



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:07 AM UTC

PDB ID : 6C08 / pdb_00006c08
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 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

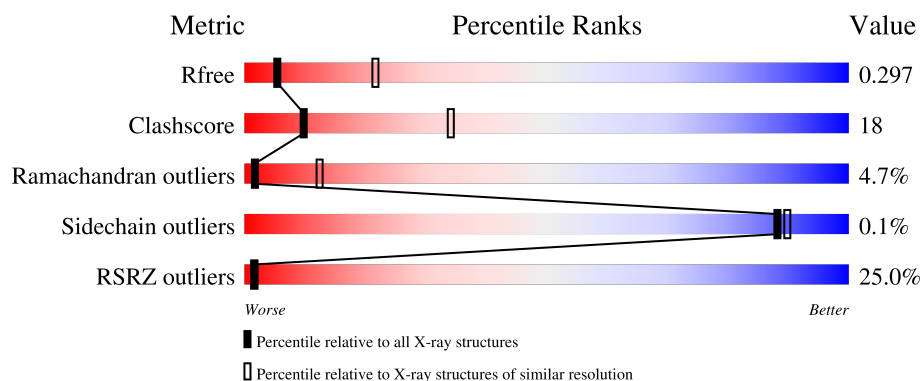
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (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 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	218	15% 79% 18% .
1	D	218	17% 78% 20% .
2	B	215	17% 78% 22%
2	E	215	21% 80% 20%
3	C	479	25% 41% 30% 5% 24%

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Mol	Chain	Length	Quality of chain
3	F	479	27% 42% 35% • 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			

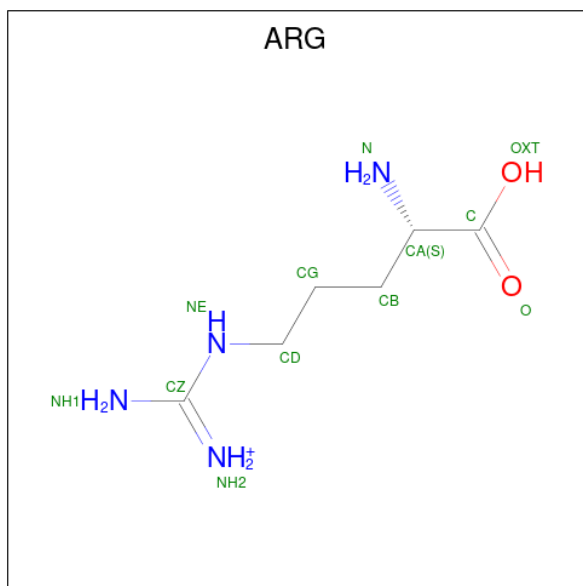
- Molecule 3 is a protein called Sodium-coupled neutral amino acid transporter 9.

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 (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).

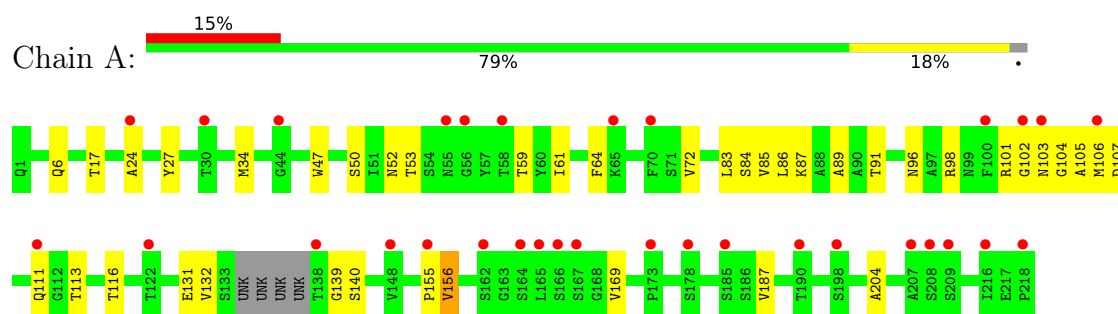


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	1	Total	C	N	O	0	0
			12	6	4	2		

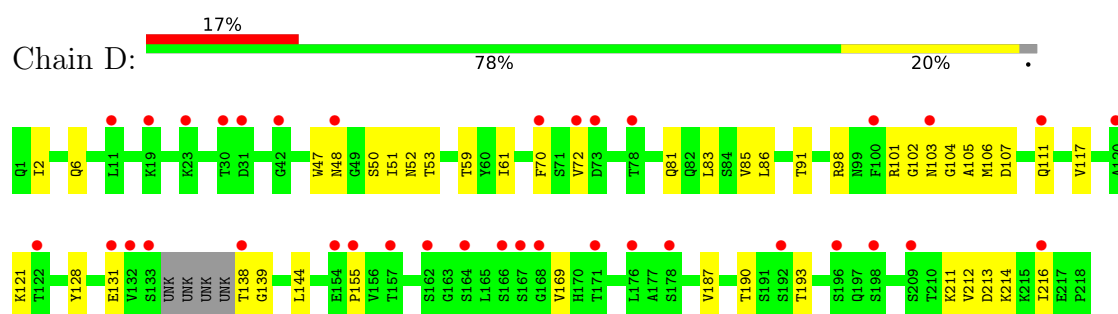
3 Residue-property plots [i](#)

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 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.

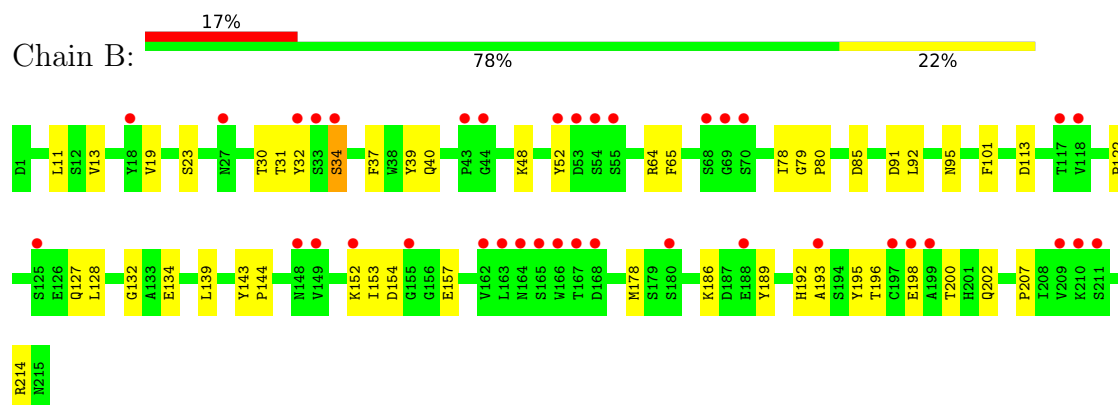
- Molecule 1: antibody Fab Heavy Chain



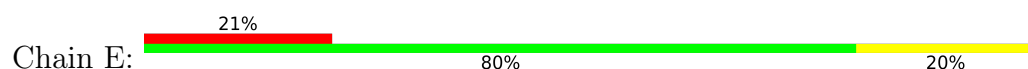
- Molecule 1: antibody Fab Heavy Chain

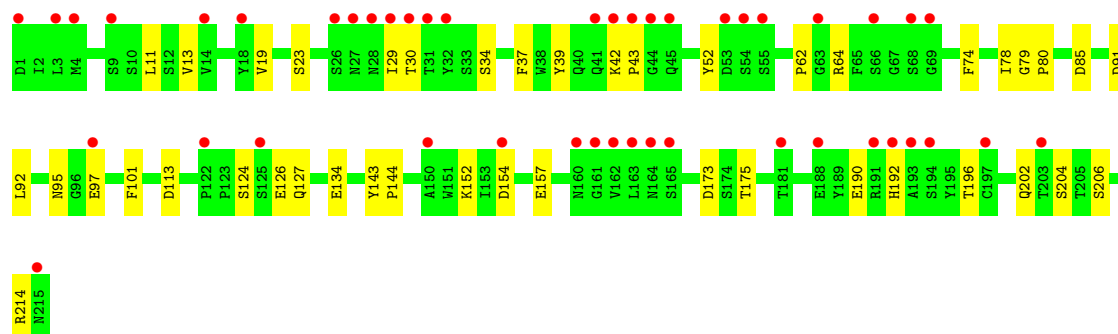


- Molecule 2: antibody Fab light chain

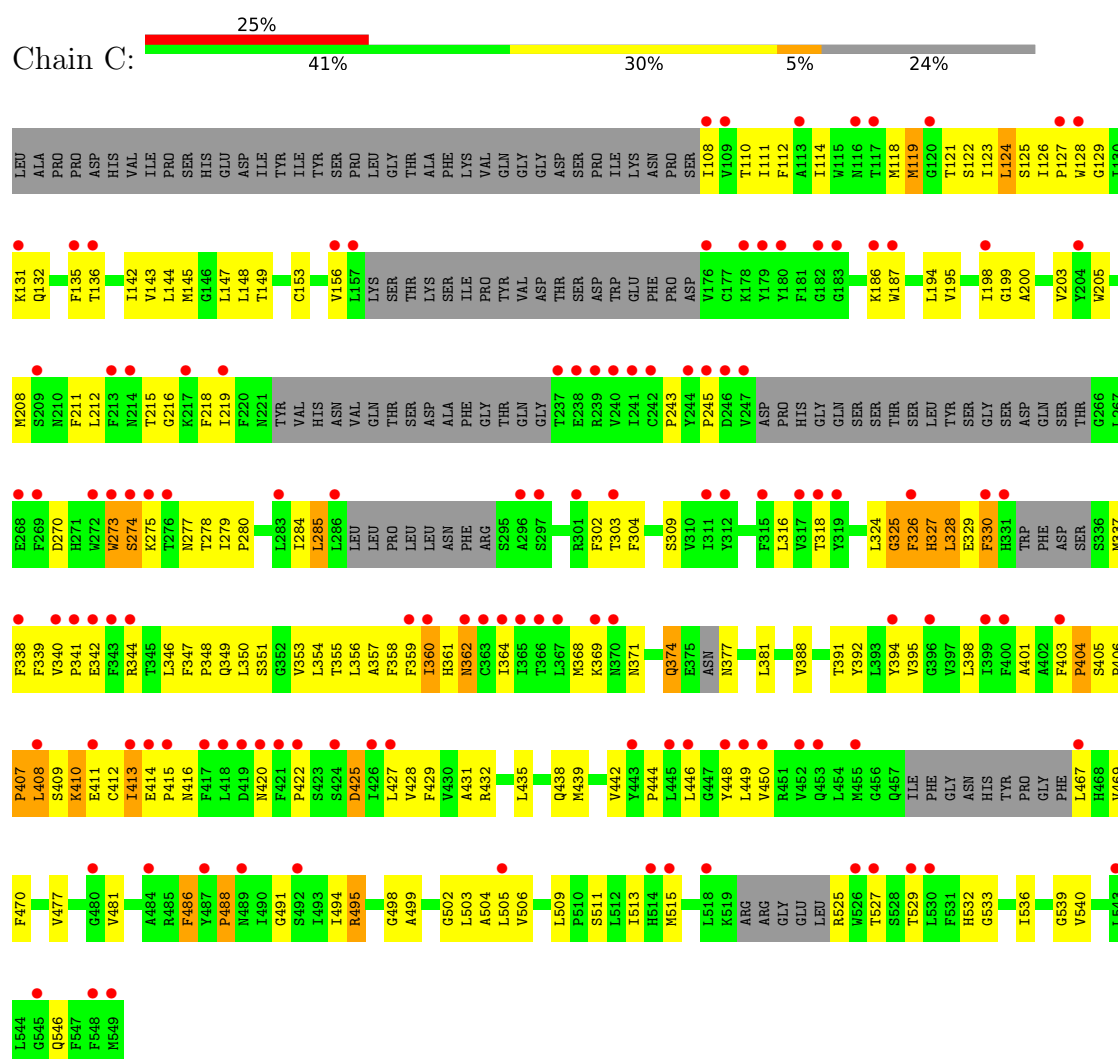


- Molecule 2: antibody Fab light chain

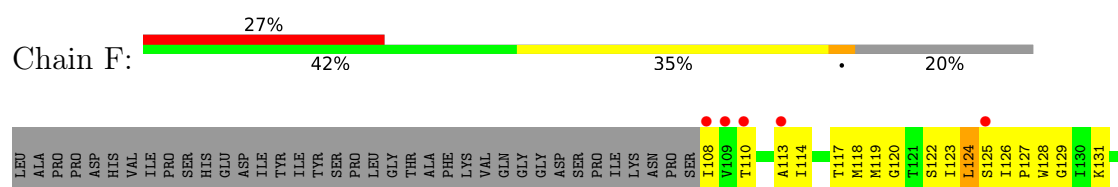




• Molecule 3: Sodium-coupled neutral amino acid transporter 9



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





4 Data and refinement statistics

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 – 3.17 156.50 – 3.17	Depositor EDS
% Data completeness (in resolution range)	99.8 (156.50-3.17) 95.0 (156.50-3.17)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.267 , 0.285 0.275 , 0.297	Depositor DCC
R_{free} test set	2000 reflections (3.14%)	wwPDB-VP
Wilson B-factor (Å ²)	105.2	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 83.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/1597	0.40	0/2178
1	D	0.18	0/1597	0.40	0/2178
2	B	0.17	0/1679	0.40	0/2285
2	E	0.17	0/1679	0.41	0/2285
3	C	0.28	0/2942	0.88	7/3998 (0.2%)
3	F	0.27	0/3145	0.88	4/4275 (0.1%)
All	All	0.23	0/12639	0.67	11/17199 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	355	THR	N-CA-C	-8.04	101.59	111.40
3	C	425	ASP	N-CA-C	-6.40	98.46	108.90
3	C	325	GLY	CA-C-N	6.21	133.41	121.54
3	C	325	GLY	C-N-CA	6.21	133.41	121.54
3	C	416	ASN	N-CA-C	-5.86	100.44	109.76
3	C	273	TRP	N-CA-C	5.41	120.25	113.43
3	F	506	VAL	CA-C-N	-5.33	111.54	122.58
3	F	506	VAL	C-N-CA	-5.33	111.54	122.58
3	F	425	ASP	N-CA-C	-5.28	101.10	109.96
3	C	274	SER	CA-C-N	5.15	129.32	120.71
3	C	274	SER	C-N-CA	5.15	129.32	120.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	32	0
1	D	1561	0	1524	35	0
2	B	1642	0	1561	32	0
2	E	1642	0	1561	34	0
3	C	2866	0	2923	153	0
3	F	3057	0	3090	158	0
4	F	12	0	12	3	0
All	All	12341	0	12195	432	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 18.

All (432) 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:368:MET:HE2	3:F:368:MET:HA	1.45	0.97
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: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:F:118:MET:HE3	3:F:388:VAL:HG21	1.64	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:C:410:LYS:C	3:C:412:CYS:H	1.90	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:205:TRP:NE1	3:F:274:SER:OG	2.18	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:F:205:TRP:HE1	3:F:274:SER:HG	1.37	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
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
3:C:273:TRP:C	3:C:275:LYS:H	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:114:ILE:HD11	3:C:368:MET:HE1	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:489:ASN:CG	3:F:492:SER:OG	2.39	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:F:368:MET:HA	3:F:368:MET:CE	2.26	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:F:360:ILE:C	3:F:362:ASN:H	2.05	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
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:119:MET:HE2	3:F:388:VAL:HG22	1.81	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:131:GLU:OE1	1:A:132:VAL:C	2.44	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
1:A:131:GLU:OE1	1:A:131:GLU:C	2.45	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: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
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
3:F:198:ILE:HA	3:F:201:MET:HE2	1.85	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:145:MET:HE3	3:C:351:SER:HB2	1.86	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: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:C:525:ARG:N	3:C:529:THR:HG1	2.03	0.57
3:F:438:GLN:NE2	3:F:442:VAL:HB	2.19	0.57
2:E:23:SER:OG	2:E:91:ASP:OD2	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
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
2:E:64:ARG:HH12	2:E:85:ASP:CG	2.15	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
1:D:47:TRP:HE1	1:D:50:SER:HG	1.56	0.54
3:F:192:PHE:O	3:F:195:VAL:HG22	2.08	0.54
2:B:23:SER:OG	2:B:91:ASP:OD2	2.25	0.53
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:204:TYR:HB3	3:F:208:MET:HE3	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:415:PRO:C	3:F:417:PHE:H	2.17	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:O	1:D:48:ASN:ND2	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
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
3:C:118:MET:HE3	3:C:358:PHE:HA	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:477:VAL:O	3:F:481:VAL:HG23	2.11	0.50
3:C:273:TRP:CE3	3:C:273:TRP:HA	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
1:A:131:GLU:C	1:A:131:GLU:CD	2.79	0.49
2:B:152:LYS:HB2	2:B:196:THR:OG1	2.12	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:120:GLY:C	3:F:122:SER:H	2.20	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
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
2:E:173:ASP:OD1	2:E:175:THR:OG1	2.18	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
3:F:360:ILE:C	3:F:362:ASN:N	2.70	0.48
2:E:192:HIS:O	2:E:214:ARG:NH2	2.42	0.48
2:B:139:LEU:HD13	2:B:178:MET:HE3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:C:410:LYS:C	3:C:412:CYS:N	2.61	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
1:A:34:MET:HE1	1:A:96:ASN:OD1	2.15	0.47
2:B:40:GLN:O	2:B:48:LYS:N	2.44	0.47
3:C:123:ILE:C	3:C:125:SER:H	2.23	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:345:THR:C	3:F:347:PHE:H	2.23	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
1:A:131:GLU:CD	1:A:131:GLU:O	2.58	0.46
3:C:318:THR:OG1	3:C:394:TYR:OH	2.22	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:416:ASN:HD22	3:F:416:ASN:C	2.19	0.46
3:F:503:LEU:HD13	3:F:540:VAL:HA	1.96	0.46
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:C:329:GLU:C	3:C:330:PHE:O	2.58	0.46
3:F:160:THR:HG23	3:F:161:LYS:HG3	1.98	0.46
3:F:123:ILE:C	3:F:125:SER:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE1	1:A:50:SER:HG	1.61	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
2:E:127:GLN:CD	2:E:134:GLU:OE2	2.59	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
2:E:95:ASN:HD22	2:E:95:ASN:C	2.21	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:273:TRP:C	3:C:275:LYS:N	2.74	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:F:517:SER:C	3:F:519:LYS:H	2.25	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
3:C:131:LYS:HE3	3:C:411:GLU:CD	2.42	0.44
3:F:205:TRP:NE1	3:F:274:SER:HG	2.05	0.44
3:C:414:GLU:O	3:C:415:PRO:C	2.60	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
3:C:515:MET:HE3	3:C:529:THR:HG22	2.00	0.43
1:D:51:ILE:CD1	1:D:72:VAL:HG23	2.43	0.43
3:F:418:LEU:O	3:F:432:ARG:NH2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:119:MET:HE2	3:C:388:VAL:HG13	2.01	0.43
3:C:369:LYS:H	3:C:369:LYS:HG2	1.63	0.43
3:C:128:TRP:HD1	3:C:413:ILE:O	2.00	0.43
3:C:144:LEU:O	3:C:148:LEU:HD13	2.19	0.43
3:C:503:LEU:HD13	3:C:539:GLY:C	2.43	0.43
1:D:131:GLU:H	1:D:131:GLU:HG3	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
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
3:F:123:ILE:C	3:F:125:SER:N	2.77	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:F:176:VAL:HG11	3:F:362:ASN:ND2	2.35	0.42
3:C:369:LYS:HE2	3:C:369:LYS:HB3	1.69	0.42
3:C:136:THR:N	3:C:342:GLU:OE1	2.46	0.42
3:C:348:PRO:C	3:C:546:GLN:HE22	2.25	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
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
3:C:405:SER:HB3	3:C:410:LYS:HZ1	1.85	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:136:THR:OG1	3:C:342:GLU:OE1	2.30	0.41
3:C:270:ASP:O	3:C:273:TRP:CD1	2.73	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
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:119:MET:HE1	3:C:391:THR:HB	2.03	0.41
3:C:145:MET:HB2	3:C:354:LEU:HD23	2.02	0.41
3:C:467:LEU:HD12	3:C:467:LEU:HA	1.81	0.41
3:C:503:LEU:HD13	3:C:540:VAL:N	2.35	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:F:153:CYS:SG	3:F:364:ILE:HG21	2.61	0.41
3:F:349:GLN:HG2	3:F:495:ARG:NH1	2.36	0.41
3:F:439:MET:HA	3:F:442:VAL:CG1	2.46	0.41
3:C:128:TRP:CB	3:C:415:PRO:HA	2.51	0.40
3:C:325:GLY:O	3:C:326:PHE:CG	2.74	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
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
2:E:91:ASP:OD1	2:E:91:ASP:N	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

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	210/218 (96%)	196 (93%)	8 (4%)	6 (3%)	3	21
1	D	210/218 (96%)	196 (93%)	10 (5%)	4 (2%)	6	30
2	B	213/215 (99%)	197 (92%)	12 (6%)	4 (2%)	6	30
2	E	213/215 (99%)	198 (93%)	13 (6%)	2 (1%)	14	45
3	C	346/479 (72%)	290 (84%)	28 (8%)	28 (8%)	1	4
3	F	369/479 (77%)	305 (83%)	34 (9%)	30 (8%)	1	4
All	All	1561/1824 (86%)	1382 (88%)	105 (7%)	74 (5%)	2	12

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	140	SER
1	A	155	PRO
3	C	122	SER
3	C	326	PHE
3	C	330	PHE
3	C	361	HIS
3	C	408	LEU
3	C	488	PRO
3	C	504	ALA
1	D	103	ASN
1	D	155	PRO
3	F	272	TRP
3	F	304	PHE
3	F	326	PHE
3	F	331	HIS
3	F	407	PRO
3	F	414	GLU
3	F	422	PRO
3	F	458	ILE

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Mol	Chain	Res	Type
3	F	504	ALA
3	F	526	TRP
1	A	85	VAL
1	A	156	VAL
2	B	79	GLY
3	C	124	LEU
3	C	187	TRP
3	C	327	HIS
3	C	362	ASN
3	C	404	PRO
3	C	407	PRO
3	C	449	LEU
3	C	527	THR
1	D	2	ILE
2	E	79	GLY
3	F	167	ASP
3	F	285	LEU
3	F	305	LEU
3	F	327	HIS
3	F	361	HIS
3	F	412	CYS
3	F	415	PRO
3	F	449	LEU
2	B	34	SER
3	C	119	MET
3	C	410	LYS
3	C	422	PRO
3	C	486	PHE
1	D	85	VAL
2	E	157	GLU
3	F	329	GLU
3	F	417	PHE
3	F	454	LEU
3	F	486	PHE
2	B	157	GLU
3	C	186	LYS
3	C	245	PRO
3	C	303	THR
3	C	324	LEU
3	C	328	LEU
3	C	346	LEU
3	C	413	ILE

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Mol	Chain	Res	Type
3	F	184	PHE
3	F	324	LEU
3	F	346	LEU
2	B	32	TYR
3	C	374	GLN
3	F	124	LEU
3	F	165	TYR
3	F	360	ILE
3	C	360	ILE
1	A	139	GLY
3	F	405	SER
3	F	185	GLY

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	174/176 (99%)	174 (100%)	0	100	100
1	D	174/176 (99%)	174 (100%)	0	100	100
2	B	184/185 (100%)	184 (100%)	0	100	100
2	E	184/185 (100%)	184 (100%)	0	100	100
3	C	311/424 (73%)	309 (99%)	2 (1%)	78	82
3	F	332/424 (78%)	332 (100%)	0	100	100
All	All	1359/1570 (87%)	1357 (100%)	2 (0%)	88	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	285	LEU
3	C	495	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
2	B	45	GLN
2	B	192	HIS
2	B	202	GLN
3	C	420	ASN
3	C	532	HIS
2	E	41	GLN
2	E	202	GLN
2	E	213	ASN
2	E	215	ASN
3	F	132	GLN
3	F	214	ASN
3	F	362	ASN
3	F	438	GLN
3	F	462	HIS
3	F	489	ASN

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 ⓘ

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	-	10,11,11	0.75	1 (10%)	9,13,13	1.10	1 (11%)

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	-	-	2/11/11/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	601	ARG	OXT-C	-2.12	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	601	ARG	OXT-C-O	-3.20	116.81	124.08

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	601	ARG	O-C-CA-N
4	F	601	ARG	OXT-C-CA-N

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 ⓘ

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, 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	214/218 (98%)	0.90	32 (14%) 5 3	61, 86, 111, 138	0
1	D	214/218 (98%)	0.90	36 (16%) 4 2	63, 85, 105, 145	0
2	B	215/215 (100%)	1.05	37 (17%) 4 3	65, 87, 123, 138	0
2	E	215/215 (100%)	1.13	45 (20%) 2 2	65, 86, 122, 141	0
3	C	364/479 (75%)	2.10	122 (33%) 1 1	92, 142, 172, 189	0
3	F	385/479 (80%)	1.93	130 (33%) 1 1	94, 144, 176, 200	0
All	All	1607/1824 (88%)	1.47	402 (25%) 2 1	61, 107, 166, 200	0

All (402) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	449	LEU	22.0
3	C	366	THR	21.3
3	F	238	GLU	15.8
3	C	363	CYS	15.6
3	F	366	THR	12.9
3	C	370	ASN	12.7
3	F	246	ASP	12.4
3	F	492	SER	11.2
3	C	453	GLN	10.1
3	F	237	THR	9.9
3	C	343	PHE	9.1
1	A	103	ASN	8.2
3	F	490	ILE	8.2
3	C	109	VAL	8.1
3	C	450	VAL	7.9
3	F	449	LEU	7.7
3	F	378	VAL	7.7
3	C	445	LEU	7.6
3	F	367	LEU	7.4

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Mol	Chain	Res	Type	RSRZ
3	C	414	GLU	7.3
3	C	362	ASN	7.2
3	C	303	THR	7.2
3	F	239	ARG	7.2
2	B	55	SER	7.2
1	D	133	SER	7.1
3	F	245	PRO	7.1
3	C	367	LEU	7.1
3	F	489	ASN	6.8
3	C	179	TYR	6.7
2	E	215	ASN	6.7
3	F	363	CYS	6.6
2	E	43	PRO	6.6
3	C	331	HIS	6.5
3	F	299	PHE	6.4
3	F	244	TYR	6.4
2	B	44	GLY	6.4
1	D	167	SER	6.4
3	F	165	TYR	6.3
1	D	138	THR	6.3
2	B	164	ASN	6.3
2	E	44	GLY	6.1
3	C	178	LYS	6.1
3	F	445	LEU	6.0
3	F	362	ASN	5.9
3	C	365	ILE	5.9
3	C	242	CYS	5.9
3	C	489	ASN	5.9
3	F	488	PRO	5.9
1	A	166	SER	5.9
3	F	240	VAL	5.8
1	D	166	SER	5.8
3	C	341	PRO	5.8
2	E	1	ASP	5.7
3	F	323	GLN	5.7
3	F	414	GLU	5.6
3	C	244	TYR	5.6
3	C	448	TYR	5.6
1	A	178	SER	5.5
1	A	209	SER	5.5
3	C	400	PHE	5.4
2	B	43	PRO	5.4

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Mol	Chain	Res	Type	RSRZ
3	C	241	ILE	5.3
3	F	419	ASP	5.3
2	B	211	SER	5.3
3	C	446	LEU	5.3
3	F	236	GLY	5.3
3	C	415	PRO	5.3
2	B	155	GLY	5.3
3	C	237	THR	5.3
3	C	274	SER	5.2
3	F	487	TYR	5.2
3	F	448	TYR	5.2
3	C	420	ASN	5.1
3	C	240	VAL	5.0
3	C	452	VAL	5.0
2	E	55	SER	5.0
2	E	54	SER	4.9
3	C	411	GLU	4.9
2	E	27	ASN	4.9
3	C	360	ILE	4.8
3	F	198	ILE	4.8
3	C	424	SER	4.7
2	E	32	TYR	4.7
2	B	163	LEU	4.7
1	D	73	ASP	4.7
2	E	31	THR	4.6
1	A	167	SER	4.6
3	C	422	PRO	4.6
3	C	272	TRP	4.6
3	C	247	VAL	4.6
3	F	331	HIS	4.5
3	F	243	PRO	4.5
3	F	209	SER	4.5
3	F	170	ASP	4.5
2	E	45	GLN	4.5
3	F	364	ILE	4.5
1	A	164	SER	4.5
3	F	420	ASN	4.4
3	F	329	GLU	4.4
3	C	296	ALA	4.4
3	C	268	GLU	4.4
2	B	166	TRP	4.4
1	D	164	SER	4.4

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Mol	Chain	Res	Type	RSRZ
3	F	332	TRP	4.3
3	C	340	VAL	4.3
2	E	30	THR	4.3
2	B	198	GLU	4.3
3	C	127	PRO	4.3
3	C	421	PHE	4.2
3	F	164	PRO	4.2
1	D	103	ASN	4.2
3	C	369	LYS	4.2
2	B	149	VAL	4.2
2	E	163	LEU	4.2
2	E	150	ALA	4.1
3	F	274	SER	4.1
3	F	319	TYR	4.1
2	B	199	ALA	4.1
3	C	239	ARG	4.1
3	C	330	PHE	4.1
3	F	163	ILE	4.1
3	F	296	ALA	4.1
2	B	53	ASP	4.0
3	C	209	SER	4.0
3	F	483	MET	4.0
3	C	394	TYR	4.0
3	F	464	PRO	4.0
3	C	116	ASN	4.0
2	E	68	SER	4.0
3	C	399	ILE	4.0
3	C	426	ILE	4.0
3	C	492	SER	4.0
1	D	131	GLU	4.0
3	C	427	LEU	4.0
3	F	422	PRO	3.9
3	F	466	PHE	3.9
3	F	242	CYS	3.9
3	C	487	TYR	3.9
3	C	136	THR	3.9
3	C	246	ASP	3.9
3	C	359	PHE	3.9
3	F	426	ILE	3.8
1	A	70	PHE	3.8
1	D	78	THR	3.8
2	B	168	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	193	ALA	3.8
2	B	162	VAL	3.8
3	C	315	PHE	3.8
2	E	26	SER	3.8
2	E	162	VAL	3.8
3	C	419	ASP	3.7
3	F	377	ASN	3.7
3	F	475	PHE	3.7
3	F	110	THR	3.7
1	A	216	ILE	3.7
1	A	138	THR	3.6
3	F	482	LEU	3.6
3	C	396	GLY	3.6
3	C	364	ILE	3.6
3	C	543	LEU	3.6
3	F	359	PHE	3.6
3	C	344	ARG	3.6
2	E	164	ASN	3.6
3	C	273	TRP	3.5
1	A	173	PRO	3.5
3	F	446	LEU	3.5
3	F	285	LEU	3.5
1	D	168	GLY	3.4
3	C	518	LEU	3.4
3	C	526	TRP	3.4
3	F	458	ILE	3.4
2	B	197	CYS	3.4
3	C	318	THR	3.4
2	B	148	ASN	3.3
2	E	97	GLU	3.3
2	E	3	LEU	3.3
3	C	108	ILE	3.3
3	F	493	ILE	3.3
3	F	268	GLU	3.3
3	F	191	VAL	3.3
3	C	187	TRP	3.3
1	A	44	GLY	3.3
3	C	319	TYR	3.2
2	E	42	LYS	3.2
3	C	514	HIS	3.2
3	F	459	PHE	3.2
2	E	69	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
3	F	125	SER	3.2
1	D	192	SER	3.2
3	F	139	ILE	3.2
3	F	303	THR	3.2
3	F	273	TRP	3.1
2	B	180	SER	3.1
3	C	527	THR	3.1
3	F	527	THR	3.1
2	E	53	ASP	3.1
3	F	197	LEU	3.1
3	F	187	TRP	3.1
3	C	408	LEU	3.1
3	F	183	GLY	3.1
3	C	176	VAL	3.1
3	F	360	ILE	3.1
3	F	455	MET	3.1
1	A	56	GLY	3.1
2	B	69	GLY	3.1
1	A	162	SER	3.1
1	D	198	SER	3.1
2	E	14	VAL	3.1
3	C	117	THR	3.0
1	D	72	VAL	3.0
3	F	284	ILE	3.0
3	C	128	TRP	3.0
1	D	70	PHE	3.0
3	C	417	PHE	3.0
3	C	238	GLU	3.0
1	D	196	SER	3.0
2	E	125	SER	3.0
3	C	530	LEU	3.0
3	F	321	ALA	3.0
3	C	182	GLY	3.0
3	C	403	PHE	3.0
2	B	33	SER	2.9
2	E	28	ASN	2.9
2	E	66	SER	2.9
3	F	517	SER	2.9
3	C	467	LEU	2.9
2	E	193	ALA	2.9
2	B	70	SER	2.9
3	F	405	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	58	THR	2.9
3	F	383	LEU	2.9
1	D	111	GLN	2.8
3	F	166	VAL	2.8
3	C	338	PHE	2.8
3	C	418	LEU	2.8
3	F	496	TYR	2.8
3	C	484	ALA	2.8
3	C	135	PHE	2.8
3	F	518	LEU	2.8
2	E	4	MET	2.8
3	F	513	ILE	2.8
3	F	528	SER	2.8
1	D	31	ASP	2.8
3	F	272	TRP	2.8
3	F	370	ASN	2.8
3	F	540	VAL	2.8
3	F	514	HIS	2.7
1	A	207	ALA	2.7
3	F	477	VAL	2.7
2	E	160	ASN	2.7
3	F	494	ILE	2.7
2	B	34	SER	2.7
3	F	282	TYR	2.7
1	A	102	GLY	2.7
2	E	188	GLU	2.7
3	C	529	THR	2.7
2	E	154	ASP	2.7
3	F	394	TYR	2.7
3	F	195	VAL	2.7
3	F	324	LEU	2.7
1	D	155	PRO	2.7
3	F	460	GLY	2.7
3	C	297	SER	2.7
2	B	209	VAL	2.7
3	F	286	LEU	2.7
3	F	436	LEU	2.7
3	F	338	PHE	2.6
2	E	161	GLY	2.6
3	F	368	MET	2.6
2	E	63	GLY	2.6
3	C	183	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	165	LEU	2.6
3	F	473	ASN	2.6
3	C	283	LEU	2.6
1	A	198	SER	2.6
2	E	194	SER	2.6
3	F	486	PHE	2.6
3	F	113	ALA	2.6
3	F	271	HIS	2.5
3	C	311	ILE	2.5
3	C	180	TYR	2.5
3	F	349	GLN	2.5
3	C	113	ALA	2.5
3	C	413	ILE	2.5
3	F	376	ASN	2.5
3	C	269	PHE	2.5
2	E	192	HIS	2.5
2	E	29	ILE	2.5
1	D	100	PHE	2.5
3	C	326	PHE	2.5
1	A	30	THR	2.5
3	F	406	PRO	2.5
2	E	18	TYR	2.5
2	B	54	SER	2.4
2	E	9	SER	2.4
1	D	154	GLU	2.4
1	D	48	ASN	2.4
1	A	122	THR	2.4
1	A	190	THR	2.4
2	B	68	SER	2.4
3	C	157	LEU	2.4
3	F	381	LEU	2.4
3	F	181	PHE	2.4
3	F	212	LEU	2.4
3	C	214	ASN	2.4
2	B	52	TYR	2.4
3	C	443	TYR	2.4
3	F	298	PHE	2.4
3	F	326	PHE	2.4
3	F	467	LEU	2.4
2	B	125	SER	2.4
3	F	109	VAL	2.4
2	B	152	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	186	LYS	2.4
3	C	548	PHE	2.4
1	A	208	SER	2.4
3	C	198	ILE	2.3
1	A	111	GLN	2.3
3	F	189	SER	2.3
3	C	217	LYS	2.3
2	B	18	TYR	2.3
1	A	155	PRO	2.3
3	F	444	PRO	2.3
3	C	120	GLY	2.3
3	C	276	THR	2.3
3	F	300	ALA	2.3
3	C	312	TYR	2.3
2	B	27	ASN	2.3
1	A	100	PHE	2.3
1	A	148	VAL	2.3
3	C	156	VAL	2.3
3	C	219	ILE	2.3
3	C	515	MET	2.3
2	B	32	TYR	2.3
2	B	118	VAL	2.3
3	F	415	PRO	2.3
1	A	185	SER	2.3
3	F	365	ILE	2.2
1	D	30	THR	2.2
1	A	55	ASN	2.2
1	D	132	VAL	2.2
2	E	122	PRO	2.2
3	F	535	LEU	2.2
1	D	122	THR	2.2
3	F	210	ASN	2.2
3	C	549	MET	2.2
2	E	203	THR	2.2
3	C	204	TYR	2.2
3	F	463	TYR	2.2
2	E	165	SER	2.2
3	F	530	LEU	2.2
1	D	23	LYS	2.2
3	C	213	PHE	2.2
2	B	117	THR	2.2
3	F	211	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	403	PHE	2.2
3	C	317	VAL	2.1
1	D	178	SER	2.1
3	C	455	MET	2.1
3	F	417	PHE	2.1
2	B	167	THR	2.1
1	D	216	ILE	2.1
3	F	241	ILE	2.1
3	F	148	LEU	2.1
1	D	120	ALA	2.1
1	A	218	PRO	2.1
1	D	42	GLY	2.1
3	F	469	VAL	2.1
1	D	11	LEU	2.1
3	C	131	LYS	2.1
3	C	245	PRO	2.1
1	D	162	SER	2.1
2	B	165	SER	2.1
1	D	19	LYS	2.1
1	D	176	LEU	2.1
3	F	108	ILE	2.1
2	E	191	ARG	2.1
3	C	301	ARG	2.1
1	A	106	MET	2.1
3	F	180	TYR	2.1
2	B	188	GLU	2.1
3	C	286	LEU	2.1
3	F	343	PHE	2.1
2	B	210	LYS	2.0
1	D	209	SER	2.0
3	F	526	TRP	2.0
2	E	181	THR	2.0
3	F	380	ASP	2.0
2	E	41	GLN	2.0
1	A	65	LYS	2.0
3	C	342	GLU	2.0
3	F	205	TRP	2.0
1	A	24	ALA	2.0
1	D	157	THR	2.0
1	D	171	THR	2.0
2	E	197	CYS	2.0
3	C	480	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	545	GLY	2.0
3	C	275	LYS	2.0
3	C	505	LEU	2.0
3	F	454	LEU	2.0
3	F	311	ILE	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($\text{\AA}^2$)	Q<0.9
4	ARG	F	601	12/12	0.65	0.15	133,144,157,163	0

6.5 Other polymers [i](#)

There are no such residues in this entry.