C:449:ARG:HG2	1.98	0.44
1:A:527:TYR:HB2	1:A:534:TRP:CE2	2.53	0.44
1:A:527:TYR:HB2	1:A:534:TRP:CD2	2.53	0.44
1:D:430:VAL:HG21	1:D:487:TRP:CZ2	2.53	0.44
2:B:370:VAL:HG21	2:B:408:VAL:HG11	2.00	0.44
2:B:497:ARG:HB2	2:B:500:LEU:CD2	2.48	0.44
1:C:415:LEU:O	1:C:433:TYR:N	2.41	0.44
1:A:587:MET:HE1	1:A:591:ARG:HG3	1.99	0.44
2:B:477:VAL:HG13	2:B:490:ILE:HB	1.99	0.44
1:D:361:SER:OG	1:D:408:VAL:HG23	2.18	0.44
1:D:437:GLU:N	1:D:437:GLU:OE1	2.50	0.44
1:D:465:VAL:HG12	1:D:500:LEU:HD21	1.99	0.44
1:D:497:ARG:HD3	1:D:513:GLY:O	2.18	0.44
2:B:377:SER:OG	2:B:378:TYR:N	2.51	0.43
1:D:358:VAL:HG21	1:D:369:ALA:HB1	2.00	0.43
3:E:403:ARG:HG2	3:E:422:ASP:HB2	2.00	0.43
1:D:458:LEU:HD12	1:D:458:LEU:HA	1.81	0.43
1:A:450:ARG:NH2	1:A:476:THR:OG1	2.50	0.43
1:A:351:MET:HE1	1:A:355:ARG:HD2	2.01	0.43
2:B:479:ARG:O	2:B:487:TRP:HB2	2.18	0.43
1:C:327:ALA:HB3	1:C:332:ILE:HD11	2.00	0.43
1:C:422:ASP:HB2	1:C:427:LEU:HD22	2.00	0.43
1:C:508:MET:SD	1:C:526:ARG:HD2	2.59	0.43
1:A:542:SER:O	1:A:544:ARG:HG3	2.18	0.43
1:C:443:VAL:HG22	1:C:444:ALA:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:ARG:HG3	1:C:516:ASP:O	2.19	0.43
1:A:461:PHE:CE1	1:A:479:ARG:HD2	2.53	0.43
1:A:562:PHE:HB2	1:A:592:LEU:HD12	2.01	0.43
1:C:547:VAL:HG23	1:C:559:VAL:O	2.18	0.43
1:D:525:GLU:HA	1:D:537:VAL:HG23	2.01	0.43
1:D:544:ARG:HH12	1:D:572:GLU:CG	2.29	0.43
3:E:333:SER:HB3	3:E:354:ARG:HG2	2.00	0.43
1:A:399:THR:HG22	1:A:440:TRP:CZ2	2.54	0.43
1:C:559:VAL:HA	1:C:571:ILE:HG22	2.00	0.43
1:D:400:SER:HB2	1:D:431:GLU:OE2	2.19	0.43
1:C:378:TYR:HE2	1:C:423:GLY:H	1.65	0.42
1:D:540:MET:CE	1:D:544:ARG:HD2	2.49	0.42
1:A:367:LEU:HD12	1:A:367:LEU:HA	1.89	0.42
3:E:467:GLY:O	3:E:474:LEU:HD23	2.19	0.42
1:D:527:TYR:HB2	1:D:534:TRP:CE2	2.54	0.42
1:C:540:MET:HB3	1:C:572:GLU:OE1	2.20	0.42
3:E:468:SER:HA	3:E:473:PRO:HA	2.01	0.42
3:E:497:ARG:HG2	3:E:521:LEU:HD13	2.02	0.42
1:A:427:LEU:HA	1:A:427:LEU:HD23	1.81	0.42
1:D:396:VAL:HG13	1:D:433:TYR:CZ	2.55	0.42
3:E:336:GLU:HG3	3:E:345:TRP:HE3	1.84	0.42
1:A:587:MET:HE2	1:A:591:ARG:HG3	2.00	0.42
2:B:411:LEU:HB3	2:B:457:VAL:HG11	2.01	0.42
1:C:337:ARG:NH2	1:C:346:ARG:HD3	2.35	0.42
1:C:429:ILE:HD13	1:C:442:ARG:HH12	1.85	0.42
1:D:362:VAL:O	1:D:410:VAL:HG11	2.19	0.42
1:D:509:ILE:HG23	1:D:527:TYR:HB3	2.01	0.42
3:E:363:LEU:HD23	3:E:364:ASP:HB2	2.01	0.42
1:A:326:TRP:CZ3	2:B:347:MET:HB2	2.55	0.42
1:A:328:SER:OG	1:A:329:GLY:N	2.51	0.42
2:B:385:TYR:HB2	2:B:392:TRP:CZ3	2.55	0.42
1:D:355:ARG:HH22	1:D:383:GLU:HG3	1.84	0.42
1:D:403:ARG:HD3	1:D:419:GLY:O	2.19	0.42
1:D:469:ASP:HB3	1:D:474:LEU:HD21	2.02	0.42
1:A:587:MET:H	1:A:587:MET:HG2	1.75	0.42
2:B:545:SER:H	2:B:562:PHE:H	1.68	0.42
2:B:570:THR:HA	2:B:586:GLY:HA3	2.01	0.42
1:A:428:ASN:HB3	1:A:449:ARG:HA	2.02	0.41
1:A:454:ALA:HB3	1:A:500:LEU:HD12	2.01	0.41
2:B:446:MET:HA	2:B:487:TRP:NE1	2.36	0.41
1:C:368:TYR:HE2	1:C:433:TYR:CE2	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:385:TYR:HD2	1:D:392:TRP:CE2	2.39	0.41
2:B:497:ARG:O	2:B:500:LEU:HD23	2.20	0.41
2:B:521:LEU:HD12	2:B:521:LEU:HA	1.79	0.41
1:C:431:GLU:HB3	1:C:440:TRP:CE3	2.55	0.41
1:D:382:VAL:HG21	1:D:440:TRP:CH2	2.56	0.41
1:D:569:LYS:HD2	1:D:587:MET:O	2.20	0.41
1:A:363:LEU:HG	1:A:364:ASP:OD1	2.21	0.41
2:B:428:ASN:OD1	2:B:428:ASN:N	2.53	0.41
2:B:475:ASN:HB3	2:B:496:ARG:HA	2.03	0.41
1:D:473:PRO:HB2	1:D:496:ARG:HB3	2.03	0.41
3:E:362:VAL:HG11	3:E:598:VAL:O	2.20	0.41
1:A:321:PHE:CE1	1:A:599:ILE:HD12	2.55	0.41
1:A:493:MET:HB3	1:A:525:GLU:OE1	2.20	0.41
1:A:522:SER:O	1:A:540:MET:HG3	2.20	0.41
2:B:338:TYR:HB2	2:B:345:TRP:CZ3	2.54	0.41
1:C:523:SER:HA	1:C:539:ALA:HA	2.02	0.41
1:D:431:GLU:HB3	1:D:440:TRP:HD1	1.84	0.41
1:A:499:HIS:HB3	1:A:546:GLY:HA2	2.03	0.41
2:B:473:PRO:HB2	2:B:496:ARG:HB3	2.02	0.41
1:D:494:GLY:N	1:D:525:GLU:OE2	2.41	0.41
1:D:498:LYS:HB3	1:D:515:ARG:O	2.21	0.41
1:D:587:MET:HE1	1:D:591:ARG:HD2	2.03	0.41
3:E:336:GLU:HG3	3:E:345:TRP:CE3	2.56	0.41
3:E:526:ARG:HG3	3:E:535:SER:HB2	2.02	0.41
1:A:527:TYR:O	1:A:529:PRO:HD3	2.21	0.41
3:E:527:TYR:OH	3:E:532:ASN:HA	2.21	0.41
2:B:370:VAL:HA	2:B:382:VAL:HG12	2.03	0.40
1:C:342:THR:HG21	1:D:421:GLN:OE1	2.20	0.40
2:B:390:ASN:ND2	2:B:390:ASN:O	2.54	0.40
3:E:589:TYR:HB3	3:E:591:ARG:HE	1.86	0.40
1:A:360:VAL:HG22	1:A:595:GLY:HA3	2.03	0.40
1:A:457:VAL:HG22	1:A:462:LEU:HA	2.02	0.40
1:D:321:PHE:CD2	1:D:367:LEU:HD22	2.56	0.40
1:D:336:GLU:OE1	1:D:587:MET:HB2	2.21	0.40
1:C:367:LEU:HD12	1:C:367:LEU:HA	1.88	0.40
1:C:461:PHE:HD2	1:C:479:ARG:HA	1.82	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	283/307 (92%)	242 (86%)	30 (11%)	11 (4%)	3 27
1	C	286/307 (93%)	260 (91%)	23 (8%)	3 (1%)	15 51
1	D	283/307 (92%)	264 (93%)	17 (6%)	2 (1%)	22 59
2	B	283/307 (92%)	253 (89%)	28 (10%)	2 (1%)	22 59
3	E	284/307 (92%)	265 (93%)	15 (5%)	4 (1%)	11 45
All	All	1419/1535 (92%)	1284 (90%)	113 (8%)	22 (2%)	9 43

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	553	ASN
3	E	343	ASN
3	E	423	GLY
1	A	328	SER
2	B	364	ASP
1	C	412	GLY
1	C	423	GLY
1	D	553	ASN
3	E	449	ARG
3	E	517	ASP
1	A	364	ASP
1	A	447	SER
1	A	448	THR
1	C	353	LYS
1	A	329	GLY
1	A	376	SER
1	A	378	TYR
1	A	418	VAL
1	A	520	GLU
1	D	327	ALA
1	A	443	VAL

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Mol	Chain	Res	Type
2	B	513	GLY

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	226/244 (93%)	225 (100%)	1 (0%)	91 95
1	C	226/244 (93%)	224 (99%)	2 (1%)	78 88
1	D	226/244 (93%)	225 (100%)	1 (0%)	91 95
2	B	226/244 (93%)	226 (100%)	0	100 100
3	E	227/244 (93%)	226 (100%)	1 (0%)	91 95
All	All	1131/1220 (93%)	1126 (100%)	5 (0%)	91 95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	PHE
1	C	320	LEU
1	C	480	TYR
1	D	440	TRP
3	E	440	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	421	GLN
1	C	588	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 95^{th} 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	285/307 (92%)	0.06	1 (0%) 92 91	47, 66, 84, 100	0
1	C	288/307 (93%)	-0.04	0 100 100	59, 89, 111, 138	0
1	D	285/307 (92%)	0.37	4 (1%) 75 69	67, 91, 117, 138	0
2	B	285/307 (92%)	0.17	2 (0%) 87 85	55, 76, 102, 123	0
3	E	286/307 (93%)	0.07	0 100 100	68, 96, 121, 128	0
All	All	1429/1535 (93%)	0.12	7 (0%) 91 89	47, 84, 115, 138	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	556	LEU	2.8
1	A	326	TRP	2.6
1	D	509	ILE	2.5
2	B	464	ALA	2.5
2	B	416	TYR	2.5
1	D	368	TYR	2.3
1	D	465	VAL	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.