



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:30 PM UTC

PDB ID : 3LTG / pdb_00003ltg
Title : Crystal structure of the Drosophila Epidermal Growth Factor Receptor ectodomain complexed with a low affinity Spitz mutant
Authors : Alvarado, D.; Klein, D.E.; Lemmon, M.A.
Deposited on : 2010-02-15
Resolution : 3.40 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
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

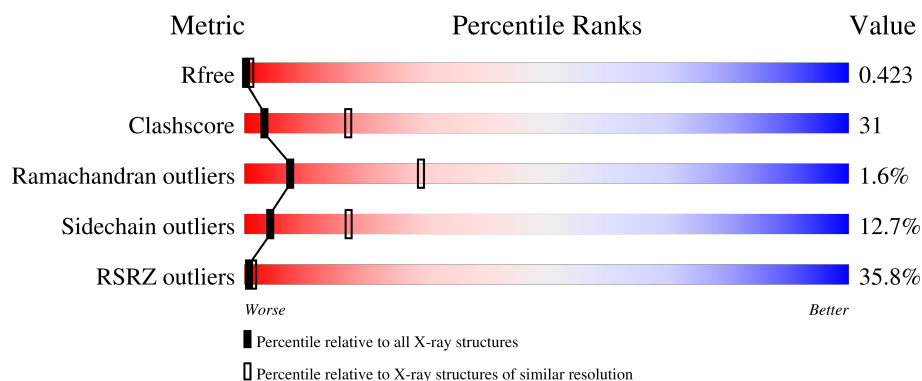
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	601	
1	C	601	
2	D	52	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8529 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4013	2497	709	759	48			
1	C	531	Total	C	N	O	S	0	1	0
			4115	2565	732	768	50			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP P04412
A	-4	HIS	-	expression tag	UNP P04412
A	-3	HIS	-	expression tag	UNP P04412
A	-2	HIS	-	expression tag	UNP P04412
A	-1	HIS	-	expression tag	UNP P04412
A	0	HIS	-	expression tag	UNP P04412
A	38	GLU	LYS	conflict	UNP P04412
A	230	GLY	ALA	conflict	UNP P04412
A	232	CYS	SER	conflict	UNP P04412
A	359	LEU	ARG	conflict	UNP P04412
A	493	ASN	THR	conflict	UNP P04412
A	590	HIS	-	expression tag	UNP P04412
A	591	HIS	-	expression tag	UNP P04412
A	592	HIS	-	expression tag	UNP P04412
A	593	HIS	-	expression tag	UNP P04412
A	594	HIS	-	expression tag	UNP P04412
A	595	HIS	-	expression tag	UNP P04412
C	-5	HIS	-	expression tag	UNP P04412
C	-4	HIS	-	expression tag	UNP P04412
C	-3	HIS	-	expression tag	UNP P04412
C	-2	HIS	-	expression tag	UNP P04412
C	-1	HIS	-	expression tag	UNP P04412
C	0	HIS	-	expression tag	UNP P04412
C	38	GLU	LYS	conflict	UNP P04412
C	230	GLY	ALA	conflict	UNP P04412

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Chain	Residue	Modelled	Actual	Comment	Reference
C	232	CYS	SER	conflict	UNP P04412
C	359	LEU	ARG	conflict	UNP P04412
C	493	ASN	THR	conflict	UNP P04412
C	590	HIS	-	expression tag	UNP P04412
C	591	HIS	-	expression tag	UNP P04412
C	592	HIS	-	expression tag	UNP P04412
C	593	HIS	-	expression tag	UNP P04412
C	594	HIS	-	expression tag	UNP P04412
C	595	HIS	-	expression tag	UNP P04412

- Molecule 2 is a protein called Protein spitz.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	51	Total	C	N	O	S	0	0	0
			401	259	62	73	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	52	ASP	-	expression tag	UNP Q01083

- Molecule 1: Epidermal growth factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.75Å 120.15Å 274.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.40 50.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	82.7 (50.00-3.40) 82.8 (50.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.406 , 0.427 0.399 , 0.423	Depositor DCC
R_{free} test set	2887 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å ²)	109.4	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 0.0	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	0.78	EDS
Total number of atoms	8529	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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

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	0.95	5/4103 (0.1%)	1.20	27/5566 (0.5%)
1	C	0.86	4/4211 (0.1%)	1.15	23/5707 (0.4%)
2	D	0.76	0/413	1.12	4/560 (0.7%)
All	All	0.90	9/8727 (0.1%)	1.17	54/11833 (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
1	C	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	490	GLN	C-N	18.08	1.58	1.33
1	A	181	PHE	C-N	14.34	1.53	1.33
1	A	383	ASN	CG-ND2	-12.83	1.06	1.33
1	A	470	ASN	CG-ND2	-12.10	1.07	1.33
1	C	436	ASP	CG-OD1	11.22	1.46	1.25
1	C	436	ASP	CB-CG	6.87	1.69	1.52
1	C	436	ASP	CA-CB	6.26	1.61	1.53
1	A	470	ASN	CB-CG	5.38	1.65	1.52
1	C	383	ASN	CG-ND2	-5.10	1.22	1.33

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	GLY	N-CA-C	-16.45	92.58	112.48
1	A	490	GLN	CA-C-N	-15.97	100.69	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	GLN	C-N-CA	-15.97	100.69	122.72
1	A	490	GLN	O-C-N	10.86	136.40	122.39
1	C	435	ARG	N-CA-C	8.94	120.63	111.07
1	A	267	CYS	CA-CB-SG	-7.46	97.24	114.40
1	C	159	CYS	CA-CB-SG	-7.28	97.66	114.40
2	D	16	CYS	N-CA-C	7.01	121.10	109.46
2	D	16	CYS	CA-CB-SG	-6.94	98.44	114.40
2	D	35	CYS	N-CA-C	6.77	120.56	109.06
1	C	436	ASP	CB-CG-OD2	-6.71	102.97	118.40
1	C	165	SER	CA-C-N	-6.63	112.41	122.81
1	C	165	SER	C-N-CA	-6.63	112.41	122.81
1	A	159	CYS	N-CA-C	6.59	120.15	109.15
1	A	134	ILE	N-CA-C	6.19	116.82	110.82
1	A	232	CYS	N-CA-C	6.15	118.43	108.41
1	C	302	LYS	N-CA-C	-6.12	101.87	110.50
1	C	12	VAL	N-CA-C	6.11	115.92	109.01
1	C	248	VAL	N-CA-C	6.10	116.40	108.35
1	C	423	GLN	N-CA-C	6.04	119.08	108.75
1	A	355	ASP	CA-C-N	5.91	126.32	119.47
1	A	355	ASP	C-N-CA	5.91	126.32	119.47
1	C	219	ASP	N-CA-C	5.90	120.47	113.28
1	A	423	GLN	N-CA-C	5.85	119.01	108.48
1	C	436	ASP	CB-CG-OD1	5.82	131.79	118.40
1	C	190	CYS	CA-CB-SG	-5.79	101.09	114.40
1	A	495	LYS	N-CA-C	-5.76	101.99	110.52
1	A	129	CYS	N-CA-C	5.74	117.69	109.14
1	A	159	CYS	CA-CB-SG	-5.74	101.21	114.40
1	C	337	GLY	N-CA-C	-5.70	105.59	112.48
1	C	436	ASP	N-CA-CB	5.60	119.08	110.79
1	A	477	GLN	N-CA-C	-5.58	103.01	110.55
1	A	236	CYS	CA-CB-SG	-5.54	101.66	114.40
1	C	12	VAL	CB-CA-C	-5.41	104.05	109.89
1	C	473	ILE	N-CA-C	5.40	118.34	113.10
1	C	197	GLY	N-CA-C	-5.40	101.33	112.34
1	A	440	VAL	N-CA-C	5.40	116.77	110.62
1	A	470	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	C	220	CYS	N-CA-CB	5.30	118.47	110.42
1	A	174	GLY	CA-C-N	5.27	126.43	119.84
1	A	174	GLY	C-N-CA	5.27	126.43	119.84
1	C	79	ILE	N-CA-C	5.25	117.32	108.81
1	C	218	LYS	N-CA-C	-5.24	106.39	112.89
1	A	267	CYS	CB-CA-C	5.23	116.24	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	177	ASN	N-CA-C	5.16	119.42	113.18
2	D	5	TYR	N-CA-C	5.15	117.69	109.81
1	A	440	VAL	CB-CA-C	-5.13	105.32	112.04
1	A	361	VAL	CB-CA-C	-5.09	104.02	112.26
1	A	197	GLY	CA-C-N	5.07	124.56	119.19
1	A	197	GLY	C-N-CA	5.07	124.56	119.19
1	A	3	CYS	CB-CA-C	-5.01	101.53	109.80
1	C	329	ARG	CA-C-N	-5.01	116.61	123.12
1	C	329	ARG	C-N-CA	-5.01	116.61	123.12
1	A	352	ILE	CB-CA-C	-5.00	102.25	111.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	PHE	Mainchain
1	C	158	GLU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4013	0	3753	243	2
1	C	4115	0	3906	281	6
2	D	401	0	362	19	0
All	All	8529	0	8021	506	8

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 31.

All (506) 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:354:LEU:HD12	1:A:355:ASP:N	1.12	1.44
1:A:354:LEU:CD1	1:A:355:ASP:O	1.76	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:HIS:CE1	1:C:351:TYR:CE1	2.21	1.28
1:A:354:LEU:HD12	1:A:355:ASP:CA	1.67	1.25
1:C:311:HIS:CE1	1:C:351:TYR:HE1	1.56	1.23
1:A:354:LEU:HD12	1:A:354:LEU:C	1.64	1.20
1:A:354:LEU:CD1	1:A:355:ASP:N	2.06	1.19
1:A:354:LEU:CD1	1:A:355:ASP:C	2.16	1.19
1:A:524:CYS:SG	1:A:531:CYS:SG	1.37	1.17
1:C:340:ASP:HB2	1:C:351:TYR:CE2	1.82	1.14
1:C:373:ASN:CG	1:C:399:MET:HE1	1.73	1.13
1:C:340:ASP:HB2	1:C:351:TYR:HE2	1.05	1.11
1:C:341:VAL:HG23	2:D:45:ARG:NH1	1.67	1.09
1:A:354:LEU:HD11	1:A:355:ASP:O	1.52	1.08
1:A:352:ILE:HG13	1:A:352:ILE:O	1.41	1.07
1:C:36:ASN:OD1	1:C:61:TYR:CE1	2.09	1.05
1:A:524:CYS:SG	1:A:531:CYS:CB	2.43	1.05
1:A:354:LEU:HD11	1:A:355:ASP:C	1.79	1.04
1:C:15:ASN:HD22	1:C:18:HIS:HB2	1.22	1.04
1:C:287:MET:HE2	1:C:301:PRO:HD2	1.40	1.04
1:C:477:GLN:C	1:C:495:LYS:HB2	1.82	1.04
1:C:531:CYS:SG	1:C:539:CYS:HB3	1.97	1.03
1:C:477:GLN:O	1:C:495:LYS:N	1.93	1.00
1:C:499:PHE:HB3	1:C:504:ILE:HD12	1.45	0.99
1:C:473:ILE:O	1:C:474:CYS:HB2	1.62	0.99
1:A:352:ILE:HD12	1:A:353:PRO:O	1.63	0.98
1:A:324:ILE:HD13	1:A:328:ILE:HD11	1.46	0.96
1:C:130:HIS:H	1:C:132:ARG:HH11	1.14	0.96
1:A:524:CYS:CB	1:A:531:CYS:SG	2.54	0.95
1:A:163:HIS:HD2	1:A:165:SER:H	1.12	0.94
1:A:194:ARG:O	1:A:204:CYS:HB2	1.68	0.94
1:C:227:PHE:CZ	1:C:230:GLY:HA2	2.02	0.94
1:C:113:ARG:HG3	1:C:113:ARG:HH11	1.33	0.94
1:C:12:VAL:HG11	1:C:41:TRP:CD1	2.04	0.93
1:A:287:MET:HB2	1:A:296:CYS:HB3	1.49	0.93
1:C:373:ASN:CB	1:C:399:MET:HE1	1.99	0.92
1:A:466:LEU:O	1:A:470:ASN:HB2	1.68	0.92
1:A:354:LEU:HD13	1:A:355:ASP:O	1.66	0.91
1:C:400:GLU:HG3	2:D:51:ILE:HD12	1.49	0.91
1:C:476:ASP:O	1:C:495:LYS:HD3	1.72	0.90
1:C:12:VAL:CG1	1:C:41:TRP:CD1	2.56	0.89
1:A:73:VAL:HG12	1:A:108:GLU:HB2	1.55	0.89
1:C:227:PHE:CE2	1:C:230:GLY:HA2	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:HIS:H	1:C:132:ARG:NH1	1.73	0.86
1:A:354:LEU:HD12	1:A:355:ASP:C	1.91	0.86
1:C:307:VAL:HG11	1:C:314:ASN:HD22	1.43	0.84
1:A:354:LEU:CD1	1:A:354:LEU:C	2.29	0.84
1:C:371:TYR:CE1	1:C:399:MET:HE3	2.13	0.83
1:A:24:ARG:HH11	1:A:24:ARG:HG2	1.43	0.82
1:C:287:MET:CE	1:C:301:PRO:HD2	2.09	0.82
1:C:311:HIS:HE1	1:C:351:TYR:HE1	1.22	0.81
1:A:193:GLY:HA3	1:C:201:ARG:HH12	1.43	0.81
1:A:163:HIS:CD2	1:A:165:SER:H	1.99	0.81
1:A:448:ILE:HD11	1:A:484:TRP:HZ2	1.45	0.81
1:C:138:GLU:OE1	1:C:184:LEU:HG	1.81	0.80
1:C:373:ASN:HB2	1:C:399:MET:HE1	1.60	0.80
1:A:100:THR:HG22	1:A:123:HIS:HB3	1.63	0.80
1:C:21:ARG:HG3	1:C:24:ARG:NH2	1.97	0.80
1:C:311:HIS:CE1	1:C:351:TYR:CD1	2.69	0.80
1:A:113:ARG:NH2	1:A:182:SER:OG	2.14	0.80
1:A:352:ILE:CD1	1:A:353:PRO:O	2.30	0.80
1:C:478:CYS:N	1:C:495:LYS:HB2	1.95	0.80
1:A:138:GLU:HB2	1:A:184:LEU:HG	1.65	0.79
1:A:514:TYR:HB2	1:A:532:ASN:C	2.09	0.78
1:A:274:ASP:OD2	1:C:240:ARG:NH2	2.16	0.78
1:C:15:ASN:ND2	1:C:18:HIS:HB2	1.98	0.77
1:C:311:HIS:ND1	1:C:351:TYR:CD1	2.52	0.77
1:C:138:GLU:HB2	1:C:184:LEU:CD1	2.14	0.77
1:A:402:MET:HE2	1:A:430:VAL:HG22	1.66	0.77
1:C:477:GLN:C	1:C:495:LYS:CB	2.57	0.77
1:C:287:MET:HE3	1:C:296:CYS:CB	2.15	0.77
1:C:476:ASP:O	1:C:495:LYS:CD	2.34	0.76
1:A:225:ASN:HD22	1:A:225:ASN:H	1.30	0.75
1:A:248:VAL:HA	1:C:279:VAL:HG22	1.68	0.75
1:C:373:ASN:HB2	1:C:399:MET:CE	2.16	0.74
1:A:402:MET:HE2	1:A:430:VAL:CG2	2.16	0.74
1:A:193:GLY:HA3	1:C:201:ARG:NH1	2.01	0.74
1:C:287:MET:HE3	1:C:296:CYS:HB3	1.68	0.74
1:C:339:GLN:NE2	1:C:350[B]:ARG:NH2	2.36	0.74
1:C:340:ASP:OD2	1:C:351:TYR:OH	2.05	0.74
1:A:411:SER:OG	1:A:413:LEU:HD13	1.87	0.74
1:C:127:ASN:O	1:C:157:ARG:NH1	2.20	0.73
1:C:514:TYR:CZ	1:C:534:ALA:HB2	2.23	0.73
1:A:104:MET:HE2	1:A:128:LEU:HG	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:VAL:HG22	1:C:122:PHE:CD2	2.23	0.73
1:C:180:LYS:C	1:C:181:PHE:HD1	1.96	0.73
1:C:347:MET:HE1	2:D:15:TYR:HA	1.70	0.73
1:A:87:SER:HB2	1:A:93:GLU:O	1.89	0.73
1:C:15:ASN:HD22	1:C:18:HIS:CB	2.00	0.72
1:C:239:MET:CE	1:C:257:TYR:CE1	2.71	0.72
1:C:477:GLN:HB3	1:C:503:CYS:HB3	1.72	0.72
1:C:132:ARG:H	1:C:132:ARG:HD3	1.55	0.72
1:A:351:TYR:O	1:A:352:ILE:C	2.31	0.71
1:C:433:HIS:CE1	1:C:460:GLU:HG3	2.25	0.71
1:A:484:TRP:HB2	1:A:490:GLN:HG3	1.71	0.71
1:A:433:HIS:HB2	1:A:460:GLU:OE1	1.91	0.71
1:A:163:HIS:HD2	1:A:165:SER:N	1.88	0.71
1:C:113:ARG:HG3	1:C:113:ARG:NH1	2.05	0.70
1:C:189:GLN:OE1	1:C:200:PRO:HB3	1.92	0.70
1:C:36:ASN:HD21	1:C:84:THR:HB	1.56	0.70
1:A:138:GLU:HB2	1:A:184:LEU:CG	2.22	0.70
1:A:411:SER:CB	1:A:413:LEU:HD13	2.22	0.70
1:C:102:SER:H	1:C:125:ASN:HB3	1.55	0.70
1:C:12:VAL:HG13	1:C:41:TRP:CD1	2.27	0.69
1:C:345:TYR:O	2:D:11:PHE:HZ	1.75	0.69
1:A:448:ILE:HD11	1:A:484:TRP:CZ2	2.27	0.69
1:C:477:GLN:O	1:C:495:LYS:CB	2.40	0.69
1:C:330:ILE:HD11	1:C:381:PHE:CZ	2.28	0.69
1:C:180:LYS:C	1:C:181:PHE:CD1	2.71	0.69
1:A:15:ASN:ND2	1:A:18:HIS:H	1.92	0.68
1:A:33:VAL:HG13	1:A:58:VAL:HG22	1.75	0.68
1:C:181:PHE:HD1	1:C:181:PHE:N	1.91	0.68
1:C:65:SER:OG	1:C:66:HIS:HD2	1.77	0.68
1:C:208:CYS:HB3	1:C:222:ALA:O	1.93	0.68
1:A:277:ALA:HB1	1:C:242:TYR:CD1	2.29	0.68
1:A:451:GLU:HB3	1:A:453:GLU:OE2	1.94	0.68
1:C:496:ASN:ND2	1:C:505:ALA:O	2.27	0.68
1:A:402:MET:HE3	1:A:457:TRP:CD2	2.29	0.67
1:A:433:HIS:ND1	1:A:460:GLU:OE1	2.27	0.67
1:C:181:PHE:CD1	1:C:181:PHE:N	2.60	0.67
1:C:341:VAL:CG2	2:D:45:ARG:NH1	2.54	0.67
1:C:417:GLU:OE1	1:C:490:GLN:NE2	2.27	0.67
1:C:114:ASP:CG	1:C:194:ARG:NH1	2.53	0.67
1:A:33:VAL:CG1	1:A:58:VAL:HG22	2.25	0.67
1:C:347:MET:HE3	2:D:14:TRP:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ILE:CD1	1:A:328:ILE:HD11	2.23	0.66
1:C:44:ASN:O	1:C:47:LEU:HD23	1.94	0.66
1:C:183:LYS:HG2	1:C:184:LEU:HD23	1.76	0.66
1:A:336:SER:O	1:A:353:PRO:HG3	1.95	0.66
1:A:484:TRP:NE1	1:A:492:LEU:CD2	2.59	0.66
1:A:191:ALA:O	1:C:201:ARG:HD2	1.96	0.66
1:C:228:ASP:OD2	1:C:233:LYS:HE3	1.96	0.65
1:A:327:ASN:OD1	1:A:371:TYR:CE2	2.50	0.65
1:A:270:HIS:HA	1:A:396:ARG:HG2	1.79	0.65
1:C:77:LEU:C	1:C:77:LEU:HD23	2.22	0.65
1:C:239:MET:CE	1:C:257:TYR:CZ	2.80	0.65
1:C:114:ASP:OD2	1:C:194:ARG:NH1	2.30	0.64
1:C:114:ASP:CG	1:C:194:ARG:HH12	2.05	0.64
1:C:12:VAL:HG11	1:C:41:TRP:CG	2.32	0.64
1:C:344:ASN:N	1:C:344:ASN:OD1	2.30	0.64
1:A:405:ALA:HB2	1:A:427:GLY:HA3	1.80	0.64
1:C:400:GLU:HG3	2:D:51:ILE:CD1	2.24	0.64
1:C:319:ARG:HA	1:C:361:VAL:HG13	1.79	0.63
1:A:383:ASN:HA	1:A:415:SER:O	1.97	0.63
1:A:57:GLU:HG3	1:A:79:ILE:HB	1.81	0.63
1:C:44:ASN:OD1	1:C:47:LEU:HD22	1.98	0.63
1:C:77:LEU:HD23	1:C:78:GLN:N	2.14	0.63
1:C:138:GLU:HB2	1:C:184:LEU:HD11	1.79	0.63
1:C:14:SER:OG	2:D:36:GLU:OE2	2.15	0.63
1:A:477:GLN:O	1:A:478:CYS:SG	2.56	0.63
1:C:477:GLN:O	1:C:495:LYS:HB2	1.97	0.63
1:A:411:SER:HB2	1:A:413:LEU:CD1	2.28	0.63
1:C:327:ASN:HB3	1:C:371:TYR:H	1.62	0.63
1:A:374:ILE:HD13	1:A:384:LEU:HD21	1.80	0.62
1:A:411:SER:HB2	1:A:413:LEU:HD13	1.81	0.62
1:A:267:CYS:SG	1:A:268:PRO:HD2	2.39	0.62
1:A:391:GLU:HA	1:A:420:ASN:O	1.99	0.62
1:C:306:GLY:N	1:C:325:ASP:O	2.32	0.62
1:A:138:GLU:HB2	1:A:184:LEU:CD1	2.30	0.62
1:C:514:TYR:OH	1:C:534:ALA:HB2	1.99	0.62
1:A:354:LEU:O	1:A:354:LEU:HG	1.99	0.62
1:C:383:ASN:HB2	1:C:417:GLU:HG3	1.82	0.62
1:C:483:CYS:HB3	1:C:491:CYS:HA	1.82	0.61
1:C:482:GLY:C	1:C:483:CYS:SG	2.83	0.61
1:A:81:ARG:NH2	1:A:223:CYS:O	2.18	0.61
1:C:36:ASN:OD1	1:C:61:TYR:CZ	2.52	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LEU:HD11	1:A:440:VAL:HG13	1.82	0.61
1:C:49:LEU:HD22	1:C:69:VAL:HG11	1.83	0.61
1:C:130:HIS:N	1:C:132:ARG:HH11	1.93	0.61
1:A:226:PHE:HB2	1:A:233:LYS:O	2.00	0.61
1:A:354:LEU:CD1	1:A:355:ASP:CA	2.49	0.61
1:C:294:VAL:HG13	1:C:295:PRO:HD2	1.83	0.61
1:A:413:LEU:HB2	1:A:437:LEU:HD23	1.82	0.61
2:D:27:ILE:O	2:D:27:ILE:HG13	1.98	0.61
1:A:279:VAL:HA	1:C:247:TYR:O	2.01	0.60
1:A:378:HIS:HD2	1:A:380:GLN:H	1.50	0.60
1:C:36:ASN:OD1	1:C:61:TYR:CD1	2.52	0.60
1:C:45:GLU:O	1:C:46:ASN:HB2	2.01	0.60
1:C:275:ASN:OD1	1:C:276:GLY:N	2.35	0.60
1:A:410:LYS:HG3	1:A:433:HIS:HD2	1.66	0.60
1:A:437:LEU:HD12	1:A:440:VAL:HG22	1.84	0.60
1:C:311:HIS:ND1	1:C:351:TYR:HD1	1.97	0.60
1:C:228:ASP:O	1:C:231:VAL:HG13	2.02	0.59
1:C:183:LYS:HG2	1:C:184:LEU:N	2.18	0.59
1:A:378:HIS:CD2	1:A:380:GLN:H	2.19	0.59
1:C:473:ILE:O	1:C:474:CYS:CB	2.39	0.59
1:C:186:CYS:HB3	1:C:198:PRO:HA	1.85	0.59
1:C:374:ILE:HD13	1:C:384:LEU:HD21	1.84	0.59
1:A:15:ASN:C	1:A:15:ASN:HD22	2.11	0.58
1:A:402:MET:HE3	1:A:457:TRP:CG	2.38	0.58
1:C:163:HIS:ND1	1:C:165:SER:HB3	2.17	0.58
1:C:200:PRO:O	1:C:201:ARG:CB	2.51	0.58
1:C:211:GLY:O	1:C:220:CYS:HB3	2.04	0.58
1:C:340:ASP:CG	1:C:351:TYR:HH	2.12	0.58
1:A:484:TRP:NE1	1:A:492:LEU:HD23	2.19	0.57
2:D:16:CYS:HB3	2:D:20:ALA:HB3	1.86	0.57
1:A:437:LEU:HD13	1:A:438:CYS:H	1.68	0.57
1:A:524:CYS:SG	1:A:531:CYS:HB2	2.40	0.57
1:C:36:ASN:N	1:C:36:ASN:HD22	2.02	0.57
1:C:109:ILE:HG22	1:C:112:LEU:HB2	1.87	0.57
1:C:51:PHE:CD2	1:C:52:LEU:HD13	2.39	0.57
1:C:504:ILE:HG22	1:C:506:ASP:H	1.70	0.57
1:C:199:LYS:HB2	1:C:202:GLU:OE2	2.04	0.57
1:C:341:VAL:HG23	2:D:45:ARG:CZ	2.33	0.57
1:C:451:GLU:O	1:C:454:GLN:HG3	2.05	0.57
1:A:191:ALA:O	1:C:201:ARG:CD	2.53	0.57
1:A:225:ASN:OD1	1:A:233:LYS:C	2.48	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:GLY:C	1:A:327:ASN:HD22	2.13	0.57
1:C:37:LEU:C	1:C:37:LEU:HD12	2.30	0.57
1:A:295:PRO:HG3	1:C:295:PRO:HG3	1.86	0.56
1:A:335:PHE:HE1	1:A:376:GLY:HA3	1.69	0.56
1:A:351:TYR:O	1:A:352:ILE:O	2.23	0.56
1:A:453:GLU:CD	1:A:453:GLU:H	2.12	0.56
1:A:416:LEU:HD21	1:A:440:VAL:HG12	1.88	0.56
1:C:340:ASP:HB3	1:C:349:PRO:HD2	1.86	0.56
1:A:302:LYS:O	1:A:322:THR:HG22	2.04	0.56
1:A:87:SER:HB3	1:A:94:LYS:HA	1.87	0.56
1:C:200:PRO:O	1:C:201:ARG:HB2	2.04	0.56
1:A:319:ARG:HA	1:A:361:VAL:HG12	1.87	0.56
1:C:42:LEU:HD23	1:C:49:LEU:HD11	1.87	0.56
1:C:342:TYR:HD1	1:C:346:THR:HG23	1.70	0.56
1:A:182:SER:HB2	1:A:194:ARG:HD3	1.88	0.56
1:C:195:CYS:HB3	1:C:203:CYS:SG	2.46	0.56
1:A:433:HIS:CG	1:A:460:GLU:OE1	2.58	0.55
1:A:303:THR:CG2	1:A:304:CYS:N	2.68	0.55
1:A:189:GLN:OE1	1:A:200:PRO:HB2	2.07	0.55
1:C:239:MET:HE1	1:C:257:TYR:CE1	2.40	0.55
1:C:53:ASP:HA	1:C:75:PRO:HD2	1.87	0.55
1:A:323:VAL:HG22	1:A:367:GLU:HB2	1.89	0.55
1:C:307:VAL:HG11	1:C:314:ASN:ND2	2.17	0.55
1:A:437:LEU:HD13	1:A:438:CYS:N	2.22	0.55
1:C:330:ILE:HD11	1:C:381:PHE:CE1	2.40	0.55
1:A:433:HIS:CB	1:A:460:GLU:OE1	2.54	0.55
1:A:242:TYR:CE2	1:C:277:ALA:HB1	2.41	0.55
1:A:247:TYR:O	1:C:279:VAL:HA	2.06	0.55
1:A:259:TYR:O	1:A:262:THR:HB	2.07	0.55
1:A:343:ALA:C	1:A:345:TYR:H	2.14	0.55
1:C:478:CYS:CA	1:C:495:LYS:HB2	2.37	0.55
1:A:262:THR:HG22	1:A:264:VAL:HG13	1.89	0.54
1:A:274:ASP:CG	1:C:240:ARG:HH22	2.13	0.54
1:A:228:ASP:HB3	1:A:233:LYS:HD3	1.88	0.54
1:A:327:ASN:HD22	1:A:327:ASN:N	2.06	0.54
1:A:233:LYS:HG3	1:A:235:GLU:O	2.08	0.54
1:A:283:PRO:HG3	1:C:240:ARG:NH2	2.23	0.54
1:C:300:CYS:O	1:C:301:PRO:C	2.51	0.54
1:C:163:HIS:ND1	1:C:175:PRO:HG3	2.23	0.54
1:A:274:ASP:O	1:C:249:LEU:HD11	2.08	0.54
1:C:369:THR:HA	1:C:394:HIS:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ASN:HD21	1:C:275:ASN:ND2	2.05	0.53
1:A:225:ASN:HD22	1:A:225:ASN:N	2.01	0.53
1:A:477:GLN:C	1:A:478:CYS:SG	2.92	0.53
1:C:478:CYS:HA	1:C:495:LYS:N	2.24	0.53
1:A:100:THR:HA	1:A:123:HIS:O	2.07	0.53
1:C:163:HIS:ND1	1:C:165:SER:CB	2.71	0.53
1:A:242:TYR:CD2	1:C:277:ALA:HB1	2.44	0.53
1:A:477:GLN:O	1:A:478:CYS:CB	2.55	0.53
1:C:21:ARG:CG	1:C:24:ARG:NH2	2.71	0.53
1:C:341:VAL:CG2	2:D:45:ARG:CZ	2.87	0.53
1:A:437:LEU:HD12	1:A:440:VAL:CG2	2.39	0.53
1:A:451:GLU:H	1:A:454:GLN:NE2	2.07	0.53
1:A:22:ASN:OD1	1:A:401:SER:HB3	2.09	0.53
1:A:109:ILE:HG22	1:A:112:LEU:HB2	1.90	0.53
1:A:211:GLY:C	1:A:212:CYS:SG	2.92	0.53
1:A:351:TYR:C	1:A:352:ILE:O	2.49	0.53
1:C:163:HIS:CE1	1:C:175:PRO:HG3	2.44	0.53
1:A:134:ILE:O	1:A:135:GLN:HB3	2.09	0.53
1:C:274:ASP:O	1:C:275:ASN:C	2.51	0.53
1:C:319:ARG:HG3	1:C:319:ARG:HH11	1.74	0.52
2:D:26:LYS:HA	2:D:30:LEU:O	2.09	0.52
1:A:134:ILE:O	1:A:179:GLN:OE1	2.27	0.52
1:A:484:TRP:HE1	1:A:492:LEU:CD2	2.22	0.52
1:C:33:VAL:CG1	1:C:58:VAL:HG22	2.39	0.52
1:A:280:ARG:N	1:C:247:TYR:O	2.40	0.52
1:A:409:VAL:HG12	1:A:410:LYS:HD3	1.91	0.52
1:A:338:PHE:O	1:A:338:PHE:CD1	2.63	0.52
1:A:444:ARG:HG2	1:A:481:ASP:HA	1.92	0.52
1:A:335:PHE:O	1:A:353:PRO:HB3	2.10	0.52
1:C:218:LYS:HE2	1:C:230:GLY:O	2.10	0.52
1:C:339:GLN:NE2	1:C:350[B]:ARG:HH22	2.08	0.52
1:A:193:GLY:CA	1:C:201:ARG:NH1	2.71	0.52
1:A:496:ASN:O	1:A:497:PHE:CB	2.57	0.52
1:A:24:ARG:HH11	1:A:24:ARG:CG	2.21	0.51
1:C:138:GLU:O	1:C:183:LYS:HD3	2.10	0.51
1:A:514:TYR:CB	1:A:532:ASN:C	2.83	0.51
1:A:437:LEU:CD1	1:A:440:VAL:HG13	2.40	0.51
1:C:333:GLN:HE22	2:D:47:GLU:HB2	1.75	0.51
1:A:193:GLY:CA	1:C:201:ARG:HH12	2.17	0.51
1:A:377:THR:HA	1:A:412:SER:OG	2.10	0.51
1:A:20:TYR:CD1	1:A:47:LEU:HD22	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:GLN:HG3	1:A:338:PHE:HB2	1.92	0.51
1:C:33:VAL:HG13	1:C:58:VAL:HG22	1.92	0.51
1:A:474:CYS:SG	1:A:483:CYS:N	2.84	0.51
1:C:217:GLN:HB2	1:C:231:VAL:HG23	1.93	0.51
1:C:347:MET:HE1	2:D:15:TYR:CA	2.39	0.51
1:A:181:PHE:CE2	1:A:184:LEU:HD12	2.46	0.50
1:A:344:ASN:OD1	1:A:344:ASN:N	2.35	0.50
1:C:499:PHE:HB3	1:C:504:ILE:CD1	2.29	0.50
1:A:208:CYS:SG	1:A:212:CYS:HB3	2.51	0.50
1:C:77:LEU:C	1:C:77:LEU:CD2	2.84	0.50
1:C:444:ARG:NH1	1:C:447:ALA:HB2	2.26	0.50
1:C:340:ASP:HB2	1:C:351:TYR:CZ	2.41	0.50
1:C:492:LEU:O	1:C:493:ASN:ND2	2.37	0.50
1:A:421:LEU:HD23	1:A:484:TRP:CH2	2.47	0.50
1:C:207:PHE:CE1	1:C:234:GLU:HB2	2.47	0.49
1:A:247:TYR:HB2	1:C:280:ARG:HG3	1.95	0.49
1:C:37:LEU:HD12	1:C:38:GLU:N	2.28	0.49
1:C:504:ILE:HD13	1:C:510:ILE:HD12	1.94	0.49
1:A:240:ARG:NH1	1:A:249:LEU:HD13	2.28	0.49
1:C:20:TYR:CD1	1:C:47:LEU:HD12	2.46	0.49
1:C:315:ILE:HD12	1:C:354:LEU:HD11	1.95	0.49
1:C:492:LEU:C	1:C:493:ASN:HD22	2.20	0.49
1:C:350[A]:ARG:HG2	1:C:350[A]:ARG:HH11	1.78	0.48
1:A:374:ILE:CD1	1:A:384:LEU:HD21	2.42	0.48
1:C:130:HIS:N	1:C:132:ARG:NH1	2.54	0.48
1:C:325:ASP:C	1:C:325:ASP:OD1	2.55	0.48
1:A:99:VAL:HG11	1:A:104:MET:HE1	1.95	0.48
1:A:142:ASN:HB2	1:A:144:THR:HG22	1.95	0.48
1:A:355:ASP:HB2	1:A:356:PRO:HD2	1.96	0.48
1:C:347:MET:HE1	2:D:14:TRP:C	2.38	0.48
1:C:484:TRP:CE2	1:C:492:LEU:HD11	2.47	0.48
1:A:416:LEU:HD21	1:A:440:VAL:CG1	2.42	0.48
1:A:489:ASP:OD1	1:A:489:ASP:N	2.30	0.48
1:A:356:PRO:HG3	1:A:381:PHE:HB2	1.95	0.48
1:C:465:ASP:N	1:C:465:ASP:OD1	2.47	0.48
1:A:164:GLU:OE1	1:A:164:GLU:HA	2.13	0.48
1:C:130:HIS:HA	1:C:133:THR:HG23	1.94	0.48
1:A:228:ASP:HA	1:A:263:CYS:HB2	1.95	0.48
1:A:283:PRO:HG3	1:C:240:ARG:HH21	1.77	0.48
1:A:287:MET:SD	1:A:296:CYS:HB2	2.54	0.48
1:C:15:ASN:ND2	1:C:18:HIS:CB	2.69	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ARG:O	1:C:158:GLU:O	2.32	0.48
1:C:310:LEU:HA	1:C:314:ASN:HD21	1.79	0.48
1:A:134:ILE:O	1:A:135:GLN:CB	2.61	0.47
1:A:329:ARG:HD3	1:A:371:TYR:HE1	1.79	0.47
1:A:484:TRP:NE1	1:A:492:LEU:HD21	2.28	0.47
1:C:44:ASN:O	1:C:47:LEU:CD2	2.62	0.47
1:A:43:PRO:HD2	1:A:44:ASN:H	1.79	0.47
1:A:336:SER:C	1:A:337:GLY:O	2.55	0.47
1:A:343:ALA:C	1:A:345:TYR:N	2.72	0.47
1:C:239:MET:HE3	1:C:257:TYR:CZ	2.49	0.47
1:C:477:GLN:O	1:C:495:LYS:CA	2.62	0.47
1:A:26:ARG:HG2	1:A:27:TYR:CD1	2.48	0.47
1:C:99:VAL:CG2	1:C:122:PHE:CD2	2.97	0.47
1:C:183:LYS:HE2	1:C:184:LEU:CD2	2.44	0.47
1:A:270:HIS:CD2	1:A:270:HIS:H	2.32	0.47
1:C:64:ILE:HG23	1:C:67:VAL:HG11	1.96	0.47
1:C:445:TRP:N	1:C:446:PRO:HD2	2.29	0.47
1:C:287:MET:CE	1:C:301:PRO:CD	2.90	0.47
1:A:484:TRP:HE1	1:A:492:LEU:HD23	1.80	0.47
1:C:187:SER:HB3	1:C:188:PRO:HD2	1.96	0.47
1:C:70:LYS:HG2	1:C:105:TYR:CD1	2.51	0.46
1:C:97:LEU:HD23	1:C:98:PHE:N	2.31	0.46
1:C:479:ASN:OD1	1:C:481:ASP:HB2	2.14	0.46
2:D:8:PRO:HD2	2:D:33:TYR:CE2	2.50	0.46
1:A:228:ASP:CB	1:A:233:LYS:HD3	2.45	0.46
1:A:240:ARG:NH2	1:C:283:PRO:HG3	2.30	0.46
1:A:407:ALA:HA	1:A:430:VAL:O	2.16	0.46
1:A:413:LEU:CB	1:A:437:LEU:HD23	2.44	0.46
1:C:260:GLY:O	1:C:261:ALA:HB3	2.15	0.46
1:A:283:PRO:CG	1:C:240:ARG:NH2	2.78	0.46
1:A:338:PHE:HD1	1:A:338:PHE:H	1.63	0.46
1:A:432:GLN:HA	1:A:459:ASN:O	2.15	0.46
1:C:239:MET:HE2	1:C:257:TYR:CE1	2.50	0.46
1:C:57:GLU:HG3	1:C:79:ILE:HG12	1.98	0.46
1:C:499:PHE:HB2	1:C:521:CYS:HB2	1.97	0.46
1:C:342:TYR:CE1	1:C:348:GLY:HA2	2.51	0.46
1:C:78:GLN:HA	1:C:112:LEU:HA	1.96	0.46
1:A:195:CYS:HA	1:A:203:CYS:HA	1.97	0.46
1:A:410:LYS:HD2	1:A:433:HIS:HB3	1.98	0.46
1:A:517:ASP:HB3	1:A:520:THR:H	1.80	0.46
1:C:99:VAL:HG22	1:C:122:PHE:HD2	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:LYS:HE2	1:C:184:LEU:HD21	1.98	0.46
1:A:484:TRP:CE2	1:A:492:LEU:HD21	2.51	0.45
1:A:363:SER:O	1:A:389:ASN:ND2	2.48	0.45
1:A:402:MET:HE2	1:A:430:VAL:HG21	1.96	0.45
1:A:419:ARG:C	1:A:421:LEU:H	2.25	0.45
1:C:157:ARG:O	1:C:158:GLU:C	2.59	0.45
1:C:392:THR:HG22	1:C:423:GLN:HB3	1.99	0.45
1:A:240:ARG:HB3	1:A:249:LEU:HD22	1.98	0.45
1:C:174:GLY:H	1:C:177:ASN:HD22	1.63	0.45
1:A:444:ARG:HD3	1:A:481:ASP:OD1	2.17	0.45
1:C:512:ASN:O	1:C:524:CYS:N	2.50	0.45
1:C:190:CYS:O	1:C:191:ALA:C	2.58	0.45
1:C:205:HIS:HD2	1:C:207:PHE:H	1.63	0.45
1:C:373:ASN:HB2	1:C:399:MET:HE3	1.98	0.45
1:A:333:GLN:HB3	1:A:338:PHE:HB3	1.97	0.45
1:C:483:CYS:HA	1:C:492:LEU:HD12	1.99	0.45
1:C:138:GLU:CB	1:C:184:LEU:HD11	2.46	0.45
1:C:216:THR:O	1:C:219:ASP:HB2	2.17	0.45
1:C:476:ASP:O	1:C:495:LYS:HD2	2.16	0.45
1:A:15:ASN:ND2	1:A:15:ASN:C	2.75	0.45
1:A:381:PHE:O	1:A:412:SER:O	2.35	0.45
1:C:7:LYS:O	1:C:7:LYS:HG3	2.17	0.45
1:C:350[A]:ARG:HH11	1:C:350[A]:ARG:CG	2.30	0.45
1:C:40:THR:HA	1:C:65:SER:O	2.17	0.44
1:C:99:VAL:CG2	1:C:122:PHE:HD2	2.30	0.44
1:C:286:LYS:HA	1:C:295:PRO:HA	1.97	0.44
1:A:288:ASP:OD1	1:A:288:ASP:C	2.60	0.44
1:A:514:TYR:HB3	1:A:532:ASN:H	1.82	0.44
1:C:36:ASN:HD21	1:C:84:THR:CB	2.28	0.44
1:C:138:GLU:HB2	1:C:184:LEU:HD12	1.98	0.44
1:C:239:MET:HE2	1:C:257:TYR:CZ	2.52	0.44
1:C:246:THR:OG1	1:C:248:VAL:HG12	2.17	0.44
1:C:327:ASN:HB3	1:C:371:TYR:N	2.28	0.44
1:A:3:CYS:HB2	1:A:33:VAL:HA	2.00	0.44
1:C:407:ALA:HA	1:C:430:VAL:O	2.17	0.44
1:C:374:ILE:CD1	1:C:384:LEU:HD21	2.48	0.44
1:A:109:ILE:CG2	1:A:112:LEU:HB2	2.46	0.44
1:A:316:ASP:OD1	1:A:358:ARG:NH2	2.51	0.44
1:C:404:ALA:HB2	1:C:430:VAL:CG1	2.48	0.44
1:A:138:GLU:HB2	1:A:184:LEU:HD11	2.00	0.44
1:A:433:HIS:HA	1:A:460:GLU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:HD2	1:A:78:GLN:HE21	1.83	0.44
1:A:39:LEU:HD11	1:A:52:LEU:HD11	2.00	0.44
1:C:67:VAL:HG13	1:C:102:SER:OG	2.18	0.44
1:A:367:GLU:OE1	1:A:394:HIS:HE1	2.01	0.43
1:A:445:TRP:HB2	1:A:456:VAL:HG11	2.00	0.43
1:C:528:CYS:HB2	1:C:539:CYS:HB2	1.88	0.43
1:A:163:HIS:CD2	1:A:164:GLU:N	2.86	0.43
1:C:338:PHE:O	1:C:351:TYR:HD2	2.01	0.43
1:C:512:ASN:OD1	1:C:512:ASN:N	2.50	0.43
1:A:50:SER:O	1:A:53:ASP:HB2	2.18	0.43
1:A:181:PHE:HB2	1:A:185:THR:OG1	2.18	0.43
1:C:373:ASN:ND2	1:C:399:MET:HE1	2.28	0.43
1:A:335:PHE:CZ	1:A:381:PHE:CD1	3.07	0.43
1:C:329:ARG:HG2	1:C:373:ASN:HB3	2.01	0.43
1:A:252:ASN:OD1	1:A:254:GLU:N	2.51	0.43
1:C:53:ASP:HA	1:C:75:PRO:CD	2.47	0.43
1:C:212:CYS:HA	1:C:220:CYS:HA	2.00	0.43
1:C:339:GLN:HE22	1:C:350[B]:ARG:HH22	1.67	0.43
1:A:138:GLU:CB	1:A:184:LEU:HD11	2.48	0.43
1:A:512:ASN:HB2	1:A:524:CYS:SG	2.58	0.43
1:C:279:VAL:HG13	1:C:281:SER:H	1.84	0.43
1:C:350[B]:ARG:NH1	1:C:350[B]:ARG:HB2	2.33	0.43
1:C:514:TYR:OH	1:C:534:ALA:CB	2.66	0.43
1:A:15:ASN:ND2	1:A:17:GLU:N	2.66	0.43
1:A:332:ASP:O	1:A:336:SER:HB3	2.18	0.43
1:C:110:PRO:O	1:C:111:ASP:CB	2.67	0.43
1:C:138:GLU:OE2	1:C:183:LYS:HB3	2.18	0.43
1:A:279:VAL:CA	1:C:247:TYR:O	2.66	0.43
1:C:325:ASP:OD1	1:C:326:GLY:N	2.52	0.43
1:C:451:GLU:H	1:C:454:GLN:NE2	2.17	0.43
1:A:46:ASN:OD1	1:A:47:LEU:N	2.51	0.42
1:C:62:ILE:HD11	1:C:77:LEU:HD11	2.01	0.42
1:C:273:ARG:HD3	1:C:292:GLU:OE2	2.19	0.42
1:C:374:ILE:HD13	1:C:384:LEU:HD11	2.00	0.42
1:A:252:ASN:OD1	1:A:252:ASN:C	2.62	0.42
1:A:314:ASN:O	1:A:317:SER:OG	2.22	0.42
1:A:59:THR:O	1:A:81:ARG:HB2	2.19	0.42
1:A:236:CYS:SG	1:A:237:PRO:HD2	2.59	0.42
1:C:344:ASN:HB2	1:C:346:THR:HG22	2.01	0.42
1:A:292:GLU:HG2	1:A:294:VAL:HG23	2.01	0.42
1:A:444:ARG:O	1:A:444:ARG:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:TRP:N	1:A:446:PRO:CD	2.82	0.42
1:A:1:LYS:HG2	1:A:30:CYS:HA	2.02	0.42
1:C:416:LEU:O	1:C:417:GLU:HB2	2.20	0.42
1:C:477:GLN:NE2	1:C:504:ILE:C	2.77	0.42
1:A:336:SER:OG	1:A:337:GLY:O	2.30	0.42
1:A:338:PHE:CD1	1:A:338:PHE:N	2.87	0.42
1:C:34:ASP:C	1:C:34:ASP:OD1	2.63	0.42
1:C:325:ASP:HA	1:C:369:THR:OG1	2.20	0.42
1:C:331:LEU:O	1:C:334:THR:HB	2.19	0.42
1:A:-2:HIS:HB3	1:A:-1:HIS:H	1.58	0.42
1:C:531:CYS:CB	1:C:539:CYS:HB3	2.50	0.42
1:C:2:ILE:CG2	1:C:3:CYS:N	2.82	0.41
1:C:159:CYS:SG	1:C:160:PRO:HD2	2.60	0.41
1:C:498:ASN:HD22	1:C:499:PHE:N	2.18	0.41
1:A:311:HIS:CD2	1:A:338:PHE:CE1	3.09	0.41
2:D:42:MET:HG2	2:D:50:GLU:HG2	2.01	0.41
1:C:45:GLU:O	1:C:46:ASN:CB	2.68	0.41
1:A:15:ASN:ND2	1:A:17:GLU:H	2.19	0.41
1:A:134:ILE:HD13	1:A:134:ILE:HA	1.87	0.41
1:A:308:THR:O	1:A:329:ARG:HG3	2.20	0.41
1:C:53:ASP:HA	1:C:75:PRO:HG2	2.03	0.41
1:C:432:GLN:HA	1:C:459:ASN:O	2.20	0.41
1:C:15:ASN:ND2	1:C:18:HIS:H	2.18	0.41
1:C:285:ASP:OD1	1:C:285:ASP:N	2.54	0.41
1:A:15:ASN:HB3	1:A:18:HIS:CD2	2.55	0.41
1:A:71:LYS:HG2	1:A:106:THR:HG23	2.03	0.41
1:A:243:ASN:HA	1:A:244:PRO:HD2	1.93	0.41
1:A:339:GLN:CD	1:A:347:MET:HE2	2.45	0.41
1:C:288:ASP:OD2	1:C:289:LYS:O	2.39	0.41
1:C:304:CYS:HA	1:C:305:PRO:HD2	1.90	0.41
1:C:329:ARG:CZ	1:C:399:MET:HE2	2.50	0.41
1:A:339:GLN:OE1	1:A:348:GLY:O	2.39	0.41
1:C:369:THR:O	1:C:396:ARG:HB2	2.21	0.41
1:A:87:SER:CB	1:A:93:GLU:O	2.65	0.41
1:A:335:PHE:CE1	1:A:376:GLY:HA3	2.54	0.41
1:A:429:VAL:HG13	1:A:456:VAL:HB	2.02	0.41
1:C:45:GLU:HA	1:C:69:VAL:HA	2.03	0.41
1:C:477:GLN:NE2	1:C:505:ALA:HA	2.36	0.41
1:A:329:ARG:HD3	1:A:371:TYR:CE1	2.56	0.41
1:A:141:SER:O	1:A:142:ASN:CB	2.69	0.40
1:A:514:TYR:CB	1:A:532:ASN:O	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:SER:O	1:C:91:GLU:O	2.38	0.40
1:C:183:LYS:CG	1:C:184:LEU:N	2.81	0.40
1:C:188:PRO:C	1:C:190:CYS:H	2.30	0.40
1:A:327:ASN:OD1	1:A:371:TYR:CZ	2.75	0.40
1:A:382:ARG:O	1:A:383:ASN:O	2.40	0.40
1:A:477:GLN:O	1:A:478:CYS:HB2	2.21	0.40
1:C:394:HIS:O	1:C:425:SER:HB2	2.21	0.40
1:A:15:ASN:CG	1:A:18:HIS:CD2	2.99	0.40
1:A:163:HIS:O	1:A:166:CYS:HB2	2.22	0.40
1:C:210:GLY:O	1:C:221:ILE:HD12	2.22	0.40
1:C:228:ASP:O	1:C:229:GLU:HB2	2.22	0.40
2:D:47:GLU:OE1	2:D:47:GLU:N	2.51	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:THR:O	1:C:313:GLY:CA[3_554]	1.18	1.02
1:A:48:ASP:CB	1:A:350:ARG:O[4_545]	1.91	0.29
1:C:181:PHE:CD2	1:C:352:ILE:CG2[3_554]	1.99	0.21
1:C:167:THR:O	1:C:313:GLY:C[3_554]	2.02	0.18
1:C:168:HIS:CE1	1:C:352:ILE:N[3_554]	2.03	0.17
1:C:168:HIS:NE2	1:C:352:ILE:N[3_554]	2.04	0.16
1:A:46:ASN:CG	1:A:351:TYR:CE2[4_545]	2.12	0.08
1:C:135:GLN:NE2	1:C:358:ARG:CD[3_554]	2.14	0.06

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	514/601 (86%)	466 (91%)	38 (7%)	10 (2%)	6 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	528/601 (88%)	494 (94%)	27 (5%)	7 (1%)	9	33
2	D	49/52 (94%)	46 (94%)	3 (6%)	0	100	100
All	All	1091/1254 (87%)	1006 (92%)	68 (6%)	17 (2%)	7	29

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	ASN
1	A	478	CYS
1	C	158	GLU
1	A	212	CYS
1	A	344	ASN
1	A	420	ASN
1	A	497	PHE
1	A	511	SER
1	C	92	GLU
1	C	201	ARG
1	C	260	GLY
1	C	127	ASN
1	C	474	CYS
1	A	155	PRO
1	C	159	CYS
1	A	43	PRO
1	A	13	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	440/531 (83%)	392 (89%)	48 (11%)	6	22
1	C	454/531 (86%)	386 (85%)	68 (15%)	3	11
2	D	42/45 (93%)	38 (90%)	4 (10%)	8	29
All	All	936/1107 (85%)	816 (87%)	120 (13%)	4	17

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	9	ARG
1	A	11	SER
1	A	12	VAL
1	A	15	ASN
1	A	24	ARG
1	A	33	VAL
1	A	69	VAL
1	A	106	THR
1	A	128	LEU
1	A	129	CYS
1	A	138	GLU
1	A	141	SER
1	A	144	THR
1	A	159	CYS
1	A	182	SER
1	A	190	CYS
1	A	225	ASN
1	A	233	LYS
1	A	249	LEU
1	A	262	THR
1	A	267	CYS
1	A	287	MET
1	A	303	THR
1	A	322	THR
1	A	323	VAL
1	A	336	SER
1	A	338	PHE
1	A	344	ASN
1	A	352	ILE
1	A	354	LEU
1	A	361	VAL
1	A	364	THR
1	A	375	GLU
1	A	384	LEU
1	A	410	LYS
1	A	416	LEU
1	A	429	VAL
1	A	436	ASP
1	A	437	LEU
1	A	448	ILE
1	A	453	GLU

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Mol	Chain	Res	Type
1	A	456	VAL
1	A	463	ARG
1	A	470	ASN
1	A	476	ASP
1	A	489	ASP
1	A	531	CYS
1	C	8	SER
1	C	12	VAL
1	C	14	SER
1	C	31	THR
1	C	33	VAL
1	C	36	ASN
1	C	37	LEU
1	C	42	LEU
1	C	44	ASN
1	C	52	LEU
1	C	67	VAL
1	C	79	ILE
1	C	84	THR
1	C	92	GLU
1	C	97	LEU
1	C	99	VAL
1	C	102	SER
1	C	107	LEU
1	C	113	ARG
1	C	125	ASN
1	C	127	ASN
1	C	128	LEU
1	C	132	ARG
1	C	133	THR
1	C	137	SER
1	C	157	ARG
1	C	159	CYS
1	C	166	CYS
1	C	181	PHE
1	C	182	SER
1	C	185	THR
1	C	186	CYS
1	C	201	ARG
1	C	208	CYS
1	C	220	CYS
1	C	231	VAL

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Mol	Chain	Res	Type
1	C	235	GLU
1	C	246	THR
1	C	265	LYS
1	C	279	VAL
1	C	285	ASP
1	C	286	LYS
1	C	293	CYS
1	C	303	THR
1	C	307	VAL
1	C	322	THR
1	C	325	ASP
1	C	327	ASN
1	C	330	ILE
1	C	331	LEU
1	C	344	ASN
1	C	350[A]	ARG
1	C	350[B]	ARG
1	C	354	LEU
1	C	398	LEU
1	C	406	LEU
1	C	430	VAL
1	C	456	VAL
1	C	462	LEU
1	C	465	ASP
1	C	483	CYS
1	C	492	LEU
1	C	511	SER
1	C	512	ASN
1	C	528	CYS
1	C	531	CYS
1	C	532	ASN
1	C	539	CYS
2	D	4	THR
2	D	6	LYS
2	D	27	ILE
2	D	42	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	18	HIS

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Mol	Chain	Res	Type
1	A	119	GLN
1	A	163	HIS
1	A	168	HIS
1	A	179	GLN
1	A	217	GLN
1	A	225	ASN
1	A	270	HIS
1	A	275	ASN
1	A	311	HIS
1	A	327	ASN
1	A	378	HIS
1	A	394	HIS
1	A	433	HIS
1	A	449	GLN
1	A	454	GLN
1	A	477	GLN
1	A	490	GLN
1	C	15	ASN
1	C	36	ASN
1	C	66	HIS
1	C	117	ASN
1	C	333	GLN
1	C	339	GLN
1	C	373	ASN
1	C	380	GLN
1	C	394	HIS
1	C	420	ASN
1	C	432	GLN
1	C	449	GLN
1	C	477	GLN
1	C	493	ASN
1	C	498	ASN
2	D	44	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	522/601 (86%)	1.87	204 (39%)  	35, 60, 83, 106	0
1	C	531/601 (88%)	1.70	171 (32%)  	27, 56, 80, 97	1 (0%)
2	D	51/52 (98%)	1.80	20 (39%)  	41, 50, 58, 61	0
All	All	1104/1254 (88%)	1.78	395 (35%)  	27, 58, 81, 106	1 (0%)

All (395) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	153	THR	8.3
1	C	3	CYS	7.4
1	A	46	ASN	7.0
1	A	433	HIS	6.9
1	A	432	GLN	6.7
1	A	-2	HIS	6.6
1	A	56	ARG	6.3
1	A	357	GLU	6.2
1	A	98	PHE	6.2
1	C	421	LEU	5.8
1	A	89	SER	5.8
1	A	147	TYR	5.8
1	A	274	ASP	5.5
1	C	523	ILE	5.4
1	A	155	PRO	5.4
1	C	192	GLY	5.3
1	C	506	ASP	5.3
1	C	393	ILE	5.2
1	C	350[A]	ARG	5.2
1	A	105	TYR	5.1
1	C	55	ILE	5.0
2	D	19	ASP	5.0
1	C	23	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	402	MET	4.9
1	C	27	TYR	4.8
1	C	51	PHE	4.8
1	A	260	GLY	4.7
1	C	30	CYS	4.7
1	A	295	PRO	4.7
1	A	409	VAL	4.7
1	C	424	ILE	4.7
1	C	0	HIS	4.7
1	A	430	VAL	4.6
1	C	401	SER	4.6
1	C	271	LEU	4.5
1	A	457	TRP	4.5
1	C	154	ALA	4.5
1	A	235	GLU	4.5
1	A	114	ASP	4.5
2	D	15	TYR	4.5
1	A	31	THR	4.5
1	A	47	LEU	4.5
1	A	272	LEU	4.4
1	A	521	CYS	4.4
1	A	48	ASP	4.4
1	A	-1	HIS	4.4
1	C	507	CYS	4.4
1	A	394	HIS	4.3
1	C	352	ILE	4.3
1	C	525	HIS	4.2
1	C	448	ILE	4.2
1	C	524	CYS	4.2
1	A	368	ILE	4.2
1	A	276	GLY	4.2
1	A	405	ALA	4.2
1	A	396	ARG	4.1
1	A	328	ILE	4.0
1	C	484	TRP	4.0
1	A	283	PRO	4.0
1	A	419	ARG	3.9
1	C	315	ILE	3.9
1	A	342	TYR	3.9
1	A	262	THR	3.9
2	D	14	TRP	3.9
1	A	158	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	373	ASN	3.8
1	C	12	VAL	3.8
1	C	10	LEU	3.8
1	A	277	ALA	3.8
1	A	481	ASP	3.8
1	A	279	VAL	3.8
1	C	443	ILE	3.8
1	A	199	LYS	3.7
1	C	74	PHE	3.7
1	A	282	CYS	3.7
1	A	287	MET	3.7
1	C	155	PRO	3.7
1	A	514	TYR	3.7
1	A	99	VAL	3.7
1	A	398	LEU	3.7
1	C	41	TRP	3.7
1	A	209	ALA	3.7
1	C	483	CYS	3.7
1	A	480	GLU	3.6
1	C	33	VAL	3.6
1	A	324	ILE	3.6
2	D	18	ASN	3.6
1	C	20	TYR	3.6
1	C	168	HIS	3.5
1	C	69	VAL	3.5
1	A	469	LYS	3.5
1	C	422	LYS	3.5
2	D	17	LEU	3.5
1	C	462	LEU	3.5
1	A	393	ILE	3.5
1	A	113	ARG	3.5
1	A	349	PRO	3.5
1	A	259	TYR	3.5
1	A	226	PHE	3.5
1	A	387	PHE	3.5
1	C	160	PRO	3.5
2	D	51	ILE	3.5
1	A	343	ALA	3.5
1	A	431	ILE	3.5
1	A	210	GLY	3.4
1	A	52	LEU	3.4
1	C	416	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	349	PRO	3.4
1	A	285	ASP	3.4
1	C	476	ASP	3.4
1	C	387	PHE	3.4
1	A	280	ARG	3.4
1	A	459	ASN	3.4
1	A	126	TYR	3.4
1	C	341	VAL	3.4
1	C	456	VAL	3.4
1	A	448	ILE	3.4
1	C	170	CYS	3.4
1	A	429	VAL	3.4
1	A	120	VAL	3.3
1	C	42	LEU	3.3
1	A	421	LEU	3.3
1	C	347	MET	3.3
1	A	185	THR	3.3
1	C	440	VAL	3.3
1	C	76	LYS	3.3
2	D	34	SER	3.2
1	C	53	ASP	3.2
1	A	307	VAL	3.2
1	A	154	ALA	3.2
1	C	13	PRO	3.2
1	A	74	PHE	3.2
1	A	397	GLN	3.2
1	A	372	LEU	3.2
1	A	347	MET	3.2
1	A	125	ASN	3.2
1	A	225	ASN	3.2
1	C	503	CYS	3.2
1	A	532	ASN	3.1
1	A	329	ARG	3.1
1	C	62	ILE	3.1
1	A	261	ALA	3.1
1	A	369	THR	3.1
1	C	47	LEU	3.1
2	D	52	ASP	3.1
1	A	79	ILE	3.1
1	A	269	GLY	3.1
1	C	316	ASP	3.1
1	C	429	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	110	PRO	3.1
1	C	139	ILE	3.1
1	C	297	ASN	3.1
1	A	516	PHE	3.1
1	C	510	ILE	3.1
1	C	191	ALA	3.0
1	A	293	CYS	3.0
1	C	143	GLY	3.0
1	A	410	LYS	3.0
1	A	460	GLU	3.0
1	C	134	ILE	3.0
1	A	423	GLN	3.0
1	C	284	GLN	3.0
1	C	173	GLU	3.0
1	C	162	CYS	3.0
1	A	348	GLY	3.0
1	A	55	ILE	3.0
1	C	97	LEU	2.9
1	C	92	GLU	2.9
1	C	480	GLU	2.9
1	A	281	SER	2.9
1	C	225	ASN	2.9
1	C	452	PRO	2.9
1	C	87	SER	2.9
1	A	78	GLN	2.9
1	A	346	THR	2.9
1	C	318	PHE	2.9
1	A	327	ASN	2.9
1	C	129	CYS	2.9
1	C	261	ALA	2.9
2	D	25	VAL	2.9
1	A	509	TYR	2.9
1	C	230	GLY	2.9
1	C	310	LEU	2.9
1	A	268	PRO	2.9
1	C	96	ALA	2.9
1	A	136	TRP	2.9
2	D	20	ALA	2.8
1	A	44	ASN	2.8
1	A	390	LEU	2.8
1	C	4	ILE	2.8
1	C	372	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	426	SER	2.8
2	D	28	ALA	2.8
1	C	482	GLY	2.8
1	C	432	GLN	2.8
1	C	464	ALA	2.8
1	A	362	PHE	2.8
1	C	249	LEU	2.8
1	A	182	SER	2.8
1	A	440	VAL	2.8
1	C	38	GLU	2.8
1	A	484	TRP	2.8
2	D	48	TYR	2.8
1	A	341	VAL	2.8
1	C	354	LEU	2.8
1	A	370	GLY	2.7
1	A	507	CYS	2.7
1	A	310	LEU	2.7
1	C	88	LEU	2.7
1	A	411	SER	2.7
1	A	192	GLY	2.7
1	C	26	ARG	2.7
1	A	275	ASN	2.7
1	A	96	ALA	2.7
1	A	416	LEU	2.7
1	C	467	CYS	2.7
1	A	227	PHE	2.7
1	A	193	GLY	2.7
1	A	21	ARG	2.7
1	A	344	ASN	2.7
1	A	107	LEU	2.7
1	C	188	PRO	2.7
1	A	223	CYS	2.7
1	C	267	CYS	2.7
1	A	258	ALA	2.7
1	A	498	ASN	2.7
1	A	499	PHE	2.7
1	A	4	ILE	2.6
1	C	431	ILE	2.6
1	A	121	GLY	2.6
1	A	278	CYS	2.6
1	C	377	THR	2.6
1	C	530	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	312	ALA	2.6
1	C	390	LEU	2.6
1	A	383	ASN	2.6
1	C	86	PHE	2.6
1	C	31	THR	2.6
1	C	414	TYR	2.6
1	C	251	THR	2.6
1	C	201	ARG	2.6
1	A	408	ILE	2.6
1	A	270	HIS	2.6
1	A	305	PRO	2.6
1	A	290	GLY	2.6
1	A	309	VAL	2.6
1	C	40	THR	2.6
1	A	381	PHE	2.6
1	A	306	GLY	2.6
1	A	54	ASN	2.6
1	A	340	ASP	2.6
1	A	184	LEU	2.6
1	C	206	LEU	2.5
1	A	350	ARG	2.5
1	C	56	ARG	2.5
1	C	436	ASP	2.5
1	C	465	ASP	2.5
1	A	2	ILE	2.5
1	A	520	THR	2.5
1	C	308	THR	2.5
1	A	345	TYR	2.5
1	C	159	CYS	2.5
1	A	326	GLY	2.5
1	C	275	ASN	2.5
1	A	5	GLY	2.5
1	A	189	GLN	2.5
1	A	304	CYS	2.5
1	A	376	GLY	2.5
1	C	126	TYR	2.5
1	C	529	ARG	2.5
1	C	90	VAL	2.5
1	C	400	GLU	2.5
1	C	283	PRO	2.5
1	C	281	SER	2.4
1	C	242	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	180	LYS	2.4
2	D	41	PHE	2.4
1	A	116	LEU	2.4
1	C	37	LEU	2.4
1	C	184	LEU	2.4
1	A	288	ASP	2.4
1	A	351	TYR	2.4
1	A	375	GLU	2.4
1	C	367	GLU	2.4
1	A	220	CYS	2.4
1	A	263	CYS	2.4
1	A	308	THR	2.4
1	A	0	HIS	2.4
1	C	481	ASP	2.4
1	A	374	ILE	2.4
1	C	164	GLU	2.4
1	C	508	GLY	2.3
1	A	367	GLU	2.3
1	A	365	VAL	2.3
1	C	174	GLY	2.3
1	C	298	GLY	2.3
1	C	479	ASN	2.3
1	C	274	ASP	2.3
1	A	128	LEU	2.3
1	A	331	LEU	2.3
1	C	331	LEU	2.3
1	C	295	PRO	2.3
1	A	139	ILE	2.3
1	C	270	HIS	2.3
1	A	178	CYS	2.3
2	D	11	PHE	2.3
1	A	35	GLY	2.3
1	A	330	ILE	2.3
1	C	535	GLY	2.3
1	A	418	MET	2.3
1	A	112	LEU	2.3
1	C	248	VAL	2.3
1	C	172	GLY	2.3
2	D	40	GLY	2.3
1	A	206	LEU	2.3
1	C	130	HIS	2.3
1	A	366	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	83	ARG	2.3
2	D	45	ARG	2.3
1	A	315	ILE	2.2
1	A	406	LEU	2.2
1	C	362	PHE	2.2
1	A	50	SER	2.2
1	A	401	SER	2.2
1	A	29	ASN	2.2
1	C	179	GLN	2.2
1	C	504	ILE	2.2
1	A	403	PHE	2.2
1	C	366	LYS	2.2
2	D	23	PHE	2.2
1	C	382	ARG	2.2
1	A	57	GLU	2.2
1	C	473	ILE	2.2
1	C	402	MET	2.2
1	C	437	LEU	2.2
1	C	534	ALA	2.2
1	C	338	PHE	2.2
1	A	97	LEU	2.2
1	C	357	GLU	2.2
1	A	129	CYS	2.2
1	A	447	ALA	2.2
1	C	268	PRO	2.2
1	C	428	SER	2.2
1	A	413	LEU	2.2
1	A	224	LYS	2.2
1	C	513	ALA	2.2
1	A	427	GLY	2.2
1	A	171	TRP	2.2
2	D	21	HIS	2.2
1	C	334	THR	2.1
1	A	77	LEU	2.1
1	C	329	ARG	2.1
1	C	493	ASN	2.1
1	A	25	ASP	2.1
1	C	120	VAL	2.1
1	C	409	VAL	2.1
1	A	6	THR	2.1
1	A	322	THR	2.1
1	C	330	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	514	TYR	2.1
1	A	176	LYS	2.1
1	C	406	LEU	2.1
1	A	87	SER	2.1
1	C	75	PRO	2.1
1	C	356	PRO	2.1
2	D	50	GLU	2.1
1	A	494	CYS	2.1
1	A	23	LEU	2.1
1	A	80	ILE	2.1
1	C	374	ILE	2.1
1	A	518	ASN	2.1
1	A	359	LEU	2.1
1	A	490	GLN	2.1
1	C	449	GLN	2.1
1	A	181	PHE	2.1
1	A	318	PHE	2.1
1	C	9	ARG	2.1
1	C	193	GLY	2.1
1	C	487	GLY	2.1
1	A	51	PHE	2.1
1	C	360	GLU	2.1
1	A	264	VAL	2.0
2	D	6	LYS	2.0
1	A	10	LEU	2.0
1	C	109	ILE	2.0
1	C	445	TRP	2.0
1	A	236	CYS	2.0
1	C	536	ALA	2.0
1	C	210	GLY	2.0
1	C	269	GLY	2.0
1	A	173	GLU	2.0
1	C	247	TYR	2.0
1	C	351	TYR	2.0
1	C	340	ASP	2.0
1	A	384	LEU	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.