Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:56 am BST

PDB ID	:	4Q9U
Title	:	Crystal structure of the Rab5, Rabex-5delta and Rabaptin-5C21 complex
Authors	:	Zhang, Z.; Zhang, T.; Ding, J.
Deposited on	:	2014-05-01
Resolution	:	4.62 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 following versions of software and data (see references ①) were used in the production of this report:

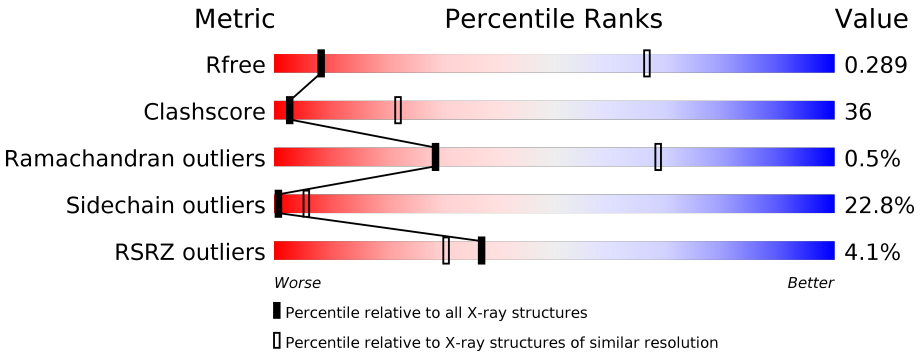
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.62 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1062 (5.40-3.80)
Clashscore	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)
Sidechain outliers	138945	1055 (5.40-3.80)
RSRZ outliers	127900	1114 (5.54-3.70)

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

Mol	Chain	Length	Quality of chain
1	A	317	28% 53% 15%
1	E	317	2% 35% 44% 14% 7%
2	B	171	8% 35% 47% 7% 11%
2	F	171	18% 38% 29% 30%
3	C	92	26% 43% 20% 10%
3	D	92	29% 41% 10% 18%

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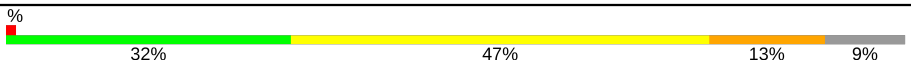
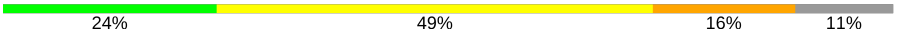
Mol	Chain	Length	Quality of chain
3	G	92	
3	H	92	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9679 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 Rab5 GDP/GTP exchange factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2492	1573	426	474	19			
1	E	296	Total	C	N	O	S	0	0	0
			2441	1541	419	462	19			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	MET	-	EXPRESSION TAG	UNP Q9UJ41
A	125	GLY	-	EXPRESSION TAG	UNP Q9UJ41
A	126	HIS	-	EXPRESSION TAG	UNP Q9UJ41
A	127	HIS	-	EXPRESSION TAG	UNP Q9UJ41
A	128	HIS	-	EXPRESSION TAG	UNP Q9UJ41
A	129	HIS	-	EXPRESSION TAG	UNP Q9UJ41
A	130	HIS	-	EXPRESSION TAG	UNP Q9UJ41
A	131	HIS	-	EXPRESSION TAG	UNP Q9UJ41
A	?	-	LYS	DELETION	UNP Q9UJ41
A	?	-	GLN	DELETION	UNP Q9UJ41
A	?	-	GLU	DELETION	UNP Q9UJ41
A	?	-	ALA	DELETION	UNP Q9UJ41
A	?	-	GLU	DELETION	UNP Q9UJ41
A	?	-	SER	DELETION	UNP Q9UJ41
A	?	-	TRP	DELETION	UNP Q9UJ41
A	?	-	SER	DELETION	UNP Q9UJ41
A	?	-	PRO	DELETION	UNP Q9UJ41
A	?	-	ASP	DELETION	UNP Q9UJ41
A	?	-	ALA	DELETION	UNP Q9UJ41
A	?	-	CYS	DELETION	UNP Q9UJ41
A	?	-	LEU	DELETION	UNP Q9UJ41
A	?	-	GLY	DELETION	UNP Q9UJ41
A	?	-	VAL	DELETION	UNP Q9UJ41
E	124	MET	-	EXPRESSION TAG	UNP Q9UJ41
E	125	GLY	-	EXPRESSION TAG	UNP Q9UJ41

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Chain	Residue	Modelled	Actual	Comment	Reference
E	126	HIS	-	EXPRESSION TAG	UNP Q9UJ41
E	127	HIS	-	EXPRESSION TAG	UNP Q9UJ41
E	128	HIS	-	EXPRESSION TAG	UNP Q9UJ41
E	129	HIS	-	EXPRESSION TAG	UNP Q9UJ41
E	130	HIS	-	EXPRESSION TAG	UNP Q9UJ41
E	131	HIS	-	EXPRESSION TAG	UNP Q9UJ41
E	?	-	LYS	DELETION	UNP Q9UJ41
E	?	-	GLN	DELETION	UNP Q9UJ41
E	?	-	GLU	DELETION	UNP Q9UJ41
E	?	-	ALA	DELETION	UNP Q9UJ41
E	?	-	GLU	DELETION	UNP Q9UJ41
E	?	-	SER	DELETION	UNP Q9UJ41
E	?	-	TRP	DELETION	UNP Q9UJ41
E	?	-	SER	DELETION	UNP Q9UJ41
E	?	-	PRO	DELETION	UNP Q9UJ41
E	?	-	ASP	DELETION	UNP Q9UJ41
E	?	-	ALA	DELETION	UNP Q9UJ41
E	?	-	CYS	DELETION	UNP Q9UJ41
E	?	-	LEU	DELETION	UNP Q9UJ41
E	?	-	GLY	DELETION	UNP Q9UJ41
E	?	-	VAL	DELETION	UNP Q9UJ41

- Molecule 2 is a protein called Ras-related protein Rab-5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1194	759	201	229	5			
2	F	120	Total	C	N	O	S	0	0	0
			948	607	160	177	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	14	SER	-	EXPRESSION TAG	UNP P20339
F	14	SER	-	EXPRESSION TAG	UNP P20339

- Molecule 3 is a protein called Rab GTPase-binding effector protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	83	Total	C	N	O	S	0	0	0
			667	406	119	138	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	75	Total	C	N	O	S	0	0	0
			601	369	106	122	4			
3	G	84	Total	C	N	O	S	0	0	0
			678	412	123	139	4			
3	H	82	Total	C	N	O	S	0	0	0
			658	401	118	135	4			

There are 4 discrepancies between the modelled and reference sequences:

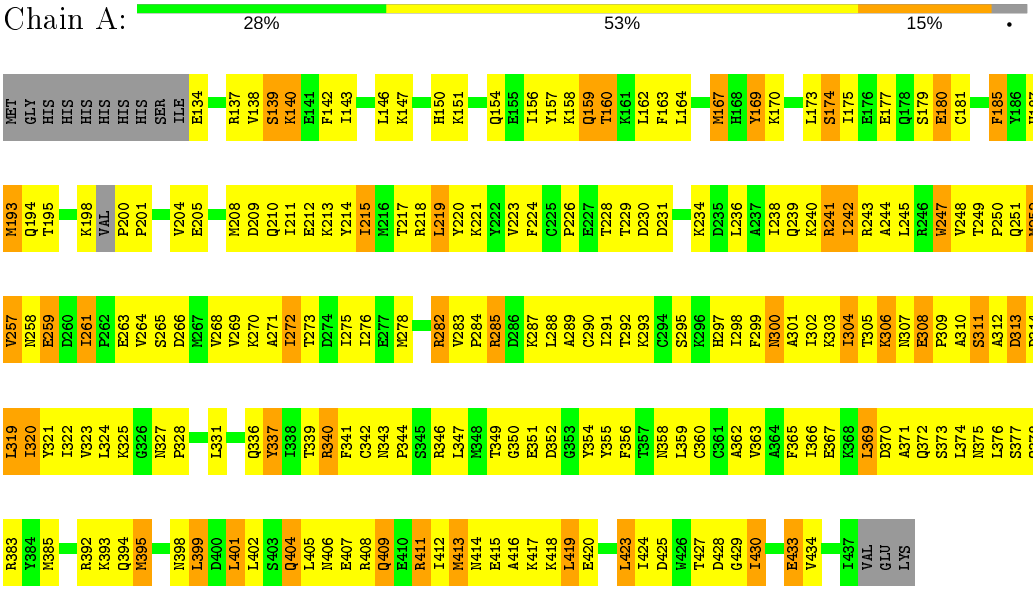
Chain	Residue	Modelled	Actual	Comment	Reference
C	551	MET	-	EXPRESSION TAG	UNP Q15276
D	551	MET	-	EXPRESSION TAG	UNP Q15276
G	551	MET	-	EXPRESSION TAG	UNP Q15276
H	551	MET	-	EXPRESSION TAG	UNP Q15276

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

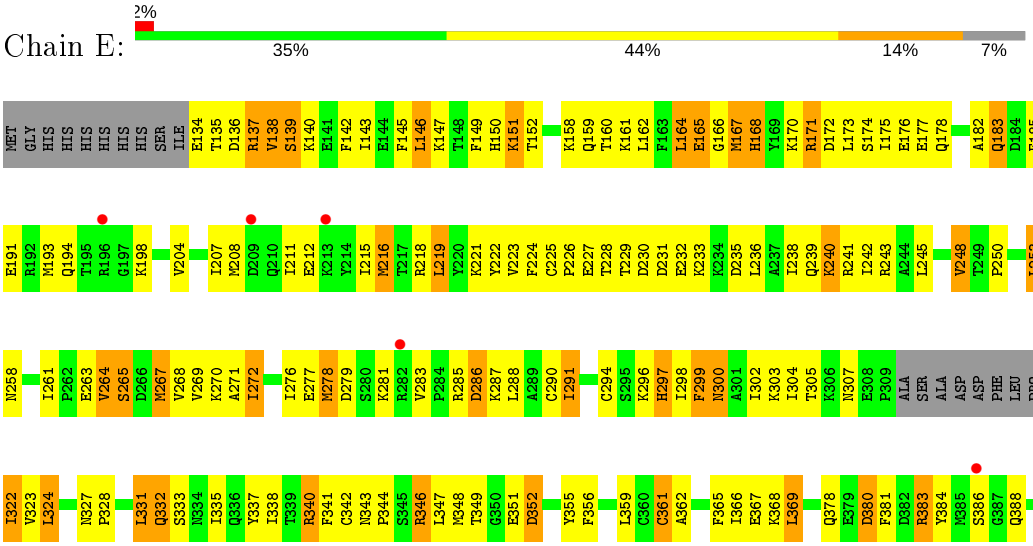
- Molecule 1: Rab5 GDP/GTP exchange factor

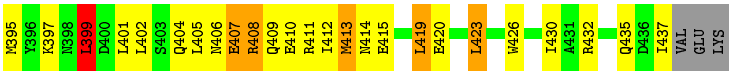
Chain A:



- Molecule 1: Rab5 GDP/GTP exchange factor

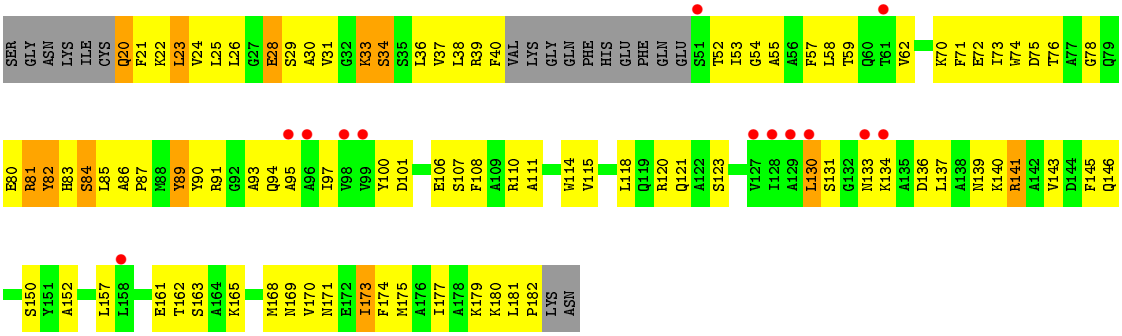
Chain E:





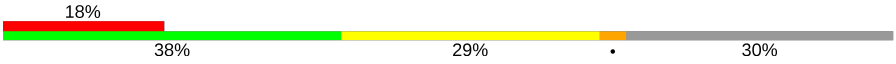
• Molecule 2: Ras-related protein Rab-5A

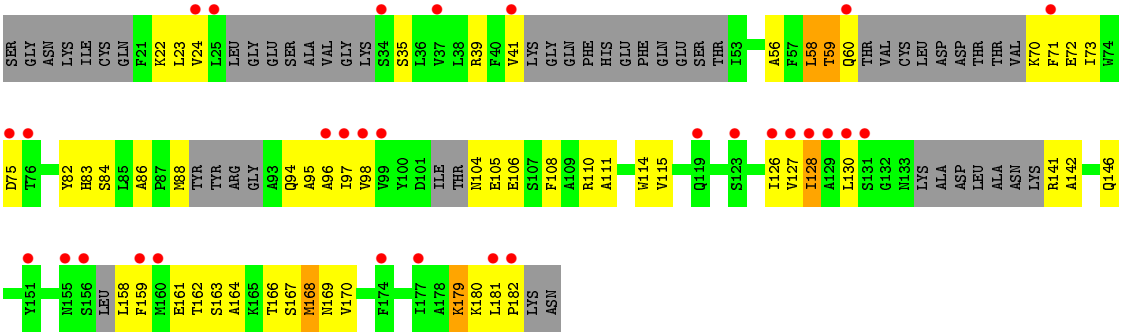
Chain B:



• Molecule 2: Ras-related protein Rab-5A

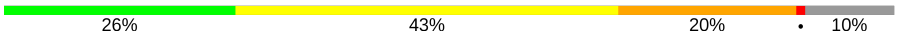
Chain F:

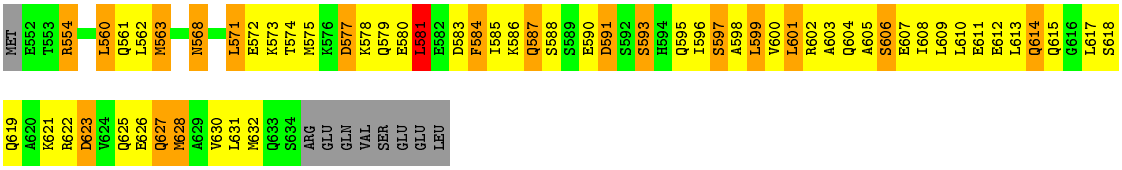




• Molecule 3: Rab GTPase-binding effector protein 1

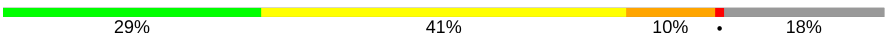
Chain C:

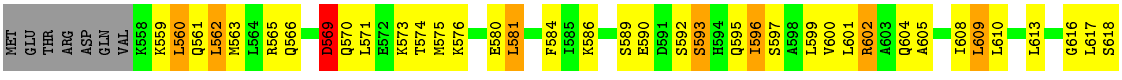




• Molecule 3: Rab GTPase-binding effector protein 1

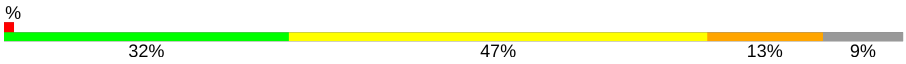
Chain D:

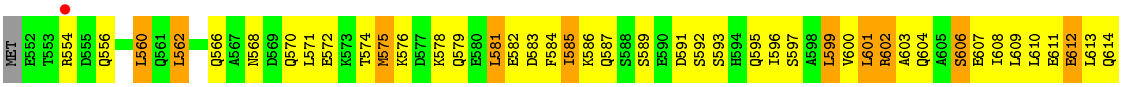


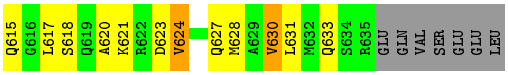


• Molecule 3: Rab GTPase-binding effector protein 1

Chain G:

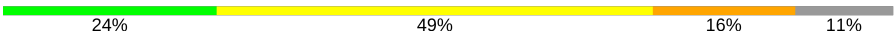


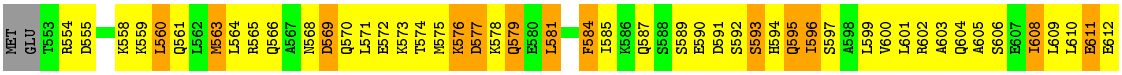




• Molecule 3: Rab GTPase-binding effector protein 1

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	174.82Å 174.82Å 149.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.78 – 4.62 48.49 – 4.62	Depositor EDS
% Data completeness (in resolution range)	95.9 (40.78-4.62) 95.9 (48.49-4.62)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 4.64Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.251 , 0.343 0.258 , 0.289	Depositor DCC
R_{free} test set	621 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	172.7	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 208.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9679	wwPDB-VP
Average B, all atoms (Å^2)	187.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.71	0/2535	0.92	2/3410 (0.1%)
1	E	0.60	0/2482	0.84	2/3338 (0.1%)
2	B	0.52	0/1213	0.71	0/1639
2	F	0.48	1/959 (0.1%)	0.60	0/1285
3	C	0.84	0/668	1.04	1/890 (0.1%)
3	D	0.82	0/602	1.09	1/801 (0.1%)
3	G	0.84	0/679	1.00	0/904
3	H	0.74	0/659	0.99	0/878
All	All	0.67	1/9797 (0.0%)	0.88	6/13145 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	86	ALA	CA-CB	5.09	1.63	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	581	LEU	CB-CG-CD1	-5.56	101.54	111.00
1	E	399	LEU	CB-CG-CD2	5.20	119.84	111.00
1	A	399	LEU	CB-CG-CD2	5.17	119.78	111.00
1	E	253	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	308	GLU	N-CA-C	-5.14	97.11	111.00
3	D	569	ASP	CB-CG-OD1	-5.14	113.68	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2492	0	2502	226	0
1	E	2441	0	2460	185	0
2	B	1194	0	1192	81	0
2	F	948	0	937	36	0
3	C	667	0	678	61	0
3	D	601	0	618	50	0
3	G	678	0	691	60	0
3	H	658	0	672	70	0
All	All	9679	0	9750	692	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 36.

All (692) 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:A:395:MET:HG3	1:A:399:LEU:HD23	1.45	0.99
1:A:250:PRO:HA	1:A:253:LEU:HG	1.49	0.92
1:A:238:ILE:HD13	1:A:331:LEU:HD23	1.53	0.89
1:E:258:ASN:H	1:E:305:THR:HG21	1.41	0.85
1:E:216:MET:HA	1:E:219:LEU:HD22	1.57	0.85
1:E:271:ALA:HA	1:E:297:HIS:CE1	2.12	0.84
1:A:365:PHE:HB2	2:B:85:LEU:HD21	1.60	0.84
1:A:261:ILE:HD11	1:A:263:GLU:HB3	1.58	0.83
1:A:312:ALA:HA	1:A:315:PHE:HB3	1.62	0.82
2:B:174:PHE:HA	2:B:177:ILE:HD12	1.64	0.79
3:D:569:ASP:N	3:D:569:ASP:OD1	2.09	0.79
3:H:593:SER:O	3:H:596:ILE:HG13	1.83	0.79
1:A:282:ARG:H	1:A:282:ARG:HD3	1.48	0.78
1:E:288:LEU:HA	1:E:291:ILE:HG22	1.64	0.78
3:G:578:LYS:HE2	3:H:581:LEU:HD13	1.64	0.78
2:F:127:VAL:HG21	2:F:180:LYS:HD3	1.65	0.78
1:A:413:MET:SD	1:A:417:LYS:NZ	2.57	0.77
1:A:256:PRO:HG2	1:A:302:ILE:HD11	1.67	0.77
1:E:328:PRO:HB2	1:E:331:LEU:HD21	1.65	0.76
1:E:231:ASP:HB3	1:E:333:SER:HB2	1.68	0.76
1:A:248:VAL:HG13	1:A:321:TYR:HE1	1.52	0.75
3:D:597:SER:O	3:D:601:LEU:HG	1.85	0.75
1:A:288:LEU:HA	1:A:291:ILE:HD12	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:615:GLN:OE1	3:G:578:LYS:NZ	2.20	0.75
3:C:560:LEU:HB3	3:D:560:LEU:HD22	1.68	0.74
1:E:294:CYS:HA	1:E:297:HIS:CE1	2.22	0.74
2:B:58:LEU:HB2	2:B:73:ILE:HD13	1.70	0.74
1:A:394:GLN:HB3	3:D:589:SER:OG	1.88	0.74
2:F:56:ALA:HA	2:F:75:ASP:HB3	1.68	0.73
1:A:158:LYS:HE3	1:A:162:LEU:HD21	1.70	0.73
3:G:585:ILE:HD13	3:H:585:ILE:HD11	1.71	0.72
1:A:299:PHE:O	1:A:302:ILE:HG22	1.89	0.72
1:E:404:GLN:HA	1:E:407:GLU:HB2	1.71	0.72
3:G:630:VAL:HG22	3:G:631:LEU:HD12	1.72	0.72
1:E:402:LEU:HD21	3:G:595:GLN:HB3	1.71	0.72
1:A:269:VAL:O	1:A:273:THR:HG23	1.90	0.71
3:G:608:ILE:O	3:G:611:GLU:N	2.23	0.71
3:H:597:SER:O	3:H:600:VAL:HG12	1.90	0.71
1:E:407:GLU:O	1:E:411:ARG:HB2	1.90	0.71
3:C:572:GLU:HA	3:C:575:MET:SD	2.32	0.70
1:A:134:GLU:OE1	1:A:137:ARG:NH1	2.23	0.70
1:E:183:GLN:HA	1:E:186:TYR:HD2	1.57	0.70
2:F:83:HIS:HB2	2:F:114:TRP:HH2	1.55	0.70
2:B:53:ILE:HG22	2:B:54:GLY:H	1.57	0.70
1:A:270:LYS:HB3	1:A:297:HIS:ND1	2.08	0.69
1:A:245:LEU:HA	1:A:247:TRP:HZ3	1.57	0.69
1:A:395:MET:SD	3:C:588:SER:OG	2.51	0.69
1:E:231:ASP:OD2	1:E:340:ARG:NH2	2.24	0.69
1:E:250:PRO:HA	1:E:253:LEU:HD13	1.75	0.69
1:A:220:TYR:HD1	1:A:337:TYR:HE2	1.41	0.69
3:C:611:GLU:HA	3:C:614:GLN:HB2	1.73	0.68
1:A:371:ALA:HB2	1:A:381:PHE:CG	2.28	0.68
1:E:356:PHE:HA	1:E:359:LEU:HG	1.76	0.68
1:E:361:CYS:SG	1:E:362:ALA:N	2.66	0.68
1:A:142:PHE:CD1	1:A:214:TYR:HB2	2.29	0.68
1:E:291:ILE:HG13	1:E:359:LEU:HD11	1.76	0.68
1:E:135:THR:O	1:E:139:SER:HB2	1.93	0.68
1:A:229:THR:HG23	1:A:231:ASP:H	1.59	0.67
2:B:28:GLU:HG3	2:B:110:ARG:HG3	1.76	0.67
1:A:354:TYR:O	1:A:358:ASN:ND2	2.27	0.67
1:E:143:ILE:HG12	1:E:147:LYS:HE3	1.76	0.67
1:A:175:ILE:HD12	1:A:226:PRO:HG2	1.76	0.67
1:E:235:ASP:O	1:E:238:ILE:HG13	1.95	0.67
1:A:257:VAL:HG12	1:A:305:THR:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:608:ILE:HA	3:C:611:GLU:OE2	1.95	0.67
1:E:189:VAL:O	1:E:193:MET:HG3	1.95	0.66
3:C:602:ARG:O	3:C:606:SER:HB3	1.95	0.66
3:G:581:LEU:HD23	3:G:582:GLU:N	2.10	0.66
1:A:245:LEU:HA	1:A:247:TRP:CZ3	2.31	0.66
3:G:578:LYS:HG3	3:H:578:LYS:HG3	1.77	0.66
1:E:265:SER:HA	1:E:268:VAL:HB	1.78	0.66
2:B:24:VAL:HG23	2:B:74:TRP:HB2	1.76	0.66
3:G:617:LEU:HD12	3:G:618:SER:N	2.11	0.66
3:H:596:ILE:HA	3:H:599:LEU:HD12	1.78	0.66
1:A:398:ASN:ND2	3:D:596:ILE:HD11	2.12	0.65
2:F:96:ALA:HB2	2:F:126:ILE:HD11	1.78	0.65
1:A:240:LYS:HA	1:A:243:ARG:HH11	1.61	0.65
3:G:624:VAL:HA	3:G:627:GLN:HB2	1.76	0.65
1:E:346:ARG:NH1	1:E:352:ASP:OD2	2.29	0.65
3:C:598:ALA:HA	3:C:601:LEU:HD23	1.77	0.65
1:E:300:ASN:ND2	1:E:300:ASN:H	1.93	0.65
2:F:95:ALA:HB2	2:F:181:LEU:HD21	1.77	0.65
1:A:213:LYS:HG2	1:A:283:VAL:HG21	1.79	0.65
1:A:320:ILE:HG12	1:A:366:ILE:HD11	1.79	0.65
2:B:152:ALA:HA	2:B:157:LEU:HD12	1.80	0.64
3:D:586:LYS:O	3:D:589:SER:HB3	1.97	0.64
3:G:597:SER:O	3:G:601:LEU:HB3	1.97	0.64
1:A:419:LEU:O	1:A:423:LEU:HB3	1.97	0.64
1:E:384:TYR:HA	1:E:388:GLN:HE22	1.63	0.64
3:G:610:LEU:HD21	3:H:606:SER:HB3	1.79	0.64
3:G:608:ILE:HG13	3:G:609:LEU:HD22	1.78	0.63
3:D:573:LYS:HE3	3:G:618:SER:HB3	1.81	0.63
1:A:160:THR:HA	1:A:163:PHE:CE2	2.33	0.63
3:G:592:SER:O	3:G:596:ILE:HB	1.99	0.63
1:E:331:LEU:O	1:E:335:ILE:HG13	1.99	0.63
3:H:571:LEU:HG	3:H:572:GLU:N	2.14	0.63
1:E:232:GLU:OE2	3:H:568:ASN:HB3	1.98	0.63
2:B:100:TYR:HB2	2:B:108:PHE:HA	1.81	0.63
3:G:593:SER:O	3:G:596:ILE:N	2.31	0.63
3:G:603:ALA:O	3:G:606:SER:N	2.29	0.63
1:A:401:LEU:O	1:A:404:GLN:N	2.30	0.63
3:D:602:ARG:HH11	3:D:602:ARG:HG2	1.64	0.63
1:E:412:ILE:HA	1:E:415:GLU:OE2	1.99	0.63
2:F:98:VAL:HG21	2:F:115:VAL:HG22	1.81	0.63
3:C:610:LEU:HD13	3:D:609:LEU:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ILE:HD13	1:A:322:ILE:HG23	1.82	0.62
2:B:33:LYS:NZ	2:B:75:ASP:OD1	2.32	0.62
3:G:608:ILE:HD12	3:G:612:GLU:OE2	1.99	0.62
1:E:270:LYS:HG2	1:E:297:HIS:HD2	1.63	0.62
2:B:23:LEU:HG	2:B:24:VAL:N	2.13	0.62
1:E:183:GLN:O	1:E:186:TYR:HB2	1.99	0.62
1:A:324:LEU:HD23	1:A:324:LEU:O	1.99	0.62
1:E:135:THR:HG23	1:E:218:ARG:HH21	1.64	0.62
2:B:23:LEU:HB2	2:B:95:ALA:HB3	1.82	0.62
3:H:568:ASN:HA	3:H:571:LEU:HD23	1.82	0.62
3:H:592:SER:O	3:H:596:ILE:HG23	2.00	0.62
3:D:602:ARG:HD2	3:H:591:ASP:HB2	1.82	0.62
3:D:631:LEU:O	1:E:134:GLU:N	2.33	0.62
1:A:363:VAL:O	1:A:366:ILE:N	2.32	0.62
1:A:405:LEU:HD21	3:D:600:VAL:HB	1.82	0.62
2:B:22:LYS:HB2	2:B:93:ALA:HA	1.82	0.61
1:A:351:GLU:HA	2:B:57:PHE:CZ	2.35	0.61
1:E:227:GLU:HB3	3:H:561:GLN:HB3	1.81	0.61
2:F:83:HIS:HB2	2:F:114:TRP:CH2	2.35	0.61
3:H:584:PHE:O	3:H:587:GLN:HG2	2.00	0.61
1:E:139:SER:HA	1:E:142:PHE:CE2	2.35	0.61
1:E:216:MET:N	1:E:216:MET:SD	2.73	0.61
3:G:575:MET:SD	3:H:574:THR:HG21	2.40	0.61
3:H:595:GLN:O	3:H:599:LEU:HG	1.99	0.61
1:E:255:VAL:HG21	1:E:321:TYR:CD2	2.35	0.61
3:C:580:GLU:O	3:C:583:ASP:HB2	2.00	0.61
3:G:608:ILE:HG13	3:G:609:LEU:N	2.16	0.61
1:A:241:ARG:NH2	1:A:367:GLU:O	2.34	0.60
1:A:359:LEU:O	1:A:363:VAL:HG23	2.02	0.60
1:A:319:LEU:O	1:A:323:VAL:HG23	2.02	0.60
1:E:235:ASP:OD1	1:E:332:GLN:N	2.33	0.60
3:D:597:SER:O	3:D:600:VAL:HG12	2.02	0.60
1:E:378:GLN:HA	1:E:381:PHE:HB3	1.84	0.60
1:A:320:ILE:O	1:A:324:LEU:HB2	2.01	0.60
3:G:623:ASP:O	3:G:627:GLN:HG2	2.02	0.60
3:G:603:ALA:O	3:G:607:GLU:HG2	2.02	0.60
1:E:414:ASN:N	1:E:414:ASN:OD1	2.35	0.60
3:C:583:ASP:O	3:C:587:GLN:HG3	2.02	0.59
1:A:287:LYS:O	1:A:290:CYS:N	2.34	0.59
1:A:342:CYS:SG	1:A:343:ASN:N	2.75	0.59
1:E:236:LEU:O	1:E:240:LYS:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:581:LEU:O	3:H:584:PHE:HB3	2.02	0.59
3:H:605:ALA:O	3:H:608:ILE:HG22	2.02	0.59
3:H:596:ILE:O	3:H:599:LEU:HB2	2.02	0.59
1:A:242:ILE:HB	1:A:327:ASN:OD1	2.03	0.59
1:E:242:ILE:HD13	1:E:327:ASN:HA	1.83	0.59
1:E:166:GLY:O	1:E:170:LYS:HG3	2.03	0.58
1:E:392:ARG:HB3	3:G:584:PHE:CZ	2.37	0.58
1:A:354:TYR:HA	2:B:74:TRP:CZ3	2.37	0.58
1:E:378:GLN:HA	1:E:381:PHE:CB	2.33	0.58
1:A:258:ASN:H	1:A:305:THR:HG21	1.68	0.58
1:A:249:THR:HB	1:A:251:GLN:OE1	2.04	0.58
1:E:149:PHE:HB3	1:E:151:LYS:HG3	1.85	0.58
3:G:581:LEU:O	3:G:585:ILE:HG23	2.04	0.58
1:A:292:THR:HG22	1:A:355:TYR:CD2	2.39	0.58
2:F:106:GLU:OE2	2:F:110:ARG:NH1	2.36	0.58
2:B:162:THR:HG22	2:B:169:ASN:HB2	1.86	0.57
2:B:59:THR:HA	2:B:71:PHE:O	2.03	0.57
2:F:58:LEU:HD12	2:F:73:ILE:HB	1.85	0.57
1:A:223:VAL:HB	1:A:341:PHE:CE2	2.38	0.57
1:E:298:ILE:HD13	1:E:322:ILE:HG21	1.85	0.57
3:D:601:LEU:HA	3:D:604:GLN:HE22	1.70	0.57
3:C:581:LEU:O	3:C:584:PHE:HB3	2.05	0.57
1:A:356:PHE:O	1:A:359:LEU:HB3	2.03	0.57
1:A:284:PRO:HA	1:A:287:LYS:HB2	1.86	0.57
1:E:351:GLU:HB2	1:E:355:TYR:CE2	2.40	0.57
1:E:239:GLN:HG2	1:E:243:ARG:HH22	1.70	0.57
2:B:39:ARG:NH1	2:B:39:ARG:O	2.36	0.56
1:E:136:ASP:OD1	1:E:137:ARG:N	2.33	0.56
2:B:22:LYS:CB	2:B:93:ALA:HA	2.35	0.56
3:C:603:ALA:O	3:C:607:GLU:N	2.26	0.56
3:H:608:ILE:HA	3:H:611:GLU:OE1	2.05	0.56
1:A:226:PRO:O	1:A:229:THR:HG22	2.06	0.56
2:B:133:ASN:ND2	2:B:134:LYS:H	2.03	0.56
1:E:170:LYS:HB3	1:E:173:LEU:HD23	1.88	0.56
3:C:571:LEU:HD23	3:C:572:GLU:HG3	1.86	0.56
1:A:220:TYR:CD1	1:A:337:TYR:HE2	2.23	0.56
1:A:409:GLN:HG3	1:A:412:ILE:HD11	1.88	0.56
1:A:351:GLU:HA	2:B:57:PHE:HZ	1.71	0.56
1:E:328:PRO:O	1:E:331:LEU:HG	2.06	0.56
1:A:193:MET:HG2	1:A:194:GLN:N	2.21	0.56
2:B:23:LEU:HD21	2:B:25:LEU:HD21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:MET:SD	1:E:194:GLN:N	2.79	0.56
1:A:223:VAL:HB	1:A:341:PHE:HE2	1.71	0.56
3:C:563:MET:SD	3:C:563:MET:N	2.79	0.56
2:F:60:GLN:HB3	2:F:71:PHE:HB2	1.88	0.56
1:A:255:VAL:HG21	1:A:318:THR:HA	1.88	0.56
1:A:321:TYR:O	1:A:325:LYS:HG2	2.06	0.56
3:G:602:ARG:HB3	3:G:602:ARG:CZ	2.36	0.56
1:A:242:ILE:HA	1:A:245:LEU:HG	1.88	0.55
1:E:283:VAL:HG22	1:E:285:ARG:H	1.71	0.55
1:E:320:ILE:O	1:E:324:LEU:HB2	2.07	0.55
1:E:344:PRO:O	1:E:348:MET:HG2	2.07	0.55
1:A:193:MET:O	1:A:198:LYS:N	2.38	0.55
1:A:423:LEU:HD23	3:D:617:LEU:HD22	1.88	0.55
1:A:354:TYR:CD1	1:A:354:TYR:N	2.74	0.55
1:A:320:ILE:HG13	1:A:362:ALA:HB1	1.88	0.55
2:F:23:LEU:HD11	2:F:97:ILE:HG23	1.89	0.55
2:B:133:ASN:CG	2:B:134:LYS:H	2.10	0.55
1:E:272:ILE:O	1:E:276:ILE:HD13	2.06	0.55
3:H:555:ASP:O	3:H:559:LYS:HG2	2.07	0.55
1:A:261:ILE:HG13	1:A:264:VAL:H	1.71	0.55
1:A:258:ASN:H	1:A:305:THR:CG2	2.19	0.55
1:A:303:LYS:HD2	1:A:309:PRO:HA	1.89	0.55
1:A:401:LEU:O	1:A:404:GLN:HB2	2.07	0.55
1:A:261:ILE:HG13	1:A:261:ILE:O	2.07	0.55
1:A:164:LEU:O	1:A:167:MET:HG2	2.07	0.54
1:A:303:LYS:HE2	1:A:309:PRO:HD3	1.89	0.54
1:E:270:LYS:HG2	1:E:297:HIS:CD2	2.42	0.54
2:F:105:GLU:HA	2:F:108:PHE:CD1	2.42	0.54
3:G:581:LEU:O	3:G:584:PHE:HB3	2.08	0.54
1:A:309:PRO:HG2	2:B:38:LEU:HD13	1.89	0.54
3:C:585:ILE:HA	3:C:588:SER:HB3	1.88	0.54
1:E:419:LEU:HD21	3:H:613:LEU:HD21	1.90	0.54
1:A:238:ILE:O	1:A:242:ILE:HG13	2.08	0.54
1:E:365:PHE:CD2	1:E:366:ILE:HG13	2.42	0.54
2:B:169:ASN:O	2:B:173:ILE:N	2.24	0.54
3:H:589:SER:O	3:H:593:SER:HB2	2.07	0.54
1:A:137:ARG:O	1:A:140:LYS:HD2	2.07	0.54
1:A:405:LEU:O	1:A:408:ARG:N	2.40	0.54
3:C:606:SER:HA	3:C:609:LEU:HG	1.90	0.54
1:A:247:TRP:HE3	1:A:247:TRP:H	1.56	0.54
3:C:618:SER:O	3:C:621:LYS:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:629:ALA:HA	1:E:137:ARG:HH22	1.73	0.54
1:E:409:GLN:HE21	3:H:603:ALA:HA	1.72	0.54
2:B:22:LYS:HB2	2:B:94:GLN:H	1.73	0.54
3:H:587:GLN:HA	3:H:590:GLU:OE1	2.08	0.54
1:A:212:GLU:HA	1:A:215:ILE:HD11	1.88	0.54
3:C:603:ALA:O	3:C:607:GLU:HG2	2.08	0.54
3:G:578:LYS:HE3	3:H:577:ASP:OD2	2.07	0.54
1:A:414:ASN:HA	1:A:417:LYS:HE2	1.91	0.53
1:E:245:LEU:O	1:E:248:VAL:HG23	2.08	0.53
1:A:220:TYR:O	1:A:224:PHE:HD1	1.90	0.53
3:D:595:GLN:O	3:D:599:LEU:HD23	2.08	0.53
3:H:620:ALA:O	3:H:624:VAL:HG22	2.08	0.53
3:C:587:GLN:O	3:C:590:GLU:HB2	2.09	0.53
3:D:590:GLU:O	3:D:593:SER:HB3	2.08	0.53
1:A:218:ARG:O	1:A:221:LYS:HE2	2.07	0.53
1:A:256:PRO:HG3	1:A:314:ASP:HA	1.91	0.53
3:D:593:SER:O	3:D:596:ILE:HG13	2.08	0.53
1:E:204:VAL:HG22	1:E:207:ILE:HG21	1.89	0.53
1:A:300:ASN:O	1:A:304:ILE:HG13	2.09	0.53
1:E:366:ILE:O	1:E:369:LEU:HB2	2.09	0.53
3:G:609:LEU:O	3:G:613:LEU:HG	2.09	0.53
1:A:292:THR:HG22	1:A:355:TYR:HD2	1.73	0.53
1:A:427:THR:O	1:A:430:ILE:HG22	2.08	0.53
3:C:596:ILE:O	3:C:599:LEU:HB3	2.09	0.53
1:E:333:SER:O	1:E:337:TYR:HB2	2.08	0.53
1:A:250:PRO:HD3	1:A:321:TYR:CZ	2.44	0.53
1:E:236:LEU:HD23	1:E:236:LEU:N	2.24	0.53
1:A:408:ARG:HH22	3:D:604:GLN:HB2	1.73	0.52
1:E:300:ASN:HA	1:E:303:LYS:HE3	1.89	0.52
1:A:427:THR:OG1	1:A:428:ASP:N	2.42	0.52
3:G:600:VAL:O	3:G:603:ALA:N	2.42	0.52
3:D:595:GLN:OE1	3:H:602:ARG:NH1	2.43	0.52
2:F:161:GLU:O	2:F:169:ASN:ND2	2.39	0.52
1:A:242:ILE:HD13	1:A:327:ASN:HA	1.91	0.52
2:B:29:SER:HB2	2:B:78:GLY:C	2.30	0.52
1:A:416:ALA:O	1:A:419:LEU:HD12	2.10	0.52
3:D:584:PHE:CD1	3:D:584:PHE:C	2.83	0.52
1:A:362:ALA:O	1:A:366:ILE:HG13	2.10	0.52
1:A:275:ILE:O	1:A:278:MET:HB3	2.10	0.52
1:A:349:THR:HA	2:B:72:GLU:OE1	2.10	0.52
2:B:141:ARG:HH12	2:B:145:PHE:H	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:560:LEU:HD22	3:H:563:MET:SD	2.50	0.52
2:B:23:LEU:O	2:B:74:TRP:HD1	1.92	0.52
3:H:601:LEU:HA	3:H:604:GLN:HE22	1.74	0.52
1:E:221:LYS:HG3	1:E:222:TYR:CD1	2.44	0.52
1:E:366:ILE:HA	1:E:369:LEU:HD12	1.92	0.51
2:F:163:SER:HB3	2:F:168:MET:SD	2.49	0.51
3:G:570:GLN:OE1	3:G:570:GLN:HA	2.10	0.51
3:H:576:LYS:HA	3:H:579:GLN:OE1	2.10	0.51
2:B:23:LEU:HD11	2:B:97:ILE:HG13	1.92	0.51
3:D:605:ALA:O	3:D:608:ILE:HG13	2.11	0.51
1:E:419:LEU:O	1:E:419:LEU:HG	2.10	0.51
3:H:584:PHE:C	3:H:584:PHE:CD1	2.83	0.51
2:B:100:TYR:HB3	2:B:111:ALA:HB2	1.92	0.51
3:C:584:PHE:CD1	3:C:584:PHE:C	2.84	0.51
1:E:229:THR:HG23	1:E:231:ASP:H	1.75	0.51
1:E:300:ASN:O	1:E:303:LYS:HG2	2.11	0.51
1:A:374:LEU:HG	1:A:376:LEU:HD13	1.93	0.51
3:D:604:GLN:N	3:D:604:GLN:OE1	2.43	0.51
1:A:285:ARG:HE	1:A:346:ARG:HH22	1.57	0.51
3:G:593:SER:HA	3:G:596:ILE:HG22	1.91	0.51
3:H:569:ASP:O	3:H:572:GLU:HB2	2.10	0.51
3:D:613:LEU:O	3:D:616:GLY:N	2.44	0.51
1:A:179:SER:HA	1:A:341:PHE:HE1	1.76	0.51
3:C:618:SER:HA	3:C:621:LYS:HD3	1.92	0.51
1:E:221:LYS:HE3	1:E:222:TYR:CE1	2.45	0.51
1:A:310:ALA:O	2:B:55:ALA:HB3	2.11	0.50
2:B:70:LYS:HG2	2:B:71:PHE:N	2.25	0.50
3:C:591:ASP:O	3:C:595:GLN:HB2	2.11	0.50
1:E:230:ASP:HA	1:E:233:LYS:HD2	1.92	0.50
1:E:296:LYS:O	1:E:300:ASN:ND2	2.43	0.50
2:F:59:THR:HG22	2:F:70:LYS:HD2	1.93	0.50
1:A:238:ILE:HD12	1:A:239:GLN:N	2.25	0.50
3:D:559:LYS:HD2	3:D:562:LEU:HD11	1.94	0.50
1:E:158:LYS:O	1:E:162:LEU:HG	2.11	0.50
1:A:344:PRO:HA	1:A:347:LEU:HD12	1.93	0.50
1:E:239:GLN:CG	1:E:243:ARG:HH22	2.25	0.50
1:E:261:ILE:HG22	1:E:263:GLU:H	1.77	0.50
2:F:98:VAL:O	2:F:130:LEU:HD12	2.12	0.50
1:A:177:GLU:HA	1:A:180:GLU:HB2	1.93	0.50
1:A:248:VAL:HG13	1:A:321:TYR:CE1	2.41	0.50
2:B:21:PHE:HB3	2:B:70:LYS:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:H	1:A:253:LEU:HD23	1.75	0.50
1:A:250:PRO:CB	1:A:255:VAL:HG12	2.42	0.50
2:B:22:LYS:O	2:B:95:ALA:N	2.44	0.50
1:E:135:THR:HG23	1:E:218:ARG:NH2	2.26	0.50
1:E:288:LEU:CA	1:E:291:ILE:HG22	2.39	0.50
3:D:584:PHE:CE2	3:G:611:GLU:HG2	2.47	0.50
1:E:232:GLU:O	1:E:235:ASP:HB2	2.12	0.50
2:B:174:PHE:O	2:B:177:ILE:HB	2.12	0.50
2:B:36:LEU:HD12	2:B:37:VAL:HG23	1.94	0.50
3:D:573:LYS:NZ	3:G:621:LYS:HE2	2.27	0.50
3:C:610:LEU:HD11	3:D:609:LEU:HD21	1.93	0.49
1:E:281:LYS:HG2	1:E:286:ASP:HB2	1.93	0.49
2:F:162:THR:HG22	2:F:169:ASN:HB2	1.93	0.49
3:H:560:LEU:HA	3:H:563:MET:SD	2.52	0.49
1:E:352:ASP:OD1	1:E:352:ASP:N	2.41	0.49
3:C:560:LEU:HD12	3:D:560:LEU:HB3	1.94	0.49
1:A:289:ALA:O	1:A:293:LYS:HB3	2.13	0.49
1:E:263:GLU:HB3	1:E:304:ILE:HD13	1.94	0.49
1:E:402:LEU:HD22	3:G:595:GLN:NE2	2.27	0.49
1:A:259:GLU:O	1:A:259:GLU:HG3	2.12	0.49
1:A:417:LYS:HG3	1:A:420:GLU:OE1	2.12	0.49
1:A:248:VAL:HG11	1:A:324:LEU:HD22	1.93	0.49
1:E:380:ASP:HB2	1:E:384:TYR:CE2	2.48	0.49
1:A:272:ILE:HG22	1:A:276:ILE:HD13	1.95	0.49
2:B:120:ARG:HB3	2:B:121:GLN:OE1	2.13	0.49
2:B:86:ALA:N	2:B:87:PRO:HD2	2.28	0.49
3:D:559:LYS:O	3:D:562:LEU:HG	2.12	0.49
1:E:159:GLN:HG3	1:E:160:THR:N	2.28	0.49
1:A:138:VAL:HG11	1:A:214:TYR:HA	1.95	0.49
1:A:285:ARG:HE	1:A:346:ARG:NH2	2.10	0.49
1:A:395:MET:HG3	1:A:399:LEU:CD2	2.31	0.49
3:C:627:GLN:O	3:C:630:VAL:HG12	2.13	0.49
1:A:240:LYS:HA	1:A:243:ARG:NH1	2.27	0.48
2:B:23:LEU:N	2:B:72:GLU:O	2.38	0.48
1:E:286:ASP:N	1:E:286:ASP:OD1	2.44	0.48
1:A:253:LEU:HD23	1:A:253:LEU:N	2.28	0.48
1:A:315:PHE:HA	1:A:318:THR:HG1	1.78	0.48
3:C:623:ASP:O	3:C:626:GLU:HB3	2.14	0.48
1:E:406:ASN:HB2	3:G:599:LEU:HD11	1.96	0.48
1:A:370:ASP:HB3	1:A:373:SER:CB	2.43	0.48
1:E:225:CYS:HB3	3:H:565:ARG:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:281:LYS:HG3	1:E:283:VAL:HG12	1.96	0.48
1:E:288:LEU:HD22	1:E:291:ILE:HG21	1.94	0.48
1:E:404:GLN:O	1:E:408:ARG:N	2.47	0.48
1:A:259:GLU:HA	1:A:264:VAL:HG12	1.96	0.48
1:E:407:GLU:HA	1:E:410:GLU:CD	2.33	0.48
1:A:138:VAL:HG12	1:A:214:TYR:HD1	1.78	0.48
1:A:317:PRO:HB3	2:B:82:TYR:OH	2.13	0.48
1:E:297:HIS:HA	1:E:300:ASN:HD21	1.78	0.48
2:F:41:VAL:HA	2:F:60:GLN:NE2	2.29	0.48
2:F:94:GLN:O	2:F:181:LEU:HD11	2.14	0.48
1:E:320:ILE:HG12	1:E:365:PHE:CE2	2.49	0.48
1:A:402:LEU:HD21	3:C:595:GLN:HG3	1.96	0.48
1:A:250:PRO:HB2	1:A:255:VAL:HG12	1.94	0.47
1:A:272:ILE:CD1	1:A:322:ILE:HG23	2.44	0.47
3:D:573:LYS:O	3:D:576:LYS:HB3	2.14	0.47
1:E:294:CYS:SG	1:E:298:ILE:HD11	2.53	0.47
1:E:383:ARG:NH1	1:E:386:SER:OG	2.47	0.47
2:F:158:LEU:HB2	2:F:180:LYS:NZ	2.29	0.47
1:A:193:MET:HE3	1:A:193:MET:HB3	1.71	0.47
1:E:232:GLU:CD	3:H:568:ASN:HB3	2.33	0.47
1:A:366:ILE:O	1:A:369:LEU:HD22	2.13	0.47
2:B:37:VAL:O	2:B:40:PHE:HB3	2.14	0.47
3:C:577:ASP:O	3:C:581:LEU:HB2	2.14	0.47
3:C:600:VAL:O	3:C:603:ALA:N	2.47	0.47
3:D:563:MET:O	3:D:566:GLN:HB2	2.13	0.47
3:H:569:ASP:HA	3:H:572:GLU:OE1	2.15	0.47
1:A:285:ARG:HA	1:A:288:LEU:HG	1.95	0.47
2:B:100:TYR:CE1	2:B:143:VAL:HG11	2.50	0.47
3:D:561:GLN:O	3:D:565:ARG:HG2	2.15	0.47
1:A:301:ALA:HA	1:A:304:ILE:HD12	1.96	0.47
2:B:180:LYS:HA	2:B:180:LYS:HD3	1.60	0.47
2:B:24:VAL:O	2:B:25:LEU:HD23	2.15	0.47
3:D:561:GLN:O	3:D:565:ARG:NH1	2.47	0.47
1:E:324:LEU:HD23	1:E:366:ILE:HD13	1.97	0.47
2:F:71:PHE:HB3	2:F:73:ILE:HD11	1.96	0.47
3:C:597:SER:OG	3:G:597:SER:HB3	2.15	0.47
3:G:604:GLN:HA	3:G:607:GLU:OE2	2.15	0.47
1:A:187:HIS:O	1:A:190:ALA:HB3	2.15	0.47
1:A:408:ARG:O	1:A:411:ARG:HB3	2.15	0.47
3:C:610:LEU:O	3:C:613:LEU:HB2	2.15	0.47
2:F:164:ALA:HA	2:F:170:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:565:ARG:NH2	3:H:566:GLN:OE1	2.48	0.47
2:B:82:TYR:C	2:B:84:SER:H	2.18	0.47
1:E:261:ILE:HB	1:E:264:VAL:CG1	2.45	0.47
1:E:278:MET:HE3	1:E:279:ASP:HB2	1.95	0.47
1:A:252:MET:O	2:B:81:ARG:NH2	2.42	0.47
1:A:295:SER:O	1:A:299:PHE:HD1	1.98	0.47
1:A:336:GLN:O	1:A:340:ARG:HG2	2.14	0.47
1:A:370:ASP:OD1	1:A:372:GLN:N	2.42	0.47
1:A:380:ASP:HA	1:A:383:ARG:NH1	2.30	0.47
2:B:171:ASN:HA	2:B:174:PHE:HB2	1.96	0.47
3:C:598:ALA:HA	3:C:601:LEU:CD2	2.45	0.47
1:E:261:ILE:HB	1:E:264:VAL:HG13	1.96	0.47
1:E:258:ASN:N	1:E:305:THR:HG21	2.20	0.47
1:E:419:LEU:HD23	3:G:613:LEU:HD12	1.97	0.47
1:E:419:LEU:O	1:E:423:LEU:HB2	2.15	0.47
1:E:229:THR:OG1	1:E:230:ASP:N	2.48	0.46
1:E:328:PRO:HB2	1:E:331:LEU:CD2	2.39	0.46
1:E:344:PRO:HA	1:E:347:LEU:HD12	1.98	0.46
1:A:355:TYR:CZ	2:B:57:PHE:HE1	2.33	0.46
1:A:373:SER:HB2	2:B:81:ARG:HB3	1.97	0.46
1:E:320:ILE:HD12	1:E:320:ILE:H	1.81	0.46
2:B:108:PHE:O	2:B:111:ALA:HB3	2.15	0.46
2:B:83:HIS:HB3	2:B:114:TRP:HH2	1.80	0.46
2:B:26:LEU:HA	2:B:76:THR:OG1	2.16	0.46
1:E:136:ASP:O	1:E:140:LYS:HG3	2.15	0.46
2:F:96:ALA:O	2:F:128:ILE:HA	2.15	0.46
1:E:236:LEU:HD11	3:H:571:LEU:HD21	1.97	0.46
1:A:167:MET:H	1:A:167:MET:HG2	1.51	0.46
1:A:370:ASP:HB3	1:A:373:SER:HB3	1.96	0.46
1:A:209:ASP:O	1:A:213:LYS:HG3	2.15	0.46
2:B:111:ALA:O	2:B:115:VAL:HG23	2.16	0.46
2:B:181:LEU:HG	2:B:182:PRO:N	2.29	0.46
2:B:91:ARG:HD2	2:B:91:ARG:HA	1.68	0.46
3:C:581:LEU:HA	3:C:581:LEU:HD22	1.62	0.46
1:E:173:LEU:HD12	1:E:174:SER:H	1.81	0.46
1:A:402:LEU:HD21	3:C:595:GLN:CG	2.46	0.46
1:A:417:LYS:O	1:A:420:GLU:HB3	2.16	0.46
1:E:346:ARG:HH11	1:E:352:ASP:CG	2.18	0.46
1:E:391:PRO:C	1:E:393:LYS:H	2.18	0.46
1:A:191:GLU:O	1:A:195:THR:HG23	2.15	0.46
1:E:204:VAL:O	1:E:208:MET:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:PHE:HD1	1:E:337:TYR:CD1	2.34	0.46
2:F:114:TRP:HA	2:F:114:TRP:CE3	2.50	0.46
1:E:168:HIS:O	1:E:171:ARG:HB3	2.16	0.46
3:G:562:LEU:O	3:G:566:GLN:HG3	2.14	0.46
3:H:604:GLN:OE1	3:H:604:GLN:N	2.44	0.46
1:A:138:VAL:HG21	1:A:217:THR:OG1	2.15	0.46
2:B:80:GLU:O	2:B:83:HIS:HB2	2.16	0.46
3:C:628:MET:HA	3:C:631:LEU:HG	1.98	0.46
3:H:633:GLN:HG3	3:H:634:SER:N	2.30	0.46
3:C:631:LEU:HD11	3:D:631:LEU:HG	1.97	0.46
1:E:407:GLU:HA	1:E:410:GLU:OE2	2.16	0.46
3:H:600:VAL:O	3:H:603:ALA:HB3	2.16	0.46
1:A:170:LYS:HB3	1:A:173:LEU:HG	1.97	0.45
1:A:201:PRO:HA	1:A:204:VAL:HG13	1.97	0.45
3:C:607:GLU:O	3:C:610:LEU:HG	2.16	0.45
1:A:256:PRO:HG3	1:A:314:ASP:CA	2.47	0.45
1:E:142:PHE:O	1:E:146:LEU:HG	2.15	0.45
1:A:212:GLU:OE1	1:A:284:PRO:HG2	2.17	0.45
1:A:315:PHE:O	1:A:318:THR:OG1	2.30	0.45
3:C:610:LEU:HD12	3:C:611:GLU:N	2.31	0.45
1:E:349:THR:HA	2:F:72:GLU:OE2	2.16	0.45
3:G:608:ILE:CG1	3:G:609:LEU:HD22	2.46	0.45
1:A:395:MET:O	1:A:399:LEU:HD23	2.16	0.45
2:B:22:LYS:HB2	2:B:94:GLN:N	2.31	0.45
3:D:610:LEU:O	3:D:610:LEU:HD13	2.17	0.45
1:E:256:PRO:HB2	1:E:302:ILE:HG23	1.99	0.45
3:C:574:THR:HA	3:C:577:ASP:OD2	2.17	0.45
3:D:600:VAL:O	3:D:604:GLN:OE1	2.34	0.45
1:E:239:GLN:HE22	3:H:572:GLU:HG2	1.81	0.45
1:A:265:SER:HA	1:A:268:VAL:HB	1.99	0.45
1:A:358:ASN:HB3	2:B:89:TYR:OH	2.17	0.45
1:E:241:ARG:O	1:E:245:LEU:HG	2.16	0.45
1:E:380:ASP:O	1:E:383:ARG:HB3	2.16	0.45
1:E:395:MET:O	1:E:399:LEU:HD22	2.17	0.45
1:E:225:CYS:SG	3:H:565:ARG:HG3	2.57	0.45
3:D:608:ILE:HD13	1:E:269:VAL:CG2	2.47	0.45
1:A:311:SER:HB2	1:A:313:ASP:OD1	2.17	0.45
2:B:25:LEU:HG	2:B:73:ILE:HG23	1.99	0.45
3:D:602:ARG:HH11	3:D:602:ARG:CG	2.28	0.45
3:D:608:ILE:HD13	1:E:269:VAL:HG21	1.99	0.45
3:D:618:SER:HA	3:D:621:LYS:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:586:LYS:O	3:C:590:GLU:HG2	2.17	0.45
1:E:161:LYS:HA	1:E:164:LEU:HB2	1.98	0.45
1:E:226:PRO:O	1:E:229:THR:HG22	2.17	0.45
3:G:596:ILE:HA	3:G:596:ILE:HD12	1.71	0.45
3:H:627:GLN:O	3:H:631:LEU:HD12	2.17	0.45
1:A:226:PRO:HD2	1:A:229:THR:HG21	1.97	0.44
1:A:399:LEU:HA	1:A:399:LEU:HD13	1.85	0.44
1:A:304:ILE:H	1:A:304:ILE:HG13	1.70	0.44
1:E:238:ILE:HG12	1:E:331:LEU:HB2	2.00	0.44
3:H:600:VAL:HG13	3:H:601:LEU:HD12	1.98	0.44
1:A:248:VAL:CG1	1:A:324:LEU:HD22	2.47	0.44
2:B:101:ASP:N	2:B:107:SER:OG	2.47	0.44
1:E:241:ARG:NE	1:E:367:GLU:O	2.49	0.44
1:E:319:LEU:O	1:E:323:VAL:HG23	2.17	0.44
1:E:404:GLN:CA	1:E:407:GLU:HB2	2.45	0.44
2:F:39:ARG:HB3	2:F:170:VAL:HG11	2.00	0.44
1:A:288:LEU:HA	1:A:291:ILE:CD1	2.44	0.44
2:B:130:LEU:HG	2:B:131:SER:N	2.32	0.44
3:G:609:LEU:O	3:G:612:GLU:HG3	2.16	0.44
1:A:327:ASN:N	1:A:328:PRO:HD3	2.32	0.44
1:A:379:GLU:O	1:A:383:ARG:HB2	2.17	0.44
1:E:395:MET:SD	3:H:589:SER:HA	2.58	0.44
1:E:402:LEU:HD23	1:E:402:LEU:C	2.38	0.44
3:H:569:ASP:HA	3:H:572:GLU:CD	2.38	0.44
3:H:601:LEU:HA	3:H:604:GLN:OE1	2.18	0.44
1:A:298:ILE:HG12	1:A:322:ILE:HG13	1.99	0.44
2:B:87:PRO:HA	2:B:90:TYR:CZ	2.53	0.44
3:H:596:ILE:HG13	3:H:596:ILE:H	1.59	0.44
3:H:601:LEU:HA	3:H:604:GLN:NE2	2.33	0.44
1:E:415:GLU:O	1:E:419:LEU:N	2.48	0.44
3:G:568:ASN:O	3:G:572:GLU:HG2	2.18	0.44
1:A:349:THR:HG22	2:B:20:GLN:HG3	2.00	0.44
3:C:598:ALA:O	3:C:601:LEU:HG	2.18	0.44
1:E:162:LEU:O	1:E:165:GLU:HG2	2.17	0.44
1:A:272:ILE:HB	3:H:608:ILE:HD13	1.99	0.44
1:A:220:TYR:CD1	1:A:224:PHE:HB3	2.53	0.43
1:A:355:TYR:HH	2:B:57:PHE:HE1	1.65	0.43
2:F:179:LYS:HE2	2:F:179:LYS:HB2	1.79	0.43
3:D:609:LEU:HD12	3:D:613:LEU:HG	2.00	0.43
1:E:243:ARG:CZ	1:E:243:ARG:HB2	2.48	0.43
3:H:569:ASP:OD1	3:H:570:GLN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:SER:O	1:A:177:GLU:HB2	2.18	0.43
1:A:288:LEU:O	1:A:292:THR:HG23	2.17	0.43
2:B:106:GLU:OE2	2:B:110:ARG:NH1	2.50	0.43
1:E:255:VAL:HG21	1:E:321:TYR:HD2	1.79	0.43
1:E:365:PHE:HD2	1:E:366:ILE:HG13	1.82	0.43
2:F:41:VAL:HG21	2:F:58:LEU:HD13	1.99	0.43
3:G:618:SER:O	3:G:621:LYS:HG2	2.18	0.43
3:H:584:PHE:HA	3:H:587:GLN:HG2	2.01	0.43
3:H:593:SER:O	3:H:594:HIS:C	2.56	0.43
3:H:612:GLU:O	3:H:615:GLN:HB2	2.18	0.43
1:A:150:HIS:O	1:A:150:HIS:CG	2.71	0.43
1:A:406:ASN:HD22	3:C:599:LEU:HB2	1.84	0.43
3:C:584:PHE:HD1	3:C:585:ILE:N	2.16	0.43
1:E:426:TRP:HE1	3:H:621:LYS:HA	1.84	0.43
3:G:610:LEU:HD13	3:H:609:LEU:HB2	2.01	0.43
1:A:336:GLN:HB3	1:A:340:ARG:NH2	2.33	0.43
1:A:425:ASP:O	1:A:429:GLY:HA3	2.19	0.43
1:E:413:MET:HE1	3:G:609:LEU:HD23	2.01	0.43
3:G:617:LEU:O	3:G:620:ALA:N	2.51	0.43
1:A:423:LEU:HD13	1:A:424:ILE:N	2.34	0.43
1:A:306:LYS:HB3	1:A:308:GLU:CG	2.49	0.43
1:A:380:ASP:HA	1:A:383:ARG:HH11	1.83	0.43
2:B:21:PHE:CE1	2:B:181:LEU:HD13	2.54	0.43
3:G:585:ILE:CG2	3:H:585:ILE:HG12	2.49	0.43
1:A:258:ASN:O	1:A:264:VAL:HG11	2.19	0.43
2:B:145:PHE:HD1	2:B:161:GLU:OE1	2.01	0.43
1:E:409:GLN:HA	1:E:412:ILE:HD12	2.01	0.43
2:F:111:ALA:O	2:F:115:VAL:HG23	2.18	0.43
1:A:158:LYS:O	1:A:162:LEU:HG	2.19	0.43
1:A:261:ILE:HD12	1:A:263:GLU:H	1.84	0.43
1:A:261:ILE:CD1	1:A:263:GLU:HB3	2.41	0.43
2:B:137:LEU:HD13	2:B:140:LYS:NZ	2.34	0.43
2:B:80:GLU:HA	2:B:83:HIS:ND1	2.34	0.43
3:C:593:SER:O	3:C:596:ILE:HG22	2.19	0.43
1:A:302:ILE:HA	1:A:302:ILE:HD12	1.88	0.43
3:C:588:SER:O	3:C:591:ASP:N	2.52	0.43
1:E:300:ASN:ND2	1:E:300:ASN:N	2.64	0.43
1:E:405:LEU:HA	1:E:405:LEU:HD12	1.57	0.43
3:G:560:LEU:HD22	3:H:560:LEU:HB3	2.00	0.43
1:A:137:ARG:HA	1:A:140:LYS:NZ	2.34	0.42
1:A:175:ILE:CD1	1:A:226:PRO:HG2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLY:O	1:A:354:TYR:HE1	2.02	0.42
3:C:608:ILE:HG13	3:C:609:LEU:N	2.33	0.42
3:D:596:ILE:H	3:D:596:ILE:HG13	1.57	0.42
3:D:608:ILE:HD12	3:D:609:LEU:N	2.34	0.42
1:E:296:LYS:HA	1:E:299:PHE:CZ	2.54	0.42
3:G:585:ILE:CD1	3:H:585:ILE:HD11	2.46	0.42
1:A:242:ILE:HA	1:A:245:LEU:CD1	2.49	0.42
1:A:312:ALA:HB1	1:A:316:LEU:HD13	2.00	0.42
1:A:342:CYS:HB3	1:A:347:LEU:HD11	2.01	0.42
2:F:130:LEU:HD23	2:F:159:PHE:CD1	2.54	0.42
3:G:618:SER:HA	3:G:621:LYS:HD3	2.00	0.42
1:A:375:ASN:C	1:A:376:LEU:HD12	2.40	0.42
2:B:146:GLN:O	2:B:150:SER:OG	2.31	0.42
3:C:568:ASN:ND2	3:C:572:GLU:OE2	2.44	0.42
1:E:362:ALA:O	1:E:366:ILE:HG13	2.19	0.42
3:G:582:GLU:HB2	3:H:581:LEU:CD2	2.50	0.42
1:A:252:MET:HB2	1:A:253:LEU:HD23	2.01	0.42
3:C:604:GLN:O	3:G:589:SER:OG	2.30	0.42
1:E:384:TYR:HA	1:E:388:GLN:NE2	2.31	0.42
3:C:613:LEU:O	3:C:614:GLN:C	2.56	0.42
3:D:581:LEU:O	3:D:584:PHE:HB3	2.19	0.42
1:E:216:MET:HE3	1:E:341:PHE:HB3	2.01	0.42
3:C:596:ILE:HA	3:C:596:ILE:HD12	1.51	0.42
1:E:278:MET:HA	1:E:290:CYS:SG	2.59	0.42
1:E:346:ARG:HD3	1:E:352:ASP:OD2	2.19	0.42
3:G:600:VAL:HG13	3:G:601:LEU:N	2.34	0.42
1:A:156:ILE:HD12	1:A:157:TYR:N	2.34	0.42
1:A:343:ASN:O	1:A:347:LEU:HG	2.19	0.42
2:B:29:SER:C	2:B:31:VAL:H	2.22	0.42
2:B:29:SER:O	2:B:31:VAL:N	2.53	0.42
2:B:39:ARG:HD2	2:B:39:ARG:HA	1.73	0.42
3:G:600:VAL:CG1	3:G:601:LEU:N	2.83	0.42
1:E:239:GLN:HE22	3:H:572:GLU:CB	2.33	0.42
1:A:200:PRO:HA	1:A:201:PRO:HD3	1.79	0.42
1:A:261:ILE:HG13	1:A:264:VAL:HB	2.02	0.42
2:B:152:ALA:O	2:B:157:LEU:HG	2.20	0.42
3:C:631:LEU:HD12	3:C:632:MET:N	2.35	0.42
3:D:592:SER:O	3:D:593:SER:C	2.58	0.42
1:E:142:PHE:HA	1:E:145:PHE:HB3	2.02	0.42
1:E:170:LYS:O	1:E:173:LEU:HB3	2.20	0.42
1:E:281:LYS:O	1:E:287:LYS:NZ	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:420:GLU:O	1:E:423:LEU:HB3	2.20	0.42
3:H:597:SER:O	3:H:600:VAL:N	2.53	0.42
1:A:257:VAL:HG21	1:A:318:THR:HG23	2.02	0.42
1:E:134:GLU:O	1:E:138:VAL:HG23	2.20	0.42
1:E:186:TYR:HE1	1:E:343:ASN:ND2	2.17	0.42
1:E:277:GLU:HG2	1:E:277:GLU:O	2.20	0.42
1:E:321:TYR:O	1:E:321:TYR:CD1	2.73	0.42
2:F:141:ARG:HB3	2:F:142:ALA:H	1.48	0.42
3:G:585:ILE:HG13	3:G:586:LYS:N	2.35	0.42
3:C:604:GLN:HB3	3:G:589:SER:OG	2.20	0.42
1:E:175:ILE:HG23	1:E:176:GLU:N	2.35	0.42
1:E:294:CYS:O	1:E:297:HIS:ND1	2.51	0.42
1:E:391:PRO:C	1:E:393:LYS:N	2.74	0.42
1:A:212:GLU:HA	1:A:215:ILE:CD1	2.50	0.41
1:A:226:PRO:HB2	1:A:229:THR:HG22	2.01	0.41
1:A:303:LYS:HE2	1:A:309:PRO:CD	2.50	0.41
1:A:271:ALA:HB3	1:A:322:ILE:HD12	2.01	0.41
1:A:336:GLN:HB3	1:A:340:ARG:CZ	2.50	0.41
2:F:110:ARG:NE	2:F:110:ARG:HA	2.35	0.41
1:A:159:GLN:HG2	1:A:160:THR:N	2.34	0.41
1:A:169:TYR:HD1	1:A:169:TYR:HA	1.72	0.41
1:A:272:ILE:HA	1:A:275:ILE:HG22	2.02	0.41
1:A:401:LEU:HA	1:A:401:LEU:HD22	1.54	0.41
3:D:629:ALA:O	1:E:137:ARG:NH1	2.53	0.41
3:H:570:GLN:O	3:H:571:LEU:C	2.58	0.41
1:A:374:LEU:CG	1:A:376:LEU:HD13	2.50	0.41
3:C:554:ARG:HB3	3:C:554:ARG:CZ	2.50	0.41
1:E:288:LEU:HD11	1:E:342:CYS:SG	2.61	0.41
1:E:378:GLN:HA	1:E:381:PHE:HB2	2.02	0.41
1:A:255:VAL:HG22	1:A:257:VAL:HG23	2.01	0.41
1:A:369:LEU:HD12	1:A:369:LEU:HA	1.85	0.41
1:A:429:GLY:O	1:A:433:GLU:HB3	2.21	0.41
3:C:605:ALA:O	3:C:609:LEU:HD11	2.20	0.41
1:E:216:MET:CE	1:E:341:PHE:HB3	2.50	0.41
1:E:324:LEU:HA	1:E:324:LEU:HD22	1.81	0.41
3:G:602:ARG:O	3:G:606:SER:HB3	2.21	0.41
3:G:614:GLN:O	3:G:617:LEU:HG	2.20	0.41
3:C:621:LYS:HZ1	3:H:576:LYS:HE2	1.85	0.41
1:A:139:SER:O	1:A:143:ILE:HG12	2.21	0.41
1:A:142:PHE:HE1	1:A:210:GLN:O	2.03	0.41
1:A:242:ILE:HG13	1:A:242:ILE:H	1.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:MET:HG3	2:B:169:ASN:H	1.85	0.41
3:C:578:LYS:HE2	3:C:578:LYS:HB3	1.86	0.41
3:C:611:GLU:HA	3:C:614:GLN:H	1.85	0.41
1:E:219:LEU:HD23	1:E:219:LEU:C	2.40	0.41
1:E:335:ILE:O	1:E:338:ILE:HB	2.21	0.41
2:F:106:GLU:OE2	2:F:110:ARG:HG2	2.20	0.41
2:F:141:ARG:HA	2:F:141:ARG:HD3	1.79	0.41
3:H:554:ARG:O	3:H:558:LYS:HB3	2.20	0.41
1:A:215:ILE:HG12	1:A:215:ILE:H	1.72	0.41
1:A:242:ILE:HG23	1:A:245:LEU:HD12	2.02	0.41
1:A:413:MET:HG3	3:C:606:SER:HB2	2.02	0.41
1:E:368:LYS:HA	1:E:368:LYS:HD3	1.72	0.41
1:A:163:PHE:CZ	1:A:185:PHE:CD1	3.09	0.41
1:A:310:ALA:HB1	1:A:314:ASP:HB2	2.02	0.41
3:C:622:ARG:HH22	3:H:573:LYS:HB3	1.84	0.41
1:E:167:MET:HE2	1:E:170:LYS:HE3	2.02	0.41
1:E:174:SER:HB3	1:E:177:GLU:HG3	2.03	0.41
3:H:623:ASP:HA	3:H:626:GLU:HG2	2.01	0.41
1:E:233:LYS:HG3	1:E:233:LYS:H	1.72	0.41
1:A:220:TYR:HD1	1:A:337:TYR:CE2	2.30	0.41
1:A:319:LEU:HG	1:A:320:ILE:N	2.36	0.41
1:A:249:THR:O	1:A:252:MET:SD	2.79	0.41
1:A:263:GLU:O	1:A:266:ASP:HB2	2.21	0.41
1:A:265:SER:O	1:A:269:VAL:HG23	2.21	0.41
1:A:295:SER:HA	1:A:298:ILE:HD12	2.02	0.41
1:A:365:PHE:CB	2:B:85:LEU:HD21	2.40	0.41
1:E:267:MET:HB3	1:E:267:MET:HE3	1.89	0.41
1:E:250:PRO:HB3	1:E:321:TYR:CE2	2.56	0.41
1:E:303:LYS:HA	1:E:307:ASN:HA	2.03	0.41
1:E:351:GLU:HG2	1:E:351:GLU:H	1.66	0.41
2:B:80:GLU:HA	2:B:83:HIS:CE1	2.56	0.40
1:E:212:GLU:O	1:E:215:ILE:HG13	2.21	0.40
3:H:595:GLN:HG3	3:H:599:LEU:HD11	2.03	0.40
1:A:163:PHE:CD1	1:A:163:PHE:C	2.94	0.40
1:A:230:ASP:O	1:A:234:LYS:NZ	2.55	0.40
1:A:242:ILE:HA	1:A:245:LEU:HD12	2.02	0.40
1:A:359:LEU:HD23	1:A:360:CYS:N	2.36	0.40
1:A:244:ALA:HB1	1:A:385:MET:HE2	2.03	0.40
2:B:26:LEU:HD11	2:B:114:TRP:CE2	2.56	0.40
2:B:134:LYS:HD3	2:B:165:LYS:NZ	2.36	0.40
1:E:182:ALA:O	1:E:185:PHE:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:VAL:HG23	1:A:205:GLU:N	2.36	0.40
1:E:230:ASP:HA	1:E:233:LYS:CD	2.51	0.40
2:F:181:LEU:HA	2:F:182:PRO:HD3	1.92	0.40
1:A:219:LEU:O	1:A:223:VAL:HG22	2.22	0.40
1:A:415:GLU:OE2	1:A:418:LYS:HD3	2.21	0.40
2:B:100:TYR:HE1	2:B:143:VAL:HG11	1.86	0.40
3:D:624:VAL:O	3:D:628:MET:HG2	2.21	0.40
1:E:174:SER:O	1:E:178:GLN:N	2.54	0.40
1:E:264:VAL:HG11	1:E:305:THR:CG2	2.52	0.40
3:G:576:LYS:HD2	3:G:576:LYS:HA	1.81	0.40
3:D:559:LYS:CD	3:D:562:LEU:HD11	2.51	0.40
1:E:281:LYS:HG2	1:E:286:ASP:CB	2.52	0.40
2:F:39:ARG:NE	2:F:167:SER:HB3	2.37	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	299/317 (94%)	279 (93%)	20 (7%)	0	100 100
1	E	292/317 (92%)	272 (93%)	18 (6%)	2 (1%)	22 62
2	B	149/171 (87%)	129 (87%)	17 (11%)	3 (2%)	7 40
2	F	104/171 (61%)	100 (96%)	3 (3%)	1 (1%)	15 54
3	C	81/92 (88%)	77 (95%)	4 (5%)	0	100 100
3	D	73/92 (79%)	73 (100%)	0	0	100 100
3	G	82/92 (89%)	80 (98%)	2 (2%)	0	100 100
3	H	80/92 (87%)	78 (98%)	2 (2%)	0	100 100
All	All	1160/1344 (86%)	1088 (94%)	66 (6%)	6 (0%)	29 68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	170	VAL
2	B	30	ALA
2	B	34	SER
1	E	391	PRO
2	F	168	MET
1	E	186	TYR

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	281/294 (96%)	217 (77%)	64 (23%)	1 6
1	E	276/294 (94%)	217 (79%)	59 (21%)	1 6
2	B	127/143 (89%)	106 (84%)	21 (16%)	2 14
2	F	100/143 (70%)	87 (87%)	13 (13%)	4 20
3	C	76/85 (89%)	49 (64%)	27 (36%)	0 1
3	D	68/85 (80%)	48 (71%)	20 (29%)	0 2
3	G	77/85 (91%)	54 (70%)	23 (30%)	0 2
3	H	75/85 (88%)	56 (75%)	19 (25%)	0 4
All	All	1080/1214 (89%)	834 (77%)	246 (23%)	1 6

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	SER
1	A	140	LYS
1	A	146	LEU
1	A	147	LYS
1	A	151	LYS
1	A	154	GLN
1	A	159	GLN
1	A	160	THR

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Mol	Chain	Res	Type
1	A	167	MET
1	A	169	TYR
1	A	174	SER
1	A	180	GLU
1	A	181	CYS
1	A	185	PHE
1	A	191	GLU
1	A	193	MET
1	A	208	MET
1	A	211	ILE
1	A	215	ILE
1	A	219	LEU
1	A	228	THR
1	A	236	LEU
1	A	241	ARG
1	A	242	ILE
1	A	247	TRP
1	A	252	MET
1	A	253	LEU
1	A	257	VAL
1	A	259	GLU
1	A	261	ILE
1	A	272	ILE
1	A	282	ARG
1	A	285	ARG
1	A	300	ASN
1	A	304	ILE
1	A	306	LYS
1	A	307	ASN
1	A	311	SER
1	A	313	ASP
1	A	316	LEU
1	A	318	THR
1	A	319	LEU
1	A	320	ILE
1	A	337	TYR
1	A	339	THR
1	A	340	ARG
1	A	352	ASP
1	A	369	LEU
1	A	377	SER
1	A	378	GLN

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Mol	Chain	Res	Type
1	A	392	ARG
1	A	393	LYS
1	A	395	MET
1	A	401	LEU
1	A	404	GLN
1	A	407	GLU
1	A	409	GLN
1	A	411	ARG
1	A	413	MET
1	A	419	LEU
1	A	423	LEU
1	A	430	ILE
1	A	433	GLU
1	A	434	VAL
2	B	20	GLN
2	B	23	LEU
2	B	28	GLU
2	B	33	LYS
2	B	34	SER
2	B	52	THR
2	B	62	VAL
2	B	81	ARG
2	B	82	TYR
2	B	84	SER
2	B	89	TYR
2	B	118	LEU
2	B	123	SER
2	B	130	LEU
2	B	136	ASP
2	B	139	ASN
2	B	141	ARG
2	B	163	SER
2	B	173	ILE
2	B	175	MET
2	B	179	LYS
3	C	554	ARG
3	C	560	LEU
3	C	561	GLN
3	C	562	LEU
3	C	563	MET
3	C	568	ASN
3	C	571	LEU

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Mol	Chain	Res	Type
3	C	573	LYS
3	C	577	ASP
3	C	579	GLN
3	C	581	LEU
3	C	584	PHE
3	C	587	GLN
3	C	591	ASP
3	C	593	SER
3	C	597	SER
3	C	599	LEU
3	C	601	LEU
3	C	606	SER
3	C	612	GLU
3	C	614	GLN
3	C	617	LEU
3	C	619	GLN
3	C	623	ASP
3	C	625	GLN
3	C	627	GLN
3	C	628	MET
3	D	560	LEU
3	D	562	LEU
3	D	569	ASP
3	D	570	GLN
3	D	571	LEU
3	D	574	THR
3	D	575	MET
3	D	580	GLU
3	D	581	LEU
3	D	593	SER
3	D	596	ILE
3	D	602	ARG
3	D	609	LEU
3	D	619	GLN
3	D	622	ARG
3	D	624	VAL
3	D	626	GLU
3	D	630	VAL
3	D	631	LEU
3	D	632	MET
1	E	137	ARG
1	E	138	VAL

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Mol	Chain	Res	Type
1	E	139	SER
1	E	146	LEU
1	E	150	HIS
1	E	151	LYS
1	E	152	THR
1	E	164	LEU
1	E	165	GLU
1	E	167	MET
1	E	168	HIS
1	E	171	ARG
1	E	172	ASP
1	E	183	GLN
1	E	191	GLU
1	E	198	LYS
1	E	211	ILE
1	E	216	MET
1	E	219	LEU
1	E	223	VAL
1	E	228	THR
1	E	240	LYS
1	E	248	VAL
1	E	257	VAL
1	E	264	VAL
1	E	265	SER
1	E	267	MET
1	E	272	ILE
1	E	278	MET
1	E	286	ASP
1	E	291	ILE
1	E	297	HIS
1	E	299	PHE
1	E	300	ASN
1	E	318	THR
1	E	319	LEU
1	E	322	ILE
1	E	324	LEU
1	E	331	LEU
1	E	332	GLN
1	E	340	ARG
1	E	346	ARG
1	E	352	ASP
1	E	361	CYS

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Mol	Chain	Res	Type
1	E	369	LEU
1	E	380	ASP
1	E	383	ARG
1	E	397	LYS
1	E	399	LEU
1	E	401	LEU
1	E	407	GLU
1	E	408	ARG
1	E	413	MET
1	E	419	LEU
1	E	423	LEU
1	E	430	ILE
1	E	432	ARG
1	E	435	GLN
1	E	437	ILE
2	F	22	LYS
2	F	24	VAL
2	F	35	SER
2	F	58	LEU
2	F	59	THR
2	F	82	TYR
2	F	84	SER
2	F	88	MET
2	F	104	ASN
2	F	128	ILE
2	F	146	GLN
2	F	166	THR
2	F	179	LYS
3	G	554	ARG
3	G	556	GLN
3	G	560	LEU
3	G	562	LEU
3	G	571	LEU
3	G	574	THR
3	G	575	MET
3	G	579	GLN
3	G	581	LEU
3	G	583	ASP
3	G	585	ILE
3	G	587	GLN
3	G	591	ASP
3	G	599	LEU

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Mol	Chain	Res	Type
3	G	601	LEU
3	G	602	ARG
3	G	606	SER
3	G	612	GLU
3	G	615	GLN
3	G	624	VAL
3	G	628	MET
3	G	630	VAL
3	G	633	GLN
3	H	560	LEU
3	H	563	MET
3	H	564	LEU
3	H	569	ASP
3	H	575	MET
3	H	576	LYS
3	H	577	ASP
3	H	579	GLN
3	H	581	LEU
3	H	584	PHE
3	H	593	SER
3	H	595	GLN
3	H	596	ILE
3	H	608	ILE
3	H	610	LEU
3	H	611	GLU
3	H	627	GLN
3	H	630	VAL
3	H	631	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	358	ASN
1	A	398	ASN
1	A	409	GLN
2	B	133	ASN
1	E	300	ASN
1	E	388	GLN
3	G	595	GLN
3	H	627	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	303/317 (95%)	-0.37	0 100 100	45, 133, 270, 349	0
1	E	296/317 (93%)	-0.16	5 (1%) 70 61	39, 209, 344, 447	0
2	B	153/171 (89%)	0.29	13 (8%) 10 10	112, 238, 333, 441	0
2	F	120/171 (70%)	1.24	30 (25%) 0 1	137, 300, 407, 493	0
3	C	83/92 (90%)	-0.24	0 100 100	36, 120, 264, 425	0
3	D	75/92 (81%)	-0.43	0 100 100	71, 130, 262, 343	0
3	G	84/92 (91%)	-0.45	1 (1%) 79 70	54, 108, 252, 324	0
3	H	82/92 (89%)	-0.32	0 100 100	37, 116, 263, 327	0
All	All	1196/1344 (88%)	-0.07	49 (4%) 37 31	36, 178, 336, 493	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	130	LEU	6.1
2	B	128	ILE	4.9
2	F	98	VAL	4.8
2	F	76	THR	4.8
2	F	128	ILE	4.1
2	F	25	LEU	4.0
2	F	99	VAL	3.9
2	F	75	ASP	3.8
2	F	181	LEU	3.5
1	E	209	ASP	3.5
2	B	158	LEU	3.4
2	F	129	ALA	3.3
2	F	155	ASN	3.2
2	F	177	ILE	3.0
2	F	127	VAL	2.9
2	B	61	THR	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	129	ALA	2.9
2	F	96	ALA	2.9
2	B	98	VAL	2.8
2	F	174	PHE	2.8
2	F	97	ILE	2.7
2	F	24	VAL	2.6
2	F	131	SER	2.6
2	B	133	ASN	2.6
2	B	51	SER	2.5
2	F	119	GLN	2.5
1	E	196	ARG	2.5
2	B	134	LYS	2.4
2	B	127	VAL	2.4
2	F	156	SER	2.4
2	F	37	VAL	2.4
2	F	60	GLN	2.3
2	B	99	VAL	2.3
2	F	160	MET	2.3
1	E	282	ARG	2.3
2	F	123	SER	2.3
2	B	95	ALA	2.3
2	B	96	ALA	2.2
2	B	130	LEU	2.2
2	F	41	VAL	2.1
2	F	126	ILE	2.1
2	F	34	SER	2.1
2	F	71	PHE	2.1
1	E	213	LYS	2.1
2	F	151	TYR	2.1
3	G	554	ARG	2.1
2	F	182	PRO	2.1
2	F	159	PHE	2.0
1	E	386	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.