



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:35 PM UTC

PDB ID : 5CTR / pdb_00005ctr
Title : Crystal structure of human SART3 HAT-C domain-human USP4 DUSP-UBL domain complex
Authors : Park, J.K.; Kim, E.E.
Deposited on : 2015-07-24
Resolution : 3.01 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

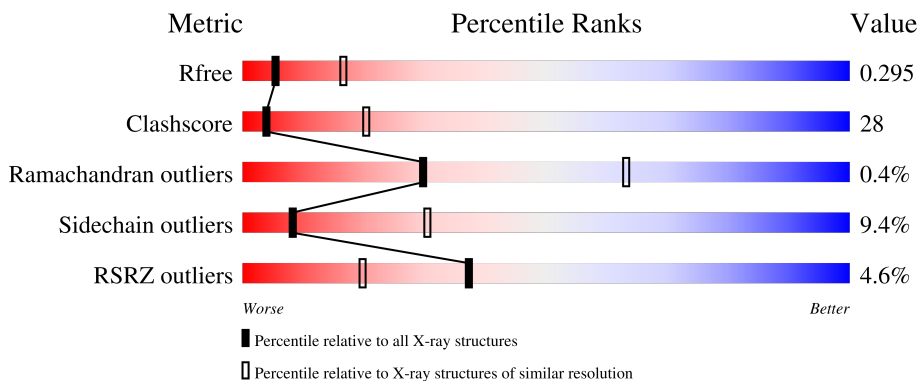
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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}	180053	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	338	
1	B	338	
2	C	233	
2	D	233	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8577 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 Squamous cell carcinoma antigen recognized by T-cells 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	308	2563	1615	457	476	15	0	0	0
1	B	305	2536	1599	453	469	15	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	GLY	-	expression tag	UNP Q15020
A	275	SER	-	expression tag	UNP Q15020
A	276	HIS	-	expression tag	UNP Q15020
A	277	MET	-	expression tag	UNP Q15020
B	274	GLY	-	expression tag	UNP Q15020
B	275	SER	-	expression tag	UNP Q15020
B	276	HIS	-	expression tag	UNP Q15020
B	277	MET	-	expression tag	UNP Q15020

- Molecule 2 is a protein called Ubiquitin carboxyl-terminal hydrolase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	206	1694	1085	284	317	8	0	0	0
2	D	212	1745	1114	294	328	9	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q13107
C	-1	SER	-	expression tag	UNP Q13107
C	0	HIS	-	expression tag	UNP Q13107
D	-2	GLY	-	expression tag	UNP Q13107

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	SER	-	expression tag	UNP Q13107
D	0	HIS	-	expression tag	UNP Q13107

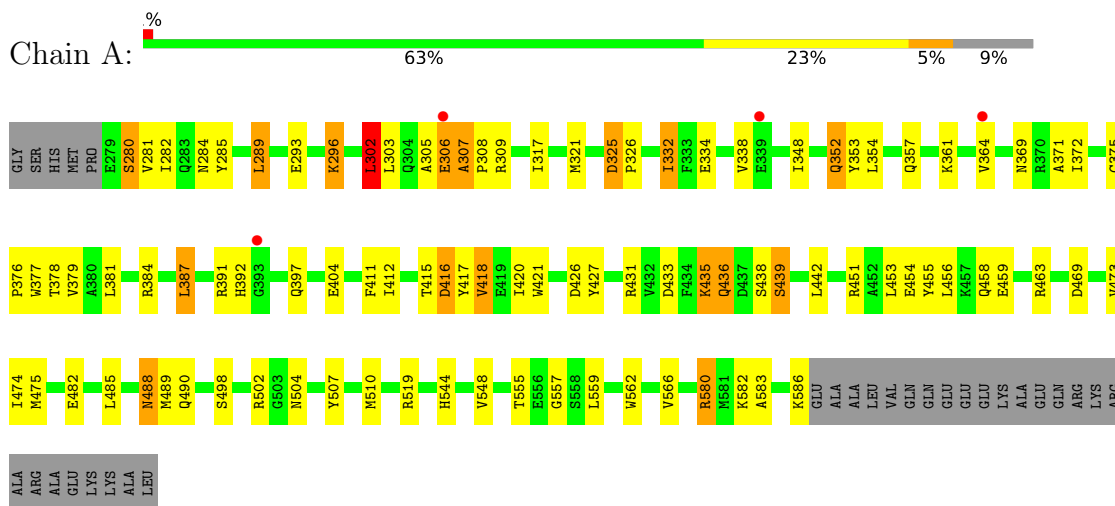
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	7	Total O 7 7	0	0
3	B	21	Total O 21 21	0	0
3	C	4	Total O 4 4	0	0
3	D	7	Total O 7 7	0	0

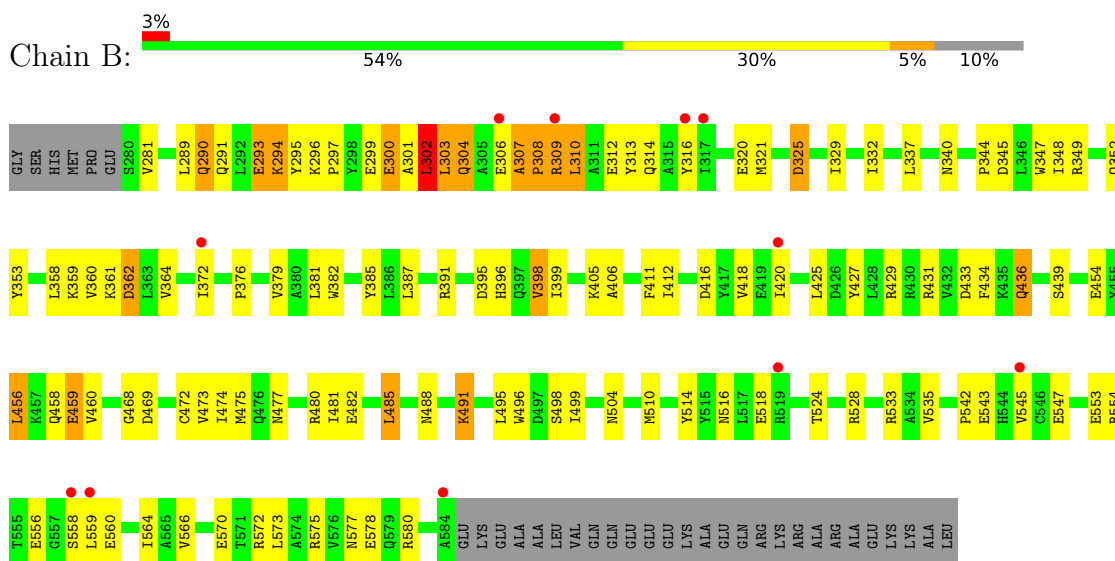
3 Residue-property plots [i](#)

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: Squamous cell carcinoma antigen recognized by T-cells 3

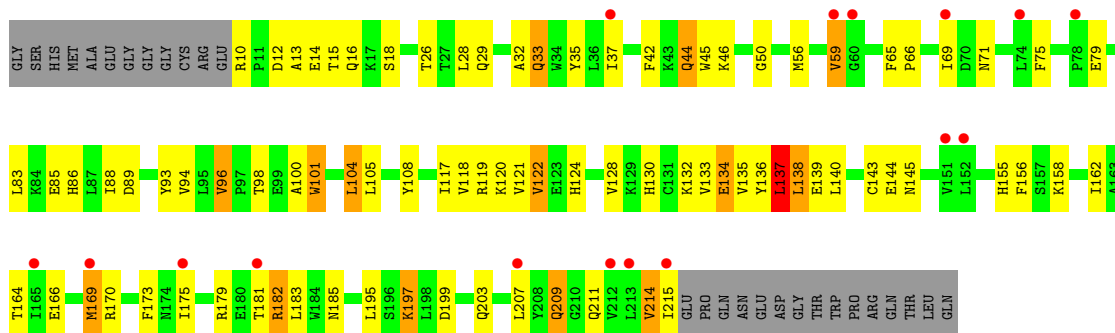


- Molecule 1: Squamous cell carcinoma antigen recognized by T-cells 3

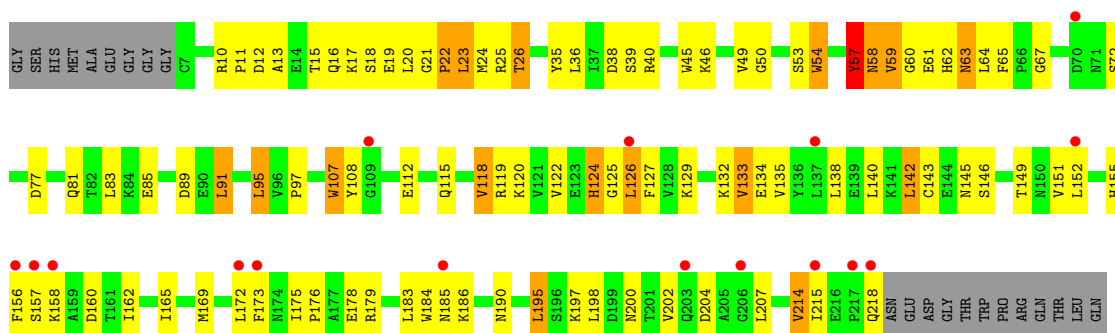


- Molecule 2: Ubiquitin carboxyl-terminal hydrolase 4





• Molecule 2: Ubiquitin carboxyl-terminal hydrolase 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	115.20Å 115.20Å 306.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.01 50.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-3.01) 98.1 (50.00-3.01)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.309 , 0.334 0.296 , 0.295	Depositor DCC
R_{free} test set	2064 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtrriage
Anisotropy	0.131	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 11.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8577	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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	0.52	1/2615 (0.0%)	1.04	16/3535 (0.5%)
1	B	0.51	0/2588	1.07	14/3500 (0.4%)
2	C	0.43	0/1737	0.85	3/2357 (0.1%)
2	D	0.39	0/1789	0.78	4/2427 (0.2%)
All	All	0.48	1/8729 (0.0%)	0.97	37/11819 (0.3%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	489	MET	CA-C	5.75	1.60	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	ALA	N-CA-C	8.47	120.69	110.19
1	B	289	LEU	N-CA-C	8.34	120.45	111.36
1	B	412	ILE	N-CA-C	7.83	118.62	110.72
1	B	293	GLU	N-CA-C	7.33	119.35	111.36
1	B	307	ALA	N-CA-C	-6.74	98.95	109.87
1	B	306	GLU	N-CA-C	6.65	123.00	114.56
1	A	412	ILE	N-CA-C	6.40	121.38	112.35
1	B	459	GLU	N-CA-C	6.37	117.88	111.07
1	A	435	LYS	O-C-N	6.34	128.84	122.12
1	A	325	ASP	CA-C-N	6.24	125.97	119.05
1	A	325	ASP	C-N-CA	6.24	125.97	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	GLU	N-CA-C	6.13	117.94	110.41
1	B	301	ALA	N-CA-C	-6.03	104.62	111.07
2	D	21	GLY	CA-C-N	6.03	127.37	119.84
2	D	21	GLY	C-N-CA	6.03	127.37	119.84
1	B	309	ARG	N-CA-C	-5.79	103.93	111.74
2	C	137	LEU	N-CA-C	-5.77	102.36	110.50
1	A	489	MET	N-CA-C	5.72	118.46	111.82
1	B	468	GLY	N-CA-C	-5.72	107.83	115.32
1	B	302	LEU	N-CA-C	-5.67	105.09	111.28
1	A	375	CYS	CA-C-N	5.62	125.23	119.56
1	A	375	CYS	C-N-CA	5.62	125.23	119.56
2	D	60	GLY	N-CA-C	-5.61	108.00	115.40
1	A	438	SER	N-CA-C	5.48	119.12	107.67
1	A	307	ALA	CA-C-N	-5.45	113.03	119.84
1	A	307	ALA	C-N-CA	-5.45	113.03	119.84
1	B	325	ASP	CA-C-N	5.39	125.03	119.05
1	B	325	ASP	C-N-CA	5.39	125.03	119.05
2	D	57	TYR	N-CA-C	5.34	117.52	111.11
1	A	302	LEU	CA-CB-CG	5.31	134.89	116.30
1	B	485	LEU	N-CA-C	5.21	119.69	112.45
1	A	580	ARG	N-CA-C	-5.20	105.69	111.36
1	B	306	GLU	O-C-N	5.13	127.54	122.10
1	A	435	LYS	CA-C-N	5.12	128.74	121.42
1	A	435	LYS	C-N-CA	5.12	128.74	121.42
2	C	10	ARG	CA-C-N	-5.08	113.48	119.84
2	C	10	ARG	C-N-CA	-5.08	113.48	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	416	ASP	Sidechain
1	A	488	ASN	Mainchain

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	2563	0	2514	84	2
1	B	2536	0	2489	170	1
2	C	1694	0	1654	143	1
2	D	1745	0	1702	87	0
3	A	7	0	0	0	0
3	B	21	0	0	0	0
3	C	4	0	0	0	0
3	D	7	0	0	0	0
All	All	8577	0	8359	476	2

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 (476) 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:320:GLU:HG3	1:B:332:ILE:CD1	1.33	1.56
2:C:138:LEU:HG	2:C:209:GLN:CD	1.36	1.48
1:A:317:ILE:CD1	1:A:332:ILE:HD12	1.45	1.45
2:C:137:LEU:HD11	2:C:156:PHE:C	1.38	1.44
2:D:175:ILE:HG23	2:D:179:ARG:NH1	1.33	1.38
2:C:137:LEU:CD1	2:C:156:PHE:O	1.72	1.35
1:B:302:LEU:HD12	1:B:303:LEU:N	1.41	1.32
1:B:310:LEU:HD12	1:B:310:LEU:O	1.34	1.27
2:D:169:MET:HG3	2:D:215:ILE:CD1	1.69	1.22
2:C:137:LEU:HD23	2:C:138:LEU:N	1.53	1.22
1:B:303:LEU:HD12	1:B:303:LEU:O	1.35	1.21
1:B:433:ASP:OD2	1:B:436:GLN:NE2	1.73	1.21
2:C:138:LEU:CG	2:C:209:GLN:CD	2.16	1.18
2:D:175:ILE:CG2	2:D:179:ARG:HH11	1.57	1.17
1:B:302:LEU:HB3	1:B:309:ARG:NH2	1.60	1.16
2:C:137:LEU:CD1	2:C:156:PHE:C	2.14	1.16
2:D:169:MET:CG	2:D:215:ILE:HD11	1.76	1.14
2:C:169:MET:SD	2:C:215:ILE:CD1	2.35	1.14
2:C:140:LEU:HD21	2:C:207:LEU:HD21	1.24	1.14
1:B:320:GLU:CG	1:B:332:ILE:CD1	2.26	1.13
2:C:138:LEU:HG	2:C:209:GLN:OE1	1.48	1.13
2:C:162:ILE:HG21	2:C:195:LEU:HD21	1.30	1.13
1:B:320:GLU:CG	1:B:332:ILE:HD12	1.80	1.11
1:A:317:ILE:HD11	1:A:332:ILE:HD12	1.33	1.10
1:B:307:ALA:O	1:B:309:ARG:N	1.84	1.10
1:A:306:GLU:O	1:A:309:ARG:HG2	1.52	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:169:MET:HB3	2:D:215:ILE:HD12	1.28	1.10
1:A:456:LEU:HD21	1:A:474:ILE:HD12	1.31	1.09
2:C:138:LEU:CG	2:C:209:GLN:OE1	1.99	1.08
1:A:317:ILE:HD13	1:A:332:ILE:HD12	1.10	1.08
1:A:281:VAL:HG23	1:A:282:ILE:N	1.68	1.08
2:D:126:LEU:N	2:D:126:LEU:HD23	1.68	1.08
1:B:309:ARG:HD2	1:B:313:TYR:CE2	1.89	1.08
1:A:317:ILE:CD1	1:A:332:ILE:CD1	2.32	1.07
1:B:307:ALA:HB1	1:B:308:PRO:HD2	1.37	1.07
2:C:137:LEU:HD11	2:C:156:PHE:O	0.89	1.07
1:B:302:LEU:HB3	1:B:309:ARG:HH22	1.17	1.06
1:B:295:TYR:C	1:B:297:PRO:HD2	1.78	1.06
1:B:299:GLU:O	1:B:302:LEU:HG	1.58	1.04
2:D:169:MET:CG	2:D:215:ILE:CD1	2.31	1.04
1:A:332:ILE:HD13	1:A:332:ILE:O	1.55	1.03
2:C:29:GLN:O	2:C:32:ALA:HB2	1.56	1.03
2:C:138:LEU:HG	2:C:209:GLN:CG	1.87	1.03
1:B:303:LEU:HD12	1:B:303:LEU:C	1.80	1.02
1:B:320:GLU:HG3	1:B:332:ILE:HD11	1.41	1.02
2:D:169:MET:CB	2:D:215:ILE:HD12	1.89	1.02
2:C:169:MET:SD	2:C:215:ILE:HG13	2.00	1.00
1:B:310:LEU:HD12	1:B:310:LEU:C	1.85	0.99
1:B:433:ASP:CG	1:B:436:GLN:NE2	2.20	0.99
2:C:183:LEU:HD13	2:C:215:ILE:HG12	1.43	0.99
2:C:169:MET:SD	2:C:215:ILE:HD12	2.00	0.98
2:D:169:MET:CB	2:D:215:ILE:CD1	2.40	0.98
2:C:138:LEU:CG	2:C:209:GLN:HB2	1.95	0.97
1:A:456:LEU:HD21	1:A:474:ILE:CD1	1.94	0.96
1:A:456:LEU:CD2	1:A:474:ILE:HD12	1.95	0.96
2:C:137:LEU:HD23	2:C:138:LEU:H	1.03	0.96
2:C:169:MET:CE	2:C:215:ILE:HD11	1.94	0.96
2:C:137:LEU:CD2	2:C:138:LEU:N	2.28	0.95
2:C:169:MET:SD	2:C:215:ILE:CG1	2.56	0.94
1:B:296:LYS:N	1:B:297:PRO:CD	2.30	0.94
1:B:296:LYS:N	1:B:297:PRO:HD2	1.83	0.94
2:C:138:LEU:HG	2:C:209:GLN:HB2	1.51	0.93
1:B:372:ILE:HD11	1:B:385:TYR:CD2	2.04	0.93
2:C:29:GLN:O	2:C:32:ALA:CB	2.18	0.92
1:B:302:LEU:HB2	1:B:309:ARG:NH1	1.85	0.92
2:C:138:LEU:HG	2:C:209:GLN:CB	1.99	0.92
1:B:309:ARG:HD2	1:B:313:TYR:CD2	2.05	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:ASP:CG	1:B:436:GLN:HE21	1.78	0.91
1:B:307:ALA:C	1:B:309:ARG:N	2.20	0.91
1:B:308:PRO:O	1:B:309:ARG:HG3	1.69	0.91
2:C:183:LEU:HD13	2:C:215:ILE:CG1	1.99	0.91
1:A:281:VAL:CG2	1:A:282:ILE:N	2.33	0.90
1:B:299:GLU:O	1:B:302:LEU:CD1	2.20	0.90
2:D:138:LEU:HD21	2:D:140:LEU:HG	1.53	0.90
1:A:332:ILE:HD13	1:A:332:ILE:C	1.96	0.90
1:A:317:ILE:HD11	1:A:332:ILE:CD1	1.97	0.89
1:A:582:LYS:HE3	1:A:586:LYS:HE3	1.53	0.89
1:B:299:GLU:O	1:B:302:LEU:CG	2.21	0.88
2:C:140:LEU:HD21	2:C:207:LEU:CD2	2.04	0.88
1:B:308:PRO:HB2	1:B:340:ASN:OD1	1.73	0.88
1:B:307:ALA:C	1:B:309:ARG:H	1.80	0.88
1:B:309:ARG:CD	1:B:313:TYR:CD2	2.56	0.88
2:C:138:LEU:CD1	2:C:209:GLN:CD	2.47	0.88
1:B:320:GLU:HG3	1:B:332:ILE:HD12	0.87	0.87
1:B:309:ARG:O	1:B:309:ARG:HD3	1.75	0.87
1:A:306:GLU:O	1:A:309:ARG:CG	2.22	0.86
1:B:302:LEU:CD1	1:B:303:LEU:N	2.36	0.86
1:B:307:ALA:CB	1:B:308:PRO:HD2	2.02	0.86
2:D:175:ILE:CG2	2:D:179:ARG:NH1	2.23	0.86
2:D:169:MET:HG3	2:D:215:ILE:HD11	0.89	0.85
1:B:302:LEU:CB	1:B:309:ARG:NH2	2.40	0.85
2:C:121:VAL:HG23	2:C:132:LYS:C	2.00	0.85
2:C:169:MET:CE	2:C:215:ILE:CD1	2.55	0.85
1:A:317:ILE:HD13	1:A:332:ILE:CD1	2.03	0.85
1:B:302:LEU:HD12	1:B:302:LEU:C	2.02	0.84
1:B:316:TYR:CD1	1:B:332:ILE:HD13	2.12	0.84
1:A:582:LYS:CE	1:A:586:LYS:HE3	2.07	0.84
1:B:309:ARG:HD3	1:B:309:ARG:C	2.04	0.83
1:B:307:ALA:O	1:B:308:PRO:C	2.19	0.83
1:B:302:LEU:HD12	1:B:303:LEU:CA	2.10	0.82
1:A:281:VAL:CG2	1:A:282:ILE:H	1.91	0.82
1:A:281:VAL:O	1:A:284:ASN:N	2.14	0.81
1:B:399:ILE:HD12	1:B:427:TYR:OH	1.78	0.81
1:B:308:PRO:O	1:B:309:ARG:CG	2.30	0.80
1:B:372:ILE:HD11	1:B:385:TYR:HD2	1.43	0.80
2:C:138:LEU:CD1	2:C:209:GLN:NE2	2.45	0.80
1:B:302:LEU:CB	1:B:309:ARG:CZ	2.58	0.80
2:D:169:MET:HE2	2:D:215:ILE:HG13	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:138:LEU:HD12	2:C:209:GLN:NE2	1.97	0.80
2:C:162:ILE:CD1	2:C:195:LEU:HD11	2.12	0.79
1:B:304:GLN:CA	1:B:304:GLN:OE1	2.30	0.79
2:D:169:MET:HB3	2:D:215:ILE:CD1	2.05	0.79
2:D:125:GLY:HA3	2:D:129:LYS:HA	1.63	0.79
1:B:309:ARG:CD	1:B:309:ARG:O	2.30	0.79
1:B:303:LEU:C	1:B:303:LEU:CD1	2.55	0.78
2:C:32:ALA:HB3	2:C:121:VAL:HG12	1.65	0.78
1:B:302:LEU:HB2	1:B:309:ARG:CZ	2.14	0.77
1:A:354:LEU:HB3	1:A:364:VAL:HG12	1.66	0.77
1:B:308:PRO:CB	1:B:340:ASN:OD1	2.32	0.77
1:A:281:VAL:HG23	1:A:282:ILE:H	1.45	0.77
2:C:29:GLN:O	2:C:121:VAL:CG1	2.33	0.76
2:D:126:LEU:HD23	2:D:126:LEU:H	1.48	0.76
1:B:293:GLU:OE1	1:B:296:LYS:NZ	2.14	0.75
2:D:175:ILE:HG23	2:D:179:ARG:HH11	0.87	0.75
1:B:379:VAL:HG23	1:B:420:ILE:HD11	1.68	0.75
2:D:169:MET:CG	2:D:215:ILE:HD12	2.13	0.75
1:B:320:GLU:CG	1:B:332:ILE:HD11	2.07	0.75
1:B:372:ILE:CD1	1:B:385:TYR:CD2	2.70	0.75
2:C:138:LEU:CD1	2:C:209:GLN:OE1	2.33	0.74
1:A:557:GLY:O	1:B:429:ARG:NH2	2.20	0.74
2:C:85:GLU:CG	2:C:136:TYR:HE1	2.01	0.74
2:D:126:LEU:N	2:D:126:LEU:CD2	2.44	0.74
1:B:302:LEU:CB	1:B:309:ARG:NH1	2.51	0.73
2:D:162:ILE:HD12	2:D:197:LYS:O	1.87	0.73
2:C:37:ILE:HA	2:C:71:ASN:HD21	1.54	0.73
1:A:555:THR:HG21	1:B:480:ARG:HH11	1.51	0.73
2:D:175:ILE:HG23	2:D:179:ARG:HH12	1.48	0.73
1:A:332:ILE:CD1	1:A:332:ILE:C	2.62	0.72
1:B:304:GLN:OE1	1:B:304:GLN:HA	1.89	0.72
2:D:202:VAL:HG13	2:D:207:LEU:HD12	1.72	0.72
1:B:302:LEU:HB3	1:B:309:ARG:CZ	2.19	0.72
2:C:140:LEU:CD2	2:C:207:LEU:HD21	2.13	0.72
2:C:88:ILE:O	2:C:93:TYR:CE2	2.43	0.72
1:A:369:ASN:O	1:A:372:ILE:HG12	1.90	0.71
2:C:138:LEU:CD2	2:C:209:GLN:OE1	2.38	0.71
1:A:379:VAL:HG21	1:A:416:ASP:HB3	1.73	0.71
2:D:124:HIS:CE1	2:D:132:LYS:HB3	2.26	0.71
2:C:121:VAL:HG23	2:C:132:LYS:O	1.90	0.70
2:C:169:MET:HE1	2:C:215:ILE:HD11	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LEU:C	1:B:310:LEU:CD1	2.60	0.70
1:B:295:TYR:HD1	1:B:316:TYR:CE1	2.10	0.69
1:B:309:ARG:HD3	1:B:313:TYR:CD2	2.26	0.69
1:B:300:GLU:O	1:B:303:LEU:HB3	1.92	0.69
2:C:85:GLU:HG2	2:C:136:TYR:HE1	1.58	0.69
2:C:138:LEU:CB	2:C:209:GLN:HB2	2.23	0.68
2:D:57:TYR:HD1	2:D:58:ASN:H	1.41	0.68
2:D:95:LEU:HD22	2:D:133:VAL:HG21	1.73	0.68
2:D:124:HIS:NE2	2:D:132:LYS:HB3	2.09	0.68
1:A:485:LEU:HD21	1:B:556:GLU:HG3	1.77	0.67
1:B:302:LEU:HD12	1:B:303:LEU:H	1.53	0.67
1:A:498:SER:OG	1:A:502:ARG:NH1	2.28	0.67
2:C:118:VAL:C	2:C:119:ARG:HG2	2.21	0.66
1:B:495:LEU:O	1:B:499:ILE:HG13	1.95	0.66
2:C:88:ILE:HG22	2:C:89:ASP:N	2.09	0.66
1:B:308:PRO:O	1:B:309:ARG:CD	2.43	0.66
1:A:307:ALA:HB3	1:A:308:PRO:HD3	1.78	0.66
2:C:137:LEU:CD2	2:C:137:LEU:C	2.68	0.66
2:D:184:TRP:HB2	2:D:214:VAL:HG13	1.78	0.66
1:B:309:ARG:CD	1:B:313:TYR:CE2	2.72	0.65
2:C:140:LEU:CD2	2:C:207:LEU:CD2	2.74	0.65
2:C:162:ILE:HD13	2:C:195:LEU:HD11	1.78	0.65
1:B:300:GLU:O	1:B:303:LEU:N	2.30	0.65
1:A:293:GLU:HG3	1:A:296:LYS:HE2	1.79	0.65
1:B:309:ARG:O	1:B:309:ARG:NE	2.30	0.65
1:A:397:GLN:OE1	1:A:397:GLN:N	2.30	0.65
1:B:304:GLN:OE1	1:B:304:GLN:N	2.30	0.65
1:B:372:ILE:CD1	1:B:385:TYR:HD2	2.09	0.64
1:B:473:VAL:O	1:B:477:ASN:ND2	2.31	0.64
1:A:307:ALA:CB	1:A:308:PRO:HD3	2.28	0.64
2:C:85:GLU:HG3	2:C:136:TYR:CE1	2.33	0.64
2:C:138:LEU:HD11	2:C:209:GLN:OE1	1.97	0.64
2:D:169:MET:CE	2:D:215:ILE:HD12	2.28	0.64
2:C:183:LEU:CD1	2:C:215:ILE:HG12	2.26	0.64
1:B:307:ALA:HB1	1:B:308:PRO:CD	2.22	0.63
2:D:122:VAL:O	2:D:124:HIS:CE1	2.51	0.63
2:C:85:GLU:CG	2:C:136:TYR:CE1	2.81	0.63
1:B:309:ARG:HH21	1:B:312:GLU:CG	2.12	0.63
1:B:295:TYR:HD1	1:B:316:TYR:CZ	2.17	0.62
1:B:302:LEU:CD1	1:B:302:LEU:C	2.68	0.62
2:C:138:LEU:N	2:C:138:LEU:HD22	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:TYR:CD1	1:B:316:TYR:CE1	2.87	0.62
1:B:456:LEU:CD1	1:B:474:ILE:HD12	2.30	0.62
2:C:12:ASP:O	2:C:15:THR:OG1	2.17	0.62
1:B:308:PRO:C	1:B:309:ARG:HG3	2.23	0.62
1:B:358:LEU:O	1:B:359:LYS:HG2	1.97	0.62
2:C:138:LEU:HB2	2:C:209:GLN:HB2	1.81	0.62
2:D:10:ARG:HB2	2:D:107:TRP:CD1	2.34	0.62
1:A:384:ARG:HA	1:A:387:LEU:HG	1.82	0.62
1:A:361:LYS:HE2	1:A:392:HIS:HB3	1.82	0.62
1:A:371:ALA:HB1	1:A:381:LEU:HD22	1.82	0.62
1:B:302:LEU:CD2	1:B:309:ARG:HH12	2.12	0.62
1:A:433:ASP:OD2	1:A:435:LYS:HG3	1.99	0.61
1:B:362:ASP:OD1	1:B:362:ASP:N	2.31	0.61
2:D:169:MET:HE2	2:D:215:ILE:CG1	2.29	0.61
1:A:482:GLU:HG3	1:A:488:ASN:HB3	1.82	0.61
1:B:379:VAL:HG23	1:B:420:ILE:CD1	2.30	0.61
1:B:379:VAL:HG23	1:B:420:ILE:CG1	2.30	0.61
2:C:124:HIS:HA	2:C:203:GLN:HG2	1.83	0.61
2:D:63:ASN:OD1	2:D:63:ASN:N	2.32	0.61
2:C:29:GLN:O	2:C:121:VAL:HG12	2.01	0.61
2:C:32:ALA:O	2:C:120:LYS:CB	2.49	0.61
1:B:458:GLN:HG3	1:B:459:GLU:OE1	2.02	0.60
2:D:65:PHE:HD2	2:D:67:GLY:H	1.49	0.60
1:A:404:GLU:OE2	1:A:451:ARG:NH2	2.34	0.60
1:B:303:LEU:O	1:B:303:LEU:CD1	2.30	0.59
2:C:32:ALA:O	2:C:120:LYS:HB2	2.03	0.59
2:C:135:VAL:HG12	2:C:136:TYR:N	2.17	0.59
2:D:185:ASN:HB2	2:D:195:LEU:HD21	1.84	0.59
2:C:137:LEU:HD11	2:C:156:PHE:CA	2.26	0.59
2:C:138:LEU:HD21	2:C:209:GLN:OE1	2.03	0.59
1:B:477:ASN:O	1:B:481:ILE:HG13	2.02	0.59
1:B:295:TYR:C	1:B:297:PRO:CD	2.62	0.59
2:C:162:ILE:HD13	2:C:195:LEU:CD1	2.33	0.59
2:C:128:VAL:O	2:C:130:HIS:HD2	1.85	0.59
2:C:138:LEU:CD2	2:C:209:GLN:HB2	2.32	0.58
2:D:107:TRP:HB3	2:D:108:TYR:HD1	1.68	0.58
1:A:490:GLN:HE22	2:C:28:LEU:HD13	1.69	0.58
2:D:118:VAL:O	2:D:119:ARG:NH1	2.33	0.58
2:C:143:CYS:HB3	2:C:214:VAL:HB	1.85	0.58
1:A:582:LYS:HE2	1:A:586:LYS:HE3	1.84	0.58
2:C:75:PHE:HE1	2:C:117:ILE:HD11	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:89:ASP:HB2	2:D:95:LEU:HD11	1.85	0.58
1:B:406:ALA:HB1	1:B:420:ILE:HD13	1.85	0.57
2:C:137:LEU:CG	2:C:156:PHE:O	2.51	0.57
1:B:379:VAL:CG2	1:B:420:ILE:HG13	2.34	0.57
1:B:488:ASN:OD1	1:B:491:LYS:HB2	2.03	0.57
1:B:299:GLU:C	1:B:302:LEU:HG	2.28	0.57
2:D:176:PRO:HD2	2:D:179:ARG:HH12	1.68	0.57
1:B:316:TYR:CD1	1:B:332:ILE:CD1	2.87	0.56
1:B:329:ILE:HD12	1:B:353:TYR:OH	2.05	0.56
2:C:175:ILE:HG12	2:C:179:ARG:HH21	1.71	0.56
1:B:302:LEU:HD22	1:B:309:ARG:HH12	1.70	0.56
1:B:472:CYS:HB2	1:B:499:ILE:HG23	1.88	0.56
2:C:143:CYS:SG	2:C:144:GLU:N	2.77	0.56
1:A:459:GLU:O	1:A:463:ARG:HG2	2.05	0.56
1:B:308:PRO:HB2	1:B:340:ASN:CG	2.30	0.55
1:B:309:ARG:HD2	1:B:313:TYR:CZ	2.39	0.55
1:B:320:GLU:OE2	1:B:332:ILE:HD11	2.06	0.55
1:B:309:ARG:HH21	1:B:312:GLU:HG3	1.71	0.55
2:C:169:MET:HE3	2:C:215:ILE:CD1	2.35	0.55
2:C:16:GLN:OE1	2:C:108:TYR:OH	2.20	0.55
1:B:307:ALA:CB	1:B:308:PRO:CD	2.81	0.55
2:C:166:GLU:O	2:C:170:ARG:HG3	2.07	0.55
2:D:169:MET:CE	2:D:215:ILE:CD1	2.85	0.55
2:D:124:HIS:CD2	2:D:158:LYS:NZ	2.75	0.54
1:B:560:GLU:O	1:B:564:ILE:HG13	2.07	0.54
1:A:302:LEU:O	1:A:309:ARG:HD3	2.08	0.54
1:B:308:PRO:O	1:B:309:ARG:HD3	2.06	0.54
1:B:299:GLU:O	1:B:302:LEU:HD11	2.08	0.54
1:B:499:ILE:O	1:B:504:ASN:HB2	2.08	0.54
2:C:122:VAL:HG13	2:C:134:GLU:HB2	1.90	0.54
2:C:197:LYS:HG3	2:C:199:ASP:H	1.73	0.53
2:D:39:SER:OG	2:D:91:LEU:O	2.24	0.53
1:B:454:GLU:O	1:B:458:GLN:HG2	2.09	0.53
1:B:456:LEU:HD11	1:B:474:ILE:CD1	2.38	0.53
1:B:295:TYR:CA	1:B:297:PRO:HD2	2.38	0.53
2:C:140:LEU:HD12	2:C:211:GLN:H	1.74	0.53
2:D:18:SER:O	2:D:22:PRO:HD2	2.09	0.53
2:D:119:ARG:HG3	2:D:135:VAL:HG22	1.89	0.53
1:A:582:LYS:HE3	1:A:586:LYS:CE	2.34	0.53
1:B:295:TYR:CD1	1:B:316:TYR:OH	2.62	0.53
2:D:179:ARG:HD3	2:D:218:GLN:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:ASP:OD1	2:C:13:ALA:N	2.41	0.53
1:B:372:ILE:HG23	1:B:382:TRP:CZ2	2.44	0.53
1:B:514:TYR:OH	1:B:518:GLU:OE1	2.19	0.53
2:D:169:MET:HE2	2:D:215:ILE:CD1	2.38	0.53
2:C:42:PHE:CE2	2:C:46:LYS:HE3	2.44	0.52
2:D:183:LEU:HB3	2:D:195:LEU:HD23	1.91	0.52
1:B:379:VAL:CG2	1:B:420:ILE:CG1	2.87	0.52
2:C:185:ASN:OD1	2:C:185:ASN:N	2.42	0.52
2:D:122:VAL:O	2:D:124:HIS:ND1	2.43	0.52
2:D:81:GLN:HE22	2:D:115:GLN:HB2	1.74	0.52
2:C:88:ILE:CG2	2:C:89:ASP:N	2.72	0.52
1:A:307:ALA:HB3	1:A:308:PRO:CD	2.39	0.52
1:B:543:GLU:O	1:B:547:GLU:HG2	2.10	0.51
2:C:124:HIS:CE1	2:C:132:LYS:HB3	2.44	0.51
1:A:387:LEU:HD13	1:A:391:ARG:HH22	1.75	0.51
1:A:458:GLN:HG2	1:A:459:GLU:OE1	2.11	0.51
2:C:101:TRP:O	2:C:105:LEU:N	2.39	0.51
2:C:162:ILE:HD13	2:C:195:LEU:HD21	1.93	0.51
2:D:183:LEU:HG	2:D:215:ILE:HG12	1.91	0.51
2:D:186:LYS:HE3	2:D:190:ASN:HA	1.93	0.51
2:C:29:GLN:O	2:C:32:ALA:HB3	2.06	0.51
2:C:88:ILE:O	2:C:93:TYR:CD2	2.64	0.51
1:B:469:ASP:OD2	1:B:473:VAL:N	2.44	0.50
2:D:124:HIS:CD2	2:D:158:LYS:HZ3	2.30	0.50
2:D:169:MET:HE3	2:D:215:ILE:HD12	1.93	0.50
2:D:134:GLU:OE1	2:D:157:SER:OG	2.25	0.50
2:C:35:TYR:HB2	2:C:96:VAL:HG13	1.93	0.50
2:C:86:HIS:H	2:C:136:TYR:HE1	1.48	0.50
2:C:169:MET:CE	2:C:215:ILE:HD12	2.37	0.49
1:A:583:ALA:O	1:A:586:LYS:O	2.30	0.49
1:B:482:GLU:HG2	1:B:491:LYS:HB3	1.94	0.49
1:B:433:ASP:CB	1:B:436:GLN:HE21	2.24	0.49
2:C:135:VAL:HG12	2:C:136:TYR:H	1.77	0.49
1:A:308:PRO:O	1:A:309:ARG:C	2.54	0.49
2:C:162:ILE:HD12	2:C:195:LEU:HD11	1.93	0.49
1:A:544:HIS:O	1:A:548:VAL:HG23	2.12	0.49
1:B:427:TYR:CZ	1:B:431:ARG:HD2	2.47	0.49
1:B:291:GLN:HA	1:B:294:LYS:HE3	1.94	0.49
2:D:15:THR:O	2:D:19:GLU:HG2	2.12	0.49
2:D:17:LYS:HB2	2:D:49:VAL:HG12	1.95	0.49
1:A:562:TRP:O	1:A:566:VAL:HG23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:183:LEU:CD1	2:C:215:ILE:CG1	2.83	0.48
2:C:32:ALA:O	2:C:120:LYS:HA	2.14	0.48
2:C:117:ILE:O	2:C:117:ILE:HG22	2.12	0.48
2:D:145:ASN:OD1	2:D:146:SER:N	2.46	0.48
2:D:12:ASP:O	2:D:16:GLN:HG3	2.14	0.48
2:C:138:LEU:HD23	2:C:209:GLN:HB2	1.94	0.48
1:A:285:TYR:O	1:A:289:LEU:HD13	2.14	0.48
1:A:302:LEU:HD12	1:A:303:LEU:N	2.29	0.48
1:B:411:PHE:CE1	1:B:420:ILE:CD1	2.97	0.48
2:C:145:ASN:OD1	2:C:182:ARG:NH2	2.47	0.48
1:A:453:LEU:HD21	1:A:475:MET:HG2	1.96	0.47
1:B:399:ILE:HD12	1:B:427:TYR:CZ	2.48	0.47
2:C:138:LEU:CD1	2:C:209:GLN:HE22	2.25	0.47
2:D:120:LYS:O	2:D:134:GLU:HG2	2.14	0.47
1:B:316:TYR:CE1	1:B:332:ILE:HD11	2.49	0.47
1:B:575:ARG:O	1:B:578:GLU:HB3	2.14	0.47
1:A:456:LEU:CD2	1:A:474:ILE:CD1	2.70	0.47
1:A:555:THR:HG21	1:B:480:ARG:HD2	1.96	0.47
1:A:379:VAL:CG2	1:A:416:ASP:HB3	2.42	0.47
2:C:75:PHE:HA	2:C:83:LEU:HA	1.97	0.47
2:C:121:VAL:HA	2:C:133:VAL:HA	1.97	0.47
1:A:417:TYR:OH	1:A:463:ARG:NH1	2.47	0.47
2:C:162:ILE:HG21	2:C:195:LEU:CD2	2.22	0.47
1:B:320:GLU:CD	1:B:332:ILE:HD11	2.40	0.46
1:B:325:ASP:O	1:B:329:ILE:HG13	2.15	0.46
2:D:126:LEU:HB2	2:D:127:PHE:CD2	2.50	0.46
1:B:300:GLU:C	1:B:303:LEU:H	2.23	0.46
1:B:302:LEU:CB	1:B:309:ARG:HH12	2.24	0.46
1:B:316:TYR:CE1	1:B:332:ILE:CD1	2.98	0.46
2:D:11:PRO:HD2	2:D:107:TRP:CE2	2.50	0.46
2:D:143:CYS:HB3	2:D:151:VAL:HG12	1.98	0.46
1:A:415:THR:O	1:A:418:VAL:HG22	2.15	0.46
2:D:16:GLN:HG2	2:D:107:TRP:CE2	2.50	0.46
1:A:348:ILE:O	1:A:352:GLN:HB3	2.15	0.46
1:A:454:GLU:HG3	1:A:455:TYR:N	2.30	0.46
1:B:290:GLN:HG2	1:B:291:GLN:N	2.31	0.46
2:C:175:ILE:HG23	2:C:179:ARG:NE	2.29	0.46
2:C:88:ILE:HG22	2:C:89:ASP:H	1.78	0.46
1:A:507:TYR:HB2	1:A:510:MET:HB2	1.97	0.46
2:D:152:LEU:HD22	2:D:172:LEU:HD21	1.97	0.46
1:A:504:ASN:HB3	1:A:510:MET:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:TYR:CD1	1:B:316:TYR:HE1	2.34	0.46
2:D:57:TYR:CD1	2:D:58:ASN:N	2.84	0.45
2:D:138:LEU:O	2:D:155:HIS:HA	2.16	0.45
1:B:496:TRP:HZ3	1:B:510:MET:HG3	1.81	0.45
2:D:198:LEU:H	2:D:198:LEU:HD23	1.80	0.45
1:B:295:TYR:CE1	1:B:316:TYR:HE1	2.35	0.45
1:B:481:ILE:HG23	1:B:485:LEU:HD12	1.97	0.45
1:B:300:GLU:HA	1:B:303:LEU:HB3	1.98	0.45
1:B:566:VAL:O	1:B:570:GLU:HG2	2.16	0.45
2:D:179:ARG:HB2	2:D:218:GLN:HB3	1.97	0.45
2:C:134:GLU:C	2:C:135:VAL:HG23	2.41	0.45
1:B:456:LEU:HD13	1:B:474:ILE:HD12	1.99	0.45
1:A:281:VAL:HG22	1:A:282:ILE:H	1.77	0.45
1:A:307:ALA:CB	1:A:308:PRO:CD	2.94	0.45
1:B:475:MET:HE1	1:B:498:SER:HB3	1.99	0.45
1:A:334:GLU:O	1:A:338:VAL:HG23	2.17	0.45
2:D:197:LYS:HE3	2:D:200:ASN:HB3	1.99	0.45
1:B:418:VAL:HG23	1:B:474:ILE:HD11	1.99	0.45
1:B:434:PHE:CD1	1:B:485:LEU:HB3	2.52	0.45
1:A:281:VAL:O	1:A:282:ILE:C	2.60	0.44
1:B:344:PRO:O	1:B:348:ILE:HG13	2.17	0.44
2:C:162:ILE:HD13	2:C:195:LEU:CD2	2.47	0.44
2:D:38:ASP:OD1	2:D:40:ARG:HG3	2.17	0.44
1:A:469:ASP:OD1	1:A:473:VAL:HG22	2.17	0.44
1:A:519:ARG:NH2	1:B:516:ASN:HB3	2.32	0.44
2:D:13:ALA:HB1	2:D:49:VAL:HA	1.98	0.44
2:D:173:PHE:HD1	2:D:173:PHE:HA	1.64	0.44
2:D:25:ARG:HG3	2:D:26:THR:N	2.31	0.44
1:B:528:ARG:HG2	1:B:553:GLU:OE2	2.16	0.44
2:C:69:ILE:HD11	2:C:104:LEU:HG	1.99	0.44
2:D:22:PRO:O	2:D:25:ARG:HG2	2.18	0.44
2:C:100:ALA:O	2:C:104:LEU:HB3	2.18	0.44
2:C:144:GLU:HB2	2:C:173:PHE:CE2	2.53	0.44
2:C:12:ASP:HB3	2:C:15:THR:HG23	1.99	0.44
2:C:88:ILE:CG2	2:C:89:ASP:H	2.31	0.44
2:C:138:LEU:N	2:C:138:LEU:CD2	2.79	0.44
1:B:308:PRO:HB2	1:B:340:ASN:ND2	2.33	0.43
2:C:124:HIS:NE2	2:C:132:LYS:HB3	2.33	0.43
2:C:29:GLN:O	2:C:121:VAL:HG11	2.11	0.43
2:C:35:TYR:CG	2:C:101:TRP:CD1	3.06	0.43
2:C:139:GLU:OE1	2:C:155:HIS:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:169:MET:HE3	2:C:169:MET:HB2	1.76	0.43
1:B:300:GLU:O	1:B:303:LEU:CB	2.64	0.43
1:B:395:ASP:HB3	1:B:398:VAL:HG12	2.01	0.43
2:C:173:PHE:O	2:C:175:ILE:HG13	2.17	0.43
1:B:295:TYR:HD1	1:B:316:TYR:OH	1.99	0.43
1:B:337:LEU:HD22	1:B:347:TRP:CE2	2.53	0.43
1:B:376:PRO:O	1:B:382:TRP:CH2	2.71	0.43
1:B:456:LEU:CD1	1:B:474:ILE:CD1	2.95	0.43
1:A:317:ILE:HG12	1:A:332:ILE:HD11	1.99	0.43
1:A:317:ILE:CG1	1:A:332:ILE:CD1	2.95	0.43
1:B:482:GLU:HG3	1:B:488:ASN:HB3	2.00	0.43
2:C:137:LEU:CD1	2:C:156:PHE:N	2.81	0.43
2:D:138:LEU:HD22	2:D:156:PHE:HD2	1.84	0.43
2:C:134:GLU:C	2:C:135:VAL:CG2	2.91	0.42
1:A:353:TYR:CE1	1:A:357:GLN:HG3	2.54	0.42
2:C:166:GLU:HA	2:C:169:MET:HE3	1.99	0.42
2:C:183:LEU:HD13	2:C:215:ILE:CD1	2.49	0.42
2:C:183:LEU:HB3	2:C:195:LEU:HD23	2.00	0.42
2:C:50:GLY:HA3	2:C:56:MET:HG2	2.00	0.42
2:C:85:GLU:HA	2:C:136:TYR:CE1	2.39	0.42
2:C:162:ILE:O	2:C:166:GLU:N	2.47	0.42
2:D:38:ASP:CG	2:D:40:ARG:HG3	2.44	0.42
1:A:387:LEU:HD13	1:A:391:ARG:NH2	2.34	0.42
1:A:427:TYR:CZ	1:A:431:ARG:HD2	2.55	0.42
1:B:314:GLN:OE1	1:B:349:ARG:NH2	2.52	0.42
2:C:121:VAL:HG22	2:C:122:VAL:N	2.34	0.42
1:A:317:ILE:O	1:A:321:MET:HG3	2.18	0.42
2:C:169:MET:HB3	2:C:215:ILE:HD12	2.02	0.42
1:A:475:MET:HE1	1:A:498:SER:HB3	2.02	0.42
2:C:75:PHE:CE1	2:C:117:ILE:HD11	2.53	0.42
2:D:160:ASP:O	2:D:202:VAL:HG23	2.19	0.42
1:B:299:GLU:O	1:B:302:LEU:HD12	2.10	0.42
2:C:89:ASP:HA	2:C:93:TYR:CZ	2.55	0.42
2:C:138:LEU:HD12	2:C:209:GLN:HE22	1.79	0.42
2:D:119:ARG:HA	2:D:119:ARG:HD3	1.81	0.42
2:D:142:LEU:H	2:D:142:LEU:HG	1.52	0.42
1:A:376:PRO:HD2	1:A:377:TRP:CE3	2.55	0.42
1:A:559:LEU:HD11	1:B:391:ARG:HG2	2.02	0.42
1:B:294:LYS:O	1:B:297:PRO:CD	2.68	0.42
2:C:44:GLN:HE21	2:C:65:PHE:C	2.27	0.42
2:C:101:TRP:HZ3	2:C:105:LEU:HG	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ILE:O	1:B:352:GLN:HB2	2.20	0.41
2:C:45:TRP:NE1	2:C:108:TYR:OH	2.51	0.41
1:A:411:PHE:HB2	1:A:417:TYR:CE1	2.56	0.41
2:D:23:LEU:HD13	2:D:97:PRO:HD2	2.02	0.41
2:D:59:VAL:C	2:D:61:GLU:H	2.27	0.41
2:C:65:PHE:CD1	2:C:66:PRO:HD2	2.55	0.41
2:D:169:MET:O	2:D:173:PHE:HB2	2.21	0.41
1:A:306:GLU:O	1:A:309:ARG:HG3	2.17	0.41
1:B:321:MET:HE3	1:B:321:MET:HB2	1.97	0.41
1:B:360:VAL:O	1:B:364:VAL:HG13	2.21	0.41
2:C:33:GLN:O	2:C:98:THR:HG23	2.20	0.41
2:D:46:LYS:O	2:D:50:GLY:N	2.52	0.41
1:A:325:ASP:HA	1:A:326:PRO:HD2	1.80	0.41
1:B:572:ARG:HH11	1:B:575:ARG:HH21	1.69	0.41
1:A:426:ASP:OD1	1:B:554:ARG:NH1	2.54	0.41
1:A:439:SER:O	1:A:442:LEU:HB3	2.20	0.41
1:A:580:ARG:HD3	1:A:580:ARG:HA	1.81	0.41
1:A:420:ILE:HG23	1:A:421:TRP:N	2.35	0.41
1:B:395:ASP:OD1	1:B:396:HIS:N	2.54	0.41
1:B:504:ASN:CG	1:B:510:MET:HE2	2.45	0.41
2:C:29:GLN:C	2:C:121:VAL:CG1	2.93	0.41
2:C:32:ALA:O	2:C:120:LYS:CA	2.68	0.41
2:C:137:LEU:HD12	2:C:156:PHE:C	2.29	0.41
2:D:54:TRP:CE3	2:D:54:TRP:N	2.89	0.41
1:B:379:VAL:HG21	1:B:416:ASP:O	2.21	0.41
1:B:456:LEU:HA	1:B:460:VAL:HG22	2.03	0.41
2:D:35:TYR:CE1	2:D:118:VAL:HG22	2.56	0.41
2:D:45:TRP:O	2:D:49:VAL:HG23	2.21	0.41
2:D:126:LEU:HB2	2:D:127:PHE:HD2	1.86	0.41
2:C:175:ILE:HG23	2:C:179:ARG:CZ	2.52	0.40
2:D:165:ILE:O	2:D:169:MET:HG2	2.20	0.40
1:B:577:ASN:HA	1:B:580:ARG:HG2	2.03	0.40
1:B:307:ALA:O	1:B:309:ARG:CB	2.70	0.40
1:B:399:ILE:CD1	1:B:427:TYR:CZ	3.04	0.40
1:B:533:ARG:HE	1:B:533:ARG:HB3	1.63	0.40
2:C:138:LEU:CG	2:C:209:GLN:CB	2.71	0.40
1:B:542:PRO:O	1:B:545:VAL:HG22	2.21	0.40
1:B:554:ARG:CZ	1:B:554:ARG:HB3	2.51	0.40
2:C:162:ILE:CG2	2:C:195:LEU:HD21	2.22	0.40
2:C:162:ILE:CD1	2:C:195:LEU:CD1	2.87	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:GLN:OE1	1:B:361:LYS:CE[5_544]	1.73	0.47
1:A:280:SER:OG	2:C:18:SER:OG[5_544]	2.08	0.12

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	306/338 (90%)	295 (96%)	11 (4%)	0	100	100
1	B	303/338 (90%)	295 (97%)	7 (2%)	1 (0%)	36	68
2	C	204/233 (88%)	184 (90%)	18 (9%)	2 (1%)	12	43
2	D	210/233 (90%)	199 (95%)	10 (5%)	1 (0%)	24	59
All	All	1023/1142 (90%)	973 (95%)	46 (4%)	4 (0%)	30	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	308	PRO
2	C	59	VAL
2	C	26	THR
2	D	22	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	271/294 (92%)	260 (96%)	11 (4%)	27	60
1	B	268/294 (91%)	244 (91%)	24 (9%)	9	32
2	C	188/209 (90%)	167 (89%)	21 (11%)	6	23
2	D	194/209 (93%)	163 (84%)	31 (16%)	2	12
All	All	921/1006 (92%)	834 (91%)	87 (9%)	8	30

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	SER
1	A	289	LEU
1	A	296	LYS
1	A	302	LEU
1	A	332	ILE
1	A	352	GLN
1	A	378	THR
1	A	387	LEU
1	A	418	VAL
1	A	436	GLN
1	A	439	SER
1	B	281	VAL
1	B	290	GLN
1	B	294	LYS
1	B	300	GLU
1	B	302	LEU
1	B	303	LEU
1	B	304	GLN
1	B	310	LEU
1	B	345	ASP
1	B	362	ASP
1	B	381	LEU
1	B	387	LEU
1	B	398	VAL
1	B	405	LYS
1	B	425	LEU
1	B	436	GLN
1	B	439	SER
1	B	456	LEU
1	B	491	LYS
1	B	524	THR
1	B	535	VAL
1	B	558	SER

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Mol	Chain	Res	Type
1	B	559	LEU
1	B	573	LEU
2	C	14	GLU
2	C	33	GLN
2	C	44	GLN
2	C	59	VAL
2	C	79	GLU
2	C	94	VAL
2	C	96	VAL
2	C	101	TRP
2	C	104	LEU
2	C	122	VAL
2	C	134	GLU
2	C	137	LEU
2	C	138	LEU
2	C	158	LYS
2	C	164	THR
2	C	169	MET
2	C	181	THR
2	C	182	ARG
2	C	197	LYS
2	C	209	GLN
2	C	214	VAL
2	D	20	LEU
2	D	23	LEU
2	D	24	MET
2	D	26	THR
2	D	36	LEU
2	D	53	SER
2	D	54	TRP
2	D	57	TYR
2	D	58	ASN
2	D	59	VAL
2	D	62	HIS
2	D	63	ASN
2	D	64	LEU
2	D	72	SER
2	D	77	ASP
2	D	83	LEU
2	D	85	GLU
2	D	91	LEU
2	D	95	LEU

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Mol	Chain	Res	Type
2	D	107	TRP
2	D	112	GLU
2	D	118	VAL
2	D	124	HIS
2	D	126	LEU
2	D	133	VAL
2	D	142	LEU
2	D	149	THR
2	D	178	GLU
2	D	195	LEU
2	D	204	ASP
2	D	214	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	GLN
1	A	465	ASN
1	B	291	GLN
1	B	396	HIS
1	B	476	GLN
1	B	525	GLN
2	C	130	HIS
2	D	33	GLN
2	D	124	HIS
2	D	185	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 oligosaccharides 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, 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	308/338 (91%)	0.05	4 (1%) 75 53	24, 74, 127, 201	0
1	B	305/338 (90%)	0.23	11 (3%) 46 26	24, 89, 149, 191	0
2	C	206/233 (88%)	0.72	16 (7%) 19 10	24, 147, 215, 238	0
2	D	212/233 (90%)	0.49	16 (7%) 20 10	24, 111, 203, 227	0
All	All	1031/1142 (90%)	0.33	47 (4%) 37 20	24, 96, 196, 238	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	215	ILE	4.6
1	B	559	LEU	4.3
2	C	59	VAL	4.3
2	D	172	LEU	4.2
2	C	207	LEU	3.9
2	D	217	PRO	3.6
1	B	372	ILE	3.5
2	C	213	LEU	3.5
2	D	126	LEU	3.4
1	B	584	ALA	3.3
2	D	218	GLN	3.3
2	C	169	MET	3.1
2	C	212	VAL	3.1
1	A	393	GLY	3.0
2	D	203	GLN	3.0
2	D	157	SER	3.0
2	D	206	GLY	2.9
1	A	339	GLU	2.9
2	C	152	LEU	2.9
2	D	173	PHE	2.9
2	D	152	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	316	TYR	2.8
1	A	364	VAL	2.7
1	B	545	VAL	2.7
1	B	309	ARG	2.6
1	B	306	GLU	2.6
2	C	78	PRO	2.5
1	A	306	GLU	2.5
1	B	558	SER	2.5
2	D	185	ASN	2.4
2	D	70	ASP	2.4
1	B	420	ILE	2.3
2	C	175	ILE	2.3
2	C	60	GLY	2.2
2	D	156	PHE	2.2
2	C	165	ILE	2.2
2	D	215	ILE	2.2
1	B	317	ILE	2.1
2	D	158	LYS	2.1
2	C	69	ILE	2.1
2	D	137	LEU	2.1
1	B	519	ARG	2.1
2	C	37	ILE	2.1
2	C	74	LEU	2.1
2	C	151	VAL	2.1
2	C	181	THR	2.0
2	D	109	GLY	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 oligosaccharides in this entry.

6.4 Ligands [\(i\)](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.