



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:42 PM UTC

PDB ID : 2ZU6 / pdb_00002zu6
Title : crystal structure of the eIF4A-PDCD4 complex
Authors : Cho, Y.; Chang, J.H.; Sohn, S.Y.
Deposited on : 2008-10-13
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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

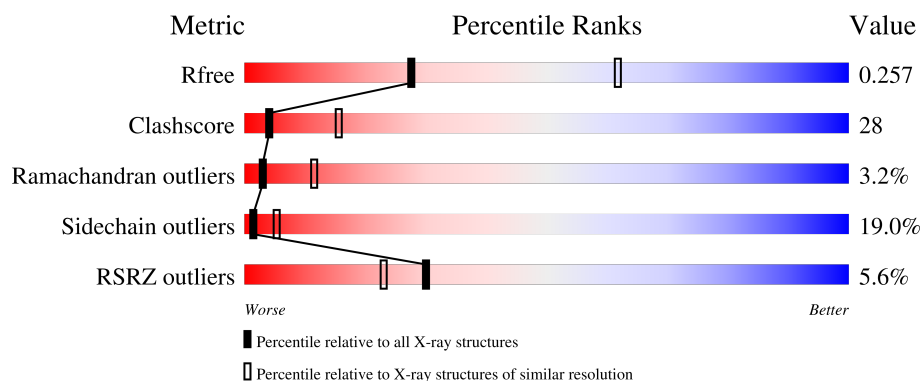
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	388	3% 43% 35% 10% • 12%
1	C	388	9% 38% 39% 13% • 10%
1	D	388	6% 41% 34% 12% • 11%
1	F	388	8% 30% 31% 7% • 30%
2	B	307	• 53% 35% 5% 7%

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Mol	Chain	Length	Quality of chain
2	E	307	 A horizontal bar chart showing the quality of chain E. The bar is divided into four segments: green (46%), yellow (38%), orange (8%), and grey (8%).

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14986 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 Eukaryotic initiation factor 4A-I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2743	1734	477	514	18			
1	C	351	Total	C	N	O	S	0	0	0
			2819	1778	492	531	18			
1	D	345	Total	C	N	O	S	0	0	0
			2756	1742	480	516	18			
1	F	271	Total	C	N	O	S	0	0	0
			2196	1389	381	411	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	expression tag	UNP P60842
C	19	MET	-	expression tag	UNP P60842
D	19	MET	-	expression tag	UNP P60842
F	19	MET	-	expression tag	UNP P60842

- Molecule 2 is a protein called Programmed cell death protein 4.

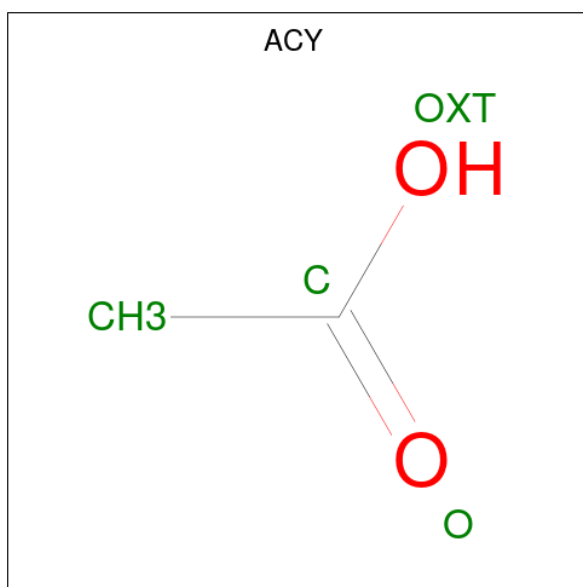
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	284	Total	C	N	O	S	Se	0	0	0
			2218	1403	366	434	6	9			
2	E	282	Total	C	N	O	S	Se	0	0	0
			2201	1393	363	430	6	9			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		

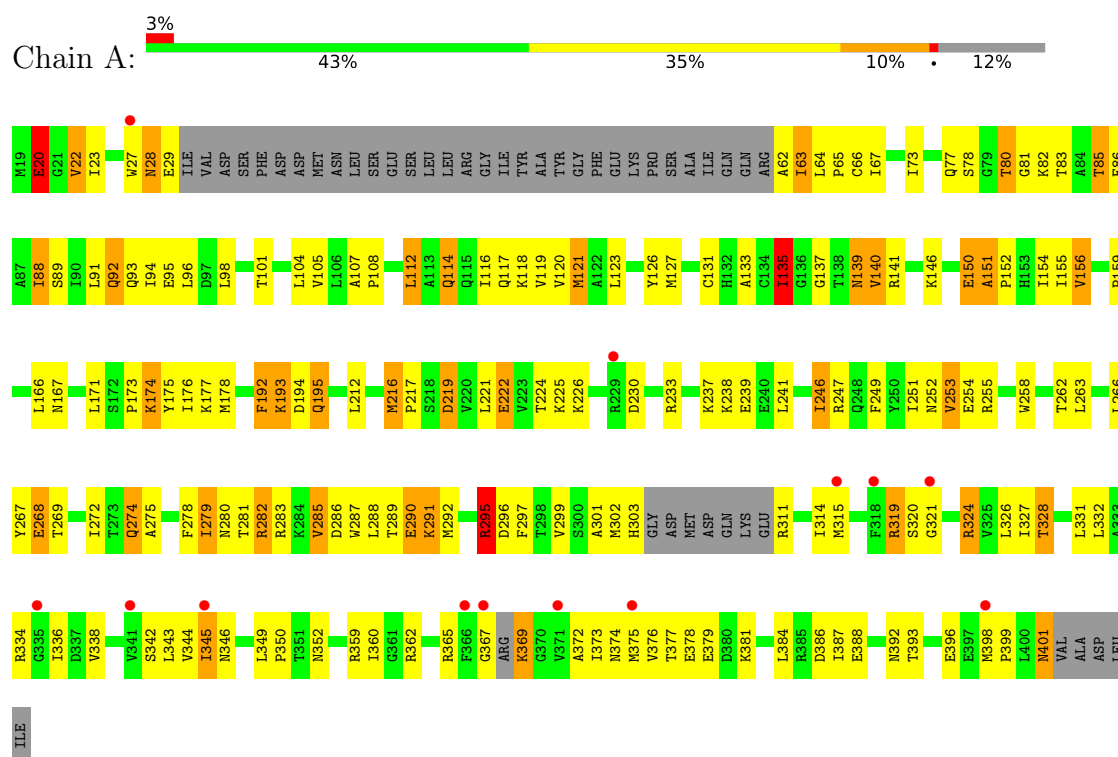
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	6	Total	O	0	0
			6	6		
5	C	3	Total	O	0	0
			3	3		
5	D	11	Total	O	0	0
			11	11		
5	E	2	Total	O	0	0
			2	2		

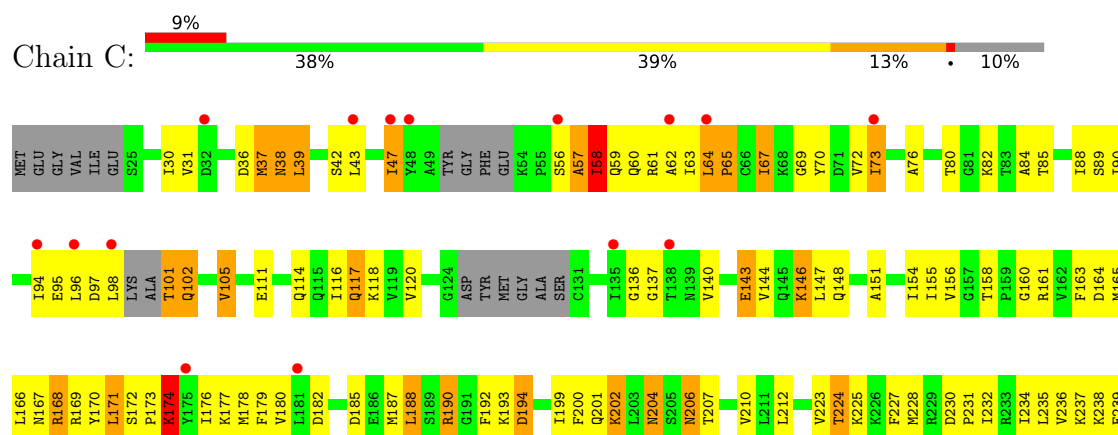
3 Residue-property plots

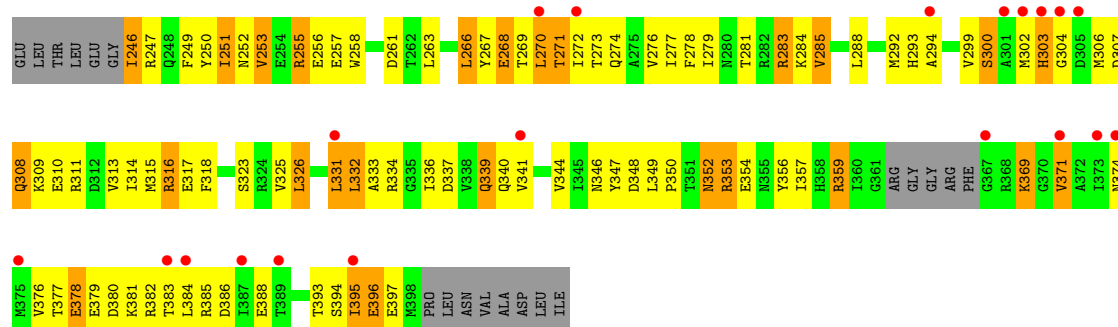
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Eukaryotic initiation factor 4A-I

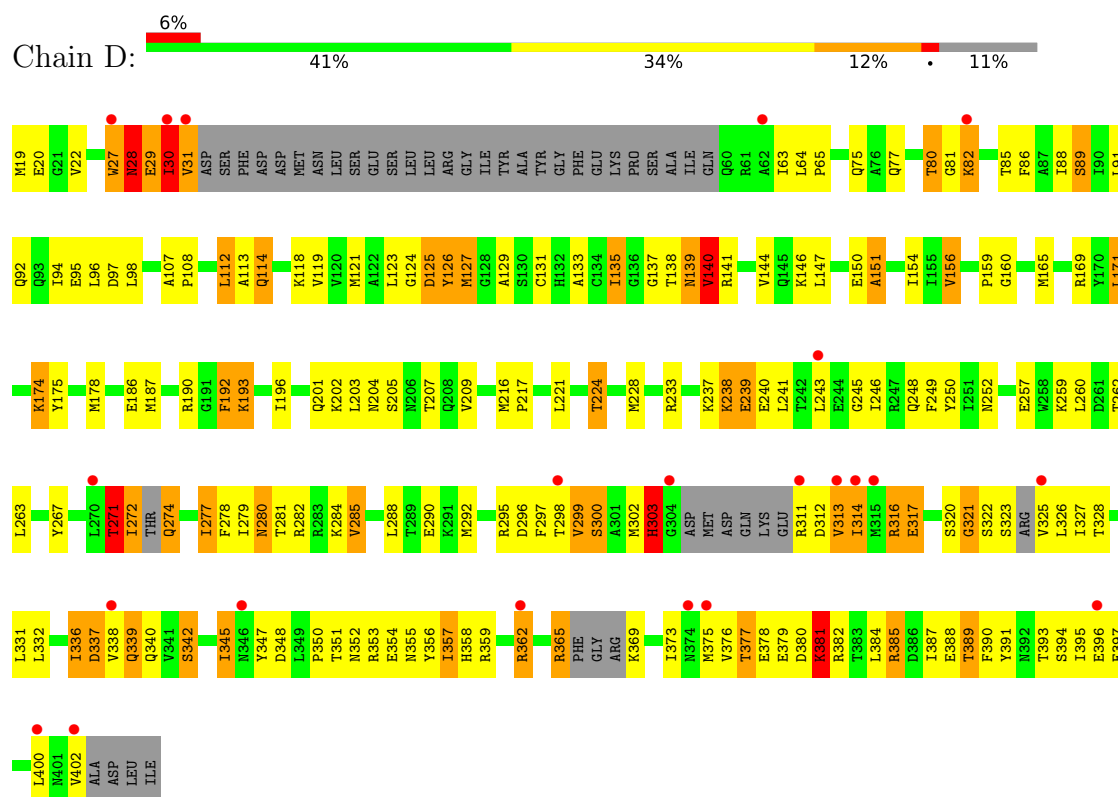


• Molecule 1: Eukaryotic initiation factor 4A-I

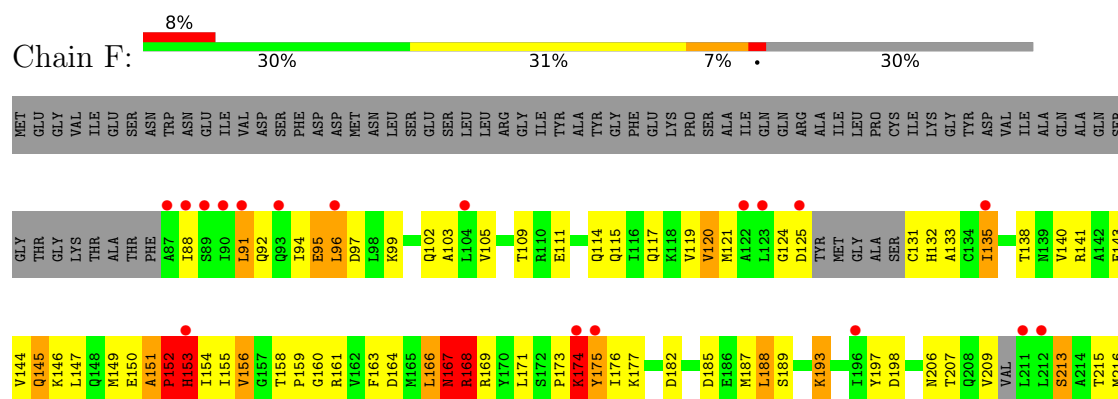


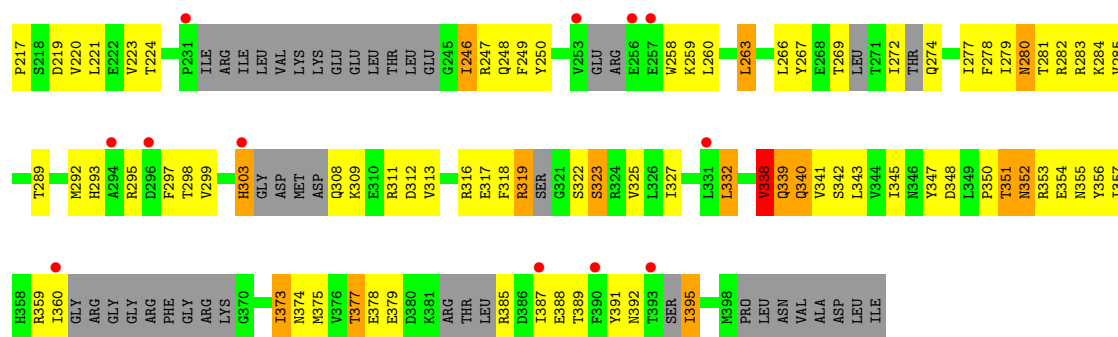


• Molecule 1: Eukaryotic initiation factor 4A-I

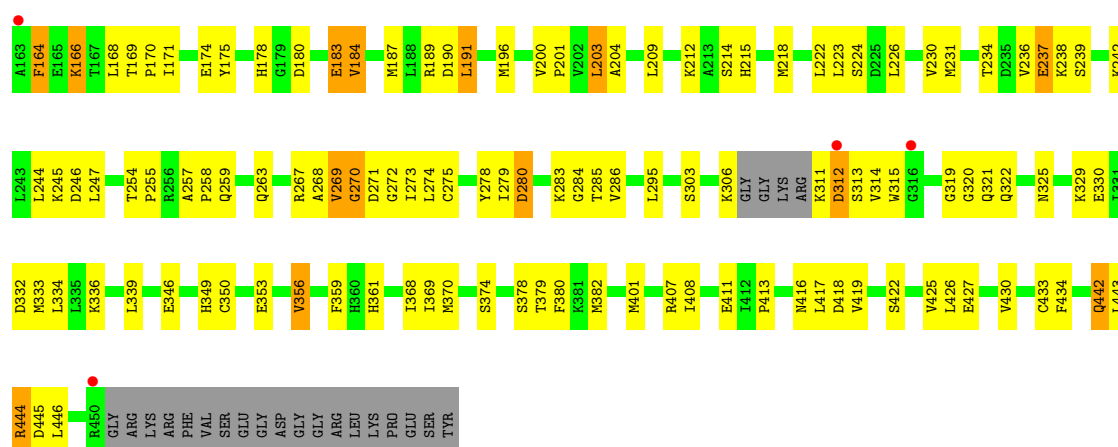


• Molecule 1: Eukaryotic initiation factor 4A-I

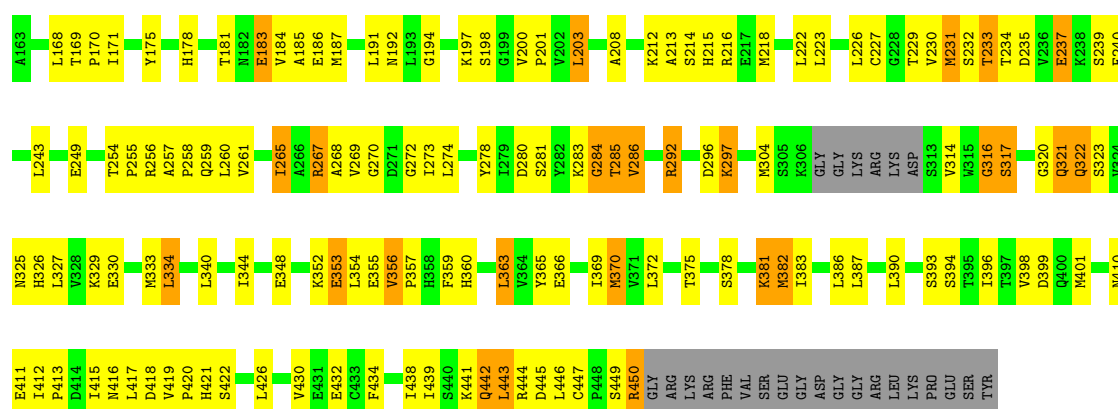




• Molecule 2: Programmed cell death protein 4



• Molecule 2: Programmed cell death protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	156.89Å 165.38Å 100.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.80) 94.1 (50.00-2.81)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.248 , 0.294 0.248 , 0.257	Depositor DCC
R_{free} test set	3260 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	60.9	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14986	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.83% 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](#)

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

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	0.98	4/2781 (0.1%)	1.18	17/3750 (0.5%)
1	C	0.52	0/2855	0.82	0/3846
1	D	0.91	1/2791 (0.0%)	1.15	13/3761 (0.3%)
1	F	0.55	0/2218	0.84	4/2978 (0.1%)
2	B	0.83	0/2244	1.01	4/3015 (0.1%)
2	E	0.81	0/2227	1.06	4/2993 (0.1%)
All	All	0.79	5/15116 (0.0%)	1.02	42/20343 (0.2%)

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	F	0	1
2	E	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	PHE	N-CA	11.53	1.60	1.46
1	A	193	LYS	C-O	7.47	1.32	1.24
1	A	107	ALA	CA-CB	-7.28	1.45	1.54
1	A	23	ILE	CA-CB	-6.26	1.46	1.54
1	D	107	ALA	CA-CB	-5.90	1.46	1.54

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	LYS	N-CA-C	12.23	124.60	111.03
1	F	151	ALA	CA-C-N	8.35	130.27	119.84
1	F	151	ALA	C-N-CA	8.35	130.27	119.84
1	D	336	ILE	N-CA-C	8.08	119.04	107.88
1	D	107	ALA	CA-C-N	-7.75	111.73	119.56
1	D	107	ALA	C-N-CA	-7.75	111.73	119.56
1	D	192	PHE	N-CA-C	7.59	126.97	110.80
1	A	107	ALA	CA-C-N	-7.33	112.13	120.04
1	A	107	ALA	C-N-CA	-7.33	112.13	120.04
1	A	226	LYS	N-CA-C	7.27	120.07	111.71
1	A	81	GLY	N-CA-C	-7.20	105.73	114.66
1	D	139	ASN	N-CA-C	7.18	120.91	112.72
2	B	313	SER	N-CA-C	6.81	119.17	107.93
2	E	285	THR	N-CA-C	-6.68	107.01	114.62
1	F	280	ASN	N-CA-C	6.54	121.41	113.17
1	A	151	ALA	CA-C-N	-6.53	113.56	120.03
1	A	151	ALA	C-N-CA	-6.53	113.56	120.03
1	A	192	PHE	CA-C-O	6.51	127.59	119.59
1	D	299	VAL	N-CA-C	6.15	116.97	107.99
1	D	81	GLY	N-CA-C	-6.12	104.94	112.77
1	D	303	HIS	N-CA-C	6.11	117.52	108.60
2	E	267	ARG	N-CA-C	-6.04	104.78	111.36
1	D	140	VAL	CB-CA-C	-6.03	104.16	111.88
1	A	139	ASN	N-CA-C	5.93	119.27	112.57
1	A	22	VAL	CB-CA-C	-5.62	100.90	111.30
1	F	248	GLN	N-CA-C	5.57	117.43	107.80
1	A	135	ILE	CB-CA-C	5.53	116.07	110.65
1	D	342	SER	N-CA-C	5.49	120.10	113.41
1	A	193	LYS	CA-C-O	5.21	126.26	120.90
2	E	356	VAL	CA-C-N	5.21	124.66	119.24
2	E	356	VAL	C-N-CA	5.21	124.66	119.24
2	B	209	LEU	N-CA-C	-5.18	106.46	112.89
1	D	205	SER	N-CA-C	5.13	119.01	112.34
1	D	193	LYS	N-CA-C	-5.10	104.99	111.11
1	A	230	ASP	CA-C-N	-5.07	115.01	120.03
1	A	230	ASP	C-N-CA	-5.07	115.01	120.03
1	A	20	GLU	N-CA-C	5.07	116.89	108.02
1	A	295	ARG	N-CA-C	-5.05	106.26	114.09
1	A	195	GLN	N-CA-CB	5.05	118.11	110.28
1	D	160	GLY	N-CA-C	5.04	118.35	112.50
2	B	315	TRP	CA-C-N	-5.02	116.07	122.19
2	B	315	TRP	C-N-CA	-5.02	116.07	122.19

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	286	VAL	Peptide
2	E	316	GLY	Peptide
1	F	152	PRO	Peptide

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	2743	0	2792	160	0
1	C	2819	0	2865	213	0
1	D	2756	0	2811	154	0
1	F	2196	0	2220	127	0
2	B	2218	0	2231	86	0
2	E	2201	0	2214	125	0
3	A	8	0	12	1	0
3	D	4	0	6	0	0
4	A	4	0	3	1	0
4	D	4	0	3	0	0
5	A	11	0	0	0	0
5	B	6	0	0	0	0
5	C	3	0	0	1	0
5	D	11	0	0	1	0
5	E	2	0	0	1	0
All	All	14986	0	15157	831	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (831) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ILE:HD13	1:C:284:LYS:HB3	1.25	1.15
1:F:115:GLN:O	1:F:119:VAL:HG23	1.48	1.14
2:E:442:GLN:H	2:E:442:GLN:NE2	1.45	1.14
2:B:339:LEU:HD11	2:B:370:MSE:HE3	1.29	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:ILE:HD12	1:C:224:THR:HG21	1.22	1.13
2:E:286:VAL:HG21	2:E:292:ARG:HE	1.10	1.10
2:E:442:GLN:HE21	2:E:442:GLN:N	1.48	1.09
1:C:369:LYS:HE2	1:C:369:LYS:HA	1.36	1.08
1:A:77:GLN:OE1	1:A:238:LYS:HD3	1.50	1.08
1:D:389:THR:HG21	5:D:18:HOH:O	1.54	1.07
1:A:121:MET:HA	1:A:121:MET:CE	1.85	1.07
1:A:121:MET:HA	1:A:121:MET:HE2	1.09	1.07
2:B:442:GLN:H	2:B:442:GLN:NE2	1.51	1.07
1:A:290:GLU:OE1	1:A:290:GLU:HA	1.55	1.06
1:A:345:ILE:HD11	1:A:375:MET:HE3	1.38	1.05
2:B:442:GLN:HE21	2:B:442:GLN:N	1.54	1.05
1:C:378:GLU:HA	1:C:381:LYS:HD3	1.37	1.05
1:A:279:ILE:HD11	1:A:327:ILE:CG2	1.87	1.04
1:A:279:ILE:HD11	1:A:327:ILE:HG22	1.39	1.04
2:B:171:ILE:HG23	2:B:187:MSE:HE3	1.40	1.03
2:E:434:PHE:HE1	2:E:441:LYS:HA	1.22	1.03
1:A:350:PRO:HD3	1:A:359:ARG:NH1	1.73	1.02
1:C:272:ILE:HG21	1:C:274:GLN:HE21	1.20	1.01
1:C:272:ILE:HG21	1:C:274:GLN:NE2	1.76	1.00
1:C:147:LEU:HA	1:C:151:ALA:HB3	1.44	1.00
1:C:272:ILE:CG2	1:C:274:GLN:HE21	1.77	0.96
2:E:212:LYS:H	2:E:215:HIS:HD2	1.10	0.96
2:B:212:LYS:H	2:B:215:HIS:HD2	1.15	0.94
2:B:442:GLN:H	2:B:442:GLN:HE21	1.03	0.93
2:E:434:PHE:CE1	2:E:441:LYS:HA	2.03	0.93
1:D:300:SER:O	1:D:326:LEU:HD12	1.68	0.92
1:D:165:MET:HB3	1:D:171:LEU:HD22	1.52	0.92
1:D:377:THR:H	1:D:380:ASP:HB2	1.31	0.91
2:E:212:LYS:H	2:E:215:HIS:CD2	1.88	0.90
2:E:286:VAL:HG21	2:E:292:ARG:NE	1.86	0.90
1:D:351:THR:CB	2:E:321:GLN:HE22	1.85	0.90
1:A:62:ALA:HB1	1:A:88:ILE:HG21	1.54	0.89
1:C:147:LEU:HA	1:C:151:ALA:CB	2.00	0.89
1:A:94:ILE:HD11	1:A:154:ILE:HD11	1.53	0.89
1:C:58:ILE:HD12	1:C:236:VAL:HG23	1.52	0.89
1:D:281:THR:HG21	2:E:183:GLU:HG3	1.55	0.88
1:F:94:ILE:HG12	1:F:95:GLU:H	1.40	0.87
1:F:395:ILE:HG13	1:F:395:ILE:O	1.71	0.87
1:D:312:ASP:O	1:D:316:ARG:HB2	1.75	0.87
1:C:82:LYS:HE2	1:C:212:LEU:HB3	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:ARG:HB2	1:D:297:PHE:HE2	1.39	0.87
1:A:377:THR:O	1:A:381:LYS:HG3	1.75	0.87
2:E:357:PRO:HA	2:E:360:HIS:CE1	2.10	0.86
1:C:73:ILE:HD12	1:C:224:THR:CG2	2.03	0.86
2:E:434:PHE:HE1	2:E:441:LYS:CA	1.89	0.85
1:C:172:SER:HB2	1:C:174:LYS:HD2	1.59	0.84
1:C:378:GLU:HA	1:C:381:LYS:CD	2.06	0.84
1:A:290:GLU:OE1	1:A:290:GLU:CA	2.26	0.83
1:A:222:GLU:HA	1:A:222:GLU:OE1	1.78	0.83
1:A:275:ALA:HB2	1:A:343:LEU:HD23	1.58	0.83
1:F:188:LEU:HD23	1:F:220:VAL:HG22	1.60	0.83
1:A:98:LEU:HD21	1:A:175:TYR:CD1	2.14	0.83
2:E:230:VAL:HG13	2:E:231:MSE:HG3	1.61	0.83
1:A:290:GLU:C	1:A:292:MET:H	1.88	0.82
2:B:311:LYS:HG3	2:B:312:ASP:H	1.44	0.82
1:A:290:GLU:O	1:A:292:MET:N	2.13	0.81
1:A:295:ARG:HG3	1:A:295:ARG:HH11	1.45	0.81
1:D:187:MET:HE3	1:D:196:ILE:HD11	1.64	0.80
1:A:350:PRO:HD3	1:A:359:ARG:HH11	1.45	0.80
1:D:28:ASN:HB2	1:D:30:ILE:HD12	1.64	0.79
1:D:351:THR:HB	2:E:321:GLN:HE22	1.46	0.79
1:C:352:ASN:HA	1:C:353:ARG:NH1	1.97	0.79
1:D:302:MET:HB2	1:D:328:THR:HG22	1.63	0.79
2:B:353:GLU:OE1	1:C:283:ARG:NH2	2.14	0.79
2:B:215:HIS:HA	2:B:218:MSE:HE3	1.63	0.78
1:C:270:LEU:HD12	1:C:272:ILE:H	1.47	0.78
1:C:62:ALA:HA	1:C:65:PRO:HG2	1.66	0.78
1:C:73:ILE:CD1	1:C:224:THR:HG21	2.11	0.78
1:F:188:LEU:HD12	1:F:193:LYS:HG2	1.64	0.78
1:A:141:ARG:NH2	2:E:281:SER:OG	2.16	0.78
1:A:345:ILE:CD1	1:A:375:MET:HE3	2.14	0.77
1:A:27:TRP:CZ3	1:A:29:GLU:HB2	2.19	0.77
2:B:212:LYS:H	2:B:215:HIS:CD2	2.01	0.77
2:B:339:LEU:HD11	2:B:370:MSE:CE	2.13	0.77
1:D:282:ARG:HH21	1:D:332:LEU:HD11	1.49	0.76
1:C:178:MET:HE3	1:C:179:PHE:H	1.49	0.76
1:A:77:GLN:O	1:A:80:THR:HG22	1.85	0.76
2:E:412:ILE:HG23	2:E:413:PRO:HD3	1.68	0.76
1:C:270:LEU:HG	1:C:271:THR:H	1.51	0.76
1:D:75:GLN:HB2	1:D:216:MET:CE	2.16	0.76
1:A:377:THR:HG22	1:A:378:GLU:N	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:279:ILE:HD11	1:F:285:VAL:HG23	1.67	0.75
1:A:295:ARG:HG3	1:A:295:ARG:NH1	2.00	0.75
2:E:212:LYS:N	2:E:215:HIS:HD2	1.84	0.75
1:C:303:HIS:O	1:C:332:LEU:HD22	1.87	0.74
2:B:339:LEU:CD1	2:B:370:MSE:HE3	2.14	0.74
1:D:376:VAL:HG11	1:D:384:LEU:HD22	1.69	0.74
1:C:253:VAL:HG23	1:C:255:ARG:O	1.88	0.74
1:A:121:MET:HE2	1:A:121:MET:CA	2.05	0.73
1:C:39:LEU:HB3	1:C:43:LEU:HD13	1.69	0.73
1:D:339:GLN:HB2	1:D:362:ARG:CG	2.19	0.73
1:C:353:ARG:HH11	1:C:353:ARG:H	1.35	0.72
1:D:174:LYS:HG2	1:D:175:TYR:CE2	2.24	0.72
1:F:279:ILE:HD11	1:F:285:VAL:CG2	2.19	0.72
1:F:274:GLN:HE22	1:F:342:SER:HB2	1.55	0.72
2:B:183:GLU:O	2:B:187:MSE:HG3	1.89	0.71
1:A:274:GLN:HA	1:A:324:ARG:O	1.90	0.71
1:C:279:ILE:HD11	1:C:285:VAL:HG23	1.73	0.71
1:D:357:ILE:HB	1:D:391:TYR:CE2	2.25	0.71
1:A:239:GLU:OE1	1:A:365:ARG:HG3	1.91	0.70
1:A:275:ALA:CB	1:A:343:LEU:HD23	2.22	0.70
1:C:146:LYS:O	1:C:151:ALA:HB2	1.91	0.70
1:C:369:LYS:HE2	1:C:369:LYS:CA	2.19	0.70
1:F:91:LEU:HD11	1:F:120:VAL:HG13	1.72	0.69
1:C:190:ARG:CG	1:C:190:ARG:HH11	2.05	0.69
1:D:295:ARG:HB2	1:D:297:PHE:CE2	2.26	0.69
1:F:91:LEU:O	1:F:94:ILE:HG22	1.92	0.69
1:F:354:GLU:H	1:F:354:GLU:CD	2.01	0.69
1:A:108:PRO:HD2	1:A:112:LEU:HD12	1.73	0.69
2:B:269:VAL:O	2:B:272:GLY:N	2.21	0.68
1:D:388:GLU:HB2	1:D:395:ILE:HD12	1.73	0.68
1:F:299:VAL:HG23	1:F:325:VAL:HB	1.76	0.68
2:E:304:MSE:HA	1:F:293:HIS:CE1	2.29	0.68
2:B:166:LYS:HD3	2:B:166:LYS:N	2.07	0.68
1:C:309:LYS:HB3	1:C:310:GLU:OE1	1.93	0.68
1:F:278:PHE:HB3	1:F:359:ARG:HH21	1.59	0.68
1:C:58:ILE:HD13	1:C:76:ALA:HB2	1.76	0.67
1:D:353:ARG:HG3	1:D:353:ARG:HH11	1.59	0.67
1:F:167:ASN:HD22	1:F:168:ARG:N	1.92	0.67
1:A:62:ALA:CB	1:A:88:ILE:HG21	2.23	0.67
1:C:167:ASN:C	1:C:169:ARG:H	2.02	0.67
1:D:350:PRO:HD3	1:D:359:ARG:CZ	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:356:VAL:HG13	2:B:359:PHE:HB3	1.77	0.67
2:E:417:LEU:HB3	1:F:161:ARG:HB3	1.77	0.67
1:F:279:ILE:HD11	1:F:281:THR:O	1.94	0.67
1:F:278:PHE:HB3	1:F:359:ARG:NH2	2.10	0.67
1:C:313:VAL:O	1:C:316:ARG:HD2	1.94	0.66
1:A:290:GLU:C	1:A:292:MET:N	2.52	0.66
1:C:148:GLN:HE22	1:C:170:TYR:HA	1.60	0.66
2:E:442:GLN:H	2:E:442:GLN:HE21	0.72	0.66
1:A:62:ALA:HB3	1:A:92:GLN:NE2	2.11	0.65
1:C:64:LEU:HD12	1:C:65:PRO:HD3	1.78	0.65
1:D:288:LEU:O	1:D:292:MET:HG2	1.96	0.65
1:C:279:ILE:HD12	1:C:281:THR:H	1.61	0.65
1:F:166:LEU:HG	1:F:171:LEU:HD23	1.79	0.65
2:B:426:LEU:O	2:B:430:VAL:HG23	1.95	0.65
1:D:108:PRO:HD2	1:D:112:LEU:HD12	1.79	0.65
1:C:270:LEU:HG	1:C:271:THR:N	2.11	0.65
1:F:338:VAL:HA	1:F:341:VAL:HG21	1.79	0.65
1:A:282:ARG:O	1:A:285:VAL:HG12	1.95	0.65
1:F:272:ILE:HG21	1:F:274:GLN:HE21	1.62	0.65
1:A:251:ILE:HG22	1:A:253:VAL:HG23	1.78	0.64
1:D:385:ARG:NE	1:D:388:GLU:OE1	2.28	0.64
1:C:116:ILE:O	1:C:120:VAL:HG23	1.96	0.64
2:E:449:SER:O	2:E:450:ARG:C	2.39	0.64
1:D:339:GLN:HB2	1:D:362:ARG:HG3	1.79	0.64
1:F:131:CYS:SG	1:F:132:HIS:N	2.69	0.64
1:D:281:THR:CG2	2:E:183:GLU:HG3	2.25	0.64
2:E:240:PHE:CE1	2:E:265:ILE:HG13	2.33	0.64
1:F:132:HIS:CD2	1:F:146:LYS:NZ	2.66	0.64
1:A:83:THR:HG22	1:A:85:THR:H	1.61	0.64
1:C:247:ARG:HB3	1:C:371:VAL:HG13	1.80	0.64
1:D:302:MET:CB	1:D:328:THR:HG22	2.27	0.64
1:F:163:PHE:CE1	1:F:198:ASP:HB3	2.33	0.64
1:F:278:PHE:CB	1:F:359:ARG:HH21	2.11	0.63
2:B:418:ASP:OD2	1:C:161:ARG:NH1	2.30	0.63
1:D:250:TYR:HD2	1:D:395:ILE:HG22	1.61	0.63
2:E:240:PHE:CD1	2:E:265:ILE:HG13	2.34	0.63
1:C:57:ALA:C	1:C:59:GLN:H	2.06	0.63
1:A:94:ILE:CD1	1:A:154:ILE:HD11	2.28	0.63
1:A:222:GLU:OE1	1:A:222:GLU:CA	2.47	0.62
1:D:278:PHE:CG	1:D:359:ARG:HD3	2.34	0.62
1:A:78:SER:HA	3:A:3:EDO:H21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:MET:HB3	1:C:171:LEU:HD22	1.79	0.62
1:A:174:LYS:HG2	1:A:175:TYR:CE2	2.35	0.62
1:A:343:LEU:HD11	1:A:373:ILE:HD12	1.80	0.62
1:D:27:TRP:HA	1:D:237:LYS:O	1.99	0.62
2:B:175:TYR:HA	2:B:178:HIS:CE1	2.35	0.62
2:B:442:GLN:NE2	2:B:442:GLN:N	2.25	0.62
1:C:64:LEU:N	1:C:65:PRO:HD2	2.14	0.62
2:E:197:LYS:HD3	2:E:231:MSE:HA	1.81	0.62
2:E:198:SER:O	2:E:239:SER:OG	2.15	0.62
1:C:303:HIS:H	1:C:303:HIS:CD2	2.18	0.62
2:B:246:ASP:O	2:B:247:LEU:C	2.43	0.62
2:B:332:ASP:OD2	2:B:336:LYS:HE2	1.99	0.62
1:C:279:ILE:HD11	1:C:281:THR:O	2.00	0.62
1:A:252:ASN:OD1	1:A:252:ASN:O	2.18	0.62
1:C:251:ILE:HG13	1:C:252:ASN:N	2.13	0.61
1:A:253:VAL:HG13	1:A:258:TRP:HB3	1.82	0.61
2:E:327:LEU:O	2:E:330:GLU:N	2.32	0.61
1:D:121:MET:HA	1:D:121:MET:HE2	1.81	0.61
1:D:144:VAL:HG22	1:D:165:MET:HE1	1.82	0.61
1:D:313:VAL:O	1:D:317:GLU:OE2	2.18	0.61
1:D:376:VAL:CG1	1:D:384:LEU:HD22	2.31	0.61
2:E:426:LEU:CD2	2:E:447:CYS:SG	2.89	0.61
2:E:426:LEU:HD23	2:E:447:CYS:SG	2.40	0.61
1:C:31:VAL:HB	1:C:63:ILE:HG21	1.82	0.61
1:C:352:ASN:HA	1:C:353:ARG:HH12	1.63	0.61
1:C:377:THR:HG23	1:C:379:GLU:H	1.66	0.61
1:A:289:THR:OG1	1:A:301:ALA:HB2	2.01	0.61
1:D:30:ILE:HG21	1:D:64:LEU:HD21	1.83	0.61
2:E:215:HIS:HA	2:E:218:MSE:HE3	1.82	0.61
1:D:239:GLU:HG2	1:D:365:ARG:HG3	1.83	0.61
1:D:121:MET:HE1	1:D:129:ALA:O	2.01	0.60
1:F:103:ALA:HB3	1:F:154:ILE:HG12	1.83	0.60
1:C:266:LEU:O	1:C:270:LEU:N	2.34	0.60
1:F:332:LEU:HG	1:F:332:LEU:O	2.01	0.60
1:C:30:ILE:HG22	1:C:61:ARG:HG2	1.81	0.60
1:C:303:HIS:CE1	1:C:306:MET:HB2	2.36	0.60
1:C:279:ILE:CG1	1:C:285:VAL:HG23	2.31	0.60
1:D:388:GLU:HA	1:D:393:THR:HG22	1.83	0.60
1:F:164:ASP:O	1:F:167:ASN:HB3	2.01	0.60
1:F:102:GLN:HA	1:F:175:TYR:O	2.01	0.60
1:C:246:ILE:HG23	1:C:246:ILE:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:PHE:HD2	1:D:396:GLU:HB2	1.67	0.60
1:D:351:THR:HB	2:E:321:GLN:NE2	2.16	0.60
1:A:150:GLU:O	1:A:151:ALA:C	2.43	0.60
1:A:321:GLY:HA3	1:A:324:ARG:HD2	1.82	0.59
1:C:310:GLU:O	1:C:313:VAL:HG12	2.02	0.59
2:B:212:LYS:N	2:B:215:HIS:HD2	1.92	0.59
1:C:388:GLU:OE2	1:C:394:SER:HA	2.01	0.59
1:C:58:ILE:HD12	1:C:236:VAL:CG2	2.30	0.59
1:C:384:LEU:C	1:C:384:LEU:HD23	2.28	0.59
2:B:418:ASP:OD1	1:C:158:THR:OG1	2.19	0.59
1:D:339:GLN:CB	1:D:362:ARG:HG3	2.31	0.59
2:E:366:GLU:O	2:E:370:MSE:HG3	2.01	0.59
1:A:62:ALA:CB	1:A:88:ILE:CG2	2.81	0.59
1:D:64:LEU:HB3	1:D:65:PRO:HD2	1.85	0.59
1:C:234:ILE:HG22	1:C:235:LEU:N	2.18	0.59
1:C:250:TYR:OH	1:C:397:GLU:HG2	2.03	0.59
1:A:295:ARG:HB3	1:A:297:PHE:HE2	1.67	0.59
1:D:88:ILE:O	1:D:92:GLN:HG2	2.03	0.59
1:F:284:LYS:HE3	1:F:348:ASP:OD1	2.02	0.59
1:A:114:GLN:HE21	1:A:114:GLN:CA	2.16	0.59
1:A:377:THR:CG2	1:A:378:GLU:N	2.65	0.59
1:C:200:PHE:C	1:C:202:LYS:H	2.10	0.59
2:B:236:VAL:HG12	2:B:274:LEU:HD12	1.84	0.58
1:D:82:LYS:O	1:D:119:VAL:HG21	2.03	0.58
1:A:278:PHE:HB2	1:A:346:ASN:HD22	1.66	0.58
1:C:72:VAL:HG22	1:C:210:VAL:HG22	1.86	0.58
1:A:279:ILE:HD11	1:A:327:ILE:HG23	1.80	0.58
1:A:377:THR:O	1:A:381:LYS:CG	2.50	0.58
1:D:209:VAL:HG12	1:D:228:MET:HE3	1.83	0.58
1:C:279:ILE:CD1	1:C:285:VAL:HG23	2.34	0.58
1:F:166:LEU:HA	1:F:171:LEU:HB3	1.85	0.58
2:E:320:GLY:C	2:E:322:GLN:H	2.12	0.58
1:F:279:ILE:HD13	1:F:284:LYS:HG2	1.85	0.58
1:C:249:PHE:CD2	1:C:397:GLU:O	2.57	0.58
1:C:271:THR:O	1:C:271:THR:HG23	2.03	0.58
2:E:383:ILE:O	2:E:387:LEU:HG	2.04	0.58
1:D:80:THR:O	1:D:86:PHE:HB2	2.04	0.57
1:D:144:VAL:CG2	1:D:165:MET:HE1	2.34	0.57
1:D:320:SER:O	1:D:321:GLY:C	2.47	0.57
1:D:272:ILE:HB	1:D:274:GLN:N	2.20	0.57
2:E:208:ALA:HB1	2:E:216:ARG:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:261:VAL:HG12	2:E:265:ILE:HD12	1.86	0.57
1:F:132:HIS:CD2	1:F:146:LYS:HZ1	2.22	0.57
1:D:249:PHE:CD2	1:D:396:GLU:HB2	2.39	0.57
2:B:187:MSE:O	2:B:191:LEU:HD13	2.04	0.57
1:C:178:MET:HE3	1:C:179:PHE:N	2.19	0.57
1:D:121:MET:HE3	1:D:131:CYS:HB3	1.86	0.57
1:A:319:ARG:NE	1:A:320:SER:HB2	2.20	0.57
1:C:288:LEU:O	1:C:292:MET:HG2	2.05	0.57
1:F:168:ARG:HB2	1:F:168:ARG:HH11	1.70	0.57
1:F:168:ARG:HB2	1:F:168:ARG:NH1	2.19	0.57
2:B:164:PHE:O	2:B:168:LEU:HD23	2.04	0.57
1:C:172:SER:HB2	1:C:174:LYS:CD	2.33	0.57
2:E:222:LEU:O	2:E:226:LEU:HG	2.05	0.57
2:E:268:ALA:HB3	2:E:274:LEU:HD22	1.86	0.57
1:F:99:LYS:CE	1:F:150:GLU:HB2	2.34	0.57
1:F:357:ILE:HG23	1:F:391:TYR:OH	2.05	0.56
2:B:356:VAL:HG13	2:B:356:VAL:O	2.05	0.56
1:D:357:ILE:HB	1:D:391:TYR:HE2	1.70	0.56
2:B:180:ASP:OD1	2:B:183:GLU:HB2	2.06	0.56
1:C:167:ASN:C	1:C:169:ARG:N	2.63	0.56
1:D:221:LEU:O	1:D:224:THR:HB	2.05	0.56
1:D:238:LYS:NZ	1:D:238:LYS:HB3	2.19	0.56
1:D:279:ILE:HD11	1:D:288:LEU:HD22	1.87	0.56
1:C:173:PRO:C	1:C:176:ILE:HD13	2.31	0.56
1:C:223:VAL:O	1:C:227:PHE:HB2	2.04	0.56
2:B:333:MSE:HE3	2:B:333:MSE:HA	1.88	0.56
1:C:339:GLN:CD	1:C:340:GLN:H	2.14	0.56
1:A:167:ASN:O	1:A:167:ASN:CG	2.49	0.56
1:C:105:VAL:HG13	1:C:180:VAL:HB	1.88	0.56
1:F:206:ASN:OD1	1:F:207:THR:N	2.38	0.56
1:F:279:ILE:CG1	1:F:285:VAL:HG22	2.35	0.56
1:A:401:ASN:OD1	1:A:401:ASN:N	2.38	0.56
1:C:56:SER:HA	1:C:60:GLN:HE21	1.71	0.56
1:C:333:ALA:HA	1:C:336:ILE:HG23	1.86	0.56
2:E:365:TYR:CZ	2:E:369:ILE:HD11	2.40	0.56
2:B:283:LYS:O	2:B:285:THR:HG23	2.06	0.56
1:C:37:MET:HE2	1:C:39:LEU:HD11	1.87	0.56
1:C:353:ARG:NH1	1:C:353:ARG:H	2.04	0.56
1:D:352:ASN:HB3	1:D:355:ASN:ND2	2.21	0.56
1:F:154:ILE:HG22	1:F:155:ILE:N	2.20	0.56
1:C:57:ALA:C	1:C:59:GLN:N	2.63	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ILE:HD11	1:A:362:ARG:NE	2.21	0.55
1:C:314:ILE:HA	1:C:317:GLU:HG2	1.88	0.55
1:F:94:ILE:HG12	1:F:95:GLU:N	2.18	0.55
1:A:279:ILE:CD1	1:A:327:ILE:CG2	2.74	0.55
1:C:114:GLN:O	1:C:117:GLN:HG3	2.07	0.55
1:C:168:ARG:C	1:C:170:TYR:H	2.13	0.55
1:C:101:THR:O	1:C:176:ILE:HG13	2.06	0.55
1:C:165:MET:CB	1:C:171:LEU:HD22	2.36	0.55
1:A:319:ARG:HE	1:A:320:SER:HB2	1.72	0.55
1:A:345:ILE:C	1:A:345:ILE:HD13	2.32	0.55
1:D:377:THR:N	1:D:380:ASP:HB2	2.14	0.55
1:F:272:ILE:HD12	1:F:272:ILE:H	1.70	0.55
1:F:377:THR:HG23	1:F:379:GLU:H	1.70	0.55
1:A:350:PRO:CD	1:A:359:ARG:NH1	2.60	0.55
1:A:377:THR:HG22	1:A:379:GLU:H	1.69	0.55
1:C:72:VAL:HG12	1:C:232:ILE:HB	1.88	0.55
1:A:193:LYS:HG2	1:A:194:ASP:N	2.22	0.55
1:A:219:ASP:OD1	1:A:219:ASP:N	2.37	0.55
1:A:280:ASN:ND2	1:A:359:ARG:HH22	2.05	0.55
1:C:177:LYS:HA	1:C:207:THR:HG22	1.89	0.55
2:E:283:LYS:O	2:E:284:GLY:C	2.50	0.55
2:B:280:ASP:OD2	2:B:280:ASP:N	2.40	0.55
1:D:353:ARG:HG3	1:D:353:ARG:NH1	2.22	0.55
1:C:31:VAL:HG21	1:C:64:LEU:HD21	1.90	0.54
1:C:143:GLU:O	1:C:146:LYS:HB3	2.07	0.54
1:C:395:ILE:HG12	1:C:395:ILE:O	2.06	0.54
1:F:103:ALA:HB3	1:F:154:ILE:HG23	1.89	0.54
1:F:182:ASP:O	1:F:187:MET:HE2	2.07	0.54
1:C:167:ASN:O	1:C:169:ARG:N	2.39	0.54
1:A:254:GLU:O	1:A:377:THR:HG23	2.08	0.54
1:D:165:MET:HB3	1:D:171:LEU:CD2	2.33	0.54
2:B:356:VAL:O	2:B:356:VAL:CG1	2.56	0.54
1:C:182:ASP:O	1:C:187:MET:HE2	2.08	0.54
1:F:95:GLU:OE2	1:F:97:ASP:HB3	2.07	0.54
1:F:318:PHE:HA	1:F:323:SER:OG	2.07	0.54
1:A:114:GLN:HA	1:A:114:GLN:NE2	2.23	0.54
2:E:387:LEU:HB3	2:E:401:MSE:HE1	1.90	0.54
1:F:281:THR:O	1:F:285:VAL:HG23	2.07	0.54
1:C:267:TYR:HA	1:C:270:LEU:HD23	1.88	0.54
1:C:300:SER:HB3	1:C:326:LEU:HD23	1.89	0.54
2:B:333:MSE:HE3	2:B:333:MSE:CA	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:LEU:C	1:C:334:ARG:H	2.14	0.53
1:D:63:ILE:HG23	1:D:92:GLN:HE22	1.73	0.53
1:A:249:PHE:HA	1:A:396:GLU:O	2.08	0.53
2:E:378:SER:OG	2:E:382:MSE:HE2	2.08	0.53
1:A:221:LEU:O	1:A:224:THR:HB	2.08	0.53
1:C:333:ALA:HA	1:C:336:ILE:CG2	2.38	0.53
1:F:308:GLN:HB3	1:F:311:ARG:NH1	2.24	0.53
1:C:350:PRO:HG3	1:C:359:ARG:CZ	2.38	0.53
2:E:419:VAL:O	2:E:422:SER:HB3	2.08	0.53
1:F:152:PRO:HG3	1:F:155:ILE:HD11	1.90	0.53
1:D:281:THR:HG21	2:E:183:GLU:CG	2.36	0.53
2:E:171:ILE:HD11	2:E:187:MSE:HE2	1.90	0.53
1:C:65:PRO:O	1:C:70:TYR:HB2	2.09	0.53
1:C:346:ASN:HD22	1:C:374:ASN:ND2	2.06	0.53
1:F:246:ILE:O	1:F:246:ILE:HG13	2.07	0.53
1:A:93:GLN:O	1:A:177:LYS:NZ	2.37	0.53
2:E:393:SER:O	2:E:394:SER:HB2	2.07	0.53
1:F:152:PRO:HB3	1:F:155:ILE:HD11	1.90	0.53
1:A:27:TRP:O	1:A:28:ASN:C	2.53	0.52
1:A:344:VAL:O	1:A:372:ALA:HA	2.09	0.52
1:C:332:LEU:C	1:C:334:ARG:N	2.68	0.52
1:D:88:ILE:O	1:D:89:SER:C	2.52	0.52
1:D:353:ARG:NE	2:E:322:GLN:O	2.42	0.52
1:A:63:ILE:O	1:A:63:ILE:CG1	2.57	0.52
1:A:268:GLU:O	1:A:269:THR:C	2.52	0.52
1:D:278:PHE:HB3	1:D:359:ARG:NH1	2.24	0.52
2:E:283:LYS:O	2:E:285:THR:HG23	2.08	0.52
1:F:207:THR:O	1:F:209:VAL:HG23	2.09	0.52
1:C:206:ASN:H	1:C:206:ASN:ND2	2.07	0.52
1:C:303:HIS:CD2	1:C:303:HIS:N	2.78	0.52
1:D:75:GLN:HB2	1:D:216:MET:HE2	1.88	0.52
1:C:251:ILE:CG1	1:C:252:ASN:N	2.72	0.52
1:C:293:HIS:O	1:C:294:ALA:C	2.52	0.52
1:D:352:ASN:HB3	1:D:355:ASN:HD22	1.73	0.52
1:F:167:ASN:C	1:F:169:ARG:H	2.18	0.52
1:D:356:TYR:O	1:D:359:ARG:HB2	2.10	0.52
1:F:339:GLN:C	1:F:341:VAL:H	2.17	0.52
1:A:80:THR:O	1:A:86:PHE:HB2	2.10	0.52
1:C:57:ALA:HB3	1:C:59:GLN:HE21	1.75	0.52
1:F:247:ARG:HG2	1:F:249:PHE:HE1	1.75	0.52
2:E:412:ILE:O	2:E:416:ASN:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LEU:HG	1:A:288:LEU:O	2.10	0.52
1:D:125:ASP:N	1:D:125:ASP:OD1	2.43	0.52
1:F:117:GLN:HG2	1:F:133:ALA:HB2	1.91	0.52
1:F:279:ILE:CD1	1:F:281:THR:O	2.58	0.52
2:B:169:THR:HB	2:B:170:PRO:HD3	1.92	0.52
1:C:37:MET:HG2	1:C:39:LEU:HG	1.92	0.52
2:E:201:PRO:HG2	2:E:239:SER:OG	2.10	0.52
2:E:269:VAL:O	2:E:272:GLY:N	2.42	0.52
2:E:356:VAL:HG13	2:E:356:VAL:O	2.10	0.52
2:E:390:LEU:HD13	2:E:396:ILE:HD12	1.92	0.52
1:F:274:GLN:NE2	1:F:342:SER:HB2	2.23	0.52
1:F:105:VAL:HB	1:F:156:VAL:HB	1.92	0.52
1:A:63:ILE:O	1:A:63:ILE:HD12	2.10	0.51
1:A:302:MET:HB3	1:A:328:THR:HG23	1.91	0.51
1:C:61:ARG:HD2	1:C:234:ILE:HG23	1.91	0.51
1:D:146:LYS:O	1:D:147:LEU:C	2.53	0.51
1:D:278:PHE:CD1	1:D:359:ARG:HD3	2.45	0.51
2:E:233:THR:O	2:E:237:GLU:OE2	2.27	0.51
1:F:350:PRO:HG2	1:F:356:TYR:HB2	1.92	0.51
1:A:377:THR:HG22	1:A:378:GLU:H	1.72	0.51
1:D:98:LEU:HD21	1:D:175:TYR:CD1	2.45	0.51
1:D:385:ARG:O	1:D:389:THR:HG22	2.10	0.51
2:E:413:PRO:O	2:E:416:ASN:HB3	2.11	0.51
2:B:269:VAL:O	2:B:271:ASP:N	2.44	0.51
1:F:115:GLN:O	1:F:119:VAL:CG2	2.39	0.51
1:F:154:ILE:CG2	1:F:155:ILE:N	2.73	0.51
1:A:116:ILE:O	1:A:120:VAL:HG23	2.11	0.51
1:A:252:ASN:O	1:A:253:VAL:O	2.29	0.51
1:C:166:LEU:HD23	1:C:171:LEU:HB3	1.92	0.51
1:C:190:ARG:CG	1:C:190:ARG:NH1	2.69	0.51
1:D:147:LEU:HG	1:D:171:LEU:HD11	1.93	0.51
1:D:377:THR:CG2	1:D:378:GLU:N	2.73	0.51
1:F:279:ILE:HG22	1:F:347:TYR:HB3	1.93	0.51
2:B:189:ARG:C	2:B:191:LEU:H	2.18	0.51
2:B:236:VAL:HG12	2:B:274:LEU:CD1	2.41	0.51
2:B:319:GLY:C	2:B:321:GLN:H	2.18	0.51
1:D:190:ARG:O	2:E:255:PRO:HG2	2.11	0.51
1:A:117:GLN:NE2	1:A:121:MET:HG3	2.25	0.51
1:C:251:ILE:HD12	1:C:252:ASN:H	1.75	0.51
1:C:315:MET:SD	1:C:337:ASP:OD2	2.69	0.51
1:A:252:ASN:HA	1:A:376:VAL:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:LYS:HE3	1:D:138:THR:O	2.10	0.51
1:F:308:GLN:HA	1:F:311:ARG:HD3	1.91	0.51
1:A:63:ILE:O	1:A:63:ILE:HG13	2.09	0.51
1:D:77:GLN:O	1:D:80:THR:HG22	2.11	0.51
2:E:412:ILE:HA	2:E:415:ILE:HD12	1.92	0.51
2:B:189:ARG:HG3	2:B:189:ARG:HH11	1.74	0.51
1:C:63:ILE:HG23	1:C:64:LEU:HG	1.93	0.51
1:C:276:VAL:HG22	1:C:326:LEU:HB3	1.92	0.51
1:D:357:ILE:HG23	1:D:358:HIS:N	2.26	0.51
1:F:279:ILE:HD12	1:F:281:THR:H	1.76	0.51
1:F:319:ARG:HB2	1:F:340:GLN:OE1	2.12	0.51
1:C:94:ILE:HG12	1:C:95:GLU:N	2.26	0.50
1:D:27:TRP:O	1:D:28:ASN:C	2.54	0.50
1:D:336:ILE:HG13	1:D:337:ASP:N	2.26	0.50
1:C:270:LEU:HD12	1:C:272:ILE:N	2.22	0.50
2:E:214:SER:O	2:E:218:MSE:HG3	2.11	0.50
1:A:302:MET:HB2	1:A:326:LEU:HD11	1.92	0.50
2:E:344:ILE:HG23	2:E:386:LEU:CD1	2.41	0.50
1:A:126:TYR:N	1:A:126:TYR:CD2	2.79	0.50
1:C:246:ILE:O	1:C:246:ILE:CG2	2.60	0.50
1:D:187:MET:HE3	1:D:196:ILE:CD1	2.39	0.50
1:D:280:ASN:ND2	1:D:348:ASP:HB2	2.27	0.50
1:D:302:MET:HE3	1:D:303:HIS:H	1.76	0.50
1:D:385:ARG:O	1:D:389:THR:CG2	2.60	0.50
1:A:96:LEU:HD13	1:A:127:MET:O	2.12	0.50
1:C:37:MET:O	1:C:38:ASN:C	2.55	0.50
1:A:377:THR:CG2	1:A:378:GLU:H	2.25	0.50
1:C:37:MET:HE3	1:C:63:ILE:HD11	1.94	0.50
2:E:257:ALA:N	2:E:258:PRO:CD	2.75	0.50
1:F:163:PHE:HE1	1:F:198:ASP:HB3	1.77	0.50
1:C:308:GLN:HA	1:C:311:ARG:HB2	1.94	0.50
2:E:420:PRO:C	2:E:422:SER:H	2.19	0.50
1:A:286:ASP:O	1:A:287:TRP:C	2.55	0.49
1:F:117:GLN:HG2	1:F:133:ALA:CB	2.41	0.49
1:F:99:LYS:HE2	1:F:150:GLU:HB2	1.94	0.49
1:A:63:ILE:HG23	1:A:64:LEU:HD22	1.94	0.49
2:B:334:LEU:HG	2:B:350:CYS:HB2	1.94	0.49
1:C:279:ILE:HG22	1:C:347:TYR:HB3	1.95	0.49
1:C:281:THR:OG1	1:C:284:LYS:HB2	2.12	0.49
1:A:252:ASN:O	1:A:253:VAL:C	2.55	0.49
1:C:200:PHE:C	1:C:202:LYS:N	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:363:LEU:C	2:E:363:LEU:HD13	2.37	0.49
1:D:204:ASN:O	1:D:207:THR:OG1	2.29	0.49
2:E:237:GLU:HG3	2:E:278:TYR:CD1	2.48	0.49
1:F:151:ALA:HB1	1:F:152:PRO:HD2	1.95	0.49
1:C:36:ASP:C	1:C:38:ASN:H	2.21	0.49
1:C:187:MET:O	1:C:192:PHE:HB2	2.13	0.49
1:D:245:GLY:O	1:D:369:LYS:N	2.45	0.49
1:A:114:GLN:HE21	1:A:114:GLN:HA	1.78	0.49
2:B:425:VAL:O	2:B:426:LEU:C	2.56	0.49
1:C:84:ALA:O	1:C:88:ILE:HG12	2.12	0.49
1:C:143:GLU:HG3	1:C:144:VAL:N	2.27	0.49
1:C:279:ILE:HD12	1:C:279:ILE:C	2.38	0.49
1:C:354:GLU:O	1:C:357:ILE:HG12	2.12	0.49
1:F:177:LYS:C	1:F:207:THR:HG23	2.38	0.49
1:D:91:LEU:O	1:D:94:ILE:HD12	2.13	0.48
1:D:345:ILE:HD11	1:D:375:MET:HE3	1.95	0.48
1:A:338:VAL:HG22	1:A:338:VAL:O	2.12	0.48
1:F:279:ILE:HD12	1:F:279:ILE:C	2.38	0.48
1:D:303:HIS:O	1:D:311:ARG:NH2	2.44	0.48
2:E:215:HIS:CE1	5:E:17:HOH:O	2.65	0.48
2:B:413:PRO:O	2:B:416:ASN:HB3	2.14	0.48
1:C:249:PHE:HD2	1:C:397:GLU:O	1.94	0.48
1:D:140:VAL:O	1:D:141:ARG:C	2.56	0.48
1:A:96:LEU:HD11	1:A:127:MET:HB3	1.95	0.48
2:B:269:VAL:O	2:B:270:GLY:C	2.55	0.48
1:C:64:LEU:N	1:C:65:PRO:CD	2.76	0.48
1:C:377:THR:H	1:C:380:ASP:HB2	1.79	0.48
1:F:285:VAL:HG13	1:F:327:ILE:HG22	1.95	0.48
1:F:343:LEU:HD11	1:F:373:ILE:HD11	1.94	0.48
1:D:108:PRO:O	1:D:190:ARG:NH1	2.46	0.48
1:C:168:ARG:O	1:C:170:TYR:N	2.46	0.48
2:E:344:ILE:HG23	2:E:386:LEU:HD13	1.95	0.48
1:D:322:SER:O	1:D:323:SER:HB2	2.13	0.48
1:F:188:LEU:CD1	1:F:193:LYS:HG2	2.37	0.48
1:A:239:GLU:OE1	1:A:365:ARG:N	2.47	0.48
1:D:377:THR:HG23	1:D:378:GLU:N	2.29	0.48
1:C:311:ARG:HH22	1:C:334:ARG:HB3	1.79	0.47
2:B:215:HIS:CA	2:B:218:MSE:HE3	2.39	0.47
2:B:419:VAL:HB	2:B:422:SER:HB3	1.96	0.47
1:C:353:ARG:HH11	1:C:353:ARG:N	2.08	0.47
1:A:346:ASN:HB2	1:A:374:ASN:HD22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ASN:C	1:A:253:VAL:O	2.56	0.47
2:E:353:GLU:OE2	1:F:283:ARG:NH2	2.37	0.47
1:F:197:TYR:HE2	1:F:223:VAL:HG22	1.80	0.47
1:D:271:THR:HG23	1:D:271:THR:O	2.14	0.47
2:B:236:VAL:CG1	2:B:274:LEU:HD12	2.45	0.47
1:C:190:ARG:HH11	1:C:190:ARG:HG2	1.75	0.47
1:C:190:ARG:NH1	1:C:190:ARG:HG3	2.29	0.47
1:F:385:ARG:NE	1:F:385:ARG:HA	2.29	0.47
1:A:173:PRO:HA	1:A:176:ILE:HD12	1.95	0.47
1:A:246:ILE:HD11	1:A:362:ARG:CZ	2.45	0.47
1:C:164:ASP:OD1	1:C:168:ARG:HD2	2.14	0.47
1:C:384:LEU:C	1:C:386:ASP:N	2.72	0.47
1:D:279:ILE:HD13	1:D:347:TYR:HB3	1.97	0.47
2:E:184:VAL:HG11	2:E:222:LEU:HD11	1.97	0.47
2:E:382:MSE:O	2:E:383:ILE:C	2.57	0.47
2:E:411:GLU:O	2:E:415:ILE:HG13	2.15	0.47
2:E:441:LYS:O	2:E:442:GLN:C	2.57	0.47
1:F:105:VAL:O	1:F:156:VAL:HA	2.15	0.47
1:A:91:LEU:HA	1:A:94:ILE:HD12	1.95	0.47
1:A:155:ILE:HG13	1:A:171:LEU:HD11	1.97	0.47
1:C:247:ARG:HG2	1:C:249:PHE:HE1	1.79	0.47
1:C:331:LEU:O	1:C:333:ALA:N	2.48	0.47
1:D:94:ILE:HD11	1:D:154:ILE:HD11	1.97	0.47
1:D:240:GLU:HB2	2:E:399:ASP:OD2	2.15	0.47
1:F:267:TYR:CE2	1:F:297:PHE:HD1	2.33	0.47
1:F:308:GLN:CB	1:F:311:ARG:HH11	2.28	0.47
1:A:121:MET:CE	1:A:121:MET:CA	2.75	0.47
1:C:257:GLU:HG2	5:C:3:HOH:O	2.15	0.47
1:D:114:GLN:HE21	1:D:114:GLN:CA	2.28	0.47
1:D:137:GLY:O	1:D:140:VAL:HG22	2.15	0.47
2:E:381:LYS:HG2	2:E:382:MSE:N	2.30	0.47
1:F:166:LEU:HD21	1:F:173:PRO:HG3	1.96	0.47
1:F:354:GLU:CD	1:F:354:GLU:N	2.69	0.47
1:D:382:ARG:H	1:D:382:ARG:HD2	1.80	0.46
1:F:96:LEU:HD21	1:F:153:HIS:HE1	1.80	0.46
1:A:251:ILE:HD11	1:A:398:MET:HE1	1.97	0.46
2:B:174:GLU:O	2:B:175:TYR:C	2.58	0.46
1:F:144:VAL:CG1	1:F:145:GLN:N	2.78	0.46
1:C:314:ILE:O	1:C:318:PHE:N	2.44	0.46
1:D:159:PRO:HG2	1:D:192:PHE:CG	2.50	0.46
1:D:311:ARG:HG3	1:D:314:ILE:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:445:ASP:O	2:E:446:LEU:HD23	2.15	0.46
1:C:331:LEU:C	1:C:333:ALA:H	2.23	0.46
1:F:166:LEU:CD2	1:F:173:PRO:HG3	2.46	0.46
1:C:384:LEU:HD23	1:C:384:LEU:O	2.16	0.46
2:E:231:MSE:HE3	2:E:231:MSE:HB2	1.94	0.46
1:A:88:ILE:HD11	1:A:123:LEU:HD13	1.97	0.46
2:B:379:THR:O	2:B:380:PHE:C	2.57	0.46
1:D:135:ILE:HD12	1:D:135:ILE:HA	1.61	0.46
1:D:216:MET:N	1:D:217:PRO:CD	2.79	0.46
1:D:379:GLU:OE2	1:D:379:GLU:N	2.47	0.46
1:A:255:ARG:HB2	1:A:255:ARG:NH1	2.30	0.46
1:C:37:MET:SD	1:C:37:MET:N	2.73	0.46
1:C:168:ARG:C	1:C:170:TYR:N	2.74	0.46
1:C:279:ILE:HG13	1:C:285:VAL:HG23	1.97	0.46
1:F:152:PRO:HB3	1:F:155:ILE:CD1	2.45	0.46
1:F:263:LEU:HD12	1:F:292:MET:SD	2.56	0.46
1:A:73:ILE:HD11	1:A:224:THR:HG23	1.98	0.46
1:A:146:LYS:HG3	1:A:150:GLU:CD	2.41	0.46
1:A:311:ARG:HB2	1:A:314:ILE:HG22	1.98	0.46
1:C:31:VAL:HB	1:C:63:ILE:CG2	2.46	0.46
1:C:102:GLN:HA	1:C:176:ILE:HA	1.98	0.46
1:A:88:ILE:N	1:A:88:ILE:HD13	2.30	0.46
1:A:114:GLN:CA	1:A:114:GLN:NE2	2.78	0.46
1:A:216:MET:N	1:A:217:PRO:CD	2.78	0.46
1:C:90:ILE:HD11	1:C:180:VAL:HG21	1.97	0.46
2:E:201:PRO:HB2	2:E:239:SER:HB3	1.97	0.46
1:A:255:ARG:HH11	1:A:255:ARG:CB	2.29	0.46
1:F:295:ARG:HD3	1:F:297:PHE:HE2	1.81	0.46
1:A:82:LYS:O	1:A:119:VAL:HG21	2.16	0.45
1:A:101:THR:HA	1:A:152:PRO:O	2.16	0.45
1:A:224:THR:HG22	1:A:225:LYS:N	2.31	0.45
1:A:283:ARG:HH21	2:B:183:GLU:HG2	1.81	0.45
1:C:63:ILE:HG23	1:C:64:LEU:N	2.31	0.45
1:C:349:LEU:HD21	1:C:384:LEU:HD12	1.99	0.45
1:C:378:GLU:CA	1:C:381:LYS:HD3	2.27	0.45
1:D:390:PHE:HD2	1:D:391:TYR:CD1	2.33	0.45
1:D:390:PHE:HD2	1:D:391:TYR:CE1	2.34	0.45
1:C:117:GLN:HE21	1:C:118:LYS:HG3	1.82	0.45
1:C:396:GLU:CD	1:C:396:GLU:H	2.23	0.45
2:E:175:TYR:HA	2:E:178:HIS:CE1	2.51	0.45
2:E:227:CYS:SG	2:E:273:ILE:HG22	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:ARG:HA	1:F:144:VAL:HG12	1.98	0.45
1:F:144:VAL:HG13	1:F:145:GLN:N	2.32	0.45
2:B:303:SER:O	2:B:306:LYS:HG3	2.16	0.45
1:C:154:ILE:HG22	1:C:155:ILE:N	2.31	0.45
1:D:339:GLN:O	1:D:362:ARG:HD3	2.16	0.45
2:E:348:GLU:O	2:E:352:LYS:HD2	2.16	0.45
1:F:197:TYR:CE2	1:F:223:VAL:HG22	2.51	0.45
1:F:395:ILE:O	1:F:395:ILE:CG1	2.55	0.45
1:D:357:ILE:O	1:D:357:ILE:HG13	2.16	0.45
2:E:442:GLN:NE2	2:E:442:GLN:N	2.28	0.45
1:F:151:ALA:CB	1:F:152:PRO:HD2	2.46	0.45
2:B:184:VAL:HG11	2:B:222:LEU:HD11	1.99	0.45
2:B:339:LEU:HD22	2:B:382:MSE:HE3	1.98	0.45
1:D:150:GLU:O	1:D:151:ALA:C	2.59	0.45
1:A:135:ILE:HD12	1:A:135:ILE:HA	1.77	0.45
1:C:204:ASN:HB3	1:C:206:ASN:HD21	1.81	0.45
1:D:238:LYS:NZ	1:D:238:LYS:CB	2.80	0.45
1:D:249:PHE:O	1:D:373:ILE:HA	2.16	0.45
2:E:417:LEU:O	1:F:160:GLY:HA3	2.17	0.45
2:E:426:LEU:HD21	2:E:447:CYS:SG	2.57	0.45
1:A:105:VAL:HB	1:A:156:VAL:HB	1.99	0.45
1:A:253:VAL:HG12	1:A:254:GLU:N	2.31	0.45
2:B:283:LYS:O	2:B:284:GLY:C	2.59	0.45
1:C:136:GLY:HA2	1:C:140:VAL:CG1	2.47	0.45
2:E:256:ARG:O	2:E:260:LEU:HD12	2.16	0.45
1:A:367:GLY:O	1:A:369:LYS:HB3	2.16	0.45
1:C:279:ILE:CD1	1:C:281:THR:O	2.64	0.45
2:E:213:ALA:O	2:E:214:SER:C	2.59	0.45
1:F:260:LEU:O	1:F:260:LEU:HD12	2.17	0.45
1:F:266:LEU:HA	1:F:269:THR:HG22	1.98	0.45
1:A:166:LEU:HG	1:A:171:LEU:HD22	1.98	0.45
1:A:238:LYS:HG2	1:A:239:GLU:O	2.16	0.45
1:C:47:ILE:HD13	1:C:47:ILE:HA	1.78	0.45
1:D:126:TYR:O	1:D:127:MET:C	2.60	0.45
2:B:370:MSE:O	2:B:374:SER:HB3	2.16	0.45
1:C:82:LYS:HG3	1:C:212:LEU:HD22	1.98	0.45
1:C:194:ASP:N	1:C:194:ASP:OD2	2.50	0.45
1:C:271:THR:O	1:C:271:THR:CG2	2.65	0.45
1:C:278:PHE:CG	1:C:359:ARG:HG2	2.51	0.45
1:C:302:MET:HE3	1:C:332:LEU:CD1	2.47	0.45
1:D:75:GLN:HB2	1:D:216:MET:HE1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:390:LEU:HD13	2:E:396:ILE:CD1	2.47	0.45
1:F:219:ASP:OD1	1:F:219:ASP:N	2.49	0.45
1:A:238:LYS:CG	1:A:239:GLU:N	2.80	0.44
1:A:247:ARG:HD2	1:A:249:PHE:CZ	2.52	0.44
1:C:331:LEU:C	1:C:333:ALA:N	2.75	0.44
1:F:102:GLN:HG2	1:F:175:TYR:HB3	1.98	0.44
1:F:124:GLY:HA3	1:F:125:ASP:HA	1.72	0.44
1:C:172:SER:O	1:C:176:ILE:HD11	2.17	0.44
1:F:185:ASP:H	1:F:213:SER:HG	1.65	0.44
1:A:27:TRP:HA	1:A:237:LYS:O	2.16	0.44
1:A:155:ILE:HD12	1:A:155:ILE:HG23	1.78	0.44
1:C:76:ALA:HB3	1:C:82:LYS:HD2	2.00	0.44
1:F:303:HIS:O	1:F:332:LEU:HD22	2.17	0.44
2:E:434:PHE:HE1	2:E:441:LYS:N	2.15	0.44
1:F:279:ILE:HD11	1:F:285:VAL:HG22	1.98	0.44
2:B:361:HIS:ND1	2:B:407:ARG:NH1	2.66	0.44
1:D:267:TYR:HE1	1:D:325:VAL:HG21	1.83	0.44
2:E:320:GLY:C	2:E:322:GLN:N	2.75	0.44
1:F:135:ILE:H	1:F:135:ILE:HG13	1.56	0.44
1:F:356:TYR:O	1:F:360:ILE:HG13	2.17	0.44
2:B:200:VAL:N	2:B:201:PRO:CD	2.81	0.44
2:B:368:ILE:HG21	2:B:408:ILE:HG13	2.00	0.44
1:D:252:ASN:ND2	1:D:381:LYS:HD3	2.32	0.44
1:D:354:GLU:OE1	2:E:356:VAL:CG2	2.66	0.44
2:E:254:THR:O	2:E:255:PRO:C	2.60	0.44
2:B:268:ALA:HB1	2:B:273:ILE:HG13	2.00	0.44
1:D:114:GLN:HE21	1:D:114:GLN:HA	1.83	0.44
1:D:297:PHE:HB2	1:D:299:VAL:HG23	1.99	0.44
1:F:263:LEU:HD23	1:F:375:MET:HE1	2.00	0.44
1:C:171:LEU:HD12	1:C:171:LEU:HA	1.92	0.44
2:E:334:LEU:C	2:E:334:LEU:HD23	2.43	0.44
1:D:280:ASN:N	1:D:280:ASN:HD22	2.16	0.44
2:E:169:THR:HB	2:E:170:PRO:HD3	2.00	0.44
2:E:197:LYS:HD2	2:E:235:ASP:OD2	2.17	0.44
1:C:270:LEU:CG	1:C:271:THR:N	2.79	0.43
1:C:277:ILE:HD12	1:C:325:VAL:HG11	2.01	0.43
1:C:303:HIS:O	1:C:332:LEU:CD2	2.64	0.43
1:C:348:ASP:O	1:C:359:ARG:NH2	2.50	0.43
1:D:354:GLU:OE1	2:E:356:VAL:HG22	2.18	0.43
2:E:443:LEU:HD22	2:E:443:LEU:HA	1.80	0.43
1:A:253:VAL:HG13	1:A:258:TRP:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ASN:HD21	1:A:359:ARG:HH22	1.65	0.43
2:B:247:LEU:HD23	2:B:247:LEU:HA	1.75	0.43
1:D:121:MET:C	1:D:124:GLY:H	2.24	0.43
2:E:168:LEU:CD1	2:E:200:VAL:HG22	2.48	0.43
2:E:434:PHE:CE1	2:E:441:LYS:CA	2.80	0.43
1:A:377:THR:HG21	1:A:379:GLU:OE2	2.18	0.43
1:C:39:LEU:HD12	1:C:39:LEU:H	1.83	0.43
1:C:337:ASP:HB3	1:C:339:GLN:OE1	2.18	0.43
1:D:64:LEU:HB3	1:D:65:PRO:CD	2.48	0.43
1:D:322:SER:O	1:D:323:SER:CB	2.66	0.43
2:E:317:SER:HB3	2:E:326:HIS:HE1	1.83	0.43
2:E:354:LEU:O	2:E:355:GLU:C	2.61	0.43
1:A:295:ARG:HB3	1:A:297:PHE:CE2	2.51	0.43
2:B:263:GLN:NE2	2:B:314:VAL:HG22	2.33	0.43
1:C:137:GLY:O	1:C:140:VAL:HG13	2.18	0.43
1:C:249:PHE:CE2	1:C:397:GLU:O	2.71	0.43
1:A:91:LEU:HA	1:A:91:LEU:HD23	1.85	0.43
1:A:112:LEU:HD22	1:A:112:LEU:O	2.19	0.43
1:C:268:GLU:H	1:C:268:GLU:HG2	1.59	0.43
1:C:352:ASN:HA	1:C:353:ARG:HH11	1.79	0.43
1:A:133:ALA:HA	1:A:156:VAL:O	2.18	0.43
1:A:216:MET:N	1:A:217:PRO:HD3	2.34	0.43
1:C:224:THR:HG22	1:C:228:MET:SD	2.58	0.43
1:D:95:GLU:O	1:D:97:ASP:N	2.51	0.43
1:D:353:ARG:HH21	2:E:323:SER:HA	1.83	0.43
2:E:226:LEU:HD22	2:E:230:VAL:HG11	2.00	0.43
2:E:226:LEU:O	2:E:230:VAL:HG12	2.19	0.43
1:F:339:GLN:C	1:F:341:VAL:N	2.77	0.43
1:A:117:GLN:HG2	1:A:131:CYS:SG	2.58	0.43
2:E:322:GLN:HE21	2:E:322:GLN:HB3	1.40	0.43
2:E:418:ASP:OD1	1:F:161:ARG:HD2	2.19	0.43
1:F:277:ILE:HB	1:F:327:ILE:HG12	2.00	0.43
1:A:159:PRO:HG2	1:A:192:PHE:HB3	2.01	0.43
1:A:192:PHE:CE1	2:B:255:PRO:HD3	2.53	0.43
1:A:267:TYR:CE1	1:A:272:ILE:HD11	2.54	0.43
2:B:444:ARG:HD2	2:B:445:ASP:OD1	2.19	0.43
2:E:257:ALA:O	2:E:261:VAL:HG23	2.19	0.43
2:E:296:ASP:O	2:E:297:LYS:C	2.60	0.43
1:F:308:GLN:HA	1:F:311:ARG:HB2	2.01	0.43
1:A:399:PRO:HB2	1:A:401:ASN:OD1	2.18	0.43
1:C:237:LYS:C	1:C:239:GLU:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:LEU:O	1:D:113:ALA:C	2.62	0.43
1:A:281:THR:HG21	2:B:183:GLU:HG3	2.01	0.43
1:C:67:ILE:HD12	1:C:89:SER:HA	2.01	0.43
1:C:385:ARG:HD3	1:C:385:ARG:HA	1.67	0.43
1:D:190:ARG:HH21	2:E:254:THR:HG23	1.84	0.43
1:D:237:LYS:HD3	1:D:237:LYS:HA	1.91	0.43
1:D:277:ILE:HG12	1:D:345:ILE:HG23	2.01	0.43
2:B:203:LEU:O	2:B:204:ALA:C	2.61	0.42
1:C:234:ILE:CG2	1:C:235:LEU:N	2.82	0.42
1:D:121:MET:HE2	1:D:124:GLY:HA3	2.00	0.42
1:D:139:ASN:O	1:D:140:VAL:C	2.62	0.42
2:E:265:ILE:O	2:E:268:ALA:N	2.52	0.42
2:E:370:MSE:HE2	2:E:383:ILE:HD11	2.00	0.42
2:B:333:MSE:HE3	2:B:333:MSE:O	2.18	0.42
1:D:339:GLN:HE21	1:D:339:GLN:N	2.17	0.42
1:A:352:ASN:OD1	2:B:320:GLY:HA3	2.19	0.42
1:C:140:VAL:HA	1:C:143:GLU:HB3	1.99	0.42
1:A:63:ILE:O	1:A:63:ILE:CD1	2.66	0.42
1:A:278:PHE:HB2	1:A:346:ASN:ND2	2.33	0.42
1:A:282:ARG:HA	1:A:285:VAL:HB	2.01	0.42
1:A:295:ARG:HH11	1:A:295:ARG:CG	2.18	0.42
2:B:349:HIS:O	2:B:353:GLU:HG3	2.20	0.42
1:C:267:TYR:HA	1:C:270:LEU:CD2	2.49	0.42
1:D:29:GLU:C	1:D:31:VAL:H	2.25	0.42
1:A:251:ILE:HD11	1:A:398:MET:CE	2.48	0.42
2:B:433:CYS:O	2:B:434:PHE:C	2.61	0.42
1:C:188:LEU:HD13	1:C:188:LEU:HA	1.84	0.42
1:D:388:GLU:HB2	1:D:395:ILE:CD1	2.46	0.42
1:F:152:PRO:CB	1:F:155:ILE:HD11	2.49	0.42
1:A:139:ASN:O	1:A:140:VAL:C	2.62	0.42
2:B:346:GLU:HG2	1:C:281:THR:HG21	2.01	0.42
1:C:193:LYS:O	1:C:194:ASP:C	2.63	0.42
1:C:278:PHE:CD1	1:C:359:ARG:HG2	2.54	0.42
1:F:279:ILE:HG13	1:F:285:VAL:HG22	2.00	0.42
1:F:308:GLN:HB3	1:F:311:ARG:HH11	1.83	0.42
1:C:166:LEU:HD23	1:C:166:LEU:HA	1.91	0.42
1:D:250:TYR:CE1	1:D:397:GLU:HG3	2.55	0.42
1:A:346:ASN:HD21	1:A:359:ARG:HD3	1.84	0.42
2:B:346:GLU:OE1	1:C:283:ARG:HD2	2.19	0.42
1:C:352:ASN:O	1:C:353:ARG:C	2.63	0.42
1:C:353:ARG:O	1:C:356:TYR:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:LEU:HD13	1:D:207:THR:HG21	2.02	0.42
1:F:167:ASN:O	1:F:169:ARG:N	2.53	0.42
1:F:352:ASN:OD1	1:F:352:ASN:N	2.53	0.42
1:A:29:GLU:OE2	1:A:29:GLU:HA	2.19	0.42
2:B:237:GLU:HG2	2:B:278:TYR:CD1	2.54	0.41
1:C:253:VAL:CG2	1:C:255:ARG:O	2.64	0.41
1:D:108:PRO:CG	1:D:186:GLU:HB2	2.50	0.41
1:D:354:GLU:CG	2:E:356:VAL:HG23	2.50	0.41
2:E:398:VAL:O	2:E:401:MSE:HB2	2.20	0.41
2:B:239:SER:O	2:B:242:LYS:HB3	2.20	0.41
2:B:279:ILE:HG23	2:B:295:LEU:HD22	2.02	0.41
1:C:147:LEU:HA	1:C:151:ALA:HB2	1.98	0.41
1:C:316:ARG:H	1:C:316:ARG:HG3	1.64	0.41
1:A:251:ILE:CG2	1:A:253:VAL:HG23	2.48	0.41
2:B:254:THR:O	2:B:255:PRO:C	2.64	0.41
2:B:417:LEU:O	1:C:160:GLY:HA3	2.20	0.41
1:C:39:LEU:HD22	1:C:43:LEU:HD21	2.02	0.41
1:C:230:ASP:HA	1:C:231:PRO:HD3	1.77	0.41
1:D:124:GLY:O	1:D:125:ASP:C	2.63	0.41
1:D:259:LYS:O	1:D:260:LEU:C	2.63	0.41
1:D:336:ILE:HG13	1:D:337:ASP:H	1.85	0.41
2:E:304:MSE:HA	1:F:293:HIS:ND1	2.36	0.41
2:E:329:LYS:O	2:E:333:MSE:HB2	2.20	0.41
1:F:308:GLN:CB	1:F:311:ARG:NH1	2.83	0.41
1:A:279:ILE:CG1	1:A:285:VAL:HG23	2.50	0.41
1:A:388:GLU:HG2	1:A:393:THR:O	2.20	0.41
2:B:330:GLU:OE2	2:B:330:GLU:HA	2.21	0.41
1:C:56:SER:HA	1:C:60:GLN:NE2	2.35	0.41
2:E:197:LYS:HB3	2:E:235:ASP:OD2	2.20	0.41
2:E:340:LEU:O	1:F:351:THR:OG1	2.27	0.41
1:C:346:ASN:HD22	1:C:374:ASN:HD21	1.66	0.41
2:B:226:LEU:HD22	2:B:230:VAL:HG11	2.03	0.41
2:B:244:LEU:O	2:B:245:LYS:C	2.63	0.41
1:C:369:LYS:HA	1:C:369:LYS:CE	2.26	0.41
1:D:178:MET:HE3	1:D:178:MET:HB2	1.72	0.41
1:D:369:LYS:HA	1:D:369:LYS:HD3	1.87	0.41
2:E:200:VAL:O	2:E:201:PRO:C	2.63	0.41
1:D:279:ILE:HG21	1:D:284:LYS:HG2	2.02	0.41
1:A:20:GLU:OE2	1:A:20:GLU:HA	2.21	0.41
1:C:204:ASN:N	1:C:204:ASN:ND2	2.67	0.41
1:F:247:ARG:HG2	1:F:249:PHE:CE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LEU:HA	1:A:65:PRO:HD3	1.95	0.41
1:A:178:MET:HE2	1:A:178:MET:HB2	1.87	0.41
1:A:288:LEU:O	1:A:292:MET:CG	2.68	0.41
2:B:203:LEU:HD23	2:B:203:LEU:HA	1.74	0.41
2:B:214:SER:C	2:B:218:MSE:CE	2.94	0.41
1:C:176:ILE:O	1:C:207:THR:HG22	2.21	0.41
1:C:272:ILE:HG22	1:C:274:GLN:HE21	1.73	0.41
1:C:310:GLU:O	1:C:313:VAL:CG1	2.68	0.41
1:C:339:GLN:C	1:C:341:VAL:H	2.29	0.41
1:D:192:PHE:O	1:D:193:LYS:C	2.63	0.41
1:D:267:TYR:CZ	1:D:297:PHE:HD1	2.39	0.41
1:D:311:ARG:HG3	1:D:314:ILE:HG21	2.02	0.41
2:E:203:LEU:HD23	2:E:203:LEU:HA	1.67	0.41
2:E:292:ARG:O	2:E:292:ARG:HG3	2.19	0.41
2:E:304:MSE:HE2	2:E:304:MSE:HB3	1.92	0.41
2:E:378:SER:O	2:E:382:MSE:HG2	2.21	0.41
1:A:137:GLY:O	1:A:140:VAL:HG22	2.20	0.41
1:C:302:MET:HE1	1:C:311:ARG:HE	1.86	0.41
1:F:158:THR:O	1:F:159:PRO:C	2.64	0.41
2:B:333:MSE:HE3	2:B:333:MSE:C	2.46	0.40
1:C:117:GLN:CD	1:C:117:GLN:C	2.88	0.40
1:C:185:ASP:OD1	1:C:185:ASP:N	2.55	0.40
1:D:267:TYR:CE2	1:D:297:PHE:HD1	2.39	0.40
1:D:381:LYS:HB2	1:D:382:ARG:HH11	1.86	0.40
2:E:184:VAL:O	2:E:185:ALA:C	2.63	0.40
2:E:365:TYR:CZ	2:E:369:ILE:CD1	3.03	0.40
1:F:174:LYS:C	1:F:176:ILE:H	2.29	0.40
2:B:257:ALA:N	2:B:258:PRO:CD	2.84	0.40
1:C:154:ILE:CG2	1:C:155:ILE:N	2.84	0.40
1:D:133:ALA:HA	1:D:156:VAL:O	2.22	0.40
2:E:317:SER:HB3	2:E:326:HIS:CE1	2.57	0.40
1:A:288:LEU:O	1:A:292:MET:HG3	2.20	0.40
2:B:183:GLU:OE1	2:B:187:MSE:HE2	2.21	0.40
2:B:231:MSE:HE3	2:B:236:VAL:HG22	2.03	0.40
2:E:363:LEU:C	2:E:363:LEU:CD1	2.94	0.40
1:F:374:ASN:OD1	1:F:395:ILE:HD13	2.21	0.40
1:A:89:SER:HB3	4:A:1:ACY:C	2.51	0.40
1:A:98:LEU:HD21	1:A:175:TYR:HD1	1.75	0.40
1:C:95:GLU:C	1:C:97:ASP:H	2.30	0.40
1:D:28:ASN:O	1:D:28:ASN:ND2	2.44	0.40
1:D:285:VAL:HG22	1:D:327:ILE:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:411:GLU:O	2:E:411:GLU:HG2	2.21	0.40
1:F:155:ILE:HG13	1:F:171:LEU:HD11	2.03	0.40
1:F:277:ILE:HG12	1:F:345:ILE:HD12	2.02	0.40
1:C:163:PHE:O	1:C:164:ASP:C	2.64	0.40
2:E:333:MSE:HG3	1:F:282:ARG:CZ	2.52	0.40
2:E:357:PRO:C	2:E:359:PHE:H	2.30	0.40
1:F:152:PRO:CG	1:F:155:ILE:HD11	2.51	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	335/388 (86%)	297 (89%)	31 (9%)	7 (2%)	5	20
1	C	339/388 (87%)	265 (78%)	60 (18%)	14 (4%)	2	8
1	D	333/388 (86%)	288 (86%)	32 (10%)	13 (4%)	2	8
1	F	247/388 (64%)	198 (80%)	37 (15%)	12 (5%)	1	6
2	B	280/307 (91%)	250 (89%)	26 (9%)	4 (1%)	9	30
2	E	278/307 (91%)	226 (81%)	44 (16%)	8 (3%)	3	13
All	All	1812/2166 (84%)	1524 (84%)	230 (13%)	58 (3%)	3	11

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	253	VAL
1	A	291	LYS
1	A	296	ASP
2	B	270	GLY

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Mol	Chain	Res	Type
1	C	174	LYS
1	D	27	TRP
1	F	153	HIS
1	F	167	ASN
1	F	174	LYS
1	A	95	GLU
1	C	38	ASN
1	C	58	ILE
1	C	168	ARG
1	C	331	LEU
1	C	332	LEU
1	D	28	ASN
1	D	96	LEU
1	D	271	THR
1	D	321	GLY
1	D	381	LYS
2	E	192	ASN
2	E	284	GLY
2	E	321	GLN
1	F	309	LYS
1	A	92	GLN
2	B	190	ASP
2	B	269	VAL
2	B	312	ASP
1	C	57	ALA
1	C	69	GLY
1	C	96	LEU
1	D	89	SER
2	E	194	GLY
1	F	149	MET
1	F	152	PRO
1	F	338	VAL
1	A	268	GLU
1	C	201	GLN
1	D	126	TYR
2	E	421	HIS
1	F	175	TYR
1	F	340	GLN
1	D	296	ASP
2	E	270	GLY
1	F	168	ARG
1	C	85	THR

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Mol	Chain	Res	Type
1	C	238	LYS
1	C	304	GLY
1	D	298	THR
1	D	337	ASP
2	E	186	GLU
1	F	322	SER
1	C	65	PRO
1	F	217	PRO
2	E	316	GLY
1	D	30	ILE
1	D	151	ALA

5.3.2 Protein sidechains ⓘ

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	303/342 (89%)	247 (82%)	56 (18%)	1	6
1	C	314/342 (92%)	247 (79%)	67 (21%)	1	4
1	D	305/342 (89%)	240 (79%)	65 (21%)	1	4
1	F	245/342 (72%)	185 (76%)	60 (24%)	1	2
2	B	251/259 (97%)	222 (88%)	29 (12%)	5	18
2	E	249/259 (96%)	209 (84%)	40 (16%)	2	8
All	All	1667/1886 (88%)	1350 (81%)	317 (19%)	1	5

All (317) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	22	VAL
1	A	63	ILE
1	A	66	CYS
1	A	67	ILE
1	A	80	THR
1	A	85	THR

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Mol	Chain	Res	Type
1	A	88	ILE
1	A	104	LEU
1	A	112	LEU
1	A	114	GLN
1	A	118	LYS
1	A	121	MET
1	A	135	ILE
1	A	140	VAL
1	A	150	GLU
1	A	156	VAL
1	A	174	LYS
1	A	195	GLN
1	A	212	LEU
1	A	216	MET
1	A	219	ASP
1	A	222	GLU
1	A	233	ARG
1	A	241	LEU
1	A	246	ILE
1	A	262	THR
1	A	263	LEU
1	A	266	LEU
1	A	274	GLN
1	A	279	ILE
1	A	282	ARG
1	A	285	VAL
1	A	290	GLU
1	A	291	LYS
1	A	295	ARG
1	A	299	VAL
1	A	303	HIS
1	A	315	MET
1	A	319	ARG
1	A	324	ARG
1	A	328	THR
1	A	331	LEU
1	A	332	LEU
1	A	334	ARG
1	A	336	ILE
1	A	342	SER
1	A	345	ILE
1	A	349	LEU

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Mol	Chain	Res	Type
1	A	360	ILE
1	A	369	LYS
1	A	384	LEU
1	A	386	ASP
1	A	387	ILE
1	A	392	ASN
1	A	401	ASN
2	B	164	PHE
2	B	166	LYS
2	B	183	GLU
2	B	184	VAL
2	B	191	LEU
2	B	196	MSE
2	B	203	LEU
2	B	223	LEU
2	B	224	SER
2	B	234	THR
2	B	237	GLU
2	B	259	GLN
2	B	267	ARG
2	B	275	CYS
2	B	280	ASP
2	B	286	VAL
2	B	322	GLN
2	B	325	ASN
2	B	329	LYS
2	B	356	VAL
2	B	369	ILE
2	B	378	SER
2	B	401	MSE
2	B	411	GLU
2	B	427	GLU
2	B	442	GLN
2	B	443	LEU
2	B	444	ARG
2	B	446	LEU
1	C	37	MET
1	C	39	LEU
1	C	42	SER
1	C	47	ILE
1	C	58	ILE
1	C	64	LEU

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Mol	Chain	Res	Type
1	C	67	ILE
1	C	73	ILE
1	C	80	THR
1	C	98	LEU
1	C	101	THR
1	C	102	GLN
1	C	105	VAL
1	C	111	GLU
1	C	117	GLN
1	C	143	GLU
1	C	146	LYS
1	C	156	VAL
1	C	171	LEU
1	C	174	LYS
1	C	188	LEU
1	C	190	ARG
1	C	194	ASP
1	C	199	ILE
1	C	202	LYS
1	C	204	ASN
1	C	206	ASN
1	C	224	THR
1	C	225	LYS
1	C	246	ILE
1	C	251	ILE
1	C	253	VAL
1	C	255	ARG
1	C	256	GLU
1	C	258	TRP
1	C	261	ASP
1	C	263	LEU
1	C	266	LEU
1	C	268	GLU
1	C	269	THR
1	C	270	LEU
1	C	271	THR
1	C	273	THR
1	C	283	ARG
1	C	285	VAL
1	C	299	VAL
1	C	300	SER
1	C	303	HIS

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Mol	Chain	Res	Type
1	C	307	ASP
1	C	308	GLN
1	C	316	ARG
1	C	323	SER
1	C	326	LEU
1	C	339	GLN
1	C	344	VAL
1	C	352	ASN
1	C	353	ARG
1	C	359	ARG
1	C	369	LYS
1	C	371	VAL
1	C	376	VAL
1	C	378	GLU
1	C	382	ARG
1	C	383	THR
1	C	393	THR
1	C	395	ILE
1	C	396	GLU
1	D	19	MET
1	D	20	GLU
1	D	22	VAL
1	D	28	ASN
1	D	29	GLU
1	D	30	ILE
1	D	31	VAL
1	D	80	THR
1	D	82	LYS
1	D	85	THR
1	D	112	LEU
1	D	114	GLN
1	D	118	LYS
1	D	123	LEU
1	D	125	ASP
1	D	127	MET
1	D	135	ILE
1	D	140	VAL
1	D	156	VAL
1	D	169	ARG
1	D	171	LEU
1	D	174	LYS
1	D	201	GLN

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Mol	Chain	Res	Type
1	D	202	LYS
1	D	224	THR
1	D	233	ARG
1	D	238	LYS
1	D	239	GLU
1	D	241	LEU
1	D	243	LEU
1	D	246	ILE
1	D	248	GLN
1	D	257	GLU
1	D	262	THR
1	D	263	LEU
1	D	271	THR
1	D	272	ILE
1	D	274	GLN
1	D	277	ILE
1	D	280	ASN
1	D	285	VAL
1	D	290	GLU
1	D	300	SER
1	D	303	HIS
1	D	313	VAL
1	D	314	ILE
1	D	316	ARG
1	D	317	GLU
1	D	331	LEU
1	D	338	VAL
1	D	339	GLN
1	D	340	GLN
1	D	342	SER
1	D	345	ILE
1	D	357	ILE
1	D	362	ARG
1	D	365	ARG
1	D	377	THR
1	D	381	LYS
1	D	385	ARG
1	D	387	ILE
1	D	389	THR
1	D	394	SER
1	D	400	LEU
1	D	402	VAL

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Mol	Chain	Res	Type
2	E	181	THR
2	E	183	GLU
2	E	191	LEU
2	E	203	LEU
2	E	223	LEU
2	E	229	THR
2	E	231	MSE
2	E	232	SER
2	E	233	THR
2	E	234	THR
2	E	237	GLU
2	E	243	LEU
2	E	249	GLU
2	E	259	GLN
2	E	265	ILE
2	E	267	ARG
2	E	280	ASP
2	E	292	ARG
2	E	297	LYS
2	E	314	VAL
2	E	317	SER
2	E	322	GLN
2	E	325	ASN
2	E	334	LEU
2	E	353	GLU
2	E	363	LEU
2	E	370	MSE
2	E	372	LEU
2	E	375	THR
2	E	381	LYS
2	E	382	MSE
2	E	410	ASN
2	E	430	VAL
2	E	432	GLU
2	E	438	ILE
2	E	439	ILE
2	E	442	GLN
2	E	443	LEU
2	E	444	ARG
2	E	450	ARG
1	F	88	ILE
1	F	91	LEU

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Mol	Chain	Res	Type
1	F	92	GLN
1	F	95	GLU
1	F	96	LEU
1	F	109	THR
1	F	111	GLU
1	F	114	GLN
1	F	120	VAL
1	F	121	MET
1	F	135	ILE
1	F	138	THR
1	F	140	VAL
1	F	143	GLU
1	F	145	GLN
1	F	147	LEU
1	F	153	HIS
1	F	156	VAL
1	F	166	LEU
1	F	167	ASN
1	F	168	ARG
1	F	174	LYS
1	F	188	LEU
1	F	189	SER
1	F	193	LYS
1	F	213	SER
1	F	215	THR
1	F	216	MET
1	F	221	LEU
1	F	224	THR
1	F	246	ILE
1	F	250	TYR
1	F	258	TRP
1	F	259	LYS
1	F	263	LEU
1	F	280	ASN
1	F	289	THR
1	F	298	THR
1	F	303	HIS
1	F	312	ASP
1	F	313	VAL
1	F	316	ARG
1	F	317	GLU
1	F	319	ARG

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Mol	Chain	Res	Type
1	F	323	SER
1	F	332	LEU
1	F	338	VAL
1	F	339	GLN
1	F	351	THR
1	F	352	ASN
1	F	353	ARG
1	F	355	ASN
1	F	373	ILE
1	F	377	THR
1	F	378	GLU
1	F	387	ILE
1	F	388	GLU
1	F	389	THR
1	F	392	ASN
1	F	395	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	114	GLN
1	A	115	GLN
1	A	145	GLN
1	A	248	GLN
1	A	280	ASN
1	A	303	HIS
1	A	346	ASN
1	A	358	HIS
1	A	374	ASN
2	B	173	GLN
2	B	215	HIS
2	B	263	GLN
2	B	290	GLN
2	B	321	GLN
2	B	322	GLN
2	B	326	HIS
2	B	442	GLN
1	C	59	GLN
1	C	60	GLN
1	C	75	GLN
1	C	92	GLN

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Mol	Chain	Res	Type
1	C	93	GLN
1	C	114	GLN
1	C	117	GLN
1	C	145	GLN
1	C	148	GLN
1	C	201	GLN
1	C	204	ASN
1	C	206	ASN
1	C	248	GLN
1	C	252	ASN
1	C	274	GLN
1	C	280	ASN
1	C	303	HIS
1	C	358	HIS
1	C	374	ASN
1	D	92	GLN
1	D	114	GLN
1	D	115	GLN
1	D	204	ASN
1	D	252	ASN
1	D	280	ASN
1	D	293	HIS
1	D	339	GLN
1	D	340	GLN
1	D	355	ASN
1	D	358	HIS
2	E	182	ASN
2	E	215	HIS
2	E	321	GLN
2	E	322	GLN
2	E	360	HIS
2	E	442	GLN
1	F	132	HIS
1	F	148	GLN
1	F	153	HIS
1	F	167	ASN
1	F	201	GLN
1	F	248	GLN
1	F	280	ASN
1	F	352	ASN
1	F	355	ASN
1	F	358	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ACY	D	2	-	3,3,3	0.82	0	3,3,3	1.02	0
3	EDO	D	1	-	3,3,3	0.49	0	2,2,2	0.52	0
3	EDO	A	3	-	3,3,3	0.53	0	2,2,2	0.27	0
4	ACY	A	1	-	3,3,3	0.87	0	3,3,3	0.76	0
3	EDO	A	2	-	3,3,3	0.48	0	2,2,2	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	1	-	-	0/1/1/1	-
3	EDO	A	2	-	-	1/1/1/1	-
3	EDO	A	3	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2	EDO	O1-C1-C2-O2
3	A	3	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3	EDO	1	0
4	A	1	ACY	1	0

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	343/388 (88%)	0.21	13 (3%) 44 35	30, 64, 115, 161	0
1	C	351/388 (90%)	0.93	35 (9%) 12 9	56, 125, 160, 163	0
1	D	345/388 (88%)	0.29	22 (6%) 25 18	31, 68, 116, 160	0
1	F	271/388 (69%)	0.93	30 (11%) 10 7	69, 122, 155, 161	0
2	B	275/307 (89%)	-0.01	4 (1%) 72 63	36, 65, 90, 108	0
2	E	273/307 (88%)	0.10	0 100 100	37, 70, 92, 108	0
All	All	1858/2166 (85%)	0.42	104 (5%) 30 23	30, 84, 149, 163	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	82	LYS	5.1
1	D	402	VAL	4.8
1	C	294	ALA	4.7
1	F	87	ALA	4.4
1	C	304	GLY	4.0
1	F	88	ILE	3.9
1	A	367	GLY	3.9
1	C	384	LEU	3.6
1	F	175	TYR	3.3
1	C	387	ILE	3.2
1	C	373	ILE	3.2
1	F	331	LEU	3.2
1	D	31	VAL	3.2
1	C	367	GLY	3.1
1	F	360	ILE	3.0
1	C	374	ASN	3.0
1	C	389	THR	2.9
1	A	366	PHE	2.9
1	D	304	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	338	VAL	2.9
1	C	270	LEU	2.8
1	F	387	ILE	2.8
1	F	89	SER	2.7
1	C	181	LEU	2.7
1	C	138	THR	2.6
1	F	93	GLN	2.6
1	F	196	ILE	2.6
1	F	294	ALA	2.6
2	B	450	ARG	2.6
1	C	135	ILE	2.6
1	C	175	TYR	2.6
1	A	375	MET	2.5
1	C	371	VAL	2.5
1	D	313	VAL	2.5
1	D	270	LEU	2.5
1	A	315	MET	2.5
1	C	73	ILE	2.5
1	C	395	ILE	2.5
1	D	298	THR	2.5
1	F	212	LEU	2.4
1	F	123	LEU	2.4
1	D	315	MET	2.4
1	D	400	LEU	2.4
1	C	341	VAL	2.4
1	F	390	PHE	2.4
1	C	302	MET	2.4
1	F	153	HIS	2.4
1	F	296	ASP	2.4
1	F	122	ALA	2.4
1	C	272	ILE	2.4
1	D	314	ILE	2.4
1	A	371	VAL	2.3
1	F	125	ASP	2.3
1	C	375	MET	2.3
1	F	303	HIS	2.3
1	C	32	ASP	2.3
2	B	312	ASP	2.3
2	B	316	GLY	2.3
1	D	396	GLU	2.3
1	D	243	LEU	2.3
1	C	303	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	257	GLU	2.3
1	F	174	LYS	2.3
1	C	64	LEU	2.2
1	F	104	LEU	2.2
1	A	318	PHE	2.2
1	D	374	ASN	2.2
1	F	91	LEU	2.2
1	F	90	ILE	2.2
1	D	362	ARG	2.2
1	A	27	TRP	2.2
1	D	27	TRP	2.2
1	A	398	MET	2.2
1	A	341	VAL	2.2
1	F	253	VAL	2.2
1	C	56	SER	2.2
1	C	331	LEU	2.2
1	D	311	ARG	2.2
1	F	135	ILE	2.2
1	C	305	ASP	2.2
1	D	375	MET	2.2
1	F	393	THR	2.2
1	A	335	GLY	2.2
1	C	301	ALA	2.2
2	B	163	ALA	2.2
1	D	62	ALA	2.1
1	A	229	ARG	2.1
1	D	325	VAL	2.1
1	C	43	LEU	2.1
1	F	211	LEU	2.1
1	C	96	LEU	2.1
1	A	345	ILE	2.1
1	D	30	ILE	2.1
1	F	256	GLU	2.1
1	F	231	PRO	2.0
1	F	96	LEU	2.0
1	C	47	ILE	2.0
1	C	62	ALA	2.0
1	C	98	LEU	2.0
1	D	346	ASN	2.0
1	A	321	GLY	2.0
1	C	94	ILE	2.0
1	C	383	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	48	TYR	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](#)

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
4	ACY	A	1	4/4	0.85	0.21	78,78,79,79	0
3	EDO	D	1	4/4	0.86	0.23	67,68,69,69	0
3	EDO	A	2	4/4	0.87	0.21	81,83,84,85	0
3	EDO	A	3	4/4	0.87	0.17	57,62,64,66	0
4	ACY	D	2	4/4	0.94	0.13	75,75,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.