Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:17 pm BST

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

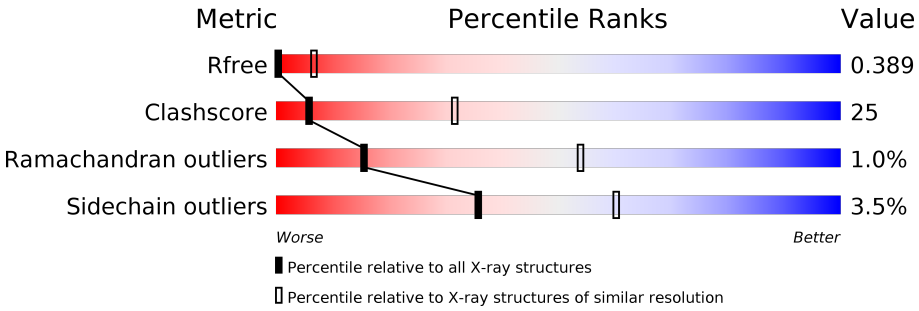
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	1083 (5.52-3.80)
Clashscore	141614	1156 (5.52-3.80)
Ramachandran outliers	138981	1092 (5.52-3.80)
Sidechain outliers	138945	1072 (5.50-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	568	71% 17% • 11%
1	B	568	73% 14% • 11%
2	C	183	39% 32% 7% 23%
2	D	183	40% 31% 6% 23%

2 Entry composition (i)

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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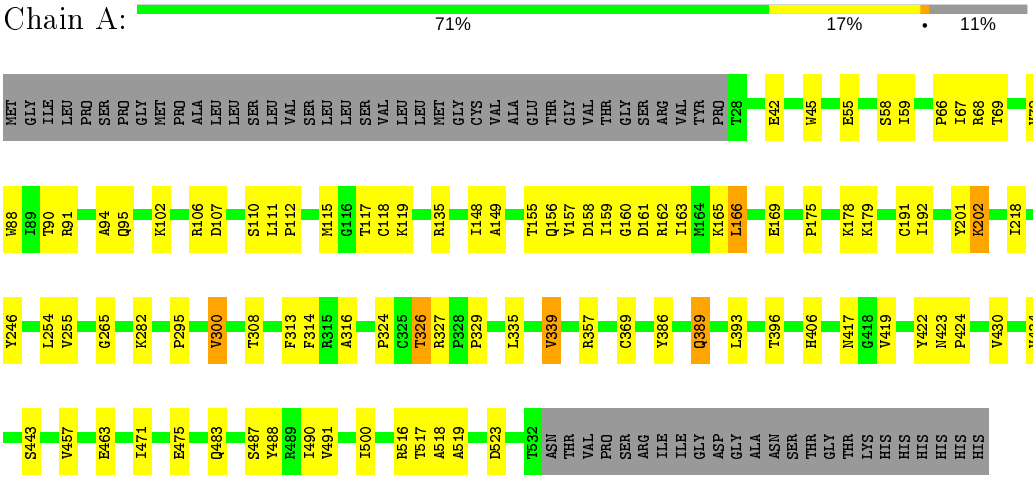
Chain	Residue	Modelled	Actual	Comment	Reference
D	11	VAL	-	expression tag	UNP Q15768
D	12	SER	-	expression tag	UNP Q15768
D	13	LEU	-	expression tag	UNP Q15768
D	14	LEU	-	expression tag	UNP Q15768
D	15	SER	-	expression tag	UNP Q15768
D	16	VAL	-	expression tag	UNP Q15768
D	17	LEU	-	expression tag	UNP Q15768
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 (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

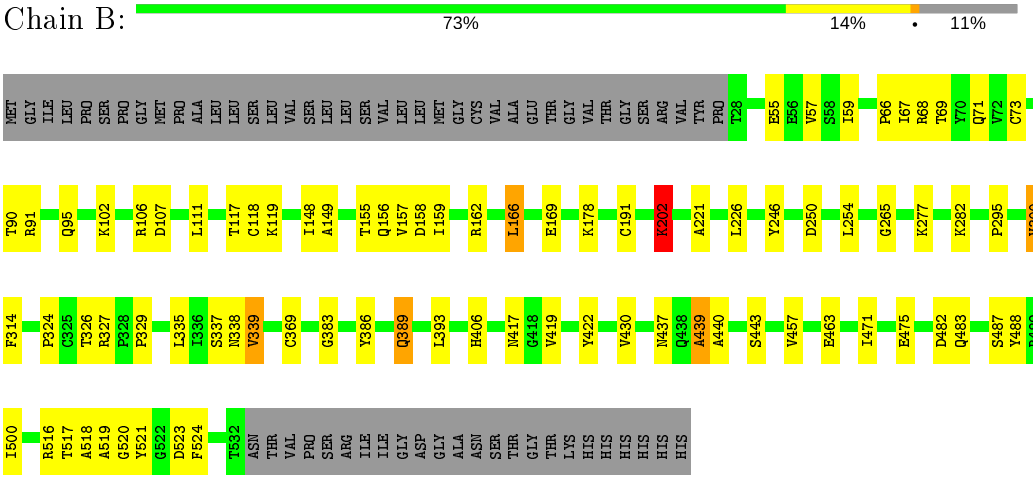
- Molecule 1: EPHRIN TYPE-A RECEPTOR 4

Chain A:



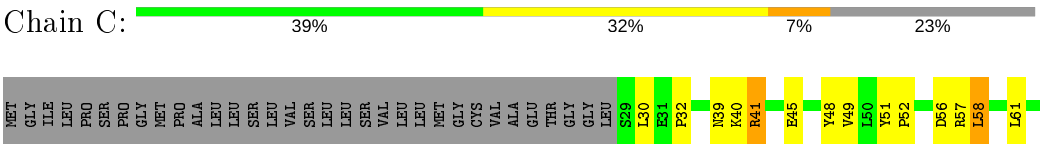
- Molecule 1: EPHRIN TYPE-A RECEPTOR 4

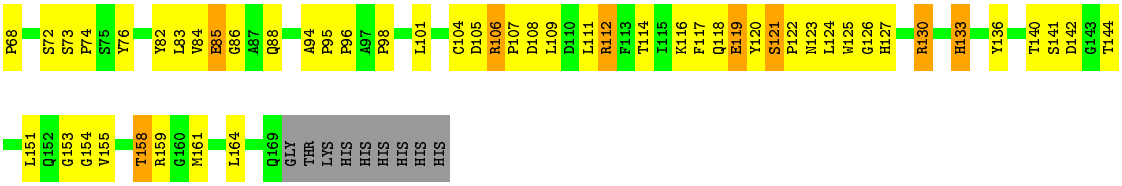
Chain B:



- Molecule 2: EPHRIN-B3

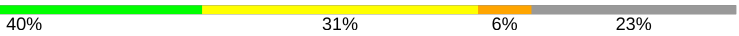
Chain C:

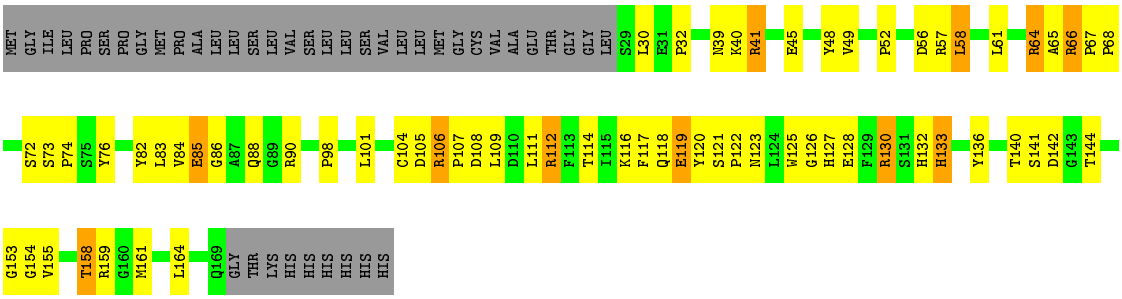




- Molecule 2: EPHRIN-B3

Chain D:





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.06 (at 4.66Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.327 , 0.351 0.363 , 0.389	Depositor DCC
R_{free} test set	1298 reflections (5.09%)	wwPDB-VP
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 , 308.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.61	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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:254:LEU:CD2	1:B:226:LEU:HD11	1.43	1.47
1:A:59:ILE:CG2	2:D:122:PRO:HB2	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:A:119:LYS:CD	1:B:117:THR:HG23	1.70	1.20
1:B:157:VAL:CB	2:C:126:GLY:N	2.03	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:B:157:VAL:C	2:C:126:GLY:N	1.99	1.16
1:A:159:ILE:HG12	2:D:127:HIS:ND1	1.58	1.16
1:A:157:VAL:HG11	2:D:123:ASN:ND2	1.54	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:A:159:ILE:HG12	2:D:127:HIS:CE1	1.80	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:111:LEU:CD2	2:D:119:GLU:HG2	1.79	1.12
1:A:159:ILE:C	2:D:125:TRP:CD2	2.22	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:149:ALA:HB2	1:B:149:ALA:HB2	1.36	1.05
1:A:157:VAL:HG11	2:D:123:ASN:HD22	1.03	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: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:B:157:VAL:C	2:C:125:TRP:C	2.26	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:86:GLY:HA2	2:D:136:TYR:HD1	1.37	0.89
2:D:66:ARG:HB3	2:D:67:PRO:HD3	1.54	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:117:THR:CB	1:B:117:THR:O	2.23	0.85
1:A:59:ILE:HG21	2:D:122:PRO:CD	1.86	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:A:117:THR:O	1:B:117:THR:C	2.18	0.81
1:B:157:VAL:HG13	2:C:125:TRP:N	1.94	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
1:A:95:GLN:NE2	1:A:221:ALA:H	1.79	0.80
2:D:118:GLN:HG2	2:D:119:GLU:N	1.96	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:B:157:VAL:HG11	2:C:123:ASN:HD22	1.47	0.79
1:A:158:ASP:CG	2:D:125:TRP:CD2	2.56	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:HH11	2:D:130:ARG:HG2	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:A:255:VAL:HG21	1:B:246:TYR:CE2	2.24	0.72
1:B:157:VAL:CG1	2:C:123:ASN:ND2	2.51	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:111:LEU:HD21	2:D:119:GLU:HG2	1.72	0.71
1:A:159:ILE:HA	2:D:127:HIS:HE2	1.53	0.71
1:A:314:PHE:HE2	1:A:424:PRO:HD3	1.53	0.71
1:A:117:THR:HG21	1:B:119:LYS:HG2	1.71	0.71
2:C:66:ARG:O	2:C:68:PRO:HD3	1.91	0.71
1:A:88:TRP:CZ3	1:A:90:THR:HG22	2.26	0.71
1:B:95:GLN:HE21	1:B:221:ALA:CB	2.04	0.71
1:A:117:THR:CG2	1:B:119:LYS:CG	2.66	0.71
1:B:157:VAL:CA	2:C:126:GLY:HA2	2.21	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:B:111:LEU:CD2	2:C:119:GLU:HG2	2.24	0.67
1:A:157:VAL:CB	2:D:127:HIS:H	2.06	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
2:C:105:ASP:HB2	2:C:106:ARG:HE	1.63	0.63
1:A:69:THR:HG21	2:D:122:PRO:CG	2.28	0.63
1:A:117:THR:HG23	1:B:119:LYS:HD3	1.80	0.63
1:A:159:ILE:N	2:D:125:TRP:CE3	2.64	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:119:LYS:CB	1:B:117:THR:CG2	2.76	0.62
1:A:117:THR:CA	1:B:117:THR:O	2.46	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:55:GLU:OE2	2:D:116:LYS:HD3	1.77	0.61
1:A:159:ILE:HG23	2:D:127:HIS:HE1	0.47	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:B:337:SER:OG	1:B:518:ALA:CA	2.49	0.60
1:A:159:ILE:CG1	2:D:127:HIS:ND1	2.45	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:91:ARG:HD3	1:A:178:LYS:O	2.03	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:69:THR:CB	2:D:122:PRO:HG3	2.32	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:A:156:GLN:HG2	2:D:126:GLY:HA3	1.86	0.57
1:B:157:VAL:N	2:C:126:GLY:CA	2.68	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:326:THR:OG1	1:A:419:VAL:HG11	2.08	0.53
1:A:119:LYS:CB	1:B:117:THR:HG21	2.38	0.53
1:A:118:CYS:HA	1:B:117:THR:HB	1.90	0.53
1:B:471:ILE:HA	1:B:517:THR:HG22	1.91	0.53
2:D:118:GLN:HG2	2:D:119:GLU:H	1.72	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
1:A:389:GLN:HB2	1:A:393:LEU:HD13	1.92	0.52
2:C:118:GLN:HG2	2:C:120:TYR:H	1.75	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:59:ILE:CD1	2:D:122:PRO:O	2.58	0.52
1:A:162:ARG:HD3	2:D:125:TRP:NE1	2.25	0.52
2:D:118:GLN:HG2	2:D:120:TYR:H	1.75	0.52
1:A:69:THR:OG1	2:D:122:PRO:HG2	2.09	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
1:A:443:SER:HB2	1:A:523:ASP:HB2	1.93	0.51
2:D:65:ALA:HB2	2:D:72:SER: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
1:A:201:TYR:CE1	1:A:218:ILE:HG22	2.47	0.50
2:C:155:VAL:HA	2:C:158:THR:HB	1.93	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:443:SER:HB2	1:B:523:ASP:HB2	1.93	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: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
2:D:104:CYS:HA	2:D:111:LEU:CD1	2.43	0.49
1:A:59:ILE:CG2	2:D:122:PRO:C	2.78	0.49
1:A:406:HIS:H	1:A:437:ASN:HB2	1.78	0.49
1:B:335:LEU:HD12	1:B:430:VAL:HG12	1.95	0.49
2:C:65:ALA:HB2	2:C:72:SER:HB2	1.93	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
2:D:32:PRO:HB3	2:D:61:LEU:HD11	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:104:CYS:HA	2:C:111:LEU:CD1	2.43	0.47
2:C:76:TYR:CD1	2:C:107:PRO:HA	2.49	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:A:88:TRP:CZ3	1:A:90:THR:CG2	2.98	0.46
1:B:339:VAL:HB	1:B:519:ALA:O	2.16	0.46
1:A:73:CYS:HA	2:D:120:TYR:HE2	1.82	0.45
1:B:102:LYS:HB3	1:B:166:LEU:HD22	1.98	0.45
2:D:85:GLU:HB2	2:D:88:GLN:CD	2.36	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:A:68:ARG:NH2	2:D:112:ARG:NH1	2.65	0.45
1:B:95:GLN:HG3	1:B:221:ALA:HA	1.99	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:102:LYS:HB3	1:A:166:LEU:HD22	1.98	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:59:ILE:HD12	2:D:122:PRO:O	2.17	0.44
2:C:140:THR:HA	2:C:154:GLY:H	1.82	0.44
2:D:56:ASP:O	2:D:117:PHE:HD1	2.00	0.44
1:A:157:VAL:HG12	2:D:127:HIS:N	2.29	0.44
1:A:94:ALA:HA	1:A:218:ILE:HD13	1.98	0.44
2:D:130:ARG:HH11	2:D:130:ARG:CG	2.22	0.44
2:D:82:TYR:CD1	2:D:98:PRO:HB2	2.52	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
1:B:326:THR:C	1:B:327:ARG:CA	2.86	0.44
2:D:140:THR:HA	2:D:154:GLY:H	1.82	0.44
1:A:314:PHE:HB3	1:A:422:TYR:CE2	2.40	0.44
1:A:326:THR:C	1:A:327:ARG:C	2.76	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:A:295:PRO:HD2	1:A:324:PRO:HB3	2.01	0.42
1:B:55:GLU:HB2	2:C:57:ARG:HH21	1.84	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
2:D:84:VAL:CG1	2:D:88:GLN:HB2	2.50	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:156:GLN:HG2	2:D:126:GLY:O	2.19	0.42
1:A:68:ARG:HH22	2:D:112:ARG:NH1	2.17	0.42
1:B:295:PRO:HD2	1:B:324:PRO:HB3	2.01	0.42
2:D:159:ARG:HD2	2:D:161:MET:HE3	2.02	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:C:155:VAL:HG12	2:C:161:MET:HB2	2.02	0.41
2:D:130:ARG:HG2	2:D:130:ARG:NH1	2.26	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%)	47 81
2	C	139/183 (76%)	120 (86%)	13 (9%)	6 (4%)	2 25
2	D	139/183 (76%)	120 (86%)	13 (9%)	6 (4%)	2 25
All	All	1282/1502 (85%)	1195 (93%)	74 (6%)	13 (1%)	15 54

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 (i)

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%)	50	70
1	B	437/490 (89%)	428 (98%)	9 (2%)	53	72
2	C	121/155 (78%)	111 (92%)	10 (8%)	11	36
2	D	121/155 (78%)	111 (92%)	10 (8%)	11	36
All	All	1116/1290 (86%)	1077 (96%)	39 (4%)	36	60

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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	326:THR	C	327:ARG	N	2.68
1	A	326:THR	C	327:ARG	N	1.98
1	A	439:ALA	C	440:ALA	N	1.65
1	B	439:ALA	C	440:ALA	N	0.61

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.