Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 11:27 PM BST

PDB ID	:	6C08
Title	:	Zebrafish SLC38A9 with arginine bound in the cytosol open state
Authors	:	Lei, H.-T.; Gonen, T.
Deposited on	:	2017-12-28
Resolution	:	3.17 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 ⓘ) were used in the production of this report:

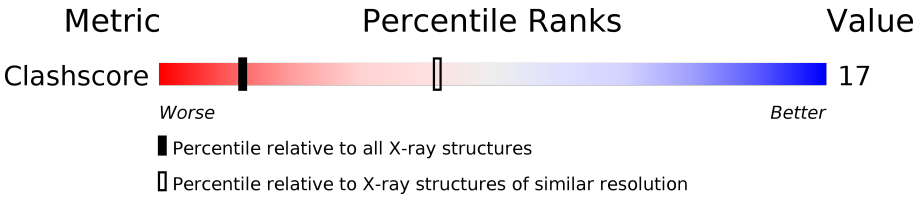
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.17 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))
Clashscore	141614	1599 (3.20-3.16)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	218	83% 16% .
1	D	218	80% 18% .
2	B	215	80% 20%
2	E	215	82% 18%
3	C	479	45% 31% 24%
3	F	479	47% 33% 20%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12341 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 antibody Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1561	983	258	316	4			
1	D	214	Total	C	N	O	S	0	0	0
			1561	983	258	316	4			

- Molecule 2 is a protein called antibody Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1642	1025	274	339	4			
2	E	215	Total	C	N	O	S	0	0	0
			1642	1025	274	339	4			

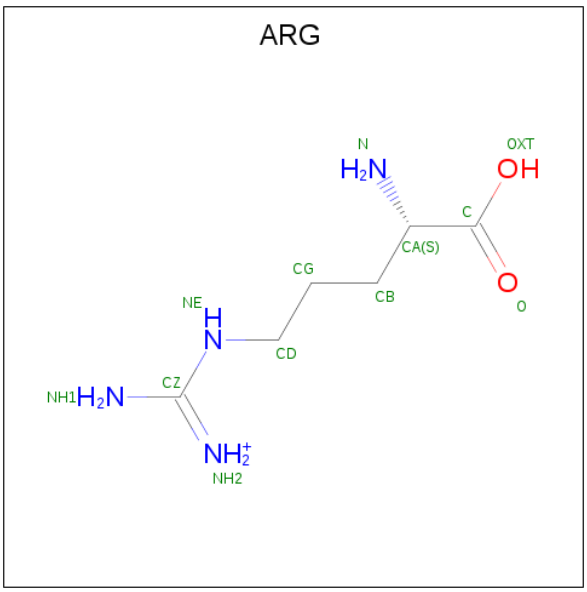
- Molecule 3 is a protein called Sodium-coupled neutral amino acid transporter 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	364	Total	C	N	O	S	0	0	0
			2866	1942	439	466	19			
3	F	385	Total	C	N	O	S	0	0	0
			3057	2066	471	501	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	227	GLN	ASN	engineered mutation	UNP Q08BA4
C	235	GLN	ASN	engineered mutation	UNP Q08BA4
C	252	GLN	ASN	engineered mutation	UNP Q08BA4
C	263	GLN	ASN	engineered mutation	UNP Q08BA4
F	227	GLN	ASN	engineered mutation	UNP Q08BA4
F	235	GLN	ASN	engineered mutation	UNP Q08BA4
F	252	GLN	ASN	engineered mutation	UNP Q08BA4
F	263	GLN	ASN	engineered mutation	UNP Q08BA4

- Molecule 4 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	1	Total	C	N	O	0	0
			12	6	4	2		

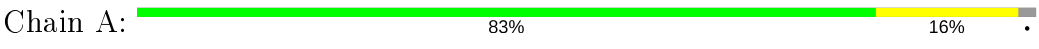
3 Residue-property plots (i)

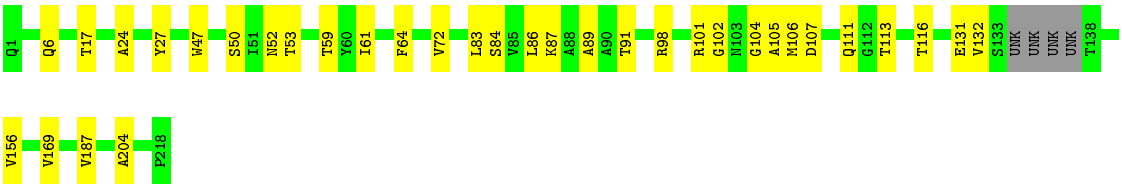
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS failed to run properly.

- Molecule 1: antibody Fab Heavy Chain

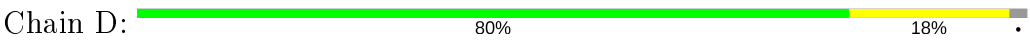
Chain A:

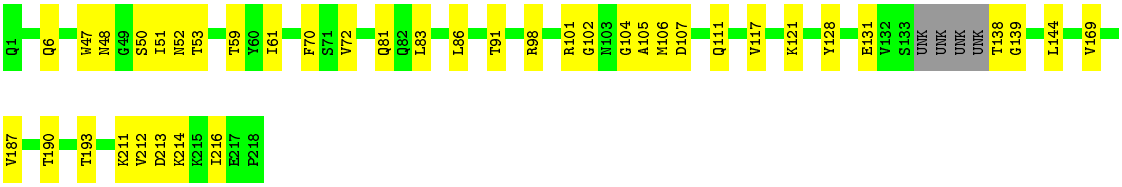




- Molecule 1: antibody Fab Heavy Chain

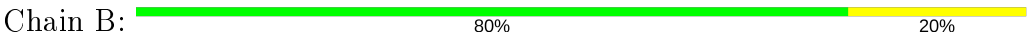
Chain D:

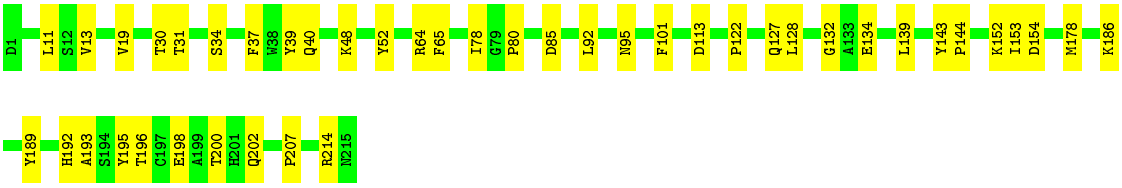




- Molecule 2: antibody Fab light chain

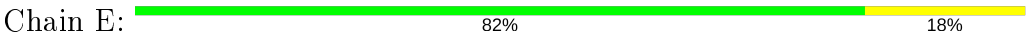
Chain B:

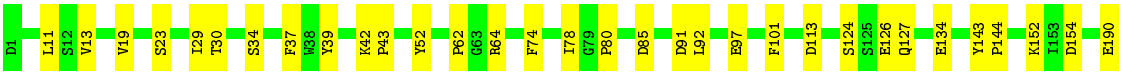


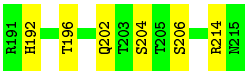


- Molecule 2: antibody Fab light chain

Chain E:

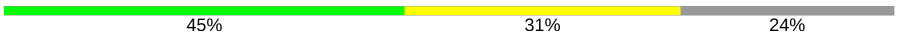


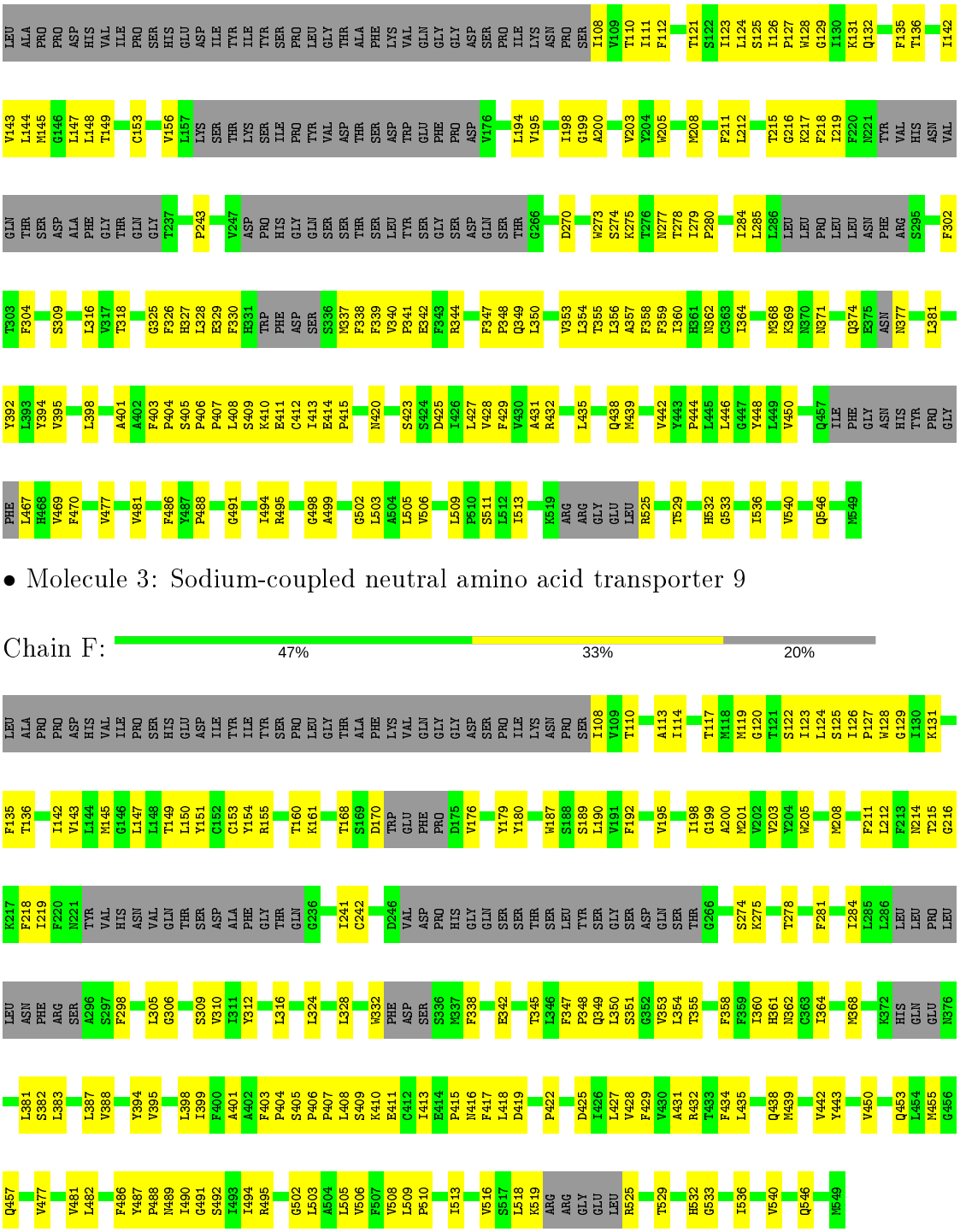




• Molecule 3: Sodium-coupled neutral amino acid transporter 9

Chain C:





• Molecule 3: Sodium-coupled neutral amino acid transporter 9

Chain F:

4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	136.61Å 82.81Å 158.92Å 90.00° 100.02° 90.00°	Depositor
Resolution (Å)	156.50 – 3.17	Depositor
% Data completeness (in resolution range)	99.8 (156.50-3.17)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.267 , 0.285	Depositor
Wilson B-factor (Å^2)	105.2	Xtriage
Anisotropy	0.042	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12341	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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	0.30	0/1597	0.51	0/2178
1	D	0.30	0/1597	0.51	0/2178
2	B	0.29	0/1679	0.50	0/2285
2	E	0.30	0/1679	0.51	0/2285
3	C	0.32	0/2942	0.70	0/3998
3	F	0.33	0/3145	0.70	0/4275
All	All	0.31	0/12639	0.61	0/17199

There are no bond length outliers.

There are no bond angle outliers.

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	1561	0	1524	31	0
1	D	1561	0	1524	34	0
2	B	1642	0	1561	31	0
2	E	1642	0	1561	31	0
3	C	2866	0	2923	143	0
3	F	3057	0	3090	153	0
4	F	12	0	12	3	0
All	All	12341	0	12195	411	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 17.

All (411) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:122:SER:HG	4:F:601:ARG:N	1.49	1.10
2:E:13:VAL:HG21	2:E:19:VAL:HG12	1.33	1.09
3:C:491:GLY:O	3:C:495:ARG:HD3	1.62	0.98
2:B:13:VAL:HG21	2:B:19:VAL:HG12	1.43	0.98
3:F:489:ASN:HB3	3:F:492:SER:HB2	1.51	0.92
3:F:489:ASN:HD22	3:F:492:SER:H	1.17	0.90
3:F:489:ASN:HD22	3:F:492:SER:N	1.69	0.88
3:F:205:TRP:HE1	3:F:274:SER:HG	1.12	0.88
3:C:284:ILE:HD13	3:C:444:PRO:HG3	1.56	0.86
1:A:131:GLU:OE2	2:B:122:PRO:HD2	1.76	0.84
3:F:150:LEU:HD11	3:F:382:SER:HA	1.59	0.83
3:C:414:GLU:HG2	3:C:415:PRO:HD2	1.61	0.82
3:F:495:ARG:NH1	3:F:546:GLN:OE1	2.11	0.82
3:C:467:LEU:HD11	3:C:470:PHE:HB2	1.61	0.81
3:F:122:SER:OG	4:F:601:ARG:N	2.14	0.80
3:C:425:ASP:HB3	3:C:428:VAL:HB	1.62	0.80
3:C:495:ARG:O	3:C:499:ALA:HB3	1.83	0.79
1:D:51:ILE:HD13	1:D:72:VAL:HG23	1.65	0.79
3:F:128:TRP:CD1	3:F:415:PRO:HD3	2.18	0.79
3:C:495:ARG:O	3:C:499:ALA:CB	2.32	0.78
3:F:425:ASP:HB3	3:F:428:VAL:HB	1.66	0.78
2:E:154:ASP:OD2	2:E:192:HIS:ND1	2.15	0.78
3:F:187:TRP:HB2	3:F:190:LEU:HD23	1.67	0.76
3:C:270:ASP:HA	3:C:273:TRP:HE1	1.48	0.76
3:F:214:ASN:HD22	3:F:432:ARG:NH1	1.81	0.76
2:E:113:ASP:OD2	2:E:202:GLN:NE2	2.18	0.76
3:F:491:GLY:HA2	3:F:494:ILE:HG12	1.68	0.76
3:C:329:GLU:O	3:C:330:PHE:O	2.04	0.75
1:D:83:LEU:HB3	1:D:86:LEU:HD11	1.68	0.75
3:F:129:GLY:HA3	3:F:350:LEU:HD13	1.68	0.74
3:F:108:ILE:HG22	3:F:110:THR:H	1.52	0.74
3:C:486:PHE:O	3:C:488:PRO:HD3	1.87	0.74
2:E:127:GLN:NE2	2:E:134:GLU:OE2	2.19	0.74
1:A:98:ARG:NH2	1:A:107:ASP:OD2	2.15	0.73
3:C:410:LYS:O	3:C:412:CYS:N	2.22	0.73
3:C:491:GLY:O	3:C:495:ARG:CD	2.36	0.72
3:F:438:GLN:O	3:F:438:GLN:NE2	2.22	0.72
2:B:64:ARG:NH2	2:B:85:ASP:OD1	2.16	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:410:LYS:C	3:C:412:CYS:H	1.90	0.72
3:C:195:VAL:HA	3:C:198:ILE:HG12	1.72	0.72
3:F:489:ASN:ND2	3:F:492:SER:N	2.39	0.70
1:A:59:THR:HG23	3:C:337:MET:H	1.57	0.70
3:F:439:MET:HA	3:F:442:VAL:HG12	1.73	0.70
1:A:17:THR:HG23	1:A:84:SER:HA	1.73	0.70
1:A:131:GLU:OE1	1:A:132:VAL:O	2.10	0.70
3:C:439:MET:HA	3:C:442:VAL:HG22	1.74	0.70
3:F:195:VAL:HA	3:F:198:ILE:HG12	1.71	0.69
3:F:489:ASN:HB3	3:F:492:SER:CB	2.22	0.69
3:F:489:ASN:ND2	3:F:492:SER:H	1.91	0.69
3:C:355:THR:HG21	3:C:502:GLY:HA3	1.75	0.69
3:F:355:THR:HG21	3:F:502:GLY:HA3	1.74	0.68
1:D:138:THR:OG1	1:D:139:GLY:N	2.25	0.68
3:C:431:ALA:O	3:C:435:LEU:HD13	1.93	0.68
3:C:491:GLY:O	3:C:495:ARG:HG2	1.93	0.68
3:F:347:PHE:CG	3:F:348:PRO:HD3	2.29	0.68
3:F:518:LEU:HD21	3:F:525:ARG:HG2	1.75	0.68
1:A:169:VAL:HG22	1:A:187:VAL:HG12	1.76	0.67
3:C:349:GLN:HG2	3:C:495:ARG:NH1	2.08	0.67
2:B:30:THR:HA	2:B:34:SER:HA	1.77	0.67
3:C:469:VAL:HG13	3:C:470:PHE:H	1.60	0.66
1:A:102:GLY:O	1:A:104:GLY:N	2.27	0.66
3:F:119:MET:HE2	3:F:388:VAL:HG22	1.77	0.66
3:F:190:LEU:HD22	3:F:457:GLN:HG3	1.76	0.66
3:C:284:ILE:HD12	3:C:285:LEU:HD22	1.77	0.66
3:C:328:LEU:HD21	3:C:401:ALA:HA	1.78	0.66
1:D:98:ARG:NH2	1:D:107:ASP:OD2	2.23	0.66
1:A:83:LEU:HB3	1:A:86:LEU:HD11	1.78	0.65
3:F:368:MET:CE	3:F:368:MET:HA	2.26	0.65
3:F:489:ASN:CB	3:F:492:SER:HB2	2.25	0.65
1:D:169:VAL:HG22	1:D:187:VAL:HG12	1.78	0.65
3:C:374:GLN:O	3:C:377:ASN:N	2.30	0.65
1:D:121:LYS:H	1:D:121:LYS:HD3	1.62	0.65
3:F:406:PRO:HG2	3:F:407:PRO:HD3	1.79	0.65
2:B:19:VAL:HG22	2:B:78:ILE:HG12	1.78	0.65
3:F:142:ILE:HG12	3:F:354:LEU:HD11	1.78	0.65
3:C:208:MET:O	3:C:212:LEU:N	2.27	0.64
3:C:406:PRO:HG2	3:C:407:PRO:HD3	1.79	0.64
3:F:502:GLY:O	3:F:506:VAL:HB	1.97	0.64
2:E:37:PHE:HD1	2:E:52:TYR:HA	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:316:LEU:HD12	3:C:427:LEU:HB3	1.78	0.64
1:D:91:THR:HG22	1:D:117:VAL:H	1.62	0.64
1:D:102:GLY:O	1:D:104:GLY:N	2.28	0.64
3:F:189:SER:HB2	3:F:505:LEU:HD11	1.80	0.63
3:F:431:ALA:O	3:F:435:LEU:HD13	1.98	0.63
3:F:438:GLN:HE22	3:F:442:VAL:HB	1.64	0.63
1:A:6:GLN:H	1:A:111:GLN:HE22	1.47	0.63
3:C:275:LYS:O	3:C:278:THR:HG22	1.99	0.63
3:F:143:VAL:O	3:F:147:LEU:HD13	1.98	0.63
3:C:110:THR:HG21	3:C:371:ASN:HB3	1.80	0.63
1:D:6:GLN:H	1:D:111:GLN:HE22	1.47	0.63
3:F:368:MET:HA	3:F:368:MET:HE2	1.79	0.62
3:F:399:ILE:HG13	3:F:417:PHE:CE1	2.33	0.62
3:F:518:LEU:HG	3:F:525:ARG:HE	1.64	0.62
3:F:508:VAL:HA	3:F:536:ILE:HG22	1.81	0.62
3:C:273:TRP:C	3:C:275:LYS:H	2.02	0.62
3:F:324:LEU:HD11	3:F:404:PRO:HD3	1.82	0.62
3:C:428:VAL:O	3:C:432:ARG:HG2	1.99	0.62
3:F:198:ILE:HA	3:F:201:MET:HE2	1.82	0.62
3:C:341:PRO:HD2	3:C:344:ARG:HD3	1.81	0.61
3:C:495:ARG:NH1	3:C:546:GLN:OE1	2.32	0.61
2:B:64:ARG:HB2	2:B:80:PRO:HD2	1.80	0.61
3:F:153:CYS:HB2	3:F:361:HIS:CE1	2.35	0.61
3:C:128:TRP:CG	3:C:415:PRO:HA	2.36	0.61
3:F:126:ILE:H	3:F:127:PRO:HD2	1.65	0.61
2:B:127:GLN:NE2	2:B:134:GLU:OE2	2.34	0.61
3:C:143:VAL:O	3:C:147:LEU:HD22	2.00	0.61
2:B:31:THR:OG1	2:B:95:ASN:ND2	2.23	0.60
2:B:37:PHE:HD1	2:B:52:TYR:HA	1.66	0.60
3:F:489:ASN:CG	3:F:492:SER:OG	2.39	0.60
3:C:347:PHE:CG	3:C:348:PRO:HD3	2.37	0.60
3:C:129:GLY:HA3	3:C:350:LEU:HD13	1.83	0.60
3:C:123:ILE:HD11	3:C:395:VAL:HG21	1.84	0.60
3:F:168:THR:O	3:F:179:TYR:OH	2.19	0.60
3:F:360:ILE:C	3:F:362:ASN:H	2.05	0.60
3:C:502:GLY:O	3:C:506:VAL:HB	2.02	0.59
3:C:505:LEU:HD23	3:C:509:LEU:HD12	1.82	0.59
3:F:416:ASN:HB2	3:F:490:ILE:HG13	1.84	0.59
3:C:126:ILE:H	3:C:127:PRO:HD2	1.67	0.59
3:F:428:VAL:HG12	3:F:432:ARG:HE	1.67	0.59
3:F:450:VAL:O	3:F:453:GLN:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:495:ARG:O	3:F:546:GLN:HG3	2.03	0.59
3:C:330:PHE:CD1	3:C:342:GLU:OE2	2.56	0.59
3:F:242:CYS:SG	3:F:408:LEU:HD22	2.42	0.59
3:C:414:GLU:CG	3:C:415:PRO:HD2	2.32	0.59
1:A:105:ALA:HB2	2:B:37:PHE:CD1	2.38	0.59
3:C:491:GLY:O	3:C:495:ARG:CG	2.51	0.58
3:F:353:VAL:HG13	3:F:494:ILE:HD12	1.85	0.58
3:F:405:SER:HB3	3:F:410:LYS:NZ	2.19	0.58
3:C:211:PHE:O	3:C:215:THR:HG23	2.04	0.58
3:C:284:ILE:CD1	3:C:285:LEU:HD22	2.33	0.58
2:B:189:TYR:O	2:B:195:TYR:OH	2.22	0.58
3:C:525:ARG:N	3:C:529:THR:HG1	2.02	0.58
3:C:446:LEU:O	3:C:450:VAL:HB	2.04	0.57
1:D:211:LYS:NZ	1:D:212:VAL:O	2.37	0.57
1:D:211:LYS:NZ	1:D:213:ASP:OD1	2.37	0.57
3:F:316:LEU:HD12	3:F:427:LEU:HB3	1.86	0.57
3:C:360:ILE:O	3:C:362:ASN:N	2.31	0.57
3:C:405:SER:HB3	3:C:410:LYS:NZ	2.19	0.57
3:F:415:PRO:HB2	3:F:490:ILE:HB	1.87	0.57
3:F:438:GLN:NE2	3:F:442:VAL:HB	2.19	0.57
3:F:353:VAL:HG22	3:F:494:ILE:HG13	1.86	0.57
3:F:208:MET:O	3:F:212:LEU:N	2.32	0.57
3:C:533:GLY:HA2	3:C:536:ILE:HD12	1.86	0.57
3:F:332:TRP:HA	3:F:342:GLU:HB2	1.86	0.56
3:F:394:TYR:O	3:F:398:LEU:HD13	2.05	0.56
3:C:121:THR:O	3:C:123:ILE:N	2.38	0.56
2:E:64:ARG:NH2	2:E:85:ASP:OD1	2.33	0.56
3:F:114:ILE:HD11	3:F:368:MET:HE1	1.88	0.56
3:F:205:TRP:NE1	3:F:274:SER:OG	2.18	0.56
3:F:416:ASN:O	3:F:416:ASN:ND2	2.34	0.56
2:E:190:GLU:O	2:E:214:ARG:NH2	2.39	0.56
3:F:142:ILE:HG12	3:F:354:LEU:CD1	2.35	0.56
1:D:101:ARG:NH1	3:F:409:SER:HB2	2.21	0.56
3:C:277:ASN:O	3:C:280:PRO:HD2	2.05	0.56
3:F:123:ILE:HD11	3:F:395:VAL:HG21	1.88	0.56
3:C:467:LEU:HD11	3:C:470:PHE:CB	2.35	0.56
1:A:131:GLU:OE1	1:A:132:VAL:C	2.44	0.56
3:F:211:PHE:O	3:F:215:THR:HG23	2.05	0.55
3:F:305:LEU:HD13	3:F:438:GLN:HA	1.86	0.55
2:E:64:ARG:HB2	2:E:80:PRO:HD2	1.88	0.55
3:F:416:ASN:HB3	3:F:419:ASP:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:281:PHE:O	3:F:284:ILE:HG22	2.07	0.55
3:C:403:PHE:O	3:C:405:SER:N	2.39	0.55
3:F:416:ASN:O	3:F:418:LEU:N	2.36	0.55
3:F:453:GLN:O	3:F:455:MET:N	2.40	0.55
1:A:131:GLU:OE1	1:A:131:GLU:C	2.45	0.55
3:C:205:TRP:HH2	3:C:278:THR:HA	1.71	0.55
3:F:410:LYS:O	3:F:413:ILE:HG12	2.07	0.55
3:F:123:ILE:HD11	3:F:395:VAL:HG11	1.89	0.54
2:B:113:ASP:OD2	2:B:202:GLN:NE2	2.39	0.54
3:C:410:LYS:C	3:C:412:CYS:N	2.61	0.54
3:F:136:THR:OG1	3:F:342:GLU:OE1	2.23	0.54
1:D:52:ASN:OD1	1:D:53:THR:N	2.41	0.54
3:F:428:VAL:CG1	3:F:432:ARG:HE	2.20	0.54
3:C:273:TRP:O	3:C:274:SER:OG	2.18	0.54
3:C:302:PHE:O	3:C:304:PHE:N	2.35	0.54
3:F:192:PHE:O	3:F:195:VAL:HG22	2.08	0.54
3:C:356:LEU:O	3:C:359:PHE:HB2	2.08	0.53
1:A:91:THR:HG23	1:A:116:THR:HA	1.91	0.53
3:C:309:SER:HB3	3:C:435:LEU:HD12	1.89	0.53
3:F:347:PHE:CD1	3:F:348:PRO:HD3	2.43	0.53
3:C:218:PHE:HD2	3:C:429:PHE:CD1	2.27	0.53
1:D:98:ARG:O	1:D:106:MET:HA	2.08	0.53
2:B:64:ARG:HD2	2:B:80:PRO:O	2.09	0.53
3:C:128:TRP:O	3:C:132:GLN:HG2	2.08	0.53
3:C:205:TRP:CH2	3:C:278:THR:HA	2.43	0.53
3:F:328:LEU:HD21	3:F:401:ALA:HA	1.90	0.53
3:C:502:GLY:HA2	3:C:506:VAL:HB	1.91	0.53
3:F:309:SER:OG	3:F:434:PHE:HB3	2.09	0.53
1:A:52:ASN:OD1	1:A:53:THR:N	2.42	0.52
3:F:135:PHE:HB3	3:F:342:GLU:OE1	2.08	0.52
3:F:364:ILE:O	3:F:368:MET:N	2.34	0.52
1:D:48:ASN:ND2	1:D:48:ASN:O	2.38	0.52
1:D:105:ALA:HB2	2:E:37:PHE:CD1	2.43	0.52
3:F:123:ILE:O	3:F:125:SER:N	2.42	0.52
2:E:13:VAL:CG2	2:E:19:VAL:HG12	2.23	0.52
3:C:135:PHE:HB3	3:C:342:GLU:OE1	2.10	0.52
3:C:149:THR:HG21	3:C:358:PHE:CD2	2.44	0.52
3:C:284:ILE:CD1	3:C:444:PRO:HG3	2.35	0.52
1:D:190:THR:OG1	1:D:193:THR:OG1	2.19	0.52
3:C:477:VAL:O	3:C:481:VAL:HG23	2.09	0.52
3:C:353:VAL:HA	3:C:494:ILE:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ALA:HB2	2:B:37:PHE:CG	2.45	0.52
3:C:243:PRO:HG2	3:C:414:GLU:OE2	2.10	0.51
3:F:119:MET:O	4:F:601:ARG:HD3	2.11	0.51
3:F:200:ALA:O	3:F:203:VAL:HG22	2.10	0.51
3:C:394:TYR:O	3:C:398:LEU:HD13	2.11	0.51
3:C:413:ILE:HA	3:C:420:ASN:HD21	1.74	0.51
3:F:145:MET:SD	3:F:351:SER:HA	2.51	0.51
3:C:357:ALA:HB1	3:C:392:TYR:CE2	2.46	0.51
3:C:364:ILE:O	3:C:368:MET:N	2.33	0.51
2:E:19:VAL:HG22	2:E:78:ILE:HG12	1.92	0.51
2:E:204:SER:OG	2:E:206:SER:O	2.19	0.51
2:B:13:VAL:CG2	2:B:19:VAL:HG12	2.29	0.51
3:C:123:ILE:HG23	3:C:124:LEU:HD12	1.92	0.51
3:C:403:PHE:HE2	3:C:409:SER:O	1.94	0.50
3:F:532:HIS:O	3:F:536:ILE:HG12	2.12	0.50
2:E:11:LEU:HD21	2:E:19:VAL:HB	1.92	0.50
3:C:205:TRP:NE1	3:C:481:VAL:HG22	2.25	0.50
3:F:155:ARG:HH11	3:F:510:PRO:HB2	1.75	0.50
3:F:416:ASN:HB2	3:F:490:ILE:CG1	2.41	0.50
3:F:477:VAL:O	3:F:481:VAL:HG23	2.11	0.50
3:C:273:TRP:HA	3:C:273:TRP:CE3	2.47	0.50
3:F:126:ILE:N	3:F:127:PRO:HD2	2.26	0.50
3:F:403:PHE:HE2	3:F:409:SER:O	1.94	0.50
3:F:205:TRP:HH2	3:F:278:THR:HA	1.76	0.50
3:F:529:THR:O	3:F:533:GLY:N	2.38	0.50
3:C:216:GLY:O	3:C:219:ILE:HG23	2.12	0.50
3:F:131:LYS:HE3	3:F:411:GLU:OE2	2.12	0.50
1:A:52:ASN:HB2	1:A:101:ARG:NH2	2.27	0.50
3:F:199:GLY:O	3:F:203:VAL:HG13	2.12	0.50
2:B:152:LYS:HB2	2:B:196:THR:OG1	2.12	0.49
2:E:64:ARG:HH12	2:E:85:ASP:CG	2.15	0.49
3:F:108:ILE:HG22	3:F:110:THR:N	2.25	0.49
3:F:241:ILE:HD12	3:F:422:PRO:HA	1.94	0.49
3:C:215:THR:HA	3:C:429:PHE:HE1	1.77	0.49
2:E:19:VAL:HG22	2:E:78:ILE:CG1	2.43	0.49
3:F:170:ASP:OD1	3:F:170:ASP:N	2.46	0.49
2:B:200:THR:HB	2:B:207:PRO:HB3	1.94	0.49
3:C:153:CYS:SG	3:C:364:ILE:HG21	2.53	0.49
3:C:285:LEU:HD12	3:C:448:TYR:CB	2.42	0.49
3:F:201:MET:HB3	3:F:443:TYR:HE1	1.77	0.49
3:C:511:SER:OG	3:C:532:HIS:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:HG23	1:A:64:PHE:HD2	1.77	0.49
3:F:509:LEU:O	3:F:513:ILE:HG12	2.13	0.49
1:A:87:LYS:HG3	1:A:89:ALA:H	1.78	0.49
3:C:284:ILE:HD12	3:C:285:LEU:N	2.27	0.49
1:D:105:ALA:HB2	2:E:37:PHE:CG	2.47	0.49
2:E:62:PRO:HB2	2:E:64:ARG:HG2	1.95	0.49
3:F:216:GLY:O	3:F:219:ILE:HG23	2.13	0.49
1:D:144:LEU:HD13	1:D:216:ILE:HG21	1.94	0.48
3:F:338:PHE:HB3	3:F:405:SER:O	2.13	0.48
3:C:126:ILE:N	3:C:127:PRO:HD2	2.28	0.48
1:A:6:GLN:H	1:A:111:GLN:NE2	2.12	0.48
2:B:92:LEU:HD13	2:B:101:PHE:CZ	2.48	0.48
2:E:192:HIS:O	2:E:214:ARG:NH2	2.42	0.48
3:F:415:PRO:C	3:F:417:PHE:H	2.17	0.48
3:C:338:PHE:HA	3:C:409:SER:HB2	1.95	0.48
3:F:281:PHE:CE2	3:F:443:TYR:CD2	3.01	0.48
3:C:194:LEU:O	3:C:198:ILE:HG23	2.13	0.48
3:C:279:ILE:HB	3:C:280:PRO:HD3	1.94	0.48
1:A:47:TRP:O	1:A:61:ILE:HG21	2.14	0.48
2:B:139:LEU:HD13	2:B:178:MET:HE3	1.95	0.48
2:B:11:LEU:HD21	2:B:19:VAL:HB	1.96	0.48
3:F:312:TYR:HE2	3:F:431:ALA:HB2	1.79	0.48
3:F:489:ASN:CB	3:F:492:SER:CB	2.88	0.47
1:A:47:TRP:HE1	1:A:50:SER:HG	1.59	0.47
3:C:435:LEU:O	3:C:439:MET:HG2	2.14	0.47
2:B:128:LEU:HD22	2:B:186:LYS:HG3	1.97	0.47
3:C:131:LYS:HE3	3:C:411:GLU:OE2	2.14	0.47
1:D:6:GLN:H	1:D:111:GLN:NE2	2.12	0.47
2:B:40:GLN:O	2:B:48:LYS:N	2.44	0.47
3:C:403:PHE:CZ	3:C:408:LEU:HD23	2.49	0.47
3:F:275:LYS:O	3:F:278:THR:HG22	2.15	0.47
1:A:52:ASN:ND2	1:A:101:ARG:HH21	2.13	0.47
2:B:153:ILE:HD12	2:B:195:TYR:CD2	2.50	0.47
3:C:340:VAL:HB	3:C:344:ARG:HH11	1.79	0.47
3:F:360:ILE:O	3:F:362:ASN:N	2.35	0.47
1:D:59:THR:OG1	2:E:97:GLU:OE1	2.29	0.46
3:F:275:LYS:HA	3:F:278:THR:HG22	1.97	0.46
3:C:347:PHE:CD2	3:C:348:PRO:HD3	2.50	0.46
3:C:495:ARG:O	3:C:499:ALA:HB2	2.14	0.46
3:F:151:TYR:O	3:F:154:TYR:HB3	2.14	0.46
3:F:503:LEU:HD13	3:F:540:VAL:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ARG:O	1:A:106:MET:HA	2.16	0.46
2:B:65:PHE:CE2	2:B:78:ILE:HD12	2.51	0.46
3:C:326:PHE:O	3:C:327:HIS:HB2	2.15	0.46
3:F:405:SER:HB3	3:F:410:LYS:HZ3	1.79	0.46
1:D:121:LYS:HD3	1:D:121:LYS:N	2.30	0.46
1:A:53:THR:HG22	1:A:72:VAL:HG11	1.98	0.46
2:B:154:ASP:OD2	2:B:192:HIS:HB3	2.15	0.46
3:C:156:VAL:HG11	3:C:364:ILE:HD11	1.97	0.46
3:F:160:THR:HG23	3:F:161:LYS:HG3	1.98	0.46
1:D:47:TRP:O	1:D:61:ILE:HG21	2.15	0.46
3:F:486:PHE:O	3:F:488:PRO:HD3	2.15	0.46
2:E:30:THR:HG22	2:E:34:SER:HA	1.98	0.46
3:C:121:THR:HA	3:C:124:LEU:HD13	1.98	0.45
3:C:123:ILE:HA	3:C:126:ILE:HD12	1.99	0.45
3:C:142:ILE:HA	3:C:354:LEU:HD21	1.98	0.45
3:F:284:ILE:HG13	3:F:298:PHE:HZ	1.82	0.45
1:A:47:TRP:NE1	1:A:50:SER:OG	2.49	0.45
3:C:111:ILE:HD12	3:C:112:PHE:N	2.31	0.45
3:C:403:PHE:CE2	3:C:409:SER:O	2.70	0.45
2:E:29:ILE:HD11	2:E:74:PHE:CE1	2.51	0.45
3:F:439:MET:O	3:F:442:VAL:HG12	2.17	0.45
2:E:64:ARG:NH1	2:E:85:ASP:OD2	2.38	0.45
3:F:153:CYS:SG	3:F:381:LEU:HD21	2.57	0.45
3:F:281:PHE:HE2	3:F:443:TYR:CD2	2.34	0.45
3:F:364:ILE:O	3:F:368:MET:HG2	2.16	0.45
1:D:53:THR:HG22	1:D:72:VAL:HG11	1.99	0.45
3:F:383:LEU:O	3:F:387:LEU:HD13	2.17	0.45
3:C:348:PRO:O	3:C:546:GLN:NE2	2.40	0.45
3:C:217:LYS:HZ3	3:C:423:SER:CB	2.28	0.45
3:F:120:GLY:C	3:F:122:SER:H	2.20	0.45
2:B:193:ALA:O	2:B:214:ARG:N	2.45	0.44
3:F:155:ARG:NH1	3:F:510:PRO:HB2	2.31	0.44
3:C:200:ALA:HA	3:C:203:VAL:HG22	1.98	0.44
3:F:205:TRP:NE1	3:F:481:VAL:HG22	2.33	0.44
3:C:404:PRO:O	3:C:407:PRO:HD2	2.17	0.44
3:C:274:SER:O	3:C:277:ASN:HB3	2.18	0.44
3:C:123:ILE:HD11	3:C:395:VAL:HG11	1.98	0.44
3:F:124:LEU:HD12	3:F:124:LEU:H	1.83	0.44
1:D:52:ASN:ND2	1:D:101:ARG:HH21	2.16	0.43
3:F:189:SER:HB3	3:F:509:LEU:CD1	2.48	0.43
3:C:153:CYS:SG	3:C:381:LEU:HD11	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:ILE:CD1	1:D:72:VAL:HG23	2.43	0.43
3:F:360:ILE:C	3:F:362:ASN:N	2.70	0.43
3:F:418:LEU:O	3:F:432:ARG:NH2	2.50	0.43
3:C:369:LYS:H	3:C:369:LYS:HG2	1.63	0.43
3:C:144:LEU:O	3:C:148:LEU:HD13	2.19	0.43
3:C:128:TRP:HD1	3:C:413:ILE:O	2.00	0.43
1:D:131:GLU:HG3	1:D:131:GLU:H	1.65	0.43
1:A:6:GLN:NE2	1:A:113:THR:OG1	2.52	0.43
2:B:152:LYS:NZ	2:B:198:GLU:OE1	2.50	0.43
3:C:329:GLU:HG3	3:C:339:PHE:CZ	2.53	0.43
3:F:114:ILE:HG23	3:F:360:ILE:CD1	2.48	0.43
3:F:149:THR:HG21	3:F:358:PHE:CD2	2.53	0.43
1:D:214:LYS:HE3	2:E:126:GLU:OE2	2.19	0.43
2:E:23:SER:OG	2:E:91:ASP:OD2	2.22	0.43
3:F:215:THR:HA	3:F:429:PHE:HE1	1.83	0.43
3:C:406:PRO:CG	3:C:407:PRO:HD3	2.48	0.43
2:E:42:LYS:HB3	2:E:43:PRO:HD2	2.01	0.43
3:C:356:LEU:HD13	3:C:498:GLY:HA2	2.00	0.43
1:D:47:TRP:NE1	1:D:50:SER:OG	2.51	0.43
3:C:410:LYS:O	3:C:411:GLU:HB2	2.19	0.43
1:D:128:TYR:HB3	2:E:124:SER:OG	2.18	0.42
3:F:215:THR:HA	3:F:429:PHE:CE1	2.54	0.42
1:A:156:VAL:HA	1:A:204:ALA:O	2.18	0.42
3:C:110:THR:HG21	3:C:371:ASN:CB	2.47	0.42
3:C:357:ALA:HB1	3:C:392:TYR:HE2	1.83	0.42
2:B:19:VAL:HG22	2:B:78:ILE:CG1	2.48	0.42
3:C:123:ILE:O	3:C:125:SER:N	2.53	0.42
3:C:123:ILE:C	3:C:125:SER:H	2.23	0.42
3:F:176:VAL:HG11	3:F:362:ASN:ND2	2.35	0.42
3:C:369:LYS:HB3	3:C:369:LYS:HE2	1.69	0.42
3:C:136:THR:N	3:C:342:GLU:OE1	2.46	0.42
3:F:345:THR:C	3:F:347:PHE:H	2.23	0.42
3:C:495:ARG:HG2	3:C:495:ARG:H	1.65	0.42
3:F:113:ALA:O	3:F:117:THR:HG22	2.19	0.42
1:A:131:GLU:O	1:A:131:GLU:CD	2.58	0.42
3:C:326:PHE:O	3:C:401:ALA:O	2.37	0.42
2:E:152:LYS:HB2	2:E:196:THR:OG1	2.20	0.42
3:F:155:ARG:HH21	3:F:532:HIS:CD2	2.38	0.42
3:F:411:GLU:O	3:F:413:ILE:N	2.52	0.42
3:C:131:LYS:HD3	3:C:132:GLN:NE2	2.35	0.42
3:C:200:ALA:O	3:C:203:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:438:GLN:NE2	3:C:442:VAL:HG11	2.34	0.42
3:F:405:SER:H	3:F:406:PRO:HD2	1.84	0.42
2:B:143:TYR:CG	2:B:144:PRO:HA	2.54	0.41
1:A:24:ALA:HB1	1:A:27:TYR:CE1	2.56	0.41
3:C:509:LEU:O	3:C:513:ILE:HG12	2.19	0.41
2:B:127:GLN:HG3	2:B:132:GLY:O	2.21	0.41
3:C:153:CYS:SG	3:C:364:ILE:HD13	2.60	0.41
2:E:143:TYR:CG	2:E:144:PRO:HA	2.55	0.41
3:C:270:ASP:O	3:C:273:TRP:CD1	2.73	0.41
3:C:136:THR:OG1	3:C:342:GLU:OE1	2.30	0.41
3:F:123:ILE:C	3:F:125:SER:H	2.24	0.41
3:F:218:PHE:HD2	3:F:429:PHE:CG	2.39	0.41
1:A:105:ALA:HB1	2:B:39:TYR:OH	2.19	0.41
3:C:156:VAL:HG11	3:C:364:ILE:CD1	2.51	0.41
3:F:180:TYR:CD2	3:F:509:LEU:HD13	2.55	0.41
3:C:318:THR:OG1	3:C:394:TYR:OH	2.22	0.41
1:D:51:ILE:HD13	1:D:72:VAL:CG2	2.43	0.41
2:E:92:LEU:HD13	2:E:101:PHE:CZ	2.56	0.41
3:F:406:PRO:CG	3:F:407:PRO:HD3	2.47	0.41
1:D:6:GLN:N	1:D:111:GLN:HE22	2.17	0.41
3:F:519:LYS:H	3:F:519:LYS:HG2	1.49	0.41
3:C:405:SER:HB3	3:C:410:LYS:HZ2	1.86	0.41
3:C:145:MET:HB2	3:C:354:LEU:HD23	2.02	0.41
3:C:329:GLU:C	3:C:330:PHE:O	2.58	0.41
1:D:70:PHE:CE1	1:D:81:GLN:HG3	2.56	0.41
3:F:123:ILE:O	3:F:126:ILE:HG12	2.21	0.41
3:C:467:LEU:HA	3:C:467:LEU:HD12	1.81	0.41
3:C:503:LEU:HD13	3:C:540:VAL:N	2.35	0.41
3:F:153:CYS:SG	3:F:364:ILE:HG21	2.61	0.41
3:F:439:MET:HA	3:F:442:VAL:CG1	2.46	0.41
3:F:349:GLN:HG2	3:F:495:ARG:NH1	2.36	0.41
3:C:325:GLY:O	3:C:326:PHE:CG	2.74	0.40
3:C:128:TRP:CB	3:C:415:PRO:HA	2.51	0.40
3:F:176:VAL:HG22	3:F:180:TYR:CE2	2.55	0.40
3:C:108:ILE:O	3:C:111:ILE:HG13	2.21	0.40
3:F:482:LEU:O	3:F:486:PHE:HB2	2.21	0.40
1:A:131:GLU:CD	1:A:131:GLU:C	2.79	0.40
3:C:408:LEU:HB3	3:C:409:SER:H	1.62	0.40
3:F:274:SER:O	3:F:278:THR:HB	2.20	0.40
3:F:516:VAL:O	3:F:519:LYS:HE2	2.21	0.40
1:D:105:ALA:HB1	2:E:39:TYR:OH	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:91:ASP:N	2:E:91:ASP:OD1	2.54	0.40
3:F:486:PHE:HB3	3:F:487:TYR:H	1.70	0.40
3:C:198:ILE:HG13	3:C:199:GLY:N	2.36	0.40
3:F:306:GLY:O	3:F:310:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry

1 ligand is 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	ARG	F	601	-	7,11,11	0.35	0	6,13,13	0.33	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
4	ARG	F	601	-	-	0/7/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	601	ARG	3	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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.