Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 02:10 PM EDT

PDB ID	:	3NJT
Title	:	Crystal structure of the R450A mutant of the membrane protein FhaC
Authors	:	Clantin, B.; Delattre, A.S.; Jacob-Dubuisson, F.; Villeret, V.
Deposited on	:	2010-06-18
Resolution	:	3.50 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:

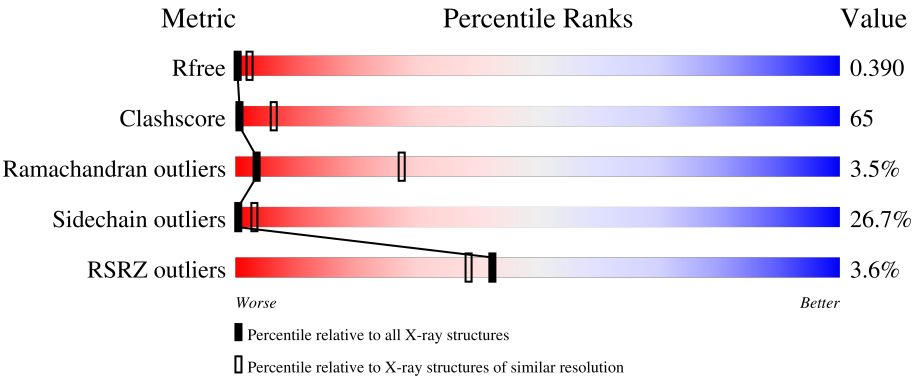
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 <=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	566	3% 28% 36% 14% · 20%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3514 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 Filamentous hemagglutinin transporter protein fhaC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	450	3514	2230	627	648	9	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

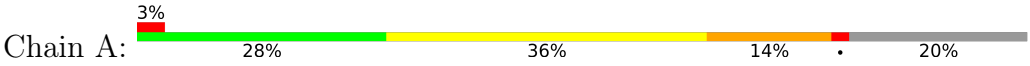
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	GLN	-	expression tag	UNP P35077
A	-10	ALA	-	expression tag	UNP P35077
A	-9	GLN	-	expression tag	UNP P35077
A	-8	GLY	-	expression tag	UNP P35077
A	-7	SER	-	expression tag	UNP P35077
A	-6	HIS	-	expression tag	UNP P35077
A	-5	HIS	-	expression tag	UNP P35077
A	-4	HIS	-	expression tag	UNP P35077
A	-3	HIS	-	expression tag	UNP P35077
A	-2	HIS	-	expression tag	UNP P35077
A	-1	HIS	-	expression tag	UNP P35077
A	0	GLY	-	expression tag	UNP P35077
A	1	PRO	-	expression tag	UNP P35077
A	2	GLY	-	expression tag	UNP P35077
A	3	SER	-	expression tag	UNP P35077
A	450	ALA	ARG	engineered mutation	UNP P35077

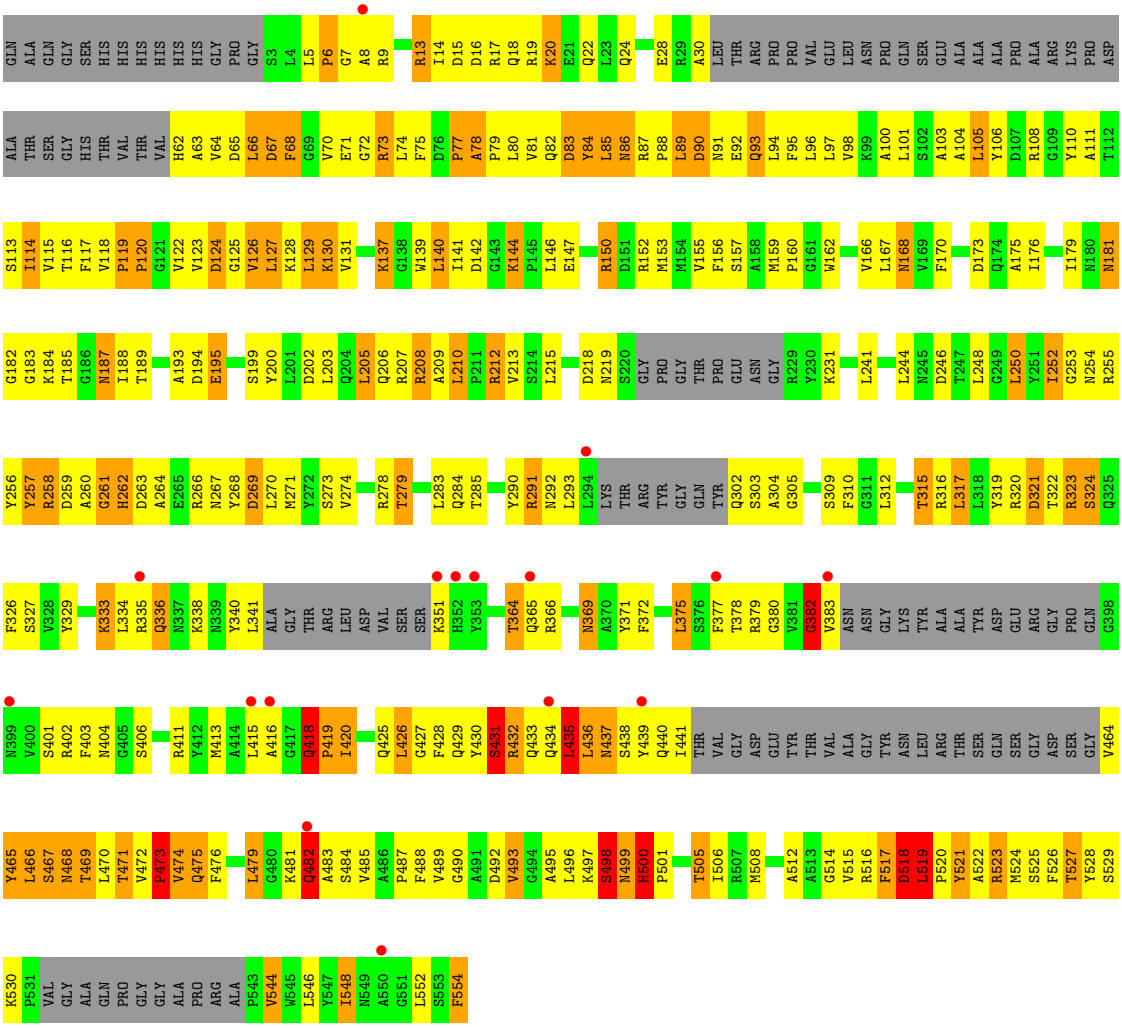
3 Residue-property plots (i)

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: Filamentous hemagglutinin transporter protein fhaC

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	107.55Å 139.39Å 113.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.56 – 3.50 48.56 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.56-3.50) 99.8 (48.56-3.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.82 (at 3.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.350 , 0.380 0.354 , 0.390	Depositor DCC
R_{free} test set	525 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å^2)	92.6	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 105.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	3514	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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	0.64	0/3584	1.00	25/4848 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	464	VAL	CB-CA-C	-10.39	91.65	111.40
1	A	499	ASN	CB-CA-C	-9.00	92.39	110.40
1	A	483	ALA	N-CA-CB	8.71	122.30	110.10
1	A	500	HIS	N-CA-C	-8.53	87.96	111.00
1	A	482	GLN	N-CA-C	8.44	133.78	111.00
1	A	261	GLY	N-CA-C	-8.19	92.63	113.10
1	A	205	LEU	CB-CA-C	-8.06	94.88	110.20
1	A	466	LEU	N-CA-C	-8.04	89.28	111.00
1	A	483	ALA	N-CA-C	-7.88	89.73	111.00
1	A	260	ALA	N-CA-C	-7.86	89.77	111.00
1	A	73	ARG	N-CA-C	-7.25	91.41	111.00
1	A	382	GLY	N-CA-C	7.08	130.81	113.10
1	A	466	LEU	N-CA-CB	-6.29	97.81	110.40
1	A	482	GLN	CB-CA-C	-6.28	97.83	110.40
1	A	6	PRO	N-CA-CB	6.11	110.63	103.30
1	A	418	GLN	C-N-CD	-5.94	107.53	120.60
1	A	6	PRO	N-CA-C	-5.77	97.09	112.10
1	A	469	THR	N-CA-C	5.72	126.45	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	467	SER	N-CA-C	-5.71	95.58	111.00
1	A	465	TYR	N-CA-CB	-5.43	100.82	110.60
1	A	498	SER	CB-CA-C	-5.42	99.81	110.10
1	A	435	LEU	N-CA-C	5.27	125.22	111.00
1	A	85	LEU	N-CA-C	5.21	125.07	111.00
1	A	206	GLN	N-CA-CB	-5.21	101.22	110.60
1	A	68	PHE	N-CA-C	-5.14	97.11	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	257	TYR	Sidechain

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	3514	0	3420	449	0
All	All	3514	0	3420	449	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 65.

All (449) 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:500:HIS:CD2	1:A:501:PRO:HD3	1.41	1.54
1:A:209:ALA:C	1:A:210:LEU:HD12	1.12	1.45
1:A:500:HIS:CG	1:A:501:PRO:HD3	1.60	1.35
1:A:64:VAL:HG22	1:A:127:LEU:CD2	1.55	1.35
1:A:209:ALA:C	1:A:210:LEU:CD1	2.07	1.22
1:A:209:ALA:O	1:A:210:LEU:HD12	1.44	1.17
1:A:64:VAL:CG1	1:A:127:LEU:HD21	1.74	1.16
1:A:500:HIS:HB3	1:A:501:PRO:CD	1.73	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:N	1:A:89:LEU:HD23	1.58	1.13
1:A:500:HIS:CD2	1:A:501:PRO:CD	2.30	1.13
1:A:89:LEU:H	1:A:89:LEU:CD2	1.56	1.11
1:A:324:SER:HB3	1:A:364:THR:HG23	1.27	1.10
1:A:500:HIS:CB	1:A:501:PRO:CD	2.31	1.09
1:A:64:VAL:HG13	1:A:127:LEU:HD21	1.17	1.07
1:A:118:VAL:O	1:A:118:VAL:HG23	1.54	1.07
1:A:441:ILE:CB	1:A:496:LEU:HD11	1.82	1.06
1:A:430:TYR:O	1:A:431:SER:HB3	1.49	1.06
1:A:64:VAL:CG2	1:A:127:LEU:HD22	1.87	1.05
1:A:418:GLN:HA	1:A:418:GLN:NE2	1.64	1.05
1:A:64:VAL:CG2	1:A:127:LEU:CD2	2.34	1.05
1:A:418:GLN:HA	1:A:418:GLN:HE21	0.90	1.04
1:A:93:GLN:OE1	1:A:93:GLN:HA	1.54	1.03
1:A:465:TYR:C	1:A:466:LEU:HG	1.73	1.03
1:A:500:HIS:HB3	1:A:501:PRO:HD2	1.38	1.02
1:A:9:ARG:CB	1:A:436:LEU:HD13	1.89	1.02
1:A:517:PHE:HD1	1:A:517:PHE:N	1.56	1.01
1:A:500:HIS:CB	1:A:501:PRO:HD3	1.90	1.00
1:A:20:LYS:HZ2	1:A:20:LYS:HB3	1.26	1.00
1:A:418:GLN:HE21	1:A:418:GLN:CA	1.70	1.00
1:A:375:LEU:HD13	1:A:403:PHE:HZ	1.28	0.99
1:A:518:ASP:C	1:A:520:PRO:HD2	1.83	0.98
1:A:89:LEU:HD23	1:A:89:LEU:H	0.82	0.98
1:A:118:VAL:HG23	1:A:120:PRO:HG2	1.46	0.98
1:A:64:VAL:HG13	1:A:127:LEU:CD2	1.94	0.97
1:A:500:HIS:HD2	1:A:501:PRO:HD3	1.17	0.97
1:A:523:ARG:C	1:A:523:ARG:CD	2.30	0.97
1:A:425:GLN:HB3	1:A:475:GLN:OE1	1.67	0.95
1:A:433:GLN:OE1	1:A:500:HIS:HA	1.67	0.95
1:A:210:LEU:HD12	1:A:210:LEU:N	1.78	0.94
1:A:258:ARG:HG2	1:A:258:ARG:HH11	1.31	0.94
1:A:124:ASP:H	1:A:126:VAL:HG23	1.32	0.94
1:A:290:TYR:CE2	1:A:305:GLY:HA3	2.03	0.94
1:A:517:PHE:N	1:A:517:PHE:CD1	2.30	0.93
1:A:500:HIS:HD2	1:A:501:PRO:CD	1.77	0.93
1:A:64:VAL:HG22	1:A:127:LEU:HD22	0.95	0.92
1:A:520:PRO:O	1:A:521:TYR:HB2	1.69	0.91
1:A:127:LEU:O	1:A:127:LEU:HD23	1.70	0.91
1:A:519:LEU:HD12	1:A:519:LEU:O	1.70	0.91
1:A:500:HIS:CG	1:A:501:PRO:CD	2.49	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:ASP:C	1:A:520:PRO:CD	2.40	0.89
1:A:30:ALA:H	1:A:365:GLN:HE22	1.18	0.89
1:A:146:LEU:O	1:A:147:GLU:HG3	1.73	0.89
1:A:466:LEU:HD12	1:A:508:MET:CE	2.03	0.88
1:A:484:SER:OG	1:A:519:LEU:HB2	1.75	0.87
1:A:209:ALA:CA	1:A:210:LEU:HD12	2.05	0.87
1:A:62:HIS:CD2	1:A:125:GLY:O	2.29	0.85
1:A:518:ASP:O	1:A:520:PRO:HD3	1.75	0.85
1:A:209:ALA:CB	1:A:210:LEU:CD1	2.55	0.85
1:A:523:ARG:HD2	1:A:523:ARG:O	1.75	0.85
1:A:20:LYS:HB3	1:A:20:LYS:NZ	1.89	0.85
1:A:375:LEU:HD13	1:A:403:PHE:CZ	2.11	0.84
1:A:505:THR:HG23	1:A:505:THR:O	1.78	0.82
1:A:432:ARG:HA	1:A:499:ASN:ND2	1.95	0.82
1:A:518:ASP:HA	1:A:522:ALA:O	1.80	0.81
1:A:118:VAL:O	1:A:120:PRO:CD	2.29	0.81
1:A:122:VAL:HG13	1:A:126:VAL:O	1.80	0.81
1:A:518:ASP:O	1:A:520:PRO:CD	2.29	0.81
1:A:466:LEU:HD13	1:A:506:ILE:HG21	1.61	0.80
1:A:116:THR:O	1:A:129:LEU:CD2	2.29	0.80
1:A:519:LEU:O	1:A:519:LEU:CD1	2.30	0.80
1:A:127:LEU:CD2	1:A:127:LEU:O	2.30	0.80
1:A:518:ASP:HB3	1:A:523:ARG:HA	1.61	0.80
1:A:505:THR:O	1:A:505:THR:CG2	2.30	0.80
1:A:210:LEU:CD1	1:A:210:LEU:N	2.39	0.80
1:A:523:ARG:CD	1:A:523:ARG:O	2.30	0.80
1:A:93:GLN:OE1	1:A:93:GLN:CA	2.30	0.79
1:A:520:PRO:O	1:A:521:TYR:CB	2.30	0.79
1:A:75:PHE:HE2	1:A:110:TYR:HH	1.29	0.79
1:A:430:TYR:CD1	1:A:470:LEU:HD22	2.17	0.79
1:A:30:ALA:N	1:A:365:GLN:HE22	1.81	0.79
1:A:427:GLY:O	1:A:473:PRO:HD2	1.82	0.79
1:A:429:GLN:O	1:A:470:LEU:HB2	1.83	0.79
1:A:432:ARG:O	1:A:469:THR:CG2	2.31	0.79
1:A:484:SER:OG	1:A:519:LEU:CB	2.31	0.78
1:A:118:VAL:O	1:A:118:VAL:CG2	2.30	0.78
1:A:118:VAL:O	1:A:120:PRO:HG2	1.83	0.78
1:A:523:ARG:O	1:A:523:ARG:CG	2.31	0.77
1:A:119:PRO:HB2	1:A:120:PRO:CD	2.15	0.77
1:A:72:GLY:HA3	1:A:75:PHE:CE1	2.20	0.77
1:A:413:MET:O	1:A:420:ILE:HG22	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:VAL:CG2	1:A:127:LEU:HD21	2.16	0.76
1:A:369:ASN:HB2	1:A:371:TYR:CZ	2.20	0.76
1:A:72:GLY:HA3	1:A:75:PHE:HE1	1.50	0.76
1:A:519:LEU:N	1:A:520:PRO:CD	2.46	0.76
1:A:418:GLN:HE21	1:A:419:PRO:CD	1.98	0.76
1:A:118:VAL:O	1:A:120:PRO:CG	2.33	0.76
1:A:162:TRP:HE3	1:A:162:TRP:O	1.67	0.75
1:A:258:ARG:HH11	1:A:258:ARG:CG	1.99	0.75
1:A:432:ARG:O	1:A:469:THR:HG21	1.87	0.75
1:A:433:GLN:N	1:A:499:ASN:HD22	1.83	0.75
1:A:439:TYR:O	1:A:467:SER:HB2	1.87	0.75
1:A:523:ARG:C	1:A:523:ARG:HD2	2.04	0.74
1:A:209:ALA:O	1:A:210:LEU:CD1	2.24	0.74
1:A:500:HIS:HD2	1:A:501:PRO:CG	1.99	0.74
1:A:64:VAL:CG1	1:A:127:LEU:CD2	2.61	0.74
1:A:433:GLN:HB3	1:A:499:ASN:HB2	1.68	0.73
1:A:415:LEU:O	1:A:416:ALA:HB3	1.89	0.73
1:A:181:ASN:ND2	1:A:183:GLY:H	1.87	0.73
1:A:465:TYR:C	1:A:466:LEU:CG	2.56	0.72
1:A:78:ALA:N	1:A:79:PRO:CD	2.51	0.72
1:A:270:LEU:O	1:A:284:GLN:HA	1.90	0.72
1:A:471:THR:HG21	1:A:496:LEU:HD23	1.71	0.72
1:A:465:TYR:O	1:A:466:LEU:HG	1.90	0.72
1:A:66:LEU:HD13	1:A:131:VAL:HG23	1.73	0.71
1:A:73:ARG:O	1:A:74:LEU:HD23	1.91	0.71
1:A:175:ALA:O	1:A:179:ILE:HG12	1.91	0.71
1:A:248:LEU:C	1:A:248:LEU:HD23	2.10	0.71
1:A:91:ASN:O	1:A:95:PHE:CD1	2.44	0.71
1:A:517:PHE:HD1	1:A:517:PHE:H	1.35	0.71
1:A:77:PRO:HB2	1:A:79:PRO:HD2	1.73	0.70
1:A:517:PHE:O	1:A:518:ASP:CG	2.30	0.70
1:A:364:THR:HG21	1:A:366:ARG:HH11	1.56	0.70
1:A:104:ALA:HB1	1:A:108:ARG:HH12	1.56	0.70
1:A:123:VAL:HG12	1:A:124:ASP:N	2.05	0.70
1:A:523:ARG:CG	1:A:523:ARG:HH11	2.05	0.70
1:A:324:SER:HB3	1:A:364:THR:CG2	2.16	0.70
1:A:90:ASP:OD2	1:A:90:ASP:C	2.30	0.70
1:A:83:ASP:C	1:A:83:ASP:OD1	2.30	0.69
1:A:418:GLN:NE2	1:A:419:PRO:HD2	2.07	0.69
1:A:369:ASN:O	1:A:371:TYR:CE1	2.46	0.69
1:A:418:GLN:NE2	1:A:419:PRO:CD	2.54	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:PRO:O	1:A:120:PRO:C	2.30	0.69
1:A:167:LEU:C	1:A:167:LEU:HD23	2.12	0.69
1:A:263:ASP:HA	1:A:291:ARG:O	1.93	0.69
1:A:466:LEU:HD12	1:A:508:MET:HE1	1.74	0.69
1:A:124:ASP:N	1:A:126:VAL:HG23	2.05	0.68
1:A:489:VAL:HG12	1:A:490:GLY:H	1.58	0.68
1:A:517:PHE:C	1:A:518:ASP:OD1	2.31	0.68
1:A:430:TYR:HA	1:A:470:LEU:HB2	1.75	0.68
1:A:523:ARG:C	1:A:523:ARG:HD3	2.14	0.68
1:A:91:ASN:O	1:A:95:PHE:HD1	1.77	0.68
1:A:93:GLN:OE1	1:A:96:LEU:HD12	1.93	0.68
1:A:465:TYR:O	1:A:466:LEU:HD23	1.94	0.68
1:A:67:ASP:C	1:A:67:ASP:OD1	2.29	0.68
1:A:523:ARG:O	1:A:523:ARG:HG3	1.93	0.68
1:A:432:ARG:HA	1:A:499:ASN:HD21	1.58	0.68
1:A:470:LEU:C	1:A:471:THR:HG22	2.14	0.67
1:A:500:HIS:HD2	1:A:501:PRO:HG3	1.59	0.67
1:A:72:GLY:O	1:A:73:ARG:C	2.30	0.67
1:A:13:ARG:NH2	1:A:439:TYR:HA	2.09	0.67
1:A:489:VAL:HG12	1:A:490:GLY:N	2.10	0.66
1:A:127:LEU:O	1:A:127:LEU:CG	2.43	0.66
1:A:465:TYR:O	1:A:466:LEU:CD2	2.44	0.66
1:A:471:THR:OG1	1:A:472:VAL:N	2.26	0.66
1:A:64:VAL:CB	1:A:127:LEU:HD21	2.25	0.66
1:A:466:LEU:CD1	1:A:508:MET:CE	2.72	0.66
1:A:122:VAL:HG12	1:A:123:VAL:N	2.09	0.66
1:A:91:ASN:OD1	1:A:92:GLU:N	2.30	0.65
1:A:209:ALA:HB3	1:A:210:LEU:CD1	2.25	0.65
1:A:118:VAL:O	1:A:120:PRO:N	2.30	0.65
1:A:466:LEU:O	1:A:496:LEU:CD1	2.44	0.65
1:A:62:HIS:CE1	1:A:85:LEU:O	2.49	0.65
1:A:85:LEU:C	1:A:86:ASN:OD1	2.34	0.65
1:A:413:MET:C	1:A:420:ILE:HG22	2.16	0.65
1:A:90:ASP:OD2	1:A:92:GLU:N	2.29	0.65
1:A:90:ASP:OD2	1:A:91:ASN:N	2.30	0.65
1:A:250:LEU:HA	1:A:269:ASP:O	1.96	0.64
1:A:516:ARG:HA	1:A:524:MET:O	1.97	0.64
1:A:213:VAL:HG12	1:A:554:PHE:O	1.98	0.64
1:A:78:ALA:N	1:A:79:PRO:HD2	2.11	0.64
1:A:150:ARG:NH2	1:A:241:LEU:O	2.30	0.64
1:A:317:LEU:HD23	1:A:326:PHE:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:LEU:O	1:A:496:LEU:HD13	1.97	0.64
1:A:78:ALA:O	1:A:81:VAL:HB	1.98	0.64
1:A:162:TRP:O	1:A:162:TRP:CE3	2.49	0.64
1:A:465:TYR:O	1:A:466:LEU:CG	2.46	0.64
1:A:369:ASN:N	1:A:369:ASN:OD1	2.30	0.63
1:A:20:LYS:NZ	1:A:20:LYS:CB	2.59	0.63
1:A:364:THR:CB	1:A:366:ARG:NH1	2.61	0.63
1:A:65:ASP:OD1	1:A:128:LYS:NZ	2.31	0.63
1:A:119:PRO:HB2	1:A:120:PRO:HD2	1.78	0.63
1:A:17:ARG:HH12	1:A:440:GLN:CB	2.11	0.63
1:A:430:TYR:O	1:A:431:SER:CB	2.33	0.63
1:A:62:HIS:ND1	1:A:85:LEU:O	2.32	0.62
1:A:320:ARG:HG2	1:A:321:ASP:H	1.64	0.62
1:A:167:LEU:HD23	1:A:167:LEU:O	1.99	0.62
1:A:515:VAL:HG12	1:A:516:ARG:N	2.14	0.62
1:A:122:VAL:CG1	1:A:123:VAL:N	2.61	0.62
1:A:439:TYR:N	1:A:468:ASN:O	2.33	0.61
1:A:471:THR:HB	1:A:496:LEU:HA	1.81	0.61
1:A:5:LEU:C	1:A:7:GLY:H	2.03	0.61
1:A:74:LEU:C	1:A:75:PHE:HD1	2.03	0.61
1:A:418:GLN:HE21	1:A:419:PRO:HD3	1.64	0.61
1:A:439:TYR:CE2	1:A:440:GLN:O	2.52	0.61
1:A:231:LYS:HB2	1:A:255:ARG:NH2	2.15	0.61
1:A:262:HIS:HB3	1:A:293:LEU:HD11	1.81	0.61
1:A:466:LEU:CD1	1:A:508:MET:HE3	2.30	0.61
1:A:187:ASN:HD21	1:A:189:THR:HG23	1.66	0.60
1:A:517:PHE:C	1:A:518:ASP:CG	2.58	0.60
1:A:279:THR:HG22	1:A:316:ARG:HH11	1.66	0.60
1:A:518:ASP:OD1	1:A:518:ASP:N	2.30	0.60
1:A:64:VAL:CB	1:A:127:LEU:CD2	2.78	0.60
1:A:81:VAL:HG12	1:A:81:VAL:O	2.01	0.60
1:A:257:TYR:HD1	1:A:263:ASP:O	1.84	0.60
1:A:382:GLY:O	1:A:383:VAL:C	2.39	0.60
1:A:74:LEU:O	1:A:75:PHE:HD1	1.85	0.60
1:A:86:ASN:OD1	1:A:86:ASN:N	2.33	0.60
1:A:122:VAL:HG22	1:A:127:LEU:HB2	1.83	0.59
1:A:208:ARG:HD3	1:A:210:LEU:O	2.02	0.59
1:A:517:PHE:O	1:A:518:ASP:CB	2.47	0.59
1:A:527:THR:O	1:A:546:LEU:HD12	2.02	0.59
1:A:252:ILE:HD13	1:A:252:ILE:O	2.02	0.59
1:A:474:VAL:HG12	1:A:476:PHE:CZ	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ASN:C	1:A:181:ASN:HD22	2.06	0.59
1:A:116:THR:O	1:A:129:LEU:HD23	2.01	0.59
1:A:466:LEU:HD12	1:A:508:MET:HE3	1.81	0.58
1:A:552:LEU:C	1:A:552:LEU:HD23	2.23	0.58
1:A:415:LEU:O	1:A:416:ALA:CB	2.51	0.58
1:A:15:ASP:HB3	1:A:19:ARG:NH2	2.18	0.58
1:A:146:LEU:HD21	1:A:152:ARG:HG2	1.83	0.58
1:A:364:THR:HB	1:A:366:ARG:NH1	2.19	0.58
1:A:369:ASN:HB2	1:A:371:TYR:OH	2.04	0.57
1:A:471:THR:HB	1:A:495:ALA:O	2.04	0.57
1:A:104:ALA:HB1	1:A:108:ARG:NH1	2.19	0.57
1:A:256:TYR:O	1:A:257:TYR:HD2	1.88	0.57
1:A:333:LYS:HE3	1:A:335:ARG:HH12	1.69	0.57
1:A:441:ILE:CB	1:A:496:LEU:HD21	2.34	0.57
1:A:92:GLU:O	1:A:96:LEU:HG	2.05	0.57
1:A:482:GLN:HE22	1:A:487:PRO:HD2	1.69	0.57
1:A:17:ARG:NH1	1:A:440:GLN:CB	2.67	0.57
1:A:271:MET:HG2	1:A:284:GLN:HG2	1.86	0.56
1:A:291:ARG:HG2	1:A:291:ARG:HH11	1.68	0.56
1:A:187:ASN:C	1:A:187:ASN:ND2	2.58	0.56
1:A:89:LEU:N	1:A:89:LEU:CD2	2.33	0.56
1:A:155:VAL:HG12	1:A:162:TRP:NE1	2.20	0.56
1:A:209:ALA:HB3	1:A:210:LEU:HD13	1.86	0.56
1:A:155:VAL:HG12	1:A:162:TRP:CD1	2.40	0.56
1:A:98:VAL:HG21	1:A:117:PHE:CE2	2.41	0.56
1:A:262:HIS:HB3	1:A:293:LEU:CD1	2.35	0.56
1:A:6:PRO:C	1:A:8:ALA:H	2.07	0.55
1:A:209:ALA:HB1	1:A:210:LEU:CD1	2.34	0.55
1:A:471:THR:HG21	1:A:496:LEU:CD2	2.35	0.55
1:A:519:LEU:N	1:A:520:PRO:HD2	2.17	0.55
1:A:88:PRO:HA	1:A:89:LEU:HD23	1.88	0.55
1:A:432:ARG:CA	1:A:499:ASN:ND2	2.69	0.55
1:A:122:VAL:HG22	1:A:127:LEU:CB	2.36	0.55
1:A:168:ASN:HD22	1:A:170:PHE:H	1.55	0.55
1:A:431:SER:O	1:A:470:LEU:HD23	2.07	0.55
1:A:66:LEU:HD23	1:A:129:LEU:HB3	1.89	0.54
1:A:256:TYR:CE2	1:A:257:TYR:O	2.60	0.54
1:A:74:LEU:O	1:A:75:PHE:CD1	2.60	0.54
1:A:157:SER:HB2	1:A:244:LEU:HD23	1.88	0.54
1:A:438:SER:HB3	1:A:468:ASN:CA	2.38	0.54
1:A:364:THR:HG21	1:A:366:ARG:NH1	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:LEU:CD1	1:A:508:MET:HE1	2.36	0.54
1:A:127:LEU:O	1:A:127:LEU:HG	2.07	0.53
1:A:530:LYS:HG2	1:A:544:VAL:HG22	1.90	0.53
1:A:20:LYS:O	1:A:20:LYS:HG2	2.08	0.53
1:A:479:LEU:N	1:A:479:LEU:HD23	2.23	0.53
1:A:338:LYS:HE3	1:A:340:TYR:OH	2.08	0.53
1:A:430:TYR:HA	1:A:470:LEU:CB	2.37	0.53
1:A:114:ILE:CG2	1:A:115:VAL:N	2.71	0.53
1:A:256:TYR:O	1:A:257:TYR:CD2	2.61	0.53
1:A:283:LEU:HG	1:A:312:LEU:HD12	1.90	0.53
1:A:518:ASP:CA	1:A:522:ALA:O	2.56	0.53
1:A:72:GLY:C	1:A:74:LEU:N	2.55	0.53
1:A:87:ARG:HH12	1:A:93:GLN:HG3	1.73	0.53
1:A:439:TYR:OH	1:A:473:PRO:HG3	2.09	0.53
1:A:100:ALA:O	1:A:103:ALA:HB3	2.08	0.52
1:A:94:LEU:O	1:A:97:LEU:HB3	2.08	0.52
1:A:257:TYR:CD1	1:A:263:ASP:O	2.62	0.52
1:A:520:PRO:O	1:A:521:TYR:CG	2.63	0.52
1:A:441:ILE:CB	1:A:496:LEU:CD1	2.73	0.52
1:A:523:ARG:NH1	1:A:523:ARG:HG2	2.23	0.52
1:A:162:TRP:CE3	1:A:162:TRP:C	2.83	0.52
1:A:118:VAL:O	1:A:120:PRO:HD2	2.08	0.52
1:A:369:ASN:HB2	1:A:371:TYR:CE1	2.44	0.51
1:A:105:LEU:O	1:A:110:TYR:HB2	2.11	0.51
1:A:113:SER:O	1:A:114:ILE:HD12	2.09	0.51
1:A:124:ASP:O	1:A:126:VAL:HG22	2.11	0.51
1:A:67:ASP:OD1	1:A:68:PHE:O	2.28	0.51
1:A:438:SER:HB3	1:A:468:ASN:HA	1.93	0.51
1:A:256:TYR:CZ	1:A:257:TYR:O	2.63	0.51
1:A:141:ILE:O	1:A:142:ASP:HB2	2.11	0.51
1:A:13:ARG:HH21	1:A:439:TYR:HA	1.75	0.51
1:A:181:ASN:HD22	1:A:183:GLY:H	1.59	0.51
1:A:470:LEU:C	1:A:471:THR:CG2	2.79	0.50
1:A:146:LEU:O	1:A:147:GLU:CG	2.54	0.50
1:A:369:ASN:CB	1:A:371:TYR:OH	2.59	0.50
1:A:5:LEU:CB	1:A:292:ASN:HD22	2.25	0.50
1:A:258:ARG:CG	1:A:258:ARG:NH1	2.66	0.50
1:A:554:PHE:C	1:A:554:PHE:CD2	2.85	0.50
1:A:13:ARG:NH2	1:A:438:SER:O	2.45	0.50
1:A:364:THR:CG2	1:A:366:ARG:HH11	2.23	0.50
1:A:119:PRO:O	1:A:120:PRO:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:HIS:O	1:A:293:LEU:HD13	2.12	0.50
1:A:474:VAL:CG1	1:A:476:PHE:CZ	2.95	0.50
1:A:438:SER:HB3	1:A:468:ASN:C	2.32	0.50
1:A:470:LEU:HD12	1:A:470:LEU:O	2.12	0.50
1:A:30:ALA:H	1:A:365:GLN:NE2	1.98	0.49
1:A:65:ASP:O	1:A:65:ASP:OD2	2.29	0.49
1:A:209:ALA:HB1	1:A:210:LEU:HD11	1.92	0.49
1:A:67:ASP:OD1	1:A:67:ASP:O	2.30	0.49
1:A:379:ARG:HG2	1:A:380:GLY:O	2.11	0.49
1:A:72:GLY:CA	1:A:75:PHE:HE1	2.21	0.49
1:A:515:VAL:CG1	1:A:516:ARG:N	2.75	0.49
1:A:20:LYS:HZ3	1:A:20:LYS:C	2.16	0.49
1:A:432:ARG:C	1:A:499:ASN:HD22	2.15	0.49
1:A:484:SER:OG	1:A:519:LEU:HB3	2.09	0.49
1:A:427:GLY:O	1:A:473:PRO:CD	2.58	0.49
1:A:481:LYS:C	1:A:482:GLN:HE21	2.16	0.49
1:A:71:GLU:OE2	1:A:166:VAL:HG23	2.13	0.49
1:A:113:SER:C	1:A:114:ILE:HD12	2.33	0.49
1:A:82:GLN:CG	1:A:83:ASP:N	2.75	0.48
1:A:432:ARG:C	1:A:469:THR:HG21	2.33	0.48
1:A:470:LEU:O	1:A:471:THR:HG22	2.13	0.48
1:A:479:LEU:HB3	1:A:488:PHE:HB3	1.96	0.48
1:A:246:ASP:HB3	1:A:274:VAL:HG22	1.94	0.48
1:A:83:ASP:OD1	1:A:83:ASP:O	2.29	0.48
1:A:193:ALA:HB2	1:A:200:TYR:HD1	1.78	0.48
1:A:523:ARG:HH11	1:A:523:ARG:HG3	1.78	0.48
1:A:28:GLU:O	1:A:365:GLN:NE2	2.46	0.48
1:A:94:LEU:HA	1:A:97:LEU:HB3	1.96	0.48
1:A:403:PHE:HE2	1:A:428:PHE:CZ	2.31	0.48
1:A:20:LYS:HG2	1:A:24:GLN:HE22	1.78	0.48
1:A:66:LEU:CD2	1:A:129:LEU:HB3	2.44	0.48
1:A:290:TYR:O	1:A:304:ALA:HA	2.14	0.48
1:A:466:LEU:O	1:A:496:LEU:HD11	2.13	0.48
1:A:62:HIS:CG	1:A:125:GLY:O	2.67	0.48
1:A:98:VAL:HG21	1:A:117:PHE:CZ	2.49	0.48
1:A:291:ARG:HH11	1:A:291:ARG:CG	2.27	0.48
1:A:66:LEU:CD1	1:A:131:VAL:HG23	2.42	0.47
1:A:84:TYR:N	1:A:84:TYR:CD1	2.82	0.47
1:A:181:ASN:HD22	1:A:182:GLY:N	2.12	0.47
1:A:432:ARG:H	1:A:432:ARG:HD2	1.80	0.47
1:A:437:ASN:O	1:A:438:SER:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:HD23	1:A:129:LEU:HA	1.37	0.47
1:A:291:ARG:HA	1:A:303:SER:O	2.15	0.47
1:A:413:MET:HB2	1:A:420:ILE:CG2	2.45	0.47
1:A:140:LEU:O	1:A:203:LEU:N	2.41	0.47
1:A:315:THR:HB	1:A:329:TYR:HB3	1.97	0.47
1:A:62:HIS:ND1	1:A:62:HIS:O	2.46	0.47
1:A:401:SER:O	1:A:431:SER:HB2	2.15	0.47
1:A:432:ARG:CA	1:A:499:ASN:HD22	2.27	0.47
1:A:430:TYR:CG	1:A:431:SER:N	2.83	0.47
1:A:433:GLN:H	1:A:499:ASN:HD22	1.60	0.47
1:A:5:LEU:C	1:A:7:GLY:N	2.66	0.47
1:A:285:THR:HA	1:A:309:SER:O	2.14	0.47
1:A:468:ASN:ND2	1:A:498:SER:HB3	2.30	0.47
1:A:523:ARG:CG	1:A:523:ARG:NH1	2.65	0.46
1:A:209:ALA:CB	1:A:210:LEU:HD12	2.26	0.46
1:A:212:ARG:HE	1:A:212:ARG:HB2	1.59	0.46
1:A:418:GLN:NE2	1:A:418:GLN:CA	2.44	0.46
1:A:518:ASP:O	1:A:520:PRO:HD2	2.01	0.46
1:A:81:VAL:O	1:A:81:VAL:CG1	2.64	0.46
1:A:94:LEU:O	1:A:97:LEU:N	2.48	0.46
1:A:266:ARG:HD2	1:A:268:TYR:OH	2.16	0.46
1:A:439:TYR:HB3	1:A:471:THR:HG23	1.97	0.46
1:A:66:LEU:HD13	1:A:131:VAL:CG2	2.45	0.46
1:A:118:VAL:C	1:A:120:PRO:HD2	2.36	0.46
1:A:401:SER:H	1:A:432:ARG:NH1	2.13	0.46
1:A:181:ASN:ND2	1:A:181:ASN:C	2.69	0.46
1:A:439:TYR:O	1:A:467:SER:CB	2.63	0.45
1:A:418:GLN:NE2	1:A:419:PRO:HD3	2.25	0.45
1:A:372:PHE:C	1:A:372:PHE:CD2	2.90	0.45
1:A:139:TRP:HZ3	1:A:188:ILE:HD11	1.81	0.45
1:A:124:ASP:C	1:A:126:VAL:H	2.15	0.45
1:A:137:LYS:NZ	1:A:195:GLU:HB2	2.32	0.45
1:A:321:ASP:OD2	1:A:323:ARG:NH2	2.50	0.45
1:A:418:GLN:HA	1:A:419:PRO:HD3	1.71	0.45
1:A:497:LYS:O	1:A:497:LYS:HG3	2.16	0.45
1:A:434:GLN:HG2	1:A:469:THR:HG23	1.97	0.45
1:A:75:PHE:HE2	1:A:110:TYR:OH	1.94	0.44
1:A:159:MET:O	1:A:162:TRP:HB3	2.17	0.44
1:A:520:PRO:O	1:A:521:TYR:CD1	2.70	0.44
1:A:66:LEU:HD23	1:A:66:LEU:HA	1.70	0.44
1:A:254:ASN:HB3	1:A:266:ARG:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ASN:O	1:A:371:TYR:CD1	2.70	0.44
1:A:411:ARG:HG2	1:A:413:MET:HG2	1.99	0.44
1:A:377:PHE:CE1	1:A:401:SER:HB2	2.53	0.44
1:A:66:LEU:CD1	1:A:131:VAL:CG2	2.96	0.44
1:A:257:TYR:CE1	1:A:263:ASP:HB3	2.52	0.44
1:A:167:LEU:C	1:A:167:LEU:CD2	2.83	0.44
1:A:246:ASP:HA	1:A:273:SER:O	2.18	0.44
1:A:219:ASN:HD21	1:A:548:ILE:CG1	2.31	0.44
1:A:434:GLN:HB3	1:A:435:LEU:H	1.66	0.44
1:A:470:LEU:C	1:A:470:LEU:HD12	2.38	0.44
1:A:114:ILE:HG23	1:A:115:VAL:N	2.33	0.43
1:A:219:ASN:HD21	1:A:548:ILE:HG13	1.83	0.43
1:A:519:LEU:O	1:A:519:LEU:HD13	2.15	0.43
1:A:144:LYS:HB3	1:A:144:LYS:HE2	1.67	0.43
1:A:364:THR:CG2	1:A:366:ARG:NH1	2.80	0.43
1:A:437:ASN:OD1	1:A:437:ASN:N	2.51	0.43
1:A:207:ARG:HB2	1:A:207:ARG:NH1	2.33	0.43
1:A:213:VAL:HG11	1:A:554:PHE:CZ	2.52	0.43
1:A:264:ALA:HB3	1:A:291:ARG:HE	1.84	0.43
1:A:489:VAL:CG1	1:A:490:GLY:N	2.80	0.43
1:A:124:ASP:C	1:A:126:VAL:N	2.70	0.43
1:A:433:GLN:OE1	1:A:500:HIS:CA	2.51	0.43
1:A:518:ASP:O	1:A:519:LEU:CB	2.66	0.43
1:A:63:ALA:HA	1:A:85:LEU:HD22	1.99	0.43
1:A:68:PHE:CD1	1:A:74:LEU:HD22	2.53	0.43
1:A:75:PHE:HE2	1:A:110:TYR:CZ	2.37	0.43
1:A:403:PHE:HE2	1:A:428:PHE:HZ	1.65	0.43
1:A:119:PRO:CB	1:A:120:PRO:HD2	2.45	0.43
1:A:179:ILE:O	1:A:184:LYS:HE2	2.18	0.43
1:A:493:VAL:O	1:A:493:VAL:HG12	2.18	0.43
1:A:114:ILE:HG22	1:A:116:THR:HG23	2.00	0.43
1:A:140:LEU:HB3	1:A:202:ASP:OD1	2.19	0.43
1:A:263:ASP:CA	1:A:291:ARG:O	2.65	0.43
1:A:482:GLN:HE22	1:A:487:PRO:CD	2.30	0.43
1:A:252:ILE:HG12	1:A:253:GLY:N	2.33	0.42
1:A:264:ALA:O	1:A:290:TYR:HA	2.19	0.42
1:A:19:ARG:O	1:A:22:GLN:HB2	2.20	0.42
1:A:179:ILE:HG23	1:A:184:LYS:HE3	2.00	0.42
1:A:156:PHE:O	1:A:160:PRO:HD3	2.19	0.42
1:A:105:LEU:HD12	1:A:105:LEU:HA	1.66	0.42
1:A:499:ASN:O	1:A:500:HIS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLN:HA	1:A:351:LYS:O	2.20	0.42
1:A:181:ASN:ND2	1:A:181:ASN:H	2.18	0.41
1:A:323:ARG:O	1:A:364:THR:HG22	2.20	0.41
1:A:317:LEU:C	1:A:317:LEU:CD2	2.89	0.41
1:A:426:LEU:HD12	1:A:474:VAL:HG22	2.02	0.41
1:A:512:ALA:HB2	1:A:529:SER:HB3	2.02	0.41
1:A:118:VAL:HA	1:A:119:PRO:HD2	1.72	0.41
1:A:14:ILE:O	1:A:18:GLN:HB2	2.20	0.41
1:A:68:PHE:CE2	1:A:75:PHE:HB2	2.55	0.41
1:A:426:LEU:HD12	1:A:474:VAL:HG13	2.02	0.41
1:A:369:ASN:CB	1:A:371:TYR:CZ	2.96	0.41
1:A:482:GLN:HB2	1:A:485:VAL:HG12	2.02	0.41
1:A:514:GLY:HA3	1:A:526:PHE:O	2.20	0.41
1:A:252:ILE:HD13	1:A:252:ILE:C	2.40	0.41
1:A:428:PHE:HA	1:A:471:THR:O	2.21	0.41
1:A:82:GLN:HG3	1:A:83:ASP:N	2.36	0.41
1:A:101:LEU:C	1:A:103:ALA:N	2.74	0.41
1:A:103:ALA:O	1:A:106:TYR:HB3	2.21	0.41
1:A:266:ARG:HG3	1:A:267:ASN:N	2.36	0.41
1:A:278:ARG:HD3	1:A:317:LEU:O	2.21	0.41
1:A:248:LEU:HD23	1:A:248:LEU:O	2.21	0.41
1:A:514:GLY:CA	1:A:526:PHE:O	2.68	0.41
1:A:130:LYS:CG	1:A:131:VAL:N	2.83	0.40
1:A:181:ASN:ND2	1:A:181:ASN:N	2.70	0.40
1:A:528:TYR:CD1	1:A:546:LEU:HD13	2.56	0.40
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.70	0.40
1:A:439:TYR:CB	1:A:471:THR:HG23	2.51	0.40
1:A:84:TYR:N	1:A:84:TYR:HD1	2.19	0.40
1:A:94:LEU:HD22	1:A:97:LEU:HD23	2.04	0.40
1:A:124:ASP:CA	1:A:126:VAL:HG23	2.52	0.40
1:A:256:TYR:CG	1:A:257:TYR:N	2.90	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	434/566 (77%)	374 (86%)	45 (10%)	15 (4%)	3 27

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	PRO
1	A	382	GLY
1	A	431	SER
1	A	473	PRO
1	A	500	HIS
1	A	519	LEU
1	A	261	GLY
1	A	518	ASP
1	A	521	TYR
1	A	111	ALA
1	A	120	PRO
1	A	419	PRO
1	A	78	ALA
1	A	544	VAL
1	A	77	PRO

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	359/460 (78%)	263 (73%)	96 (27%)	0 3

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	16	ASP
1	A	20	LYS
1	A	66	LEU

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Mol	Chain	Res	Type
1	A	67	ASP
1	A	70	VAL
1	A	80	LEU
1	A	83	ASP
1	A	84	TYR
1	A	86	ASN
1	A	89	LEU
1	A	90	ASP
1	A	93	GLN
1	A	105	LEU
1	A	114	ILE
1	A	124	ASP
1	A	126	VAL
1	A	127	LEU
1	A	129	LEU
1	A	130	LYS
1	A	137	LYS
1	A	140	LEU
1	A	144	LYS
1	A	150	ARG
1	A	153	MET
1	A	168	ASN
1	A	173	ASP
1	A	176	ILE
1	A	181	ASN
1	A	185	THR
1	A	187	ASN
1	A	194	ASP
1	A	195	GLU
1	A	199	SER
1	A	205	LEU
1	A	208	ARG
1	A	210	LEU
1	A	212	ARG
1	A	215	LEU
1	A	218	ASP
1	A	250	LEU
1	A	252	ILE
1	A	258	ARG
1	A	259	ASP
1	A	262	HIS
1	A	269	ASP

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Mol	Chain	Res	Type
1	A	279	THR
1	A	291	ARG
1	A	302	GLN
1	A	310	PHE
1	A	315	THR
1	A	317	LEU
1	A	319	TYR
1	A	321	ASP
1	A	322	THR
1	A	323	ARG
1	A	324	SER
1	A	327	SER
1	A	333	LYS
1	A	334	LEU
1	A	336	GLN
1	A	341	LEU
1	A	364	THR
1	A	369	ASN
1	A	375	LEU
1	A	378	THR
1	A	402	ARG
1	A	404	ASN
1	A	406	SER
1	A	418	GLN
1	A	420	ILE
1	A	426	LEU
1	A	431	SER
1	A	432	ARG
1	A	435	LEU
1	A	436	LEU
1	A	437	ASN
1	A	468	ASN
1	A	471	THR
1	A	473	PRO
1	A	474	VAL
1	A	475	GLN
1	A	479	LEU
1	A	482	GLN
1	A	492	ASP
1	A	493	VAL
1	A	498	SER
1	A	505	THR

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Mol	Chain	Res	Type
1	A	517	PHE
1	A	518	ASP
1	A	519	LEU
1	A	523	ARG
1	A	525	SER
1	A	527	THR
1	A	548	ILE
1	A	554	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	A	181	ASN
1	A	187	ASN
1	A	284	GLN
1	A	292	ASN
1	A	336	GLN
1	A	352	HIS
1	A	361	GLN
1	A	365	GLN
1	A	418	GLN
1	A	425	GLN
1	A	468	ASN
1	A	482	GLN
1	A	499	ASN
1	A	500	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	450/566 (79%)	0.11	16 (3%) 42 38	20, 107, 145, 145	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	377	PHE	4.2
1	A	353	TYR	3.6
1	A	294	LEU	3.2
1	A	416	ALA	3.1
1	A	351	LYS	3.0
1	A	399	ASN	2.9
1	A	415	LEU	2.8
1	A	434	GLN	2.8
1	A	352	HIS	2.7
1	A	482	GLN	2.4
1	A	383	VAL	2.3
1	A	365	GLN	2.2
1	A	335	ARG	2.2
1	A	439	TYR	2.2
1	A	550	ALA	2.1
1	A	8	ALA	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides 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.