



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:07 PM GMT

PDB ID : 4BKF
Title : crystal structure of the human EphA4 ectodomain in complex with human ephrinB3
Authors : Seiradake, E.; Schaupp, A.; del Toro Ruiz, D.; Kaufmann, R.; Mitakidis, N.; Harlos, K.; Aricescu, A.R.; Klein, R.; Jones, E.Y.
Deposited on : 2013-04-24
Resolution : 4.65 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

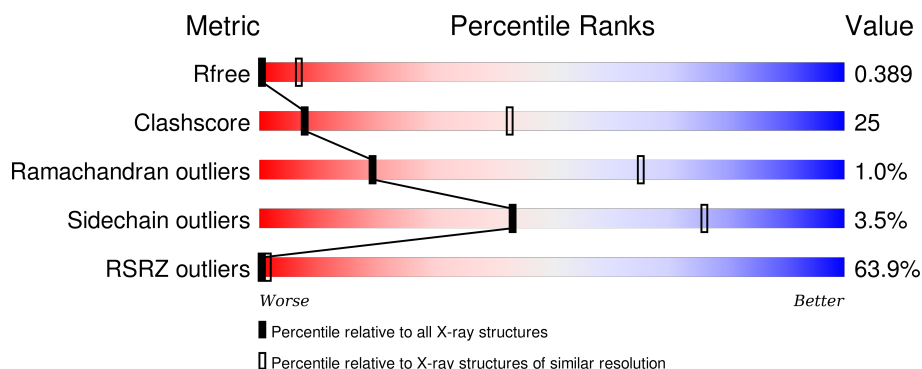
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.65 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}	91344	1093 (5.70-3.60)
Clashscore	102246	1007 (5.66-3.64)
Ramachandran outliers	100387	1135 (5.70-3.60)
Sidechain outliers	100360	1116 (5.70-3.60)
RSRZ outliers	91569	1096 (5.70-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	568	<div> <div>51%</div> <div> <div>71%</div> <div>17%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	568	<div> <div>65%</div> <div> <div>73%</div> <div>14%</div> <div>•</div> <div>11%</div> </div> </div>
2	C	183	<div> <div>56%</div> <div> <div>39%</div> <div>32%</div> <div>7%</div> <div>23%</div> </div> </div>
2	D	183	<div> <div>34%</div> <div> <div>40%</div> <div>31%</div> <div>6%</div> <div>23%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10126 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 EPHRIN TYPE-A RECEPTOR 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			3931	2451	678	776	26			
1	B	505	Total	C	N	O	S	0	0	0
			3931	2451	678	776	26			

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP P54764
A	-10	GLY	-	EXPRESSION TAG	UNP P54764
A	-9	ILE	-	EXPRESSION TAG	UNP P54764
A	-8	LEU	-	EXPRESSION TAG	UNP P54764
A	-7	PRO	-	EXPRESSION TAG	UNP P54764
A	-6	SER	-	EXPRESSION TAG	UNP P54764
A	-5	PRO	-	EXPRESSION TAG	UNP P54764
A	-4	GLY	-	EXPRESSION TAG	UNP P54764
A	-3	MET	-	EXPRESSION TAG	UNP P54764
A	-2	PRO	-	EXPRESSION TAG	UNP P54764
A	-1	ALA	-	EXPRESSION TAG	UNP P54764
A	0	LEU	-	EXPRESSION TAG	UNP P54764
A	1	LEU	-	EXPRESSION TAG	UNP P54764
A	2	SER	-	EXPRESSION TAG	UNP P54764
A	3	LEU	-	EXPRESSION TAG	UNP P54764
A	4	VAL	-	EXPRESSION TAG	UNP P54764
A	5	SER	-	EXPRESSION TAG	UNP P54764
A	6	LEU	-	EXPRESSION TAG	UNP P54764
A	7	LEU	-	EXPRESSION TAG	UNP P54764
A	8	SER	-	EXPRESSION TAG	UNP P54764
A	9	VAL	-	EXPRESSION TAG	UNP P54764
A	10	LEU	-	EXPRESSION TAG	UNP P54764
A	11	LEU	-	EXPRESSION TAG	UNP P54764
A	12	MET	-	EXPRESSION TAG	UNP P54764
A	13	GLY	-	EXPRESSION TAG	UNP P54764

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Chain	Residue	Modelled	Actual	Comment	Reference
A	14	CYS	-	EXPRESSION TAG	UNP P54764
A	15	VAL	-	EXPRESSION TAG	UNP P54764
A	16	ALA	-	EXPRESSION TAG	UNP P54764
A	17	GLU	-	EXPRESSION TAG	UNP P54764
A	18	THR	-	EXPRESSION TAG	UNP P54764
A	19	GLY	-	EXPRESSION TAG	UNP P54764
A	548	GLY	-	EXPRESSION TAG	UNP P54764
A	549	THR	-	EXPRESSION TAG	UNP P54764
A	550	LYS	-	EXPRESSION TAG	UNP P54764
A	551	HIS	-	EXPRESSION TAG	UNP P54764
A	552	HIS	-	EXPRESSION TAG	UNP P54764
A	553	HIS	-	EXPRESSION TAG	UNP P54764
A	554	HIS	-	EXPRESSION TAG	UNP P54764
A	555	HIS	-	EXPRESSION TAG	UNP P54764
A	556	HIS	-	EXPRESSION TAG	UNP P54764
A	28	THR	ALA	CONFLICT	UNP P54764
B	-11	MET	-	EXPRESSION TAG	UNP P54764
B	-10	GLY	-	EXPRESSION TAG	UNP P54764
B	-9	ILE	-	EXPRESSION TAG	UNP P54764
B	-8	LEU	-	EXPRESSION TAG	UNP P54764
B	-7	PRO	-	EXPRESSION TAG	UNP P54764
B	-6	SER	-	EXPRESSION TAG	UNP P54764
B	-5	PRO	-	EXPRESSION TAG	UNP P54764
B	-4	GLY	-	EXPRESSION TAG	UNP P54764
B	-3	MET	-	EXPRESSION TAG	UNP P54764
B	-2	PRO	-	EXPRESSION TAG	UNP P54764
B	-1	ALA	-	EXPRESSION TAG	UNP P54764
B	0	LEU	-	EXPRESSION TAG	UNP P54764
B	1	LEU	-	EXPRESSION TAG	UNP P54764
B	2	SER	-	EXPRESSION TAG	UNP P54764
B	3	LEU	-	EXPRESSION TAG	UNP P54764
B	4	VAL	-	EXPRESSION TAG	UNP P54764
B	5	SER	-	EXPRESSION TAG	UNP P54764
B	6	LEU	-	EXPRESSION TAG	UNP P54764
B	7	LEU	-	EXPRESSION TAG	UNP P54764
B	8	SER	-	EXPRESSION TAG	UNP P54764
B	9	VAL	-	EXPRESSION TAG	UNP P54764
B	10	LEU	-	EXPRESSION TAG	UNP P54764
B	11	LEU	-	EXPRESSION TAG	UNP P54764
B	12	MET	-	EXPRESSION TAG	UNP P54764
B	13	GLY	-	EXPRESSION TAG	UNP P54764
B	14	CYS	-	EXPRESSION TAG	UNP P54764

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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	VAL	-	EXPRESSION TAG	UNP P54764
B	16	ALA	-	EXPRESSION TAG	UNP P54764
B	17	GLU	-	EXPRESSION TAG	UNP P54764
B	18	THR	-	EXPRESSION TAG	UNP P54764
B	19	GLY	-	EXPRESSION TAG	UNP P54764
B	548	GLY	-	EXPRESSION TAG	UNP P54764
B	549	THR	-	EXPRESSION TAG	UNP P54764
B	550	LYS	-	EXPRESSION TAG	UNP P54764
B	551	HIS	-	EXPRESSION TAG	UNP P54764
B	552	HIS	-	EXPRESSION TAG	UNP P54764
B	553	HIS	-	EXPRESSION TAG	UNP P54764
B	554	HIS	-	EXPRESSION TAG	UNP P54764
B	555	HIS	-	EXPRESSION TAG	UNP P54764
B	556	HIS	-	EXPRESSION TAG	UNP P54764
B	28	THR	ALA	CONFLICT	UNP P54764

- Molecule 2 is a protein called EPHRIN-B3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	141	Total	C	N	O	S	0	0	0
			1132	720	201	206	5			
2	D	141	Total	C	N	O	S	0	0	0
			1132	720	201	206	5			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	MET	-	EXPRESSION TAG	UNP Q15768
C	-3	GLY	-	EXPRESSION TAG	UNP Q15768
C	-2	ILE	-	EXPRESSION TAG	UNP Q15768
C	-1	LEU	-	EXPRESSION TAG	UNP Q15768
C	0	PRO	-	EXPRESSION TAG	UNP Q15768
C	1	SER	-	EXPRESSION TAG	UNP Q15768
C	2	PRO	-	EXPRESSION TAG	UNP Q15768
C	3	GLY	-	EXPRESSION TAG	UNP Q15768
C	4	MET	-	EXPRESSION TAG	UNP Q15768
C	5	PRO	-	EXPRESSION TAG	UNP Q15768
C	6	ALA	-	EXPRESSION TAG	UNP Q15768
C	7	LEU	-	EXPRESSION TAG	UNP Q15768
C	8	LEU	-	EXPRESSION TAG	UNP Q15768
C	9	SER	-	EXPRESSION TAG	UNP Q15768
C	10	LEU	-	EXPRESSION TAG	UNP Q15768

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Chain	Residue	Modelled	Actual	Comment	Reference
C	11	VAL	-	EXPRESSION TAG	UNP Q15768
C	12	SER	-	EXPRESSION TAG	UNP Q15768
C	13	LEU	-	EXPRESSION TAG	UNP Q15768
C	14	LEU	-	EXPRESSION TAG	UNP Q15768
C	15	SER	-	EXPRESSION TAG	UNP Q15768
C	16	VAL	-	EXPRESSION TAG	UNP Q15768
C	17	LEU	-	EXPRESSION TAG	UNP Q15768
C	18	LEU	-	EXPRESSION TAG	UNP Q15768
C	19	MET	-	EXPRESSION TAG	UNP Q15768
C	20	GLY	-	EXPRESSION TAG	UNP Q15768
C	21	CYS	-	EXPRESSION TAG	UNP Q15768
C	22	VAL	-	EXPRESSION TAG	UNP Q15768
C	23	ALA	-	EXPRESSION TAG	UNP Q15768
C	24	GLU	-	EXPRESSION TAG	UNP Q15768
C	25	THR	-	EXPRESSION TAG	UNP Q15768
C	26	GLY	-	EXPRESSION TAG	UNP Q15768
C	170	GLY	-	EXPRESSION TAG	UNP Q15768
C	171	THR	-	EXPRESSION TAG	UNP Q15768
C	172	LYS	-	EXPRESSION TAG	UNP Q15768
C	173	HIS	-	EXPRESSION TAG	UNP Q15768
C	174	HIS	-	EXPRESSION TAG	UNP Q15768
C	175	HIS	-	EXPRESSION TAG	UNP Q15768
C	176	HIS	-	EXPRESSION TAG	UNP Q15768
C	177	HIS	-	EXPRESSION TAG	UNP Q15768
C	178	HIS	-	EXPRESSION TAG	UNP Q15768
C	75	SER	ASN	CONFLICT	UNP Q15768
C	85	GLU	GLY	CONFLICT	UNP Q15768
D	-4	MET	-	EXPRESSION TAG	UNP Q15768
D	-3	GLY	-	EXPRESSION TAG	UNP Q15768
D	-2	ILE	-	EXPRESSION TAG	UNP Q15768
D	-1	LEU	-	EXPRESSION TAG	UNP Q15768
D	0	PRO	-	EXPRESSION TAG	UNP Q15768
D	1	SER	-	EXPRESSION TAG	UNP Q15768
D	2	PRO	-	EXPRESSION TAG	UNP Q15768
D	3	GLY	-	EXPRESSION TAG	UNP Q15768
D	4	MET	-	EXPRESSION TAG	UNP Q15768
D	5	PRO	-	EXPRESSION TAG	UNP Q15768
D	6	ALA	-	EXPRESSION TAG	UNP Q15768
D	7	LEU	-	EXPRESSION TAG	UNP Q15768
D	8	LEU	-	EXPRESSION TAG	UNP Q15768
D	9	SER	-	EXPRESSION TAG	UNP Q15768
D	10	LEU	-	EXPRESSION TAG	UNP Q15768

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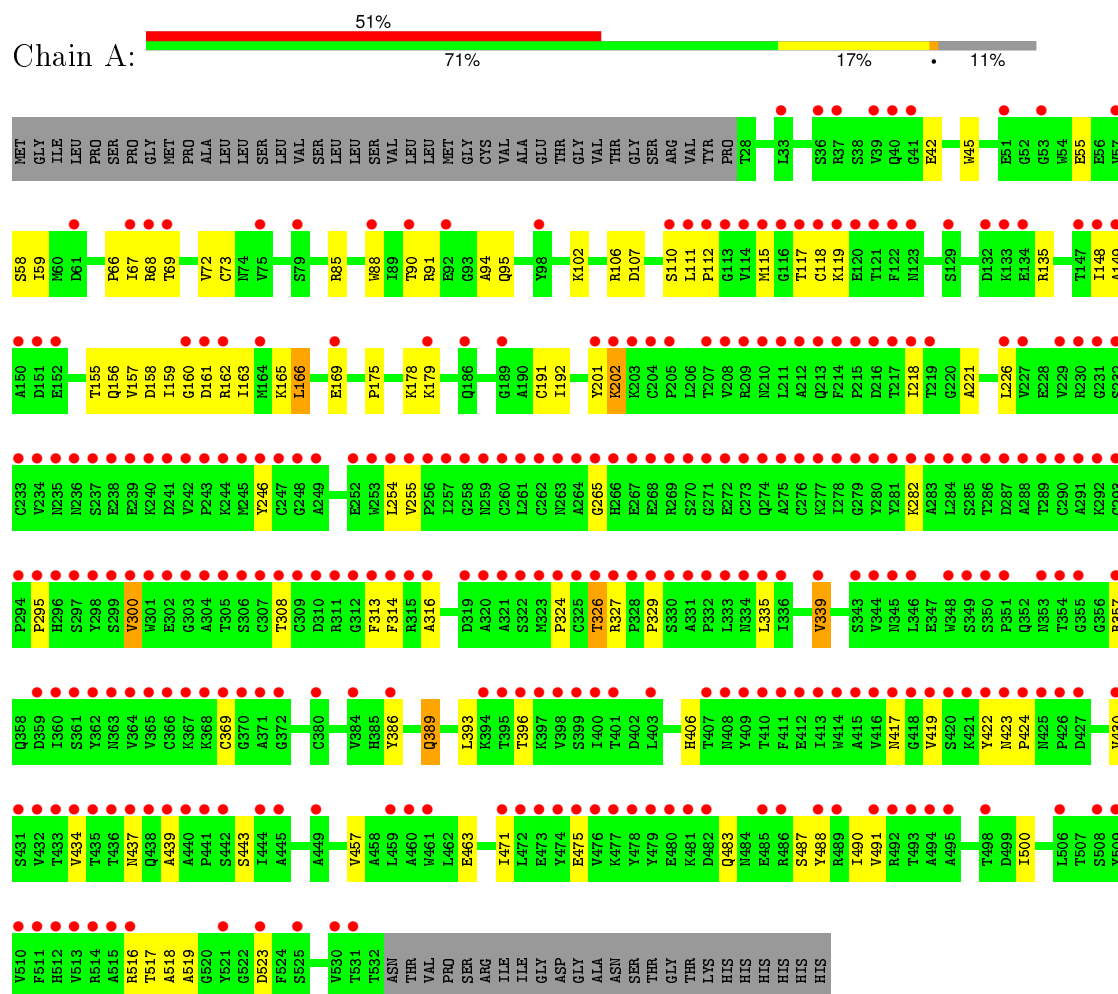
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Chain	Residue	Modelled	Actual	Comment	Reference
D	11	VAL	-	EXPRESSION TAG	UNP Q15768
D	12	SER	-	EXPRESSION TAG	UNP Q15768
D	13	LEU	-	EXPRESSION TAG	UNP Q15768
D	14	LEU	-	EXPRESSION TAG	UNP Q15768
D	15	SER	-	EXPRESSION TAG	UNP Q15768
D	16	VAL	-	EXPRESSION TAG	UNP Q15768
D	17	LEU	-	EXPRESSION TAG	UNP Q15768
D	18	LEU	-	EXPRESSION TAG	UNP Q15768
D	19	MET	-	EXPRESSION TAG	UNP Q15768
D	20	GLY	-	EXPRESSION TAG	UNP Q15768
D	21	CYS	-	EXPRESSION TAG	UNP Q15768
D	22	VAL	-	EXPRESSION TAG	UNP Q15768
D	23	ALA	-	EXPRESSION TAG	UNP Q15768
D	24	GLU	-	EXPRESSION TAG	UNP Q15768
D	25	THR	-	EXPRESSION TAG	UNP Q15768
D	26	GLY	-	EXPRESSION TAG	UNP Q15768
D	170	GLY	-	EXPRESSION TAG	UNP Q15768
D	171	THR	-	EXPRESSION TAG	UNP Q15768
D	172	LYS	-	EXPRESSION TAG	UNP Q15768
D	173	HIS	-	EXPRESSION TAG	UNP Q15768
D	174	HIS	-	EXPRESSION TAG	UNP Q15768
D	175	HIS	-	EXPRESSION TAG	UNP Q15768
D	176	HIS	-	EXPRESSION TAG	UNP Q15768
D	177	HIS	-	EXPRESSION TAG	UNP Q15768
D	178	HIS	-	EXPRESSION TAG	UNP Q15768
D	75	SER	ASN	CONFLICT	UNP Q15768
D	85	GLU	GLY	CONFLICT	UNP Q15768

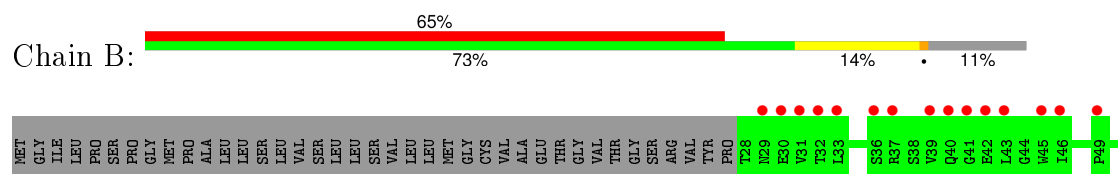
3 Residue-property plots

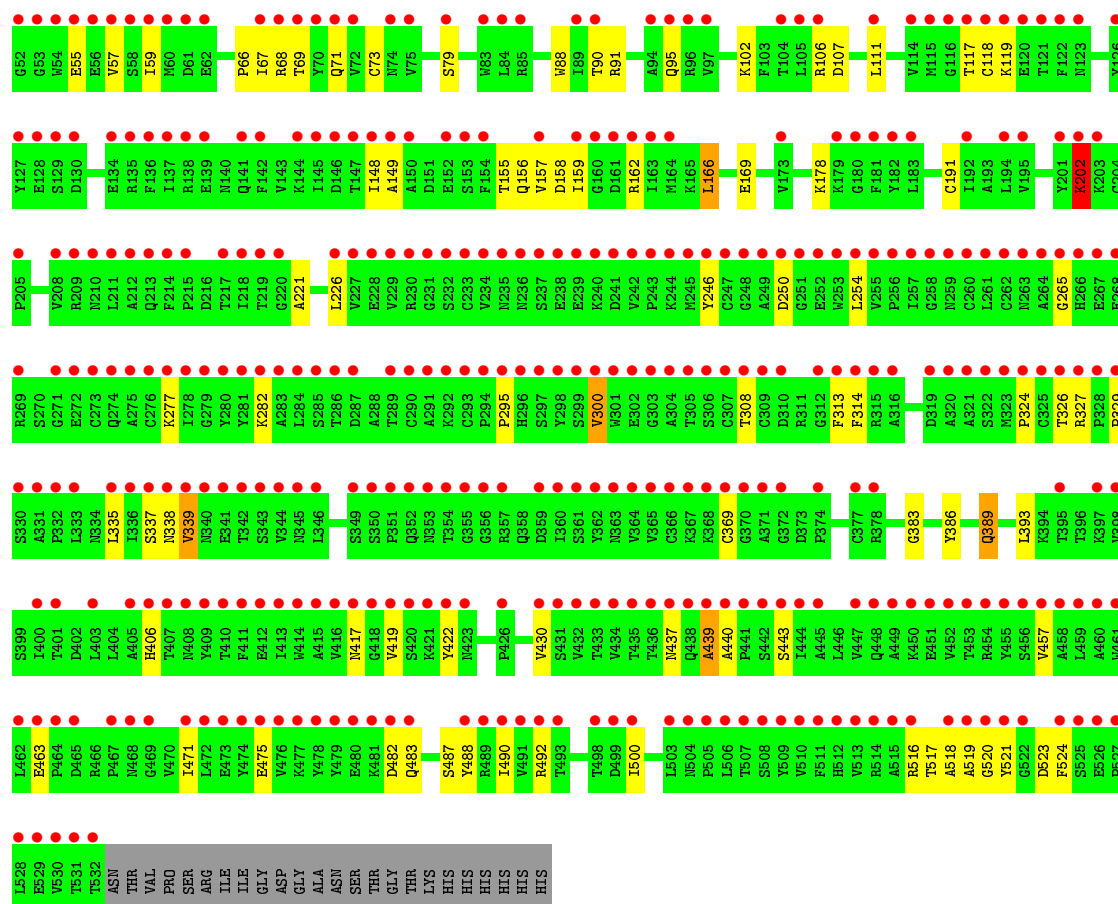
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: EPHRIN TYPE-A RECEPTOR 4

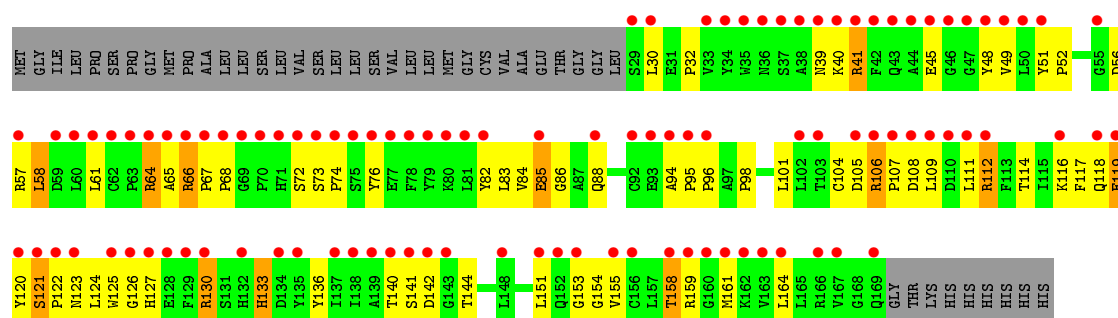


• Molecule 1: EPHRIN TYPE-A RECEPTOR 4

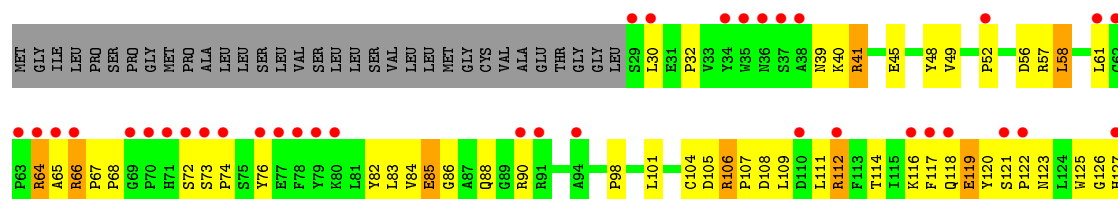




• Molecule 2: EPHRIN-B3



• Molecule 2: EPHRIN-B3





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α , β , γ	300.53Å 300.53Å 300.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.25 – 4.65 106.25 – 4.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (106.25-4.65) 99.8 (106.25-4.65)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 4.66Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.327 , 0.351 0.362 , 0.389	Depositor DCC
R_{free} test set	1296 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	209.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 303.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 25493 reflections	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	10126	wwPDB-VP
Average B, all atoms (Å ²)	221.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.61	2/4015 (0.0%)	0.85	9/5462 (0.2%)
1	B	0.61	1/4014 (0.0%)	0.60	4/5459 (0.1%)
2	C	0.37	0/1165	0.54	0/1582
2	D	0.37	0/1165	0.54	0/1582
All	All	0.57	3/10359 (0.0%)	0.69	13/14085 (0.1%)

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	B	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	439	ALA	C-N	-31.67	0.61	1.34
1	A	326	THR	C-N	28.17	1.98	1.34
1	A	439	ALA	C-N	13.50	1.65	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	THR	O-C-N	28.35	168.06	122.70
1	A	326	THR	CA-C-N	-24.38	63.57	117.20
1	A	439	ALA	O-C-N	15.91	148.15	122.70
1	A	326	THR	C-N-CA	-15.21	83.68	121.70
1	A	439	ALA	CA-C-N	-13.29	87.97	117.20
1	B	439	ALA	CA-C-N	-10.84	93.36	117.20
1	A	439	ALA	C-N-CA	-9.06	99.05	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	439	ALA	C-N-CA	-8.23	101.12	121.70
1	B	202	LYS	CA-C-N	-7.77	100.11	117.20
1	A	202	LYS	CA-C-N	-7.75	100.16	117.20
1	A	202	LYS	C-N-CA	-7.69	102.49	121.70
1	B	202	LYS	C-N-CA	-5.77	107.27	121.70
1	A	202	LYS	O-C-N	-5.01	114.69	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	LYS	Mainchain
1	B	202	LYS	Mainchain
1	B	439	ALA	Mainchain

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	3931	0	3773	251	33
1	B	3931	0	3776	220	33
2	C	1132	0	1093	124	9
2	D	1132	0	1090	169	10
All	All	10126	0	9732	501	45

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 25.

All (501) 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:159:ILE:HG23	2:D:127:HIS:CE1	1.21	1.68
1:A:159:ILE:CG2	2:D:127:HIS:HE1	1.04	1.60
1:B:314:PHE:HB3	1:B:422:TYR:CD2	1.36	1.59
1:B:157:VAL:CG1	2:C:126:GLY:H	1.05	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ILE:HG21	2:D:122:PRO:CB	1.14	1.56
1:A:59:ILE:CG2	2:D:122:PRO:CB	1.83	1.54
1:A:119:LYS:N	1:B:117:THR:CG2	1.69	1.53
1:A:59:ILE:CG2	2:D:122:PRO:HB2	1.43	1.47
1:A:254:LEU:CD2	1:B:226:LEU:HD11	1.43	1.47
1:B:157:VAL:HG12	2:C:126:GLY:N	1.29	1.43
1:B:95:GLN:CD	1:B:221:ALA:HB2	1.40	1.41
1:A:59:ILE:CG2	2:D:122:PRO:CG	1.97	1.41
1:A:119:LYS:N	1:B:117:THR:HG21	1.10	1.40
1:A:59:ILE:HG21	2:D:122:PRO:CA	1.50	1.39
1:B:95:GLN:NE2	1:B:221:ALA:HB2	1.37	1.38
1:A:254:LEU:HD23	1:B:226:LEU:CD1	1.54	1.36
1:A:326:THR:HA	1:A:327:ARG:N	1.37	1.35
1:A:59:ILE:CB	2:D:122:PRO:HB2	1.56	1.35
1:A:326:THR:CA	1:A:327:ARG:N	1.89	1.35
1:A:119:LYS:CG	1:B:117:THR:HG23	1.55	1.35
1:B:68:ARG:NH2	2:C:112:ARG:CD	1.87	1.34
1:A:226:LEU:CD1	1:B:254:LEU:HD23	1.58	1.34
1:A:59:ILE:CG2	2:D:122:PRO:CD	2.04	1.34
1:B:68:ARG:NH2	2:C:112:ARG:HD3	1.01	1.33
1:A:59:ILE:HG23	2:D:122:PRO:CG	1.51	1.33
1:A:314:PHE:HB3	1:A:422:TYR:CD2	1.63	1.33
1:B:157:VAL:HB	2:C:126:GLY:CA	1.57	1.31
1:B:159:ILE:HG13	2:C:125:TRP:O	1.30	1.31
1:B:314:PHE:HB3	1:B:422:TYR:CE2	1.65	1.31
1:A:59:ILE:CG1	2:D:122:PRO:HB2	1.59	1.31
1:A:157:VAL:CG1	2:D:123:ASN:ND2	1.93	1.30
1:A:226:LEU:HD11	1:B:254:LEU:CD2	1.61	1.28
1:B:157:VAL:CB	2:C:126:GLY:H	1.45	1.27
1:B:314:PHE:CB	1:B:422:TYR:HD2	1.48	1.26
1:A:159:ILE:C	2:D:125:TRP:CG	2.05	1.26
1:A:59:ILE:HD13	2:D:122:PRO:CB	1.66	1.26
1:B:314:PHE:CB	1:B:422:TYR:CD2	2.18	1.24
1:A:158:ASP:OD1	2:D:125:TRP:CE3	1.91	1.24
1:B:326:THR:HA	1:B:327:ARG:N	1.53	1.24
1:A:161:ASP:O	2:D:125:TRP:CH2	1.90	1.23
1:B:73:CYS:HB2	2:C:120:TYR:CD2	1.38	1.22
1:B:162:ARG:NH1	2:C:125:TRP:CD1	2.08	1.22
1:B:157:VAL:CB	2:C:126:GLY:N	2.03	1.20
1:A:119:LYS:CD	1:B:117:THR:HG23	1.70	1.20
1:A:159:ILE:CB	2:D:127:HIS:CE1	2.24	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:CYS:CB	2:C:120:TYR:CD2	2.24	1.19
1:A:119:LYS:HG2	1:B:117:THR:CG2	1.72	1.19
1:A:159:ILE:CG2	2:D:127:HIS:CE1	1.93	1.19
1:A:159:ILE:HA	2:D:127:HIS:NE2	1.59	1.17
1:A:160:GLY:N	2:D:125:TRP:CD2	2.13	1.17
1:A:326:THR:C	1:A:327:ARG:N	1.98	1.17
1:A:159:ILE:HG12	2:D:127:HIS:ND1	1.58	1.16
1:B:157:VAL:C	2:C:126:GLY:N	1.99	1.16
1:A:157:VAL:HG11	2:D:123:ASN:ND2	1.54	1.16
1:A:159:ILE:HG12	2:D:127:HIS:CE1	1.80	1.16
1:A:119:LYS:NZ	1:B:117:THR:HA	1.60	1.16
1:A:73:CYS:HB2	2:D:120:TYR:CE2	1.81	1.16
1:B:157:VAL:O	2:C:125:TRP:C	1.85	1.15
1:B:95:GLN:NE2	1:B:221:ALA:CB	2.07	1.15
1:A:95:GLN:CD	1:A:221:ALA:HB2	1.67	1.15
1:B:158:ASP:HB3	2:C:124:LEU:CB	1.62	1.13
1:A:159:ILE:C	2:D:125:TRP:CD2	2.22	1.12
1:A:111:LEU:CD2	2:D:119:GLU:HG2	1.79	1.12
1:A:59:ILE:HG23	2:D:122:PRO:HG2	1.18	1.12
1:B:157:VAL:CB	2:C:126:GLY:CA	2.28	1.11
1:A:159:ILE:CG1	2:D:127:HIS:CE1	2.34	1.10
1:B:157:VAL:CB	2:C:126:GLY:HA2	1.80	1.10
1:A:119:LYS:HG2	1:B:117:THR:HG23	1.20	1.10
1:A:59:ILE:CG2	2:D:122:PRO:HD2	1.72	1.10
1:B:326:THR:OG1	1:B:419:VAL:HG11	1.51	1.09
1:A:73:CYS:HB2	2:D:120:TYR:CD2	1.87	1.09
1:A:119:LYS:N	1:B:117:THR:HG22	1.67	1.09
1:A:314:PHE:CB	1:A:422:TYR:HD2	1.64	1.09
1:A:68:ARG:HH21	2:D:112:ARG:HD3	1.18	1.09
1:B:162:ARG:NH1	2:C:125:TRP:NE1	2.00	1.08
1:A:117:THR:O	1:B:117:THR:O	1.70	1.08
1:B:157:VAL:HG11	2:C:123:ASN:ND2	1.69	1.07
1:B:71:GLN:NE2	2:C:118:GLN:OE1	1.85	1.07
1:B:157:VAL:CG1	2:C:126:GLY:N	1.90	1.07
1:A:59:ILE:HG21	2:D:122:PRO:CG	1.72	1.07
1:A:117:THR:HG21	1:B:119:LYS:H	1.15	1.06
1:A:59:ILE:CD1	2:D:122:PRO:CB	2.33	1.06
1:A:157:VAL:HG11	2:D:123:ASN:HD22	1.03	1.05
1:A:149:ALA:HB2	1:B:149:ALA:HB2	1.36	1.05
1:B:158:ASP:HB3	2:C:124:LEU:HB3	1.38	1.04
1:A:119:LYS:HZ2	1:B:117:THR:HA	0.92	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ILE:HD13	2:D:122:PRO:HB3	1.34	1.04
1:A:59:ILE:CD1	2:D:122:PRO:HB2	1.88	1.03
1:A:160:GLY:N	2:D:125:TRP:CE3	2.27	1.02
1:A:254:LEU:CD2	1:B:226:LEU:CD1	2.24	1.01
1:A:254:LEU:HD21	1:B:226:LEU:HD11	1.37	1.01
1:A:119:LYS:CG	1:B:117:THR:CG2	2.31	1.01
1:A:117:THR:CG2	1:B:119:LYS:HG2	1.91	1.01
1:A:73:CYS:CB	2:D:120:TYR:CE2	2.43	1.01
1:A:59:ILE:CG1	2:D:122:PRO:CB	2.38	1.00
1:A:157:VAL:HB	2:D:127:HIS:N	1.75	1.00
1:A:117:THR:HG21	1:B:119:LYS:N	1.75	1.00
1:B:159:ILE:CG1	2:C:125:TRP:O	2.08	1.00
1:B:157:VAL:CG1	2:C:125:TRP:N	2.25	0.99
1:B:157:VAL:HB	2:C:126:GLY:HA2	1.01	0.99
1:A:111:LEU:HD22	2:D:119:GLU:HG2	1.41	0.99
1:A:157:VAL:CG1	2:D:123:ASN:HD22	1.65	0.98
1:A:117:THR:HG23	1:B:119:LYS:HG2	1.42	0.98
1:A:314:PHE:HB3	1:A:422:TYR:HD2	0.81	0.97
1:A:59:ILE:HG22	2:D:122:PRO:HD2	1.43	0.97
1:B:157:VAL:HG12	2:C:125:TRP:N	1.79	0.97
1:A:117:THR:O	1:B:117:THR:HB	1.64	0.97
1:B:157:VAL:HG12	2:C:125:TRP:C	1.86	0.97
1:A:95:GLN:HE21	1:A:221:ALA:H	1.12	0.96
1:A:254:LEU:HD23	1:B:226:LEU:HD11	0.99	0.96
1:A:326:THR:C	1:A:327:ARG:CA	2.33	0.96
1:A:117:THR:HB	1:B:117:THR:O	1.64	0.96
1:A:118:CYS:C	1:B:117:THR:HG22	1.86	0.96
1:A:119:LYS:CA	1:B:117:THR:CG2	2.44	0.96
1:A:68:ARG:NH2	2:D:112:ARG:HD3	1.80	0.96
1:A:119:LYS:HD3	1:B:117:THR:HG23	1.44	0.95
1:A:157:VAL:HG13	2:D:123:ASN:ND2	1.79	0.94
1:B:157:VAL:O	2:C:126:GLY:N	1.99	0.94
1:B:326:THR:CA	1:B:327:ARG:N	2.31	0.94
1:B:157:VAL:C	2:C:125:TRP:C	2.26	0.93
1:A:117:THR:C	1:B:117:THR:O	2.07	0.93
1:B:68:ARG:HH21	2:C:112:ARG:HD3	1.11	0.93
1:A:117:THR:CG2	1:B:119:LYS:N	2.30	0.93
1:B:326:THR:OG1	1:B:419:VAL:HG21	1.69	0.92
1:A:117:THR:HA	1:B:119:LYS:HZ2	1.32	0.92
1:B:95:GLN:CG	1:B:221:ALA:HB2	2.00	0.91
1:A:157:VAL:CG1	2:D:127:HIS:H	1.83	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:CYS:C	1:B:117:THR:CG2	2.38	0.91
1:A:117:THR:HG23	1:B:119:LYS:CG	2.01	0.91
1:B:157:VAL:HG12	2:C:126:GLY:H	0.77	0.90
1:B:157:VAL:HG12	2:C:125:TRP:CA	2.02	0.90
1:A:59:ILE:HG21	2:D:122:PRO:N	1.86	0.90
2:C:66:ARG:HB3	2:C:67:PRO:HD3	1.54	0.90
1:A:95:GLN:CG	1:A:221:ALA:HB2	2.00	0.89
2:D:66:ARG:HB3	2:D:67:PRO:HD3	1.54	0.89
2:D:86:GLY:HA2	2:D:136:TYR:HD1	1.37	0.89
2:C:86:GLY:HA2	2:C:136:TYR:HD1	1.37	0.89
1:A:313:PHE:HE2	1:A:327:ARG:HG3	1.36	0.89
1:A:95:GLN:HE21	1:A:221:ALA:N	1.71	0.89
1:B:159:ILE:HG23	2:C:127:HIS:CE1	2.07	0.88
2:D:118:GLN:NE2	2:D:120:TYR:HB2	1.89	0.87
1:A:159:ILE:O	2:D:125:TRP:CD1	2.26	0.87
1:A:339:VAL:HG12	1:A:519:ALA:O	1.74	0.87
1:A:159:ILE:CA	2:D:127:HIS:CE1	2.57	0.87
1:A:119:LYS:CA	1:B:117:THR:HG21	2.04	0.87
1:A:159:ILE:HA	2:D:127:HIS:CE1	2.10	0.86
2:C:118:GLN:NE2	2:C:120:TYR:HB2	1.89	0.86
1:B:157:VAL:CA	2:C:126:GLY:N	2.38	0.86
1:A:106:ARG:HB3	2:D:120:TYR:CE1	2.10	0.86
1:B:73:CYS:HB2	2:C:120:TYR:HD2	1.36	0.86
1:A:117:THR:HG23	1:B:119:LYS:CD	2.05	0.85
1:B:314:PHE:CB	1:B:422:TYR:CE2	2.53	0.85
1:A:314:PHE:HD1	1:A:422:TYR:CE2	1.94	0.85
1:A:59:ILE:HG21	2:D:122:PRO:CD	1.86	0.85
1:A:117:THR:CB	1:B:117:THR:O	2.23	0.85
1:B:157:VAL:CG1	2:C:125:TRP:H	1.87	0.84
1:B:106:ARG:HB3	2:C:120:TYR:CE1	2.13	0.84
2:D:66:ARG:HB3	2:D:67:PRO:CD	2.07	0.84
1:B:326:THR:HG1	1:B:419:VAL:HG11	1.38	0.84
2:C:66:ARG:HB3	2:C:67:PRO:CD	2.07	0.83
1:A:106:ARG:HB3	2:D:120:TYR:HE1	1.43	0.83
1:A:72:VAL:O	2:D:120:TYR:CE2	2.32	0.83
1:A:68:ARG:NH2	2:D:112:ARG:CD	2.41	0.83
1:A:157:VAL:CG1	2:D:123:ASN:HD21	1.91	0.83
2:D:86:GLY:HA2	2:D:136:TYR:CD1	2.14	0.83
1:B:158:ASP:HB3	2:C:124:LEU:HB2	1.59	0.82
1:A:68:ARG:HH21	2:D:112:ARG:CD	1.91	0.82
1:B:95:GLN:CD	1:B:221:ALA:CB	2.37	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LYS:HE2	1:B:250:ASP:O	1.78	0.82
1:B:314:PHE:HB2	1:B:422:TYR:HD2	1.42	0.82
1:A:313:PHE:CE2	1:A:327:ARG:HG3	2.14	0.81
1:B:202:LYS:CE	1:B:250:ASP:O	2.28	0.81
2:C:86:GLY:HA2	2:C:136:TYR:CD1	2.14	0.81
1:B:95:GLN:HE21	1:B:221:ALA:N	1.78	0.81
2:C:118:GLN:HG2	2:C:119:GLU:N	1.96	0.81
1:A:72:VAL:O	2:D:120:TYR:HE2	1.63	0.81
1:B:157:VAL:HG13	2:C:125:TRP:N	1.94	0.81
1:A:117:THR:O	1:B:117:THR:C	2.18	0.81
1:A:95:GLN:NE2	1:A:221:ALA:HB2	1.94	0.80
1:B:111:LEU:HD22	2:C:119:GLU:HG2	1.62	0.80
2:D:118:GLN:HG2	2:D:119:GLU:N	1.96	0.80
1:A:95:GLN:NE2	1:A:221:ALA:H	1.79	0.80
1:B:157:VAL:CA	2:C:126:GLY:CA	2.59	0.80
1:A:117:THR:O	1:B:117:THR:CB	2.30	0.80
1:A:159:ILE:CA	2:D:127:HIS:NE2	2.43	0.80
1:B:158:ASP:CB	2:C:124:LEU:HB3	2.11	0.79
1:A:158:ASP:CG	2:D:125:TRP:CD2	2.56	0.79
1:B:157:VAL:HG11	2:C:123:ASN:HD22	1.47	0.79
1:A:69:THR:OG1	2:D:122:PRO:HG3	1.82	0.79
1:A:117:THR:HA	1:B:119:LYS:NZ	1.98	0.79
1:B:314:PHE:CD1	1:B:422:TYR:CE2	2.71	0.78
1:A:59:ILE:CD1	2:D:122:PRO:HB3	2.04	0.78
1:A:314:PHE:CD2	1:A:423:ASN:HA	2.18	0.78
1:B:313:PHE:HE2	1:B:327:ARG:HG3	1.47	0.78
1:A:254:LEU:HD23	1:B:226:LEU:HD13	1.61	0.78
1:B:337:SER:OG	1:B:518:ALA:HA	1.84	0.78
1:A:314:PHE:HD1	1:A:422:TYR:HE2	1.33	0.77
1:B:326:THR:OG1	1:B:419:VAL:CG1	2.30	0.77
1:A:314:PHE:CD1	1:A:422:TYR:CE2	2.71	0.77
1:A:95:GLN:HG3	1:A:221:ALA:HB2	1.67	0.77
1:A:59:ILE:HG23	2:D:122:PRO:CD	1.87	0.77
1:A:159:ILE:O	2:D:125:TRP:CG	2.37	0.77
1:A:191:CYS:C	2:D:120:TYR:CE2	2.44	0.76
1:B:68:ARG:HH22	2:C:112:ARG:HD3	0.95	0.76
2:C:130:ARG:HH11	2:C:130:ARG:HG2	1.51	0.76
1:A:192:ILE:N	2:D:120:TYR:CE2	2.55	0.75
2:D:39:ASN:OD1	2:D:41:ARG:HB2	1.86	0.75
1:A:157:VAL:CB	2:D:127:HIS:N	2.48	0.75
1:A:117:THR:O	1:B:117:THR:CA	2.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:GLN:HE21	1:B:221:ALA:H	1.32	0.75
1:B:157:VAL:O	2:C:125:TRP:O	2.04	0.74
1:A:95:GLN:NE2	1:A:221:ALA:CB	2.50	0.74
1:A:69:THR:OG1	2:D:122:PRO:CG	2.35	0.74
2:D:130:ARG:HG2	2:D:130:ARG:HH11	1.51	0.74
1:B:68:ARG:HH22	2:C:112:ARG:CD	1.77	0.74
1:A:161:ASP:O	2:D:125:TRP:CZ2	2.20	0.73
2:C:39:ASN:OD1	2:C:41:ARG:HB2	1.86	0.73
1:A:314:PHE:CB	1:A:422:TYR:CD2	2.52	0.73
1:B:339:VAL:HG12	1:B:519:ALA:O	1.88	0.72
1:B:157:VAL:CG1	2:C:123:ASN:ND2	2.51	0.72
1:A:255:VAL:HG21	1:B:246:TYR:CE2	2.24	0.72
1:B:157:VAL:O	2:C:126:GLY:CA	2.37	0.72
1:A:111:LEU:HD22	2:D:119:GLU:CG	2.19	0.72
1:A:314:PHE:CE2	1:A:424:PRO:HD3	2.25	0.72
1:A:158:ASP:OD1	2:D:125:TRP:CD2	2.42	0.72
1:A:59:ILE:HG21	2:D:122:PRO:C	2.09	0.72
1:B:158:ASP:CB	2:C:124:LEU:CB	2.56	0.71
1:A:159:ILE:HA	2:D:127:HIS:HE2	1.53	0.71
1:A:117:THR:HG21	1:B:119:LYS:HG2	1.71	0.71
1:A:314:PHE:HE2	1:A:424:PRO:HD3	1.53	0.71
1:A:111:LEU:HD21	2:D:119:GLU:HG2	1.72	0.71
2:C:66:ARG:O	2:C:68:PRO:HD3	1.91	0.71
1:B:95:GLN:HE21	1:B:221:ALA:CB	2.04	0.71
1:A:88:TRP:CZ3	1:A:90:THR:HG22	2.26	0.71
1:B:157:VAL:CA	2:C:126:GLY:HA2	2.21	0.71
1:A:117:THR:CG2	1:B:119:LYS:CG	2.66	0.71
1:A:158:ASP:OD1	2:D:125:TRP:CZ3	2.44	0.70
1:A:119:LYS:HD3	1:B:117:THR:CG2	2.19	0.70
1:B:88:TRP:CZ3	1:B:90:THR:HG22	2.26	0.70
2:D:66:ARG:O	2:D:68:PRO:HD3	1.91	0.70
1:B:159:ILE:HG23	2:C:127:HIS:HE1	1.55	0.70
2:D:64:ARG:HD2	2:D:67:PRO:HD2	1.73	0.70
1:B:157:VAL:HG13	2:C:125:TRP:H	1.54	0.69
1:B:326:THR:CB	1:B:419:VAL:HG21	2.22	0.69
1:A:157:VAL:HG12	2:D:127:HIS:H	1.58	0.69
2:C:64:ARG:HD2	2:C:67:PRO:HD2	1.73	0.69
1:A:69:THR:HG21	2:D:122:PRO:HB3	1.75	0.69
2:D:73:SER:HB2	2:D:74:PRO:HD2	1.73	0.69
1:A:117:THR:HG23	1:B:119:LYS:NZ	2.08	0.68
1:A:59:ILE:CG2	2:D:122:PRO:CA	2.46	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:PHE:CD1	1:B:422:TYR:HE2	2.08	0.68
2:C:73:SER:HB2	2:C:74:PRO:HD2	1.73	0.68
1:A:326:THR:C	1:A:327:ARG:HA	2.14	0.68
1:B:59:ILE:HD13	2:C:122:PRO:HB3	1.76	0.68
1:B:55:GLU:CB	2:C:57:ARG:HH21	2.08	0.67
1:A:59:ILE:HG12	2:D:122:PRO:CB	2.25	0.67
1:B:69:THR:OG1	2:C:122:PRO:CG	2.43	0.67
1:A:157:VAL:CB	2:D:127:HIS:H	2.06	0.67
1:B:111:LEU:CD2	2:C:119:GLU:HG2	2.24	0.67
1:B:314:PHE:HD1	1:B:422:TYR:HE2	1.42	0.67
1:A:119:LYS:NZ	1:B:117:THR:CA	2.50	0.66
1:B:326:THR:OG1	1:B:419:VAL:CG2	2.42	0.66
1:A:326:THR:CB	1:A:327:ARG:N	2.58	0.66
1:A:117:THR:CA	1:B:119:LYS:HZ2	2.08	0.65
1:B:55:GLU:CD	2:C:116:LYS:NZ	2.43	0.65
1:A:59:ILE:CG2	2:D:122:PRO:N	2.54	0.64
1:A:326:THR:OG1	1:A:419:VAL:HG21	1.96	0.64
2:D:105:ASP:HB2	2:D:106:ARG:HE	1.62	0.64
1:A:69:THR:HG21	2:D:122:PRO:CG	2.28	0.63
2:C:105:ASP:HB2	2:C:106:ARG:HE	1.63	0.63
1:A:159:ILE:N	2:D:125:TRP:CE3	2.64	0.63
1:A:117:THR:HG23	1:B:119:LYS:HD3	1.80	0.63
1:B:157:VAL:N	2:C:126:GLY:HA2	2.14	0.63
1:B:157:VAL:O	2:C:126:GLY:HA3	1.97	0.63
1:A:88:TRP:CH2	1:A:90:THR:HG22	2.34	0.63
1:A:158:ASP:CG	2:D:125:TRP:CE3	2.71	0.63
1:B:55:GLU:HB3	2:C:57:ARG:HH21	1.62	0.63
1:A:117:THR:CA	1:B:117:THR:O	2.46	0.62
1:A:119:LYS:CB	1:B:117:THR:CG2	2.76	0.62
1:B:88:TRP:CH2	1:B:90:THR:HG22	2.34	0.62
1:A:69:THR:HG21	2:D:122:PRO:CB	2.29	0.62
2:D:66:ARG:HB2	2:D:107:PRO:O	1.98	0.62
2:C:66:ARG:HB2	2:C:107:PRO:O	1.98	0.62
1:A:160:GLY:N	2:D:125:TRP:CE2	2.66	0.62
1:B:69:THR:OG1	2:C:122:PRO:HG2	1.99	0.62
2:D:104:CYS:HA	2:D:111:LEU:HD12	1.81	0.62
1:A:73:CYS:CA	2:D:120:TYR:CE2	2.82	0.62
2:D:64:ARG:HD3	2:D:108:ASP:O	2.00	0.62
1:B:157:VAL:C	2:C:126:GLY:CA	2.69	0.61
1:B:95:GLN:HG3	1:B:221:ALA:HB2	1.82	0.61
1:B:95:GLN:HG3	1:B:221:ALA:CB	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:HG23	2:D:127:HIS:HE1	0.47	0.61
1:A:55:GLU:OE2	2:D:116:LYS:HD3	1.77	0.61
1:A:95:GLN:HG3	1:A:221:ALA:CB	2.30	0.61
2:C:104:CYS:HA	2:C:111:LEU:HD12	1.82	0.61
1:B:337:SER:HG	1:B:518:ALA:CA	2.14	0.61
2:C:118:GLN:HE22	2:C:120:TYR:HB2	1.63	0.60
2:D:118:GLN:HE22	2:D:120:TYR:HB2	1.64	0.60
1:A:159:ILE:CG1	2:D:127:HIS:ND1	2.45	0.60
1:B:337:SER:OG	1:B:518:ALA:CA	2.49	0.60
2:C:64:ARG:HD3	2:C:108:ASP:O	2.00	0.60
1:B:338:ASN:ND2	1:B:521:TYR:HB2	2.17	0.60
1:B:313:PHE:CE2	1:B:327:ARG:HG3	2.34	0.60
1:B:202:LYS:HE3	1:B:250:ASP:O	2.01	0.60
1:B:339:VAL:CG1	1:B:519:ALA:O	2.50	0.60
1:B:314:PHE:HD1	1:B:422:TYR:CE2	2.16	0.59
1:B:95:GLN:CG	1:B:221:ALA:CB	2.78	0.59
1:A:55:GLU:OE2	2:D:116:LYS:CD	2.33	0.59
1:A:59:ILE:HD13	2:D:122:PRO:CA	2.31	0.59
1:B:91:ARG:HD3	1:B:178:LYS:O	2.03	0.59
1:A:69:THR:CB	2:D:122:PRO:HG3	2.32	0.59
1:B:59:ILE:HD13	2:C:122:PRO:CB	2.32	0.59
1:B:69:THR:OG1	2:C:122:PRO:HG3	2.02	0.59
1:A:91:ARG:HD3	1:A:178:LYS:O	2.03	0.59
1:A:117:THR:HG22	1:B:119:LYS:N	2.15	0.59
1:B:314:PHE:CG	1:B:422:TYR:CE2	2.91	0.58
1:A:119:LYS:HG2	1:B:117:THR:HG21	1.75	0.58
2:C:39:ASN:O	2:C:40:LYS:HB3	2.03	0.58
1:B:73:CYS:HA	2:C:120:TYR:HE2	1.67	0.58
2:D:39:ASN:O	2:D:40:LYS:HB3	2.03	0.58
1:B:157:VAL:H	2:C:126:GLY:HA2	1.69	0.58
1:A:159:ILE:C	2:D:125:TRP:CD1	2.64	0.57
1:B:157:VAL:N	2:C:126:GLY:CA	2.68	0.57
1:A:156:GLN:HG2	2:D:126:GLY:HA3	1.86	0.57
2:D:30:LEU:HD11	2:D:52:PRO:HB3	1.87	0.57
1:B:162:ARG:HD2	2:C:124:LEU:HD12	1.87	0.57
1:B:338:ASN:HD22	1:B:521:TYR:HB2	1.71	0.56
1:A:117:THR:HG22	1:B:118:CYS:C	2.26	0.56
1:A:314:PHE:CD1	1:A:422:TYR:CD2	2.94	0.55
2:C:30:LEU:HD11	2:C:52:PRO:HB3	1.87	0.55
1:B:68:ARG:NH2	2:C:112:ARG:HD2	2.08	0.55
1:B:314:PHE:CG	1:B:422:TYR:CD2	2.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ASP:O	2:C:125:TRP:CD1	2.44	0.54
1:A:59:ILE:HG23	2:D:122:PRO:HD2	1.63	0.54
1:B:95:GLN:NE2	1:B:221:ALA:HB3	2.17	0.54
2:C:141:SER:O	2:C:155:VAL:HG23	2.08	0.54
1:A:95:GLN:NE2	1:A:221:ALA:N	2.46	0.53
1:A:457:VAL:H	1:A:500:ILE:HG13	1.73	0.53
2:D:84:VAL:HG13	2:D:88:GLN:HB2	1.90	0.53
1:A:119:LYS:CB	1:B:117:THR:HG21	2.38	0.53
1:A:326:THR:OG1	1:A:419:VAL:HG11	2.08	0.53
1:A:118:CYS:HA	1:B:117:THR:HB	1.90	0.53
2:D:118:GLN:HG2	2:D:119:GLU:H	1.72	0.53
1:B:471:ILE:HA	1:B:517:THR:HG22	1.91	0.53
1:B:457:VAL:H	1:B:500:ILE:HG13	1.73	0.53
1:B:314:PHE:HB3	1:B:422:TYR:HE2	1.57	0.53
1:A:149:ALA:CB	1:B:149:ALA:HB2	2.25	0.53
1:A:314:PHE:CG	1:A:422:TYR:CD2	2.97	0.52
1:A:58:SER:HB2	2:D:114:THR:H	1.74	0.52
2:D:141:SER:O	2:D:155:VAL:HG23	2.09	0.52
2:C:118:GLN:HG2	2:C:120:TYR:H	1.75	0.52
1:A:389:GLN:HB2	1:A:393:LEU:HD13	1.92	0.52
1:B:95:GLN:HE21	1:B:221:ALA:CA	2.23	0.52
2:C:130:ARG:CG	2:C:130:ARG:HH11	2.22	0.52
1:A:162:ARG:HD3	2:D:125:TRP:NE1	2.25	0.52
1:A:59:ILE:CD1	2:D:122:PRO:O	2.58	0.52
1:A:69:THR:OG1	2:D:122:PRO:HG2	2.09	0.52
2:D:118:GLN:HG2	2:D:120:TYR:H	1.75	0.52
1:B:57:VAL:HG13	2:C:114:THR:O	2.09	0.51
2:C:84:VAL:HG13	2:C:88:GLN:HB2	1.90	0.51
2:D:65:ALA:HB2	2:D:72:SER:HB2	1.93	0.51
1:A:443:SER:HB2	1:A:523:ASP:HB2	1.93	0.51
1:A:55:GLU:HB2	2:D:57:ARG:HH21	1.75	0.51
2:C:118:GLN:HG2	2:C:119:GLU:H	1.72	0.51
1:A:471:ILE:HA	1:A:517:THR:HG22	1.91	0.51
1:A:95:GLN:CD	1:A:221:ALA:CB	2.59	0.50
1:A:72:VAL:O	2:D:120:TYR:CD2	2.63	0.50
1:A:68:ARG:NH2	2:D:112:ARG:HH11	2.08	0.50
1:B:389:GLN:HB2	1:B:393:LEU:HD13	1.92	0.50
1:A:107:ASP:HB3	1:A:155:THR:HG22	1.93	0.50
1:B:95:GLN:NE2	1:B:221:ALA:H	2.05	0.50
2:D:155:VAL:HG11	2:D:161:MET:SD	2.52	0.50
1:A:73:CYS:HA	2:D:120:TYR:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:155:VAL:HA	2:D:158:THR:HB	1.93	0.50
2:C:155:VAL:HA	2:C:158:THR:HB	1.93	0.50
1:A:201:TYR:CE1	1:A:218:ILE:HG22	2.47	0.50
1:B:329:PRO:HG3	1:B:417:ASN:HB2	1.94	0.50
1:A:314:PHE:HB2	1:A:423:ASN:OD1	2.13	0.49
1:B:106:ARG:CB	2:C:120:TYR:CE1	2.90	0.49
2:C:155:VAL:HG11	2:C:161:MET:SD	2.52	0.49
1:B:443:SER:HB2	1:B:523:ASP:HB2	1.93	0.49
1:A:157:VAL:HB	2:D:127:HIS:H	1.60	0.49
1:B:107:ASP:HB3	1:B:155:THR:HG22	1.93	0.49
1:A:59:ILE:CG2	2:D:122:PRO:C	2.78	0.49
2:D:104:CYS:HA	2:D:111:LEU:CD1	2.43	0.49
1:A:406:HIS:H	1:A:437:ASN:HB2	1.78	0.49
2:C:65:ALA:HB2	2:C:72:SER:HB2	1.93	0.49
1:B:335:LEU:HD12	1:B:430:VAL:HG12	1.95	0.49
2:D:32:PRO:HB3	2:D:61:LEU:HD11	1.95	0.49
1:A:316:ALA:HB3	1:A:357:ARG:HH12	1.77	0.49
1:A:335:LEU:HD12	1:A:430:VAL:HG12	1.95	0.49
1:A:329:PRO:HG3	1:A:417:ASN:HB2	1.94	0.48
1:B:406:HIS:H	1:B:437:ASN:HB2	1.77	0.48
2:C:32:PRO:HB3	2:C:61:LEU:HD11	1.95	0.48
2:D:76:TYR:CD1	2:D:107:PRO:HA	2.49	0.48
2:C:64:ARG:CD	2:C:67:PRO:HD2	2.43	0.48
1:A:73:CYS:SG	2:D:120:TYR:CE2	2.96	0.48
1:B:191:CYS:HA	2:C:120:TYR:HE2	1.17	0.48
1:A:117:THR:CG2	1:B:118:CYS:C	2.82	0.47
1:A:162:ARG:NH2	2:D:123:ASN:OD1	2.46	0.47
1:A:265:GLY:H	1:A:282:LYS:HB3	1.79	0.47
2:C:76:TYR:CD1	2:C:107:PRO:HA	2.49	0.47
2:C:104:CYS:HA	2:C:111:LEU:CD1	2.43	0.47
1:A:69:THR:CG2	2:D:122:PRO:CG	2.92	0.47
1:B:326:THR:HB	1:B:419:VAL:HG21	1.95	0.47
1:B:57:VAL:CG1	2:C:114:THR:O	2.62	0.47
1:B:157:VAL:C	2:C:125:TRP:CA	2.81	0.47
1:A:158:ASP:OD2	1:A:162:ARG:HA	2.15	0.47
1:B:158:ASP:OD2	1:B:162:ARG:HA	2.15	0.46
2:C:85:GLU:HB2	2:C:88:GLN:CD	2.36	0.46
1:B:265:GLY:H	1:B:282:LYS:HB3	1.79	0.46
1:B:68:ARG:CZ	2:C:112:ARG:CD	2.84	0.46
2:D:64:ARG:CD	2:D:67:PRO:HD2	2.43	0.46
1:B:326:THR:C	1:B:327:ARG:N	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:SER:HG	1:B:518:ALA:C	2.18	0.46
1:A:157:VAL:CG1	2:D:127:HIS:N	2.62	0.46
1:B:95:GLN:NE2	1:B:221:ALA:CA	2.77	0.46
1:A:159:ILE:C	2:D:125:TRP:CE2	2.86	0.46
1:B:339:VAL:HB	1:B:519:ALA:O	2.16	0.46
1:A:88:TRP:CZ3	1:A:90:THR:CG2	2.98	0.46
1:A:73:CYS:HA	2:D:120:TYR:HE2	1.82	0.45
2:D:85:GLU:HB2	2:D:88:GLN:CD	2.36	0.45
1:B:102:LYS:HB3	1:B:166:LEU:HD22	1.98	0.45
1:A:226:LEU:HD22	1:A:246:TYR:HB3	1.98	0.45
1:A:434:VAL:HG12	1:A:518:ALA:HB1	1.97	0.45
1:B:95:GLN:HG3	1:B:221:ALA:HA	1.99	0.45
1:A:68:ARG:NH2	2:D:112:ARG:NH1	2.65	0.45
1:B:226:LEU:HD22	1:B:246:TYR:HB3	1.98	0.45
1:B:338:ASN:HA	1:B:520:GLY:HA2	1.98	0.45
2:C:56:ASP:O	2:C:117:PHE:HD1	2.00	0.45
1:A:300:VAL:HG22	1:A:308:THR:HG22	1.99	0.45
2:C:82:TYR:CD1	2:C:98:PRO:HB2	2.52	0.45
1:A:102:LYS:HB3	1:A:166:LEU:HD22	1.98	0.45
1:A:59:ILE:HD12	2:D:122:PRO:O	2.17	0.44
2:D:56:ASP:O	2:D:117:PHE:HD1	2.00	0.44
2:C:140:THR:HA	2:C:154:GLY:H	1.82	0.44
1:A:157:VAL:HG12	2:D:127:HIS:N	2.29	0.44
2:D:130:ARG:HH11	2:D:130:ARG:CG	2.22	0.44
1:A:94:ALA:HA	1:A:218:ILE:HD13	1.98	0.44
2:D:82:TYR:CD1	2:D:98:PRO:HB2	2.52	0.44
1:B:326:THR:C	1:B:327:ARG:CA	2.86	0.44
1:A:95:GLN:HG3	1:A:221:ALA:CA	2.47	0.44
1:B:300:VAL:HG22	1:B:308:THR:HG22	1.99	0.44
2:D:140:THR:HA	2:D:154:GLY:H	1.82	0.44
1:A:326:THR:C	1:A:327:ARG:C	2.76	0.44
1:A:314:PHE:HB3	1:A:422:TYR:CE2	2.40	0.44
1:A:59:ILE:HD11	1:A:67:ILE:HD11	2.00	0.43
1:B:71:GLN:OE1	2:C:121:SER:HA	2.18	0.43
2:C:130:ARG:NH1	2:C:130:ARG:HG2	2.26	0.43
2:D:49:VAL:HG22	2:D:164:LEU:HB3	2.00	0.43
1:A:148:ILE:HG23	1:A:169:GLU:HG3	2.00	0.43
1:A:159:ILE:HA	2:D:127:HIS:CD2	2.46	0.43
1:B:339:VAL:CB	1:B:519:ALA:O	2.66	0.43
2:C:49:VAL:HG22	2:C:164:LEU:HB3	2.00	0.43
2:D:83:LEU:HB2	2:D:101:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ILE:HD11	1:B:67:ILE:HD11	2.00	0.43
2:D:76:TYR:CE1	2:D:107:PRO:HA	2.54	0.43
1:B:326:THR:OG1	1:B:419:VAL:CB	2.65	0.43
2:C:76:TYR:CE1	2:C:107:PRO:HA	2.54	0.43
2:C:83:LEU:HB2	2:C:101:LEU:HD11	2.00	0.43
1:A:159:ILE:HG12	2:D:127:HIS:CG	2.44	0.43
1:B:148:ILE:HG23	1:B:169:GLU:HG3	2.00	0.43
1:A:161:ASP:O	2:D:125:TRP:CZ3	2.64	0.42
2:C:58:LEU:O	2:C:114:THR:HA	2.19	0.42
2:D:130:ARG:NH1	2:D:130:ARG:CG	2.80	0.42
1:B:55:GLU:HB2	2:C:57:ARG:HH21	1.84	0.42
1:A:295:PRO:HD2	1:A:324:PRO:HB3	2.01	0.42
2:D:84:VAL:CG1	2:D:88:GLN:HB2	2.50	0.42
2:C:151:LEU:HD23	2:C:151:LEU:HA	1.86	0.42
2:D:142:ASP:OD1	2:D:144:THR:HG23	2.20	0.42
1:A:117:THR:HG23	1:B:119:LYS:CE	2.48	0.42
1:A:326:THR:HB	1:A:327:ARG:N	2.34	0.42
1:A:68:ARG:NH2	2:D:112:ARG:HD2	2.30	0.42
1:A:68:ARG:HH22	2:D:112:ARG:NH1	2.17	0.42
1:A:156:GLN:HG2	2:D:126:GLY:O	2.19	0.42
2:D:159:ARG:HD2	2:D:161:MET:HE3	2.02	0.42
1:B:295:PRO:HD2	1:B:324:PRO:HB3	2.01	0.42
1:A:117:THR:HG23	1:B:119:LYS:HZ2	1.83	0.42
1:B:95:GLN:HG3	1:B:221:ALA:CA	2.49	0.42
2:C:84:VAL:CG1	2:C:88:GLN:HB2	2.50	0.42
1:A:59:ILE:O	1:A:66:PRO:HA	2.20	0.41
1:B:68:ARG:HH21	2:C:112:ARG:CD	1.89	0.41
1:B:88:TRP:CZ3	1:B:90:THR:CG2	2.98	0.41
2:C:159:ARG:HD2	2:C:161:MET:HE3	2.02	0.41
2:D:58:LEU:O	2:D:114:THR:HA	2.19	0.41
2:D:155:VAL:HG12	2:D:161:MET:HB2	2.02	0.41
2:C:142:ASP:OD1	2:C:144:THR:HG23	2.20	0.41
1:A:163:ILE:HG22	1:A:165:LYS:HG3	2.03	0.41
1:B:59:ILE:O	1:B:66:PRO:HA	2.20	0.41
2:D:130:ARG:HG2	2:D:130:ARG:NH1	2.26	0.41
2:C:155:VAL:HG12	2:C:161:MET:HB2	2.02	0.41
2:D:130:ARG:HB2	2:D:133:HIS:HB2	2.03	0.41
1:A:45:TRP:HB3	1:A:85:ARG:O	2.21	0.41
1:A:158:ASP:OD2	2:D:125:TRP:CE2	2.74	0.41
1:B:338:ASN:ND2	1:B:521:TYR:CB	2.83	0.41
2:C:94:ALA:HA	2:C:95:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:GLU:OE2	2:C:116:LYS:CE	2.48	0.41
2:D:105:ASP:HB2	2:D:106:ARG:NE	2.34	0.41
1:A:175:PRO:HG3	1:A:221:ALA:HB1	2.03	0.40
1:A:119:LYS:HZ3	1:B:117:THR:HA	1.71	0.40
1:A:59:ILE:HD13	2:D:122:PRO:O	2.21	0.40

All (45) 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:A:135:ARG:CZ	1:B:156:GLN:OE1[5_555]	0.38	1.82
2:C:51:TYR:CZ	2:D:64:ARG:NH2[9_555]	0.73	1.47
1:A:487:SER:OG	1:B:490:ILE:O[12_455]	1.05	1.15
1:A:135:ARG:NH1	1:B:156:GLN:OE1[5_555]	1.09	1.11
1:A:42:GLU:O	2:C:133:HIS:CE1[5_555]	1.21	0.99
1:A:487:SER:CB	1:B:490:ILE:O[12_455]	1.27	0.93
2:C:51:TYR:OH	2:D:64:ARG:NH2[9_555]	1.27	0.93
1:A:135:ARG:CD	1:B:156:GLN:NE2[5_555]	1.29	0.91
1:A:488:TYR:CE2	1:B:492:ARG:NH2[12_455]	1.35	0.85
2:C:51:TYR:CE1	2:D:64:ARG:NH2[9_555]	1.37	0.83
1:A:488:TYR:O	1:B:490:ILE:CD1[12_455]	1.37	0.83
1:A:490:ILE:O	1:B:487:SER:CB[12_455]	1.38	0.82
1:A:135:ARG:NH2	1:B:156:GLN:OE1[5_555]	1.43	0.77
1:A:135:ARG:CZ	1:B:156:GLN:CD[5_555]	1.43	0.77
1:A:135:ARG:NH1	1:B:156:GLN:CD[5_555]	1.58	0.62
1:A:135:ARG:NE	1:B:156:GLN:OE1[5_555]	1.59	0.61
1:A:490:ILE:CD1	1:B:488:TYR:CD1[12_455]	1.63	0.57
1:A:135:ARG:NE	1:B:156:GLN:CD[5_555]	1.66	0.54
1:A:42:GLU:O	2:C:133:HIS:ND1[5_555]	1.71	0.49
1:A:488:TYR:OH	1:B:475:GLU:OE2[12_455]	1.74	0.46
1:A:475:GLU:OE2	1:B:488:TYR:OH[12_455]	1.81	0.39
1:A:487:SER:CB	1:B:490:ILE:C[12_455]	1.82	0.38
2:C:51:TYR:CZ	2:D:64:ARG:CZ[9_555]	1.83	0.37
1:B:79:SER:OG	2:D:90:ARG:CB[24_555]	1.88	0.32
1:A:490:ILE:CG1	1:B:488:TYR:CE1[12_455]	1.89	0.31
1:B:383:GLY:CA	1:B:406:HIS:CE1[12_455]	1.91	0.29
1:A:135:ARG:NE	1:B:156:GLN:NE2[5_555]	1.92	0.28
1:A:490:ILE:CG2	1:B:488:TYR:CE2[12_455]	1.94	0.26
2:C:51:TYR:CE2	2:D:64:ARG:NH2[9_555]	1.98	0.22
1:A:490:ILE:O	1:B:487:SER:CA[12_455]	2.00	0.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:128:GLU:OE2	2:D:130:ARG:NE[24_555]	2.02	0.18
1:A:487:SER:OG	1:B:490:ILE:C[12_455]	2.04	0.16
1:A:490:ILE:CD1	1:B:488:TYR:CE1[12_455]	2.05	0.15
1:A:396:THR:OG1	1:B:524:PHE:CZ[12_455]	2.09	0.11
1:A:110:SER:O	2:D:133:HIS:CE1[24_555]	2.09	0.11
1:A:112:PRO:CB	2:D:132:HIS:CB[24_555]	2.09	0.11
1:A:490:ILE:CG2	1:B:488:TYR:CZ[12_455]	2.11	0.09
1:A:135:ARG:CD	1:B:156:GLN:CD[5_555]	2.12	0.08
1:B:277:LYS:NZ	1:B:482:ASP:O[22_445]	2.12	0.08
1:B:383:GLY:N	1:B:406:HIS:ND1[12_455]	2.16	0.04
1:A:179:LYS:NZ	2:C:96:PRO:CB[5_555]	2.16	0.04
2:C:51:TYR:CE1	2:D:64:ARG:CZ[9_555]	2.17	0.03
1:A:491:VAL:CG1	1:B:487:SER:OG[12_455]	2.17	0.03
1:A:490:ILE:CD1	1:B:490:ILE:CD1[12_455]	2.18	0.02
1:B:383:GLY:N	1:B:406:HIS:CE1[12_455]	2.18	0.02

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	503/568 (89%)	478 (95%)	25 (5%)	0	100	100
1	B	501/568 (88%)	477 (95%)	23 (5%)	1 (0%)	52	86
2	C	139/183 (76%)	120 (86%)	13 (9%)	6 (4%)	3	34
2	D	139/183 (76%)	120 (86%)	13 (9%)	6 (4%)	3	34
All	All	1282/1502 (85%)	1195 (93%)	74 (6%)	13 (1%)	19	65

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	440	ALA
2	C	64	ARG

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Mol	Chain	Res	Type
2	D	64	ARG
2	C	45	GLU
2	C	153	GLY
2	C	158	THR
2	D	45	GLU
2	D	153	GLY
2	D	158	THR
2	C	66	ARG
2	D	66	ARG
2	C	85	GLU
2	D	85	GLU

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	437/490 (89%)	427 (98%)	10 (2%)	58	83
1	B	437/490 (89%)	428 (98%)	9 (2%)	61	85
2	C	121/155 (78%)	111 (92%)	10 (8%)	14	51
2	D	121/155 (78%)	111 (92%)	10 (8%)	14	51
All	All	1116/1290 (86%)	1077 (96%)	39 (4%)	43	76

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	166	LEU
1	A	300	VAL
1	A	339	VAL
1	A	369	CYS
1	A	386	TYR
1	A	389	GLN
1	A	463	GLU
1	A	483	GLN
1	A	516	ARG

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Mol	Chain	Res	Type
1	B	166	LEU
1	B	300	VAL
1	B	339	VAL
1	B	369	CYS
1	B	386	TYR
1	B	389	GLN
1	B	463	GLU
1	B	483	GLN
1	B	516	ARG
2	C	41	ARG
2	C	48	TYR
2	C	58	LEU
2	C	106	ARG
2	C	109	LEU
2	C	112	ARG
2	C	119	GLU
2	C	121	SER
2	C	130	ARG
2	C	133	HIS
2	D	41	ARG
2	D	48	TYR
2	D	58	LEU
2	D	106	ARG
2	D	109	LEU
2	D	112	ARG
2	D	119	GLU
2	D	121	SER
2	D	130	ARG
2	D	133	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	B	95	GLN
1	B	338	ASN
2	C	123	ASN
2	C	127	HIS
2	D	127	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 carbohydrates 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	505/568 (88%)	3.82	291 (57%) 0 1	87, 219, 291, 295	0
1	B	505/568 (88%)	4.37	368 (72%) 0 1	103, 224, 293, 294	0
2	C	141/183 (77%)	4.26	103 (73%) 0 1	145, 217, 296, 300	0
2	D	141/183 (77%)	2.69	63 (44%) 0 2	153, 227, 295, 298	0
All	All	1292/1502 (86%)	3.96	825 (63%) 0 1	87, 221, 293, 300	0

All (825) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	CYS	23.0
1	A	282	LYS	21.8
1	A	281	TYR	19.5
1	A	267	GLU	19.3
1	A	326	THR	18.4
1	B	299	SER	18.0
1	A	307	CYS	18.0
1	B	260	CYS	17.5
1	A	260	CYS	17.5
1	B	262	CYS	16.2
1	B	232	SER	15.6
1	A	273	CYS	15.6
1	B	435	THR	15.6
1	B	259	ASN	15.3
1	A	299	SER	15.1
1	A	410	THR	15.1
1	A	266	HIS	14.7
1	B	327	ARG	14.6
1	B	326	THR	14.6
1	B	273	CYS	14.5
1	A	304	ALA	14.3

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Mol	Chain	Res	Type	RSRZ
1	B	434	VAL	14.2
1	A	259	ASN	14.2
1	A	327	ARG	14.0
1	A	262	CYS	14.0
1	B	314	PHE	13.9
2	D	139	ALA	13.6
2	D	35	TRP	13.5
1	A	366	CYS	13.5
1	A	212	ALA	13.4
1	A	306	SER	13.3
1	A	315	ARG	13.2
1	A	325	CYS	13.2
1	A	268	GLU	13.1
1	B	329	PRO	13.0
1	A	475	GLU	13.0
2	C	72	SER	13.0
1	A	409	TYR	12.9
1	B	231	GLY	12.9
1	B	236	ASN	12.8
1	B	441	PRO	12.7
1	A	264	ALA	12.7
1	A	305	THR	12.6
1	A	210	ASN	12.3
1	A	300	VAL	12.3
2	C	65	ALA	12.3
2	C	79	TYR	12.3
1	B	296	HIS	12.3
2	C	36	ASN	12.2
1	A	265	GLY	12.1
2	C	35	TRP	12.1
1	B	268	GLU	12.0
1	B	282	LYS	12.0
1	B	281	TYR	12.0
1	A	263	ASN	11.9
1	B	230	ARG	11.7
1	B	210	ASN	11.6
1	A	329	PRO	11.6
1	B	328	PRO	11.5
1	A	328	PRO	11.5
1	B	409	TYR	11.5
1	B	300	VAL	11.4
1	B	202	LYS	11.4

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Mol	Chain	Res	Type	RSRZ
1	B	315	ARG	11.3
1	B	302	GLU	11.3
1	B	267	GLU	11.2
1	B	298	TYR	11.1
1	B	303	GLY	11.0
1	A	274	GLN	11.0
1	A	473	GLU	10.9
1	B	304	ALA	10.8
1	A	303	GLY	10.8
1	A	314	PHE	10.7
1	A	302	GLU	10.7
1	B	357	ARG	10.7
1	B	368	LYS	10.6
1	B	266	HIS	10.6
1	B	127	TYR	10.5
1	A	280	TYR	10.5
1	B	235	ASN	10.4
1	A	211	LEU	10.3
1	A	289	THR	10.2
2	C	139	ALA	10.2
1	A	298	TYR	10.2
2	C	127	HIS	10.2
2	D	161	MET	10.2
1	A	213	GLN	10.2
2	D	79	TYR	10.2
1	B	355	GLY	10.2
1	A	287	ASP	10.1
1	A	415	ALA	10.1
1	A	278	ILE	10.0
2	C	63	PRO	9.9
1	B	128	GLU	9.8
1	B	277	LYS	9.8
2	C	122	PRO	9.8
1	B	233	CYS	9.8
1	A	308	THR	9.7
1	B	211	LEU	9.6
1	B	278	ILE	9.6
1	B	410	THR	9.6
1	B	212	ALA	9.6
1	A	296	HIS	9.5
1	B	258	GLY	9.5
1	B	162	ARG	9.5

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Mol	Chain	Res	Type	RSRZ
1	A	312	GLY	9.5
1	A	297	SER	9.4
1	B	276	CYS	9.4
1	B	55	GLU	9.4
1	B	261	LEU	9.4
1	B	422	TYR	9.4
1	A	276	CYS	9.4
2	C	77	GLU	9.4
1	B	280	TYR	9.3
1	A	272	GLU	9.3
2	C	78	PHE	9.3
1	B	160	GLY	9.3
1	A	203	LYS	9.2
1	A	261	LEU	9.2
1	A	291	ALA	9.2
1	B	411	PHE	9.1
2	C	141	SER	9.1
1	A	202	LYS	9.1
1	A	492	ARG	9.1
1	A	435	THR	9.1
1	B	272	GLU	9.1
1	A	149	ALA	9.1
1	B	306	SER	9.1
1	B	482	ASP	9.0
2	C	71	HIS	9.0
1	A	474	TYR	9.0
1	B	245	MET	9.0
2	D	143	GLY	8.9
1	B	203	LYS	8.9
1	B	129	SER	8.9
1	B	356	GLY	8.9
1	B	263	ASN	8.8
1	B	68	ARG	8.8
1	B	287	ASP	8.8
2	C	93	GLU	8.7
1	B	458	ALA	8.7
1	A	237	SER	8.7
1	A	309	CYS	8.7
1	A	253	TRP	8.7
1	B	369	CYS	8.7
1	B	433	THR	8.7
1	A	332	PRO	8.6

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Mol	Chain	Res	Type	RSRZ
1	B	213	GLN	8.6
2	C	161	MET	8.6
1	A	313	PHE	8.6
1	B	290	CYS	8.5
1	B	134	GLU	8.5
1	B	239	GLU	8.5
1	A	331	ALA	8.5
1	A	116	GLY	8.4
1	A	414	TRP	8.4
1	A	411	PHE	8.4
1	B	416	VAL	8.4
2	C	76	TYR	8.4
1	B	53	GLY	8.4
1	A	422	TYR	8.4
1	A	230	ARG	8.4
1	B	161	ASP	8.4
1	B	438	GLN	8.3
1	B	59	ILE	8.3
1	A	277	LYS	8.3
1	A	311	ARG	8.3
1	B	324	PRO	8.3
1	A	244	LYS	8.3
1	B	307	CYS	8.2
2	C	142	ASP	8.2
1	A	423	ASN	8.2
1	A	408	ASN	8.2
2	D	73	SER	8.2
1	B	419	VAL	8.0
1	B	279	GLY	8.0
1	B	330	SER	8.0
1	A	416	VAL	8.0
1	B	238	GLU	8.0
2	D	140	THR	8.0
1	B	58	SER	8.0
2	C	94	ALA	8.0
1	B	423	ASN	7.9
1	A	514	ARG	7.9
2	C	143	GLY	7.9
2	C	159	ARG	7.9
1	B	440	ALA	7.9
2	C	61	LEU	7.8
1	B	417	ASN	7.7

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Mol	Chain	Res	Type	RSRZ
2	D	36	ASN	7.7
1	A	245	MET	7.7
1	A	150	ALA	7.7
1	A	258	GLY	7.7
2	D	141	SER	7.7
1	A	279	GLY	7.7
1	A	269	ARG	7.7
1	A	238	GLU	7.7
1	B	71	GLN	7.6
1	A	354	THR	7.6
1	A	275	ALA	7.5
1	A	434	VAL	7.5
1	B	354	THR	7.5
2	D	63	PRO	7.5
2	C	34	TYR	7.5
1	A	283	ALA	7.5
1	B	265	GLY	7.4
2	C	121	SER	7.4
1	B	237	SER	7.4
1	B	344	VAL	7.4
1	B	283	ALA	7.4
1	A	321	ALA	7.4
1	A	293	CYS	7.4
1	B	415	ALA	7.4
2	C	169	GLN	7.4
2	C	37	SER	7.4
1	A	243	PRO	7.3
1	B	136	PHE	7.3
1	A	515	ALA	7.3
1	B	295	PRO	7.2
2	D	118	GLN	7.2
1	A	413	ILE	7.2
1	B	297	SER	7.1
1	A	294	PRO	7.1
1	B	30	GLU	7.1
1	B	301	TRP	7.0
1	B	505	PRO	7.0
1	B	246	TYR	7.0
1	B	137	ILE	7.0
1	A	41	GLY	6.9
1	B	249	ALA	6.9
1	B	229	VAL	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	439	ALA	6.9
1	A	438	GLN	6.9
1	B	67	ILE	6.9
2	D	77	GLU	6.9
1	A	419	VAL	6.8
1	B	442	SER	6.8
1	A	476	VAL	6.8
1	B	275	ALA	6.8
1	A	231	GLY	6.7
1	A	246	TYR	6.7
2	C	62	CYS	6.7
1	B	418	GLY	6.7
1	A	324	PRO	6.7
2	C	66	ARG	6.7
1	B	521	TYR	6.6
1	B	439	ALA	6.6
1	A	208	VAL	6.6
2	D	65	ALA	6.6
1	A	310	ASP	6.6
2	C	48	TYR	6.6
1	B	219	THR	6.6
2	D	72	SER	6.6
2	C	118	GLN	6.6
1	B	343	SER	6.6
1	B	430	VAL	6.5
2	D	80	LYS	6.5
1	B	40	GLN	6.5
1	A	333	LEU	6.5
1	B	325	CYS	6.5
2	D	128	GLU	6.5
1	B	432	VAL	6.5
1	B	274	GLN	6.4
2	C	57	ARG	6.4
2	D	142	ASP	6.4
2	C	73	SER	6.4
1	B	305	THR	6.4
2	C	107	PRO	6.4
1	B	408	ASN	6.4
1	B	331	ALA	6.4
1	B	339	VAL	6.3
1	B	149	ALA	6.3
1	B	370	GLY	6.3

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Mol	Chain	Res	Type	RSRZ
2	C	140	THR	6.3
1	B	234	VAL	6.3
1	B	308	THR	6.3
1	B	454	ARG	6.3
2	C	162	LYS	6.3
1	A	424	PRO	6.3
1	B	120	GLU	6.3
2	C	64	ARG	6.3
1	A	417	ASN	6.3
2	D	64	ARG	6.2
1	B	337	SER	6.2
2	C	138	ILE	6.2
1	B	367	LYS	6.2
1	B	46	ILE	6.2
1	B	515	ALA	6.1
1	A	397	LYS	6.1
1	B	37	ARG	6.1
1	B	244	LYS	6.1
1	A	531	THR	6.1
1	A	344	VAL	6.1
1	A	301	TRP	6.1
1	B	121	THR	6.1
1	B	253	TRP	6.1
1	A	430	VAL	6.1
1	A	239	GLU	6.1
1	A	330	SER	6.0
1	B	459	LEU	6.0
1	A	400	ILE	6.0
2	C	70	PRO	6.0
2	C	160	GLY	6.0
1	A	120	GLU	6.0
1	A	370	GLY	6.0
1	B	264	ALA	5.9
2	C	125	TRP	5.9
1	A	117	THR	5.9
1	B	69	THR	5.9
1	A	511	PHE	5.9
1	A	207	THR	5.9
1	B	150	ALA	5.9
1	A	292	LYS	5.9
2	C	111	LEU	5.9
1	A	255	VAL	5.8

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Mol	Chain	Res	Type	RSRZ
2	C	126	GLY	5.8
1	A	236	ASN	5.8
1	A	440	ALA	5.8
1	B	294	PRO	5.8
1	A	362	TYR	5.8
1	A	214	PHE	5.8
1	B	452	VAL	5.7
1	A	488	TYR	5.7
1	A	516	ARG	5.7
1	A	371	ALA	5.7
1	B	182	TYR	5.7
2	C	75	SER	5.7
1	A	477	LYS	5.7
2	C	49	VAL	5.7
1	B	506	LEU	5.6
2	C	112	ARG	5.6
2	C	153	GLY	5.6
1	A	162	ARG	5.6
1	A	209	ARG	5.6
1	B	228	GLU	5.6
2	D	169	GLN	5.6
1	B	504	ASN	5.6
2	C	38	ALA	5.5
2	C	69	GLY	5.5
1	B	52	GLY	5.5
2	C	85	GLU	5.5
1	A	482	ASP	5.5
1	B	437	ASN	5.5
1	B	475	GLU	5.5
1	B	85	ARG	5.5
1	B	247	CYS	5.5
1	A	493	THR	5.5
2	D	159	ARG	5.5
1	A	365	VAL	5.4
1	A	479	TYR	5.4
1	B	142	PHE	5.4
1	B	57	VAL	5.4
1	B	201	TYR	5.4
1	B	159	ILE	5.4
1	A	364	VAL	5.4
1	B	444	ILE	5.4
1	B	313	PHE	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	232	SER	5.3
1	B	312	GLY	5.3
1	A	257	ILE	5.3
1	B	350	SER	5.3
1	A	254	LEU	5.3
1	B	457	VAL	5.3
2	C	39	ASN	5.3
1	A	481	LYS	5.3
1	B	513	VAL	5.3
1	B	364	VAL	5.3
2	C	42	PHE	5.3
1	A	355	GLY	5.3
1	A	412	GLU	5.2
1	B	514	ARG	5.2
2	C	43	GLN	5.2
2	D	138	ILE	5.2
1	B	449	ALA	5.1
1	A	478	TYR	5.1
1	A	132	ASP	5.1
1	A	68	ARG	5.1
1	B	474	TYR	5.1
1	B	478	TYR	5.1
1	A	441	PRO	5.1
1	A	205	PRO	5.1
1	B	227	VAL	5.1
1	B	365	VAL	5.1
2	C	152	GLN	5.1
1	B	116	GLY	5.1
1	B	321	ALA	5.1
1	B	519	ALA	5.1
1	A	398	VAL	5.1
1	B	241	ASP	5.1
1	A	395	THR	5.1
1	B	243	PRO	5.1
1	B	254	LEU	5.0
1	A	367	LYS	5.0
1	B	460	ALA	5.0
2	C	60	LEU	5.0
2	C	80	LYS	5.0
1	B	481	LYS	5.0
1	A	350	SER	5.0
1	A	295	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	284	LEU	5.0
1	B	323	MET	5.0
2	C	130	ARG	4.9
1	B	56	GLU	4.9
1	A	509	TYR	4.9
1	B	148	ILE	4.9
1	B	371	ALA	4.9
2	D	78	PHE	4.9
2	C	47	GLY	4.9
1	A	240	LYS	4.9
1	B	366	CYS	4.9
1	B	431	SER	4.9
1	B	509	TYR	4.8
1	B	489	ARG	4.8
1	A	90	THR	4.8
2	D	37	SER	4.8
2	D	155	VAL	4.8
1	B	336	ILE	4.8
1	B	41	GLY	4.8
1	B	332	PRO	4.7
2	C	134	ASP	4.7
1	A	247	CYS	4.7
1	A	67	ILE	4.7
1	B	164	MET	4.7
1	A	426	PRO	4.6
1	B	135	ARG	4.6
2	D	66	ARG	4.6
1	B	451	GLU	4.6
1	B	412	GLU	4.6
1	A	418	GLY	4.6
1	B	54	TRP	4.6
2	D	148	LEU	4.6
2	C	128	GLU	4.5
1	B	443	SER	4.5
1	B	240	LYS	4.5
1	B	522	GLY	4.5
1	A	444	ILE	4.5
2	C	123	ASN	4.5
1	A	368	LYS	4.5
1	B	257	ILE	4.5
2	D	134	ASP	4.5
1	B	398	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	513	VAL	4.5
1	A	288	ALA	4.4
1	B	214	PHE	4.4
1	B	33	LEU	4.4
2	D	122	PRO	4.4
1	B	345	ASN	4.4
2	D	160	GLY	4.4
1	A	360	ILE	4.3
1	B	483	GLN	4.3
1	B	461	TRP	4.3
2	D	61	LEU	4.3
1	B	139	GLU	4.3
1	B	269	ARG	4.3
2	D	130	ARG	4.3
1	B	31	VAL	4.3
1	A	40	GLN	4.3
2	D	74	PRO	4.3
2	D	162	LYS	4.3
2	C	106	ARG	4.3
1	A	346	LEU	4.3
1	B	117	THR	4.3
2	C	116	LYS	4.3
1	B	138	ARG	4.2
1	B	403	LEU	4.2
2	C	151	LEU	4.2
1	A	363	ASN	4.2
2	D	116	LYS	4.2
1	B	292	LYS	4.2
1	B	507	THR	4.2
1	B	320	ALA	4.2
1	A	115	MET	4.2
1	B	413	ILE	4.2
1	A	229	VAL	4.2
1	B	39	VAL	4.1
1	B	146	ASP	4.1
2	C	132	HIS	4.1
2	C	67	PRO	4.1
1	A	334	ASN	4.1
1	B	455	TYR	4.1
1	A	491	VAL	4.1
1	B	436	THR	4.1
1	B	338	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	361	SER	4.1
1	A	335	LEU	4.1
2	C	74	PRO	4.0
2	D	149	GLU	4.0
1	B	518	ALA	4.0
1	B	414	TRP	4.0
1	A	151	ASP	4.0
1	B	309	CYS	4.0
1	A	270	SER	4.0
1	B	378	ARG	4.0
2	C	110	ASP	4.0
1	A	349	SER	4.0
1	A	361	SER	4.0
1	B	362	TYR	4.0
1	B	349	SER	4.0
1	B	464	PRO	3.9
1	B	84	LEU	3.9
2	D	29	SER	3.9
1	B	226	LEU	3.9
1	B	319	ASP	3.9
2	C	95	PRO	3.9
1	B	353	ASN	3.9
1	A	148	ILE	3.9
1	B	97	VAL	3.9
2	D	62	CYS	3.9
1	B	248	GLY	3.9
1	B	476	VAL	3.9
1	A	233	CYS	3.9
1	B	173	VAL	3.9
1	B	218	ILE	3.9
1	A	235	ASN	3.9
1	B	291	ALA	3.9
1	B	420	SER	3.9
2	C	29	SER	3.9
1	B	400	ILE	3.9
1	A	256	PRO	3.9
1	A	271	GLY	3.9
1	B	453	THR	3.9
2	D	71	HIS	3.9
2	C	120	TYR	3.9
1	B	141	GLN	3.8
1	B	491	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	360	ILE	3.8
1	B	363	ASN	3.8
1	A	285	SER	3.8
1	B	179	LYS	3.8
1	B	285	SER	3.8
1	B	293	CYS	3.8
2	C	108	ASP	3.8
1	A	485	GLU	3.8
1	A	217	THR	3.7
2	C	105	ASP	3.7
2	D	70	PRO	3.7
1	B	512	HIS	3.7
1	B	492	ARG	3.7
1	B	450	LYS	3.7
1	B	106	ARG	3.7
1	A	234	VAL	3.7
1	B	255	VAL	3.7
1	B	32	THR	3.7
1	B	118	CYS	3.7
1	B	333	LEU	3.7
2	C	33	VAL	3.7
1	A	121	THR	3.7
1	B	289	THR	3.7
1	A	489	ARG	3.6
1	B	147	THR	3.6
2	C	51	TYR	3.6
2	C	68	PRO	3.6
1	B	480	GLU	3.6
1	B	209	ARG	3.6
2	D	34	TYR	3.6
1	A	249	ALA	3.6
1	B	217	THR	3.6
1	A	320	ALA	3.6
1	B	70	TYR	3.6
1	B	126	TYR	3.6
1	A	345	ASN	3.5
1	A	530	VAL	3.5
2	C	45	GLU	3.5
1	B	448	GLN	3.5
1	A	399	SER	3.5
1	B	181	PHE	3.5
1	B	252	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	62	GLU	3.5
2	C	129	PHE	3.5
1	A	471	ILE	3.5
1	B	524	PHE	3.4
1	B	130	ASP	3.4
2	C	40	LYS	3.4
1	A	351	PRO	3.4
2	C	88	GLN	3.4
1	A	69	THR	3.4
1	B	145	ILE	3.4
1	A	357	ARG	3.4
1	B	511	PHE	3.3
1	B	152	GLU	3.3
2	D	121	SER	3.3
1	A	420	SER	3.3
2	D	110	ASP	3.3
1	A	201	TYR	3.3
1	B	74	ASN	3.3
1	B	250	ASP	3.3
1	A	380	CYS	3.3
1	A	215	PRO	3.3
1	B	153	SER	3.3
2	C	41	ARG	3.3
1	A	403	LEU	3.3
1	B	397	LYS	3.3
1	B	310	ASP	3.3
1	B	115	MET	3.3
1	A	480	GLU	3.3
1	B	516	ARG	3.2
2	D	112	ARG	3.2
2	C	50	LEU	3.2
1	A	252	GLU	3.2
1	A	521	TYR	3.2
1	B	75	VAL	3.2
1	A	372	GLY	3.2
2	C	163	VAL	3.2
2	C	167	VAL	3.2
1	A	461	TRP	3.2
1	B	493	THR	3.2
1	A	512	HIS	3.2
1	B	377	CYS	3.2
1	B	508	SER	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	109	LEU	3.2
1	B	286	THR	3.2
1	A	113	GLY	3.2
2	D	150	SER	3.2
1	A	498	THR	3.2
2	D	90	ARG	3.2
1	B	530	VAL	3.2
1	B	346	LEU	3.2
1	A	216	ASP	3.2
1	A	323	MET	3.1
1	B	463	GLU	3.1
1	B	94	ALA	3.1
1	B	477	LYS	3.1
1	B	335	LEU	3.1
1	A	495	ALA	3.1
1	B	341	GLU	3.1
1	A	161	ASP	3.1
1	A	319	ASP	3.1
2	D	133	HIS	3.1
1	A	134	GLU	3.1
1	A	226	LEU	3.1
2	C	96	PRO	3.1
1	A	112	PRO	3.1
1	B	122	PHE	3.1
2	C	30	LEU	3.1
1	A	88	TRP	3.0
1	A	437	ASN	3.0
2	C	135	TYR	3.0
1	B	406	HIS	3.0
1	B	462	LEU	3.0
1	B	183	LEU	3.0
1	B	405	ALA	2.9
1	B	503	LEU	2.9
1	A	449	ALA	2.9
1	B	468	ASN	2.9
1	B	473	GLU	2.9
1	B	488	TYR	2.9
1	A	353	ASN	2.9
1	B	111	LEU	2.9
1	A	33	LEU	2.9
1	A	227	VAL	2.9
1	A	322	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	160	GLY	2.9
2	C	166	ARG	2.9
1	B	421	LYS	2.9
1	B	529	GLU	2.9
2	D	76	TYR	2.9
1	B	520	GLY	2.9
1	B	36	SER	2.9
2	C	44	ALA	2.9
1	A	119	LYS	2.9
1	B	340	ASN	2.9
2	D	144	THR	2.9
1	B	61	ASP	2.8
2	D	153	GLY	2.8
1	A	152	GLU	2.8
1	B	525	SER	2.8
1	A	118	CYS	2.8
1	B	119	LYS	2.8
2	D	38	ALA	2.8
1	B	60	MET	2.8
1	B	532	THR	2.8
1	A	123	ASN	2.8
1	B	49	PRO	2.8
1	A	394	LYS	2.8
1	A	510	VAL	2.8
2	D	129	PHE	2.8
1	B	79	SER	2.7
1	B	498	THR	2.7
1	B	374	PRO	2.7
1	B	157	VAL	2.7
2	D	94	ALA	2.7
1	B	29	ASN	2.7
1	A	506	LEU	2.7
1	A	407	THR	2.7
1	A	51	GLU	2.7
1	A	460	ALA	2.7
2	C	148	LEU	2.7
1	B	251	GLY	2.7
1	A	241	ASP	2.7
1	A	284	LEU	2.7
1	A	369	CYS	2.7
1	A	459	LEU	2.7
1	B	105	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	114	VAL	2.7
1	A	179	LYS	2.7
1	B	479	TYR	2.6
1	B	195	VAL	2.6
1	B	242	VAL	2.6
1	A	219	THR	2.6
1	B	45	TRP	2.6
1	B	90	THR	2.6
1	B	208	VAL	2.6
1	B	194	LEU	2.6
1	B	96	ARG	2.6
1	A	386	TYR	2.6
1	B	154	PHE	2.6
1	A	242	VAL	2.6
2	D	154	GLY	2.6
1	A	336	ILE	2.5
1	B	465	ASP	2.5
1	B	395	THR	2.5
1	B	352	GLN	2.5
2	C	155	VAL	2.5
1	A	431	SER	2.5
1	A	486	ARG	2.5
1	B	456	SER	2.5
1	B	372	GLY	2.5
1	B	531	THR	2.5
1	B	192	ILE	2.5
1	B	205	PRO	2.5
1	A	36	SER	2.5
1	A	508	SER	2.5
1	B	180	GLY	2.5
2	D	167	VAL	2.5
1	A	248	GLY	2.5
1	A	147	THR	2.5
1	B	407	THR	2.5
1	A	472	LEU	2.5
1	A	421	LYS	2.5
1	B	43	LEU	2.5
1	A	39	VAL	2.5
1	A	339	VAL	2.5
1	B	469	GLY	2.5
1	B	144	LYS	2.5
1	B	271	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	114	VAL	2.5
2	D	30	LEU	2.5
1	B	42	GLU	2.5
1	A	98	TYR	2.5
1	B	95	GLN	2.4
1	B	445	ALA	2.4
1	A	37	ARG	2.4
1	A	401	THR	2.4
2	D	127	HIS	2.4
1	B	526	GLU	2.4
1	B	220	GLY	2.4
1	A	204	CYS	2.4
1	B	83	TRP	2.4
1	A	164	MET	2.4
2	C	81	LEU	2.4
1	B	499	ASP	2.4
1	A	75	VAL	2.4
2	C	137	ILE	2.4
2	C	46	GLY	2.4
1	A	286	THR	2.4
1	A	442	SER	2.4
1	B	89	ILE	2.4
1	A	133	LYS	2.4
1	A	111	LEU	2.4
1	B	351	PRO	2.4
2	D	91	ARG	2.3
1	A	523	ASP	2.3
1	A	110	SER	2.3
1	A	433	THR	2.3
1	B	490	ILE	2.3
1	B	104	THR	2.3
1	B	426	PRO	2.3
1	B	500	ILE	2.3
2	D	69	GLY	2.3
1	A	396	THR	2.3
1	B	322	SER	2.3
1	A	432	VAL	2.3
1	B	447	VAL	2.3
1	B	215	PRO	2.3
1	A	79	SER	2.3
1	A	122	PHE	2.3
1	A	445	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	467	PRO	2.2
1	B	72	VAL	2.2
1	B	510	VAL	2.2
1	B	359	ASP	2.2
1	B	163	ILE	2.2
1	A	189	GLY	2.2
1	A	425	ASN	2.2
2	C	158	THR	2.2
2	C	119	GLU	2.2
2	C	103	THR	2.2
2	C	102	LEU	2.2
1	A	525	SER	2.2
1	B	256	PRO	2.2
1	B	471	ILE	2.2
2	D	117	PHE	2.2
1	B	316	ALA	2.2
1	A	186	GLN	2.2
2	D	135	TYR	2.2
2	D	152	GLN	2.2
2	D	52	PRO	2.2
1	A	316	ALA	2.2
1	A	218	ILE	2.1
1	A	343	SER	2.1
1	A	92	GLU	2.1
2	C	82	TYR	2.1
2	C	156	CYS	2.1
1	A	61	ASP	2.1
1	B	123	ASN	2.1
1	A	436	THR	2.1
1	A	494	ALA	2.1
2	C	59	ASP	2.1
1	A	359	ASP	2.1
1	A	384	VAL	2.1
2	C	164	LEU	2.1
1	A	129	SER	2.1
1	A	57	VAL	2.1
1	B	401	THR	2.1
1	B	342	THR	2.1
2	C	55	GLY	2.1
1	B	472	LEU	2.1
1	B	527	PRO	2.1
2	C	92	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	528	LEU	2.1
2	D	156	CYS	2.0
1	A	427	ASP	2.0
1	A	53	GLY	2.0
1	A	169	GLU	2.0
1	A	348	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.