



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:50 AM UTC

PDB ID : 3P2D / pdb_00003p2d
Title : Crystal structure of arrestin-3 reveals the basis of the difference in receptor binding between two non-visual subtypes
Authors : Spiller, B.W.; Gurevich, V.V.; Zhan, X.; Gimenez, L.E.
Deposited on : 2010-10-01
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

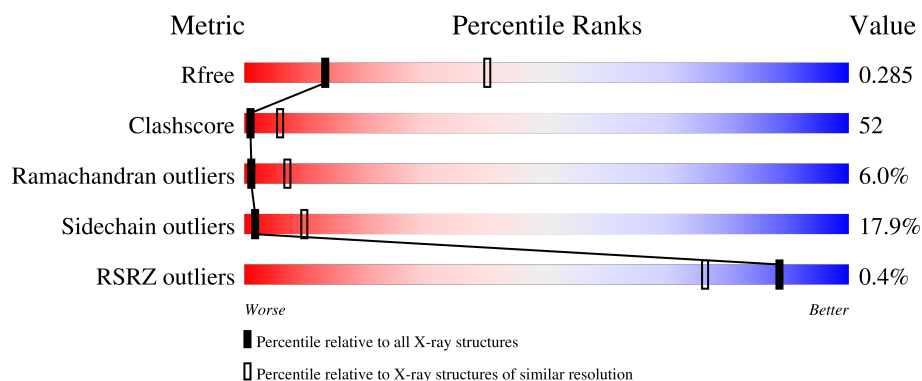
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	393	34% 41% 14% • 10%
1	B	393	31% 44% 14% • 10%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5611 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.

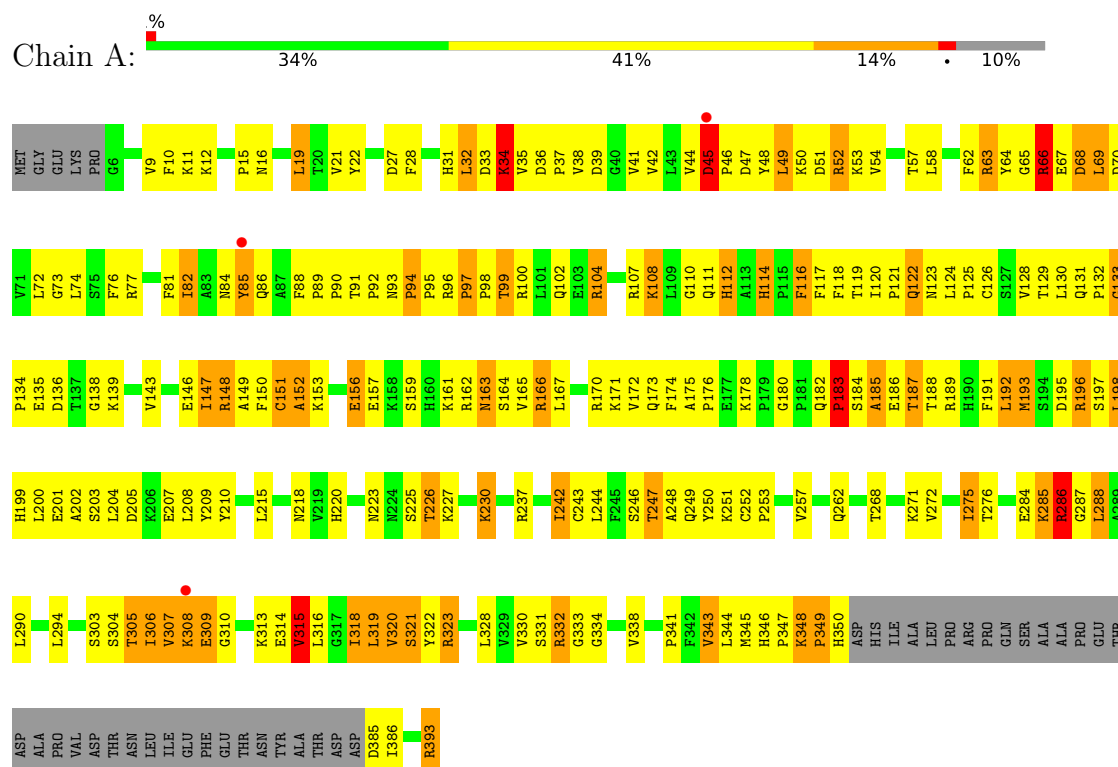
- Molecule 1 is a protein called Beta-arrestin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2814	1792	497	515	10			
1	B	352	Total	C	N	O	S	0	0	0
			2797	1781	493	513	10			

3 Residue-property plots

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

• Molecule 1: Beta-arrestin-2



• Molecule 1: Beta-arrestin-2



PRO	L288	L208
GLN		Y209
SER	D291	Y210
ALA		H211
ALA	L294	G212
PRO	K295	E213
GLU	H296	F214
THR		L215
ASP	N300	
ALA		N218
PRO	T305	V219
VAL	I306	H220
ASP	V307	
THR	K308	N223
ASN	E309	M224
LEU	G310	
ILE	A311	K227
GLU	N312	T228
PHE	K313	V229
GLU	E314	K230
THR	V315	K231
ASN	L316	
TYR	G317	T242
ALA	L318	C243
THR	L319	L244
ASP	V320	F245
ASP		S246
ASP	R323	T247
D385	V324	A248
I386	K325	Q249
V387		Y250
F388		K251
E389	L328	
D390	V329	Q256
F391	S331	V257
A392	G332	E258
R393	K333	Q259
	G334	D260
	D335	D261
	V336	Q262
	S337	V263
	V338	S264
	E339	S265
	L340	S266
		S267
	V343	T268
	L344	F269
	K345	C270
	K346	K271
	F347	
		L278
	PRO	L279
	HIS	S280
	ASP	N281
	ILE	N282
	ILE	R283
	ALA	E284
	LEU	K285
	LEU	T286
	PRO	R286
	ARG	C287

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.18Å 73.32Å 201.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.36 – 3.00 35.36 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.6 (35.36-3.00) 92.6 (35.36-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.219 , 0.286 0.220 , 0.285	Depositor DCC
R_{free} test set	1095 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å ²)	94.9	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 100.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5611	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	1/2878 (0.0%)	1.12	14/3897 (0.4%)
1	B	0.64	1/2859 (0.0%)	1.05	12/3870 (0.3%)
All	All	0.67	2/5737 (0.0%)	1.09	26/7767 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	ILE	CA-CB	-5.09	1.48	1.54
1	B	248	ALA	CA-CB	-5.01	1.45	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	16	ASN	N-CA-C	8.92	123.47	112.23
1	B	192	LEU	N-CA-C	-8.65	99.10	110.43
1	A	133	GLY	CA-C-N	8.39	130.33	119.84
1	A	133	GLY	C-N-CA	8.39	130.33	119.84
1	A	66	ARG	N-CA-C	-7.95	97.94	108.19
1	A	120	ILE	CA-C-N	-6.98	112.78	119.76
1	A	120	ILE	C-N-CA	-6.98	112.78	119.76
1	A	93	ASN	C-N-CD	-6.82	105.61	120.60
1	A	180	GLY	CA-C-N	6.65	126.41	119.76
1	A	180	GLY	C-N-CA	6.65	126.41	119.76
1	B	187	THR	N-CA-C	-6.48	99.16	109.59
1	A	136	ASP	N-CA-C	-6.37	103.85	112.26
1	B	193	MET	N-CA-C	6.15	123.90	110.80
1	A	114	HIS	CA-C-N	-6.06	114.50	120.98
1	A	114	HIS	C-N-CA	-6.06	114.50	120.98
1	B	45	ASP	CA-C-N	5.80	127.08	119.84
1	B	45	ASP	C-N-CA	5.80	127.08	119.84
1	A	322	TYR	N-CA-C	5.57	118.15	109.52
1	A	111	GLN	N-CA-C	-5.55	106.47	113.18
1	B	133	GLY	CA-C-N	5.50	126.72	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	GLY	C-N-CA	5.50	126.72	119.84
1	B	120	ILE	N-CA-C	5.24	114.23	108.05
1	B	285	LYS	N-CA-C	-5.15	105.56	111.07
1	B	316	LEU	N-CA-C	-5.10	107.03	114.12
1	A	320	VAL	N-CA-C	5.06	116.53	109.80
1	B	29	VAL	N-CA-C	5.05	115.59	108.36

There are no chirality outliers.

There are no planarity outliers.

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	2814	0	2856	296	0
1	B	2797	0	2842	298	0
All	All	5611	0	5698	590	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 52.

All (590) 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:B:41:VAL:HG22	1:B:115:PRO:HG3	1.19	1.15
1:A:53:LYS:HE2	1:A:86:GLN:HB3	1.13	1.12
1:A:49:LEU:HB2	1:A:52:ARG:HD2	1.32	1.11
1:B:40:GLY:O	1:B:115:PRO:HB3	1.53	1.07
1:A:348:LYS:HA	1:A:350:HIS:CD2	1.90	1.07
1:A:94:PRO:HB2	1:A:95:PRO:HD2	1.29	1.06
1:B:51:ASP:HB3	1:B:153:LYS:HE2	1.30	1.06
1:A:348:LYS:H	1:A:349:PRO:HD2	1.20	1.04
1:A:53:LYS:CE	1:A:86:GLN:HB3	1.88	1.03
1:A:348:LYS:HA	1:A:350:HIS:HD2	1.19	1.03
1:B:94:PRO:HB2	1:B:95:PRO:HD3	1.35	1.02
1:B:311:ALA:HA	1:B:312:ASN:C	1.85	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ARG:HD2	1:B:287:GLY:H	1.24	1.00
1:A:285:LYS:HG2	1:A:286:ARG:O	1.64	0.97
1:B:110:GLY:HA3	1:B:112:HIS:CE1	1.99	0.97
1:B:313:LYS:HG2	1:B:314:GLU:HA	1.46	0.95
1:A:286:ARG:HG3	1:A:286:ARG:HH11	1.30	0.93
1:A:19:LEU:HD13	1:A:44:VAL:HB	1.51	0.93
1:A:94:PRO:HB2	1:A:95:PRO:CD	2.00	0.92
1:B:99:THR:HG23	1:B:102:GLN:HB2	1.52	0.92
1:B:91:THR:HB	1:B:92:PRO:HD2	1.52	0.91
1:B:18:LYS:HD3	1:B:46:PRO:HG2	1.54	0.90
1:B:283:ARG:H	1:B:283:ARG:NE	1.70	0.90
1:B:45:ASP:O	1:B:47:ASP:N	2.04	0.89
1:A:66:ARG:HD3	1:A:73:GLY:HA3	1.54	0.89
1:A:85:TYR:HE2	1:A:118:PHE:CZ	1.92	0.88
1:A:183:PRO:HG2	1:A:204:LEU:HB2	1.54	0.87
1:A:53:LYS:HE2	1:A:86:GLN:CB	2.02	0.87
1:A:85:TYR:OH	1:A:116:PHE:HB2	1.75	0.87
1:B:132:PRO:C	1:B:134:PRO:HD2	1.99	0.87
1:B:312:ASN:HA	1:B:313:LYS:C	1.98	0.87
1:A:196:ARG:HE	1:A:196:ARG:HA	1.40	0.86
1:B:114:HIS:N	1:B:115:PRO:HD2	1.89	0.86
1:A:94:PRO:HD2	1:A:117:PHE:HZ	1.41	0.85
1:A:348:LYS:CA	1:A:350:HIS:HD2	1.89	0.85
1:A:123:ASN:HA	1:A:309:GLU:HG3	1.59	0.84
1:A:345:MET:HE2	1:A:345:MET:HA	1.58	0.84
1:A:200:LEU:HD13	1:A:328:LEU:HD11	1.58	0.84
1:B:330:VAL:HB	1:B:334:GLY:O	1.79	0.82
1:A:94:PRO:CB	1:A:95:PRO:HD2	2.10	0.82
1:A:348:LYS:H	1:A:349:PRO:CD	1.92	0.82
1:B:59:THR:HG23	1:B:82:ILE:HG22	1.61	0.81
1:A:66:ARG:HH11	1:A:66:ARG:HG2	1.46	0.81
1:B:283:ARG:H	1:B:283:ARG:HE	1.25	0.81
1:A:94:PRO:CD	1:A:117:PHE:HZ	1.93	0.81
1:B:117:PHE:N	1:B:117:PHE:HD2	1.81	0.79
1:B:148:ARG:HG3	1:B:166:ARG:HD2	1.66	0.78
1:B:13:SER:HA	1:B:20:THR:HA	1.66	0.78
1:A:306:ILE:O	1:A:308:LYS:N	2.18	0.77
1:B:94:PRO:HB2	1:B:95:PRO:CD	2.14	0.77
1:A:82:ILE:C	1:A:82:ILE:HD12	2.10	0.76
1:B:259:GLN:CD	1:B:271:LYS:HZ3	1.93	0.76
1:B:95:PRO:C	1:B:97:PRO:HD2	2.11	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ASP:HB3	1:A:34:LYS:HD2	1.68	0.75
1:A:133:GLY:C	1:A:135:GLU:HA	2.11	0.75
1:A:49:LEU:HB3	1:A:52:ARG:HB3	1.67	0.75
1:B:117:PHE:N	1:B:117:PHE:CD2	2.54	0.75
1:B:132:PRO:O	1:B:134:PRO:HD2	1.86	0.75
1:A:116:PHE:CD1	1:A:116:PHE:C	2.65	0.74
1:B:41:VAL:CG2	1:B:115:PRO:HG3	2.09	0.74
1:A:348:LYS:N	1:A:349:PRO:HD2	2.01	0.73
1:A:308:LYS:NZ	1:A:316:LEU:HD12	2.03	0.73
1:B:286:ARG:HD2	1:B:287:GLY:N	2.01	0.73
1:A:45:ASP:HB2	1:A:46:PRO:HD3	1.69	0.73
1:B:132:PRO:C	1:B:134:PRO:CD	2.62	0.73
1:B:134:PRO:HA	1:B:135:GLU:C	2.11	0.73
1:B:185:ALA:HA	1:B:202:ALA:O	1.87	0.73
1:A:308:LYS:C	1:A:309:GLU:HG2	2.13	0.72
1:A:308:LYS:HG2	1:A:316:LEU:HD11	1.71	0.72
1:B:200:LEU:HD13	1:B:328:LEU:HD11	1.70	0.72
1:A:246:SER:O	1:A:246:SER:OG	2.07	0.72
1:A:49:LEU:CB	1:A:52:ARG:HD2	2.16	0.72
1:B:45:ASP:H	1:B:46:PRO:HD2	1.55	0.72
1:B:284:GLU:HB3	1:B:286:ARG:HB2	1.72	0.72
1:A:286:ARG:HD3	1:A:287:GLY:H	1.56	0.71
1:B:110:GLY:HA3	1:B:112:HIS:NE2	2.04	0.71
1:B:14:SER:HB3	1:B:19:LEU:HB3	1.73	0.71
1:B:29:VAL:HG12	1:B:31:HIS:CD2	2.26	0.71
1:B:49:LEU:N	1:B:52:ARG:HB2	2.05	0.71
1:A:90:PRO:HB2	1:A:96:ARG:HH12	1.55	0.70
1:A:348:LYS:C	1:A:350:HIS:H	2.00	0.70
1:B:65:GLY:O	1:B:66:ARG:HD2	1.91	0.70
1:B:51:ASP:CB	1:B:153:LYS:HE2	2.18	0.70
1:B:149:ALA:HB3	1:B:165:VAL:CG1	2.21	0.70
1:A:218:ASN:HD21	1:B:268:THR:HG21	1.56	0.69
1:B:313:LYS:C	1:B:313:LYS:HD2	2.17	0.69
1:A:130:LEU:HD23	1:A:131:GLN:N	2.07	0.69
1:A:185:ALA:HA	1:A:202:ALA:O	1.92	0.69
1:B:43:LEU:HD11	1:B:112:HIS:HD2	1.58	0.69
1:A:65:GLY:O	1:A:66:ARG:HD2	1.91	0.69
1:B:348:LYS:HD3	1:B:348:LYS:O	1.91	0.69
1:B:19:LEU:HD22	1:B:44:VAL:HG21	1.75	0.68
1:A:183:PRO:O	1:A:184:SER:C	2.35	0.68
1:A:184:SER:C	1:A:185:ALA:O	2.35	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ARG:HH21	1:B:386:ILE:HG13	1.59	0.68
1:B:19:LEU:HA	1:B:44:VAL:HG22	1.75	0.68
1:B:91:THR:CB	1:B:92:PRO:HD2	2.21	0.68
1:A:184:SER:O	1:A:185:ALA:O	2.12	0.68
1:B:158:LYS:HD2	1:B:160:HIS:CD2	2.28	0.68
1:A:186:GLU:O	1:A:201:GLU:HA	1.93	0.67
1:A:94:PRO:CD	1:A:117:PHE:CZ	2.77	0.67
1:A:305:THR:HG23	1:A:320:VAL:O	1.94	0.67
1:B:101:LEU:HA	1:B:104:ARG:HG3	1.74	0.67
1:A:218:ASN:ND2	1:B:268:THR:HG21	2.09	0.67
1:B:134:PRO:HA	1:B:136:ASP:N	2.09	0.67
1:B:258:GLU:O	1:B:258:GLU:HG2	1.94	0.67
1:B:285:LYS:HG3	1:B:286:ARG:H	1.60	0.67
1:A:68:ASP:O	1:A:70:ASP:N	2.28	0.66
1:A:149:ALA:HB3	1:A:165:VAL:HG12	1.77	0.66
1:B:158:LYS:HG3	1:B:158:LYS:O	1.95	0.66
1:B:68:ASP:O	1:B:69:LEU:HB2	1.94	0.66
1:B:49:LEU:H	1:B:52:ARG:HB2	1.60	0.66
1:A:318:ILE:HD11	1:A:320:VAL:HG22	1.77	0.66
1:B:66:ARG:HG2	1:B:70:ASP:OD1	1.96	0.66
1:B:311:ALA:HA	1:B:312:ASN:O	1.96	0.66
1:A:108:LYS:N	1:A:108:LYS:HD3	2.10	0.66
1:B:56:VAL:HG12	1:B:118:PHE:CZ	2.30	0.66
1:B:305:THR:HG23	1:B:320:VAL:H	1.61	0.66
1:B:307:VAL:O	1:B:308:LYS:HB2	1.95	0.66
1:B:307:VAL:HG23	1:B:308:LYS:H	1.59	0.66
1:B:308:LYS:HE3	1:B:308:LYS:CA	2.24	0.66
1:A:286:ARG:HG3	1:A:286:ARG:NH1	2.04	0.66
1:A:31:HIS:HB2	1:A:34:LYS:HD3	1.76	0.65
1:A:15:PRO:HG2	1:A:162:ARG:HA	1.78	0.65
1:B:95:PRO:HD2	1:B:117:PHE:CE1	2.31	0.65
1:A:94:PRO:CB	1:A:95:PRO:CD	2.73	0.65
1:B:95:PRO:HD2	1:B:117:PHE:HE1	1.61	0.65
1:B:90:PRO:C	1:B:93:ASN:HD21	2.04	0.65
1:A:121:PRO:HB2	1:A:123:ASN:OD1	1.96	0.65
1:B:132:PRO:HD3	1:B:140:ALA:HA	1.78	0.65
1:A:91:THR:H	1:A:96:ARG:HH22	1.44	0.65
1:B:21:VAL:CG2	1:B:165:VAL:HG11	2.28	0.65
1:B:86:GLN:OE1	1:B:89:PRO:HD2	1.97	0.64
1:B:152:ALA:CB	1:B:157:GLU:HG2	2.28	0.64
1:B:96:ARG:N	1:B:97:PRO:HD2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLN:O	1:A:183:PRO:C	2.40	0.64
1:A:68:ASP:O	1:A:69:LEU:C	2.36	0.64
1:B:186:GLU:HG2	1:B:340:LEU:HG	1.80	0.64
1:A:85:TYR:OH	1:A:116:PHE:CB	2.45	0.64
1:B:19:LEU:HD13	1:B:44:VAL:HG23	1.80	0.64
1:A:66:ARG:HB3	1:A:70:ASP:OD2	1.98	0.63
1:B:313:LYS:HB3	1:B:313:LYS:HZ2	1.64	0.63
1:A:243:CYS:SG	1:A:319:LEU:HD23	2.39	0.63
1:A:104:ARG:NH2	1:A:386:ILE:HG13	2.13	0.63
1:A:306:ILE:HG23	1:A:308:LYS:H	1.62	0.63
1:A:149:ALA:HB3	1:A:165:VAL:CG1	2.29	0.63
1:A:257:VAL:HG23	1:A:275:ILE:HD12	1.81	0.63
1:B:184:SER:O	1:B:185:ALA:C	2.41	0.63
1:B:51:ASP:HB3	1:B:153:LYS:CE	2.18	0.62
1:A:285:LYS:HD2	1:A:286:ARG:N	2.14	0.62
1:B:56:VAL:HG12	1:B:118:PHE:HZ	1.64	0.62
1:B:91:THR:HB	1:B:92:PRO:CD	2.28	0.62
1:A:318:ILE:HD11	1:A:320:VAL:CG2	2.28	0.62
1:B:63:ARG:HD3	1:B:144:ASP:OD1	1.99	0.62
1:B:85:TYR:CZ	1:B:117:PHE:HE2	2.17	0.62
1:A:52:ARG:HG3	1:A:151:CYS:HB2	1.81	0.62
1:A:285:LYS:HD2	1:A:286:ARG:H	1.64	0.62
1:A:286:ARG:HH11	1:A:286:ARG:CG	2.10	0.62
1:B:99:THR:CG2	1:B:102:GLN:HB2	2.28	0.62
1:A:248:ALA:C	1:A:249:GLN:HG3	2.25	0.62
1:B:92:PRO:HG2	1:B:94:PRO:HD3	1.81	0.62
1:B:183:PRO:CG	1:B:204:LEU:HB2	2.30	0.62
1:B:313:LYS:HA	1:B:314:GLU:C	2.24	0.62
1:A:285:LYS:O	1:A:288:LEU:HB2	1.99	0.62
1:B:42:VAL:H	1:B:115:PRO:HD3	1.65	0.62
1:B:156:GLU:CD	1:B:156:GLU:H	2.08	0.62
1:B:311:ALA:HB1	1:B:313:LYS:O	2.00	0.62
1:A:331:SER:C	1:A:333:GLY:H	2.04	0.61
1:B:21:VAL:HG23	1:B:165:VAL:HG11	1.81	0.61
1:B:209:TYR:CE2	1:B:215:LEU:HG	2.36	0.61
1:B:66:ARG:NH1	1:B:72:LEU:HD23	2.15	0.61
1:B:152:ALA:HB1	1:B:157:GLU:HG2	1.83	0.61
1:B:41:VAL:HA	1:B:115:PRO:HD3	1.83	0.61
1:A:244:LEU:HD21	1:A:314:GLU:HB2	1.83	0.61
1:B:307:VAL:HG23	1:B:308:LYS:N	2.16	0.61
1:B:30:ASP:HB2	1:B:171:LYS:HE2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ILE:HD11	1:B:320:VAL:HG22	1.82	0.60
1:B:114:HIS:N	1:B:115:PRO:CD	2.62	0.60
1:A:243:CYS:O	1:A:244:LEU:HD23	2.02	0.59
1:B:128:VAL:HG21	1:B:318:ILE:HG12	1.83	0.59
1:B:111:GLN:CD	1:B:111:GLN:C	2.70	0.59
1:A:200:LEU:HD23	1:A:338:VAL:HG13	1.84	0.59
1:B:19:LEU:HD11	1:B:42:VAL:CG2	2.33	0.59
1:B:133:GLY:O	1:B:134:PRO:O	2.20	0.59
1:B:41:VAL:HG13	1:B:115:PRO:HD3	1.85	0.59
1:B:312:ASN:HA	1:B:313:LYS:O	2.03	0.59
1:B:68:ASP:O	1:B:69:LEU:CB	2.51	0.58
1:B:186:GLU:HG3	1:B:339:GLU:O	2.03	0.58
1:B:210:TYR:HA	1:B:345:MET:O	2.03	0.58
1:B:305:THR:CG2	1:B:320:VAL:H	2.15	0.58
1:A:66:ARG:HH11	1:A:66:ARG:CG	2.15	0.58
1:B:45:ASP:C	1:B:47:ASP:H	2.08	0.58
1:A:53:LYS:HE3	1:A:88:PHE:C	2.28	0.58
1:A:133:GLY:O	1:A:135:GLU:HA	2.03	0.58
1:B:208:LEU:HD21	1:B:345:MET:HB2	1.84	0.58
1:A:284:GLU:OE1	1:A:285:LYS:HD2	2.03	0.58
1:A:58:LEU:HD12	1:A:146:GLU:O	2.04	0.58
1:B:133:GLY:N	1:B:134:PRO:CD	2.67	0.58
1:A:53:LYS:HZ3	1:A:86:GLN:CD	2.12	0.58
1:A:68:ASP:C	1:A:70:ASP:N	2.60	0.57
1:A:183:PRO:CG	1:A:204:LEU:HB2	2.30	0.57
1:B:98:PRO:CB	1:B:102:GLN:HB3	2.34	0.57
1:A:348:LYS:C	1:A:350:HIS:N	2.63	0.57
1:B:313:LYS:HG2	1:B:314:GLU:CA	2.29	0.57
1:A:306:ILE:O	1:A:308:LYS:HG3	2.04	0.57
1:A:348:LYS:HG3	1:A:350:HIS:NE2	2.18	0.57
1:B:175:ALA:HB3	1:B:345:MET:HG3	1.87	0.57
1:B:182:GLN:O	1:B:183:PRO:C	2.46	0.57
1:B:306:ILE:HG13	1:B:306:ILE:O	2.03	0.57
1:B:29:VAL:HG12	1:B:31:HIS:HD2	1.70	0.57
1:A:95:PRO:C	1:A:97:PRO:HD2	2.30	0.57
1:B:200:LEU:HD22	1:B:328:LEU:HD12	1.87	0.57
1:A:96:ARG:HA	1:A:117:PHE:CE2	2.40	0.57
1:A:112:HIS:HA	1:A:114:HIS:CE1	2.40	0.57
1:A:67:GLU:HB2	1:A:68:ASP:OD1	2.05	0.56
1:A:318:ILE:HD12	1:A:319:LEU:N	2.19	0.56
1:A:91:THR:H	1:A:96:ARG:NH2	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LYS:NZ	1:A:332:ARG:HB3	2.20	0.56
1:A:227:LYS:HD3	1:A:332:ARG:HB3	1.87	0.56
1:A:331:SER:C	1:A:333:GLY:N	2.61	0.56
1:B:223:ASN:ND2	1:B:264:SER:O	2.37	0.56
1:B:189:ARG:HE	1:B:197:SER:CB	2.18	0.56
1:A:148:ARG:HE	1:A:166:ARG:NH1	2.03	0.56
1:A:315:VAL:HG13	1:A:315:VAL:O	2.04	0.56
1:B:98:PRO:HB3	1:B:102:GLN:HB3	1.86	0.56
1:B:134:PRO:HD3	1:B:136:ASP:HB2	1.87	0.56
1:A:33:ASP:HB3	1:A:34:LYS:CD	2.35	0.56
1:A:308:LYS:HZ3	1:A:316:LEU:HD12	1.68	0.56
1:A:41:VAL:HG12	1:A:42:VAL:N	2.21	0.56
1:B:10:PHE:HA	1:B:389:GLU:O	2.06	0.56
1:A:45:ASP:HB2	1:A:46:PRO:CD	2.36	0.55
1:B:294:LEU:HD12	1:B:294:LEU:O	2.05	0.55
1:A:227:LYS:CE	1:A:332:ARG:HB3	2.36	0.55
1:A:156:GLU:CD	1:A:156:GLU:H	2.13	0.55
1:A:318:ILE:HD12	1:A:319:LEU:H	1.71	0.55
1:B:203:SER:O	1:B:204:LEU:HD23	2.07	0.55
1:A:53:LYS:NZ	1:A:86:GLN:HB3	2.20	0.55
1:A:96:ARG:N	1:A:97:PRO:CD	2.69	0.55
1:A:134:PRO:HB2	1:A:135:GLU:O	2.06	0.55
1:A:132:PRO:HG3	1:A:138:GLY:O	2.07	0.55
1:A:66:ARG:CB	1:A:70:ASP:OD2	2.55	0.55
1:A:99:THR:OG1	1:A:102:GLN:HB2	2.07	0.55
1:A:95:PRO:C	1:A:97:PRO:CD	2.80	0.55
1:A:85:TYR:CE2	1:A:118:PHE:CZ	2.84	0.54
1:B:7:THR:N	1:B:385:ASP:O	2.40	0.54
1:B:43:LEU:HD11	1:B:112:HIS:CD2	2.41	0.54
1:B:184:SER:C	1:B:185:ALA:O	2.50	0.54
1:A:286:ARG:NH1	1:A:286:ARG:CG	2.70	0.54
1:B:183:PRO:HG3	1:B:204:LEU:HB2	1.89	0.54
1:A:172:VAL:HG21	1:A:346:HIS:CD2	2.43	0.54
1:B:196:ARG:HB3	1:B:224:ASN:O	2.07	0.54
1:A:19:LEU:CD1	1:A:44:VAL:HB	2.32	0.54
1:B:183:PRO:O	1:B:184:SER:C	2.50	0.54
1:A:208:LEU:HD23	1:A:209:TYR:N	2.23	0.53
1:A:307:VAL:O	1:A:308:LYS:HB2	2.07	0.53
1:B:18:LYS:O	1:B:44:VAL:HA	2.08	0.53
1:B:45:ASP:N	1:B:46:PRO:HD2	2.21	0.53
1:B:117:PHE:HD2	1:B:117:PHE:H	1.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:HIS:O	1:B:32:LEU:HB2	2.07	0.53
1:B:41:VAL:HA	1:B:115:PRO:CD	2.39	0.53
1:B:152:ALA:HB1	1:B:157:GLU:CB	2.39	0.53
1:A:148:ARG:HE	1:A:166:ARG:CD	2.22	0.53
1:A:191:PHE:CE2	1:A:197:SER:HB3	2.43	0.53
1:B:95:PRO:CD	1:B:117:PHE:HE1	2.21	0.53
1:B:40:GLY:HA3	1:B:116:PHE:CE2	2.43	0.53
1:B:134:PRO:HB3	1:B:135:GLU:HA	1.89	0.53
1:B:15:PRO:C	1:B:17:CYS:HB3	2.34	0.53
1:B:203:SER:HA	1:B:340:LEU:HD21	1.90	0.53
1:A:49:LEU:O	1:A:50:LYS:HB3	2.09	0.52
1:A:307:VAL:C	1:A:308:LYS:HG3	2.35	0.52
1:A:184:SER:O	1:A:185:ALA:C	2.52	0.52
1:B:102:GLN:HE21	1:B:115:PRO:CB	2.22	0.52
1:B:183:PRO:HD3	1:B:206:LYS:C	2.34	0.52
1:B:231:LYS:HA	1:B:261:ASP:O	2.10	0.52
1:A:148:ARG:HG3	1:A:166:ARG:HH11	1.73	0.52
1:A:167:LEU:HD12	1:A:167:LEU:C	2.34	0.52
1:B:148:ARG:CZ	1:B:166:ARG:HD3	2.39	0.52
1:A:107:ARG:HG2	1:A:107:ARG:HH11	1.74	0.52
1:B:284:GLU:HA	1:B:284:GLU:OE1	2.10	0.52
1:A:34:LYS:HD2	1:A:34:LYS:N	2.25	0.52
1:A:63:ARG:NE	1:A:67:GLU:HA	2.25	0.52
1:A:121:PRO:HG2	1:A:124:LEU:HD13	1.92	0.52
1:B:313:LYS:HB3	1:B:313:LYS:NZ	2.24	0.52
1:B:102:GLN:HE21	1:B:115:PRO:HB3	1.75	0.52
1:B:208:LEU:HD23	1:B:209:TYR:N	2.25	0.52
1:A:32:LEU:HD11	1:A:176:PRO:HD3	1.92	0.52
1:A:33:ASP:C	1:A:34:LYS:HD2	2.35	0.52
1:A:308:LYS:HZ2	1:A:316:LEU:HD12	1.73	0.52
1:B:59:THR:HG23	1:B:82:ILE:CG2	2.36	0.52
1:A:94:PRO:HG2	1:A:117:PHE:CE1	2.45	0.51
1:A:46:PRO:HB2	1:A:48:TYR:CE1	2.46	0.51
1:A:85:TYR:OH	1:A:116:PHE:CD1	2.64	0.51
1:B:19:LEU:CA	1:B:44:VAL:HG22	2.39	0.51
1:B:96:ARG:N	1:B:97:PRO:CD	2.74	0.51
1:A:85:TYR:HE2	1:A:118:PHE:CE1	2.26	0.51
1:A:246:SER:O	1:A:247:THR:C	2.52	0.51
1:A:85:TYR:OH	1:A:116:PHE:CG	2.63	0.51
1:B:329:VAL:HA	1:B:335:ASP:OD2	2.10	0.51
1:B:308:LYS:O	1:B:309:GLU:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LYS:HA	1:A:21:VAL:O	2.10	0.51
1:A:159:SER:HB2	1:A:163:ASN:OD1	2.11	0.51
1:B:158:LYS:HD2	1:B:160:HIS:NE2	2.26	0.51
1:B:285:LYS:HG3	1:B:286:ARG:N	2.24	0.51
1:A:28:PHE:CZ	1:A:38:VAL:HG22	2.46	0.51
1:A:175:ALA:HB3	1:A:345:MET:HG3	1.93	0.51
1:B:60:CYS:HB3	1:B:81:PHE:HB3	1.92	0.51
1:B:205:ASP:OD1	1:B:205:ASP:N	2.39	0.51
1:A:198:LEU:HD23	1:A:223:ASN:HA	1.92	0.50
1:A:306:ILE:C	1:A:308:LYS:N	2.69	0.50
1:A:348:LYS:C	1:A:350:HIS:HD2	2.19	0.50
1:A:27:ASP:OD1	1:A:170:ARG:HB2	2.11	0.50
1:B:53:LYS:HD3	1:B:89:PRO:HD3	1.94	0.50
1:B:282:ASN:ND2	1:B:283:ARG:HH21	2.08	0.50
1:A:76:PHE:C	1:A:76:PHE:CD2	2.89	0.50
1:A:188:THR:HG22	1:A:200:LEU:HB3	1.94	0.50
1:B:107:ARG:C	1:B:109:LEU:H	2.19	0.50
1:B:186:GLU:HB2	1:B:338:VAL:HB	1.93	0.50
1:B:305:THR:OG1	1:B:319:LEU:HD13	2.12	0.50
1:A:314:GLU:CG	1:A:315:VAL:N	2.75	0.50
1:A:10:PHE:O	1:A:22:TYR:HA	2.12	0.50
1:B:49:LEU:O	1:B:50:LYS:HB2	2.11	0.50
1:A:62:PHE:O	1:A:77:ARG:HA	2.12	0.49
1:A:88:PHE:HA	1:A:89:PRO:C	2.37	0.49
1:B:86:GLN:HG3	1:B:86:GLN:O	2.11	0.49
1:B:212:GLY:HA2	1:B:278:LEU:HD21	1.92	0.49
1:A:49:LEU:H	1:A:52:ARG:HG2	1.78	0.49
1:A:12:LYS:HD2	1:A:167:LEU:HB3	1.94	0.49
1:B:12:LYS:HD2	1:B:167:LEU:HB3	1.94	0.49
1:B:249:GLN:HB3	1:B:251:LYS:NZ	2.27	0.49
1:A:189:ARG:HG3	1:A:199:HIS:HD2	1.77	0.49
1:B:42:VAL:O	1:B:113:ALA:HA	2.11	0.49
1:A:44:VAL:HG11	1:A:54:VAL:HG21	1.95	0.49
1:B:243:CYS:SG	1:B:319:LEU:HD23	2.53	0.49
1:B:310:GLY:O	1:B:311:ALA:C	2.55	0.49
1:A:96:ARG:N	1:A:97:PRO:HD3	2.28	0.49
1:A:210:TYR:HA	1:A:345:MET:O	2.13	0.49
1:A:230:LYS:O	1:A:230:LYS:HD3	2.13	0.49
1:B:91:THR:CB	1:B:92:PRO:CD	2.87	0.49
1:B:174:PHE:HD1	1:B:346:HIS:O	1.96	0.49
1:A:85:TYR:CE2	1:A:118:PHE:CE1	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:VAL:HG13	1:B:115:PRO:CD	2.42	0.49
1:B:198:LEU:HD13	1:B:336:VAL:HG21	1.93	0.49
1:A:39:ASP:OD2	1:A:99:THR:HG21	2.13	0.48
1:B:49:LEU:C	1:B:51:ASP:H	2.20	0.48
1:B:220:HIS:HD2	1:B:269:PHE:O	1.96	0.48
1:A:53:LYS:HZ3	1:A:86:GLN:CB	2.26	0.48
1:A:130:LEU:HD23	1:A:131:GLN:CA	2.43	0.48
1:B:63:ARG:O	1:B:141:CYS:HB2	2.12	0.48
1:A:35:VAL:HG12	1:A:36:ASP:O	2.13	0.48
1:A:230:LYS:O	1:A:262:GLN:HG3	2.13	0.48
1:B:19:LEU:HD13	1:B:44:VAL:CG2	2.43	0.48
1:B:313:LYS:HD2	1:B:313:LYS:O	2.13	0.48
1:B:313:LYS:CG	1:B:314:GLU:HA	2.33	0.48
1:A:98:PRO:HA	1:A:102:GLN:OE1	2.14	0.48
1:A:116:PHE:CD1	1:A:116:PHE:O	2.67	0.48
1:A:53:LYS:HE3	1:A:89:PRO:N	2.29	0.48
1:A:131:GLN:NE2	1:A:294:LEU:HB2	2.28	0.48
1:B:92:PRO:O	1:B:96:ARG:HG2	2.13	0.48
1:A:242:ILE:HG13	1:A:248:ALA:HB3	1.95	0.48
1:B:132:PRO:CB	1:B:134:PRO:HD3	2.43	0.48
1:B:18:LYS:HB3	1:B:44:VAL:HG13	1.96	0.47
1:B:104:ARG:O	1:B:108:LYS:HG2	2.15	0.47
1:A:52:ARG:HG2	1:A:52:ARG:O	2.14	0.47
1:A:237:ARG:HH11	1:A:237:ARG:HG3	1.79	0.47
1:B:132:PRO:HB2	1:B:134:PRO:CD	2.45	0.47
1:A:227:LYS:CD	1:A:332:ARG:HB3	2.45	0.47
1:A:49:LEU:HB2	1:A:52:ARG:CD	2.23	0.47
1:B:10:PHE:CE2	1:B:26:ARG:NH1	2.82	0.47
1:B:48:TYR:C	1:B:52:ARG:HB2	2.40	0.47
1:B:242:ILE:HB	1:B:246:SER:O	2.15	0.47
1:B:96:ARG:O	1:B:98:PRO:HD3	2.15	0.47
1:A:183:PRO:HG3	1:A:207:GLU:HA	1.97	0.47
1:B:250:TYR:C	1:B:251:LYS:HE2	2.40	0.47
1:A:49:LEU:HD13	1:A:51:ASP:HB2	1.97	0.46
1:B:192:LEU:HD13	1:B:227:LYS:CG	2.44	0.46
1:A:130:LEU:HD23	1:A:130:LEU:C	2.40	0.46
1:B:76:PHE:CD1	1:B:245:PHE:CD1	3.03	0.46
1:A:323:ARG:HG3	1:A:341:PRO:HA	1.96	0.46
1:B:90:PRO:O	1:B:93:ASN:ND2	2.48	0.46
1:B:348:LYS:HD3	1:B:348:LYS:C	2.41	0.46
1:A:49:LEU:O	1:A:49:LEU:HD22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:TYR:CD1	1:A:250:TYR:N	2.84	0.46
1:A:306:ILE:O	1:A:306:ILE:CG2	2.59	0.46
1:B:41:VAL:HA	1:B:115:PRO:CG	2.46	0.46
1:A:85:TYR:CZ	1:A:116:PHE:HB2	2.50	0.46
1:A:393:ARG:H	1:A:393:ARG:HG3	1.49	0.46
1:B:98:PRO:O	1:B:99:THR:C	2.59	0.46
1:B:149:ALA:HB3	1:B:165:VAL:HG12	1.94	0.46
1:B:259:GLN:HG2	1:B:260:ASP:N	2.31	0.46
1:A:53:LYS:NZ	1:A:86:GLN:CD	2.73	0.46
1:B:140:ALA:O	1:B:141:CYS:HB3	2.16	0.46
1:A:82:ILE:HD12	1:A:82:ILE:O	2.15	0.46
1:B:19:LEU:HD12	1:B:20:THR:N	2.31	0.46
1:A:196:ARG:HA	1:A:196:ARG:NE	2.20	0.46
1:A:331:SER:O	1:A:333:GLY:N	2.48	0.46
1:A:12:LYS:HB3	1:A:167:LEU:HD23	1.98	0.46
1:A:28:PHE:CE2	1:A:38:VAL:HG22	2.51	0.46
1:A:116:PHE:C	1:A:116:PHE:HD1	2.21	0.46
1:B:111:GLN:CD	1:B:112:HIS:N	2.74	0.46
1:B:308:LYS:HE3	1:B:308:LYS:HA	1.97	0.46
1:A:58:LEU:HD13	1:A:147:ILE:HG12	1.98	0.45
1:A:307:VAL:O	1:A:308:LYS:CB	2.64	0.45
1:B:22:TYR:HB2	1:B:41:VAL:HB	1.98	0.45
1:B:158:LYS:CD	1:B:160:HIS:CD2	2.97	0.45
1:B:312:ASN:O	1:B:312:ASN:OD1	2.34	0.45
1:A:191:PHE:HE2	1:A:197:SER:HB3	1.79	0.45
1:B:7:THR:HB	1:B:385:ASP:O	2.16	0.45
1:A:315:VAL:O	1:A:315:VAL:CG1	2.64	0.45
1:B:90:PRO:C	1:B:91:THR:HG23	2.42	0.45
1:A:34:LYS:HA	1:A:122:GLN:NE2	2.31	0.45
1:A:64:TYR:CE2	1:A:139:LYS:HB2	2.51	0.45
1:A:230:LYS:HD3	1:A:230:LYS:C	2.41	0.45
1:B:62:PHE:O	1:B:77:ARG:HA	2.15	0.45
1:A:46:PRO:HD2	1:A:48:TYR:CE1	2.51	0.45
1:A:227:LYS:HD3	1:A:332:ARG:CB	2.46	0.45
1:A:148:ARG:CD	1:A:166:ARG:HH11	2.30	0.45
1:B:19:LEU:CD1	1:B:42:VAL:HG22	2.47	0.45
1:A:91:THR:HG23	1:A:92:PRO:HD2	1.98	0.45
1:A:308:LYS:NZ	1:A:319:LEU:HD21	2.31	0.45
1:B:13:SER:HB3	1:B:20:THR:HG23	1.99	0.45
1:B:14:SER:N	1:B:19:LEU:O	2.46	0.45
1:B:152:ALA:HB1	1:B:157:GLU:CG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:HIS:CD2	1:B:393:ARG:HD2	2.52	0.45
1:A:306:ILE:O	1:A:308:LYS:CA	2.64	0.45
1:B:391:PHE:C	1:B:391:PHE:CD2	2.94	0.45
1:A:183:PRO:CB	1:A:204:LEU:HD12	2.47	0.45
1:B:306:ILE:O	1:B:307:VAL:C	2.60	0.45
1:A:49:LEU:N	1:A:52:ARG:HG2	2.32	0.45
1:A:192:LEU:HD13	1:A:227:LYS:HG3	1.99	0.45
1:B:13:SER:HB3	1:B:20:THR:OG1	2.16	0.45
1:A:74:LEU:HD12	1:A:74:LEU:HA	1.66	0.44
1:B:99:THR:O	1:B:100:ARG:C	2.60	0.44
1:B:148:ARG:NE	1:B:166:ARG:HH11	2.15	0.44
1:A:46:PRO:O	1:A:48:TYR:HD1	2.01	0.44
1:B:45:ASP:C	1:B:47:ASP:N	2.74	0.44
1:B:66:ARG:HB3	1:B:70:ASP:OD2	2.17	0.44
1:B:96:ARG:O	1:B:98:PRO:CD	2.65	0.44
1:B:202:ALA:HA	1:B:218:ASN:O	2.17	0.44
1:B:261:ASP:C	1:B:262:GLN:HG3	2.41	0.44
1:B:288:LEU:HD12	1:B:288:LEU:HA	1.74	0.44
1:B:318:ILE:HD11	1:B:320:VAL:CG2	2.46	0.44
1:A:186:GLU:HB3	1:A:338:VAL:HB	1.98	0.44
1:B:66:ARG:HD3	1:B:73:GLY:HA3	1.98	0.44
1:A:128:VAL:HA	1:A:290:LEU:O	2.17	0.44
1:A:285:LYS:CD	1:A:286:ARG:N	2.80	0.44
1:B:42:VAL:N	1:B:115:PRO:HD3	2.31	0.44
1:B:151:CYS:SG	1:B:163:ASN:ND2	2.91	0.44
1:B:39:ASP:HB2	1:B:99:THR:HG21	1.98	0.44
1:B:93:ASN:N	1:B:94:PRO:CD	2.81	0.44
1:B:182:GLN:O	1:B:184:SER:N	2.50	0.44
1:B:264:SER:O	1:B:267:SER:HB3	2.18	0.44
1:A:161:LYS:HA	1:A:164:SER:OG	2.17	0.44
1:A:16:ASN:HD21	1:A:163:ASN:HA	1.83	0.44
1:A:52:ARG:CG	1:A:151:CYS:HB2	2.45	0.44
1:A:248:ALA:C	1:A:249:GLN:CG	2.91	0.44
1:A:35:VAL:O	1:A:36:ASP:C	2.60	0.44
1:A:220:HIS:CD2	1:A:220:HIS:C	2.96	0.44
1:A:271:LYS:CG	1:A:272:VAL:N	2.81	0.44
1:B:48:TYR:HA	1:B:49:LEU:HA	1.43	0.44
1:A:34:LYS:O	1:A:35:VAL:HG23	2.18	0.43
1:A:53:LYS:HG3	1:A:88:PHE:O	2.18	0.43
1:A:67:GLU:CB	1:A:68:ASP:OD1	2.65	0.43
1:B:41:VAL:CA	1:B:115:PRO:HD3	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:C	1:B:51:ASP:N	2.74	0.43
1:B:128:VAL:HG12	1:B:143:VAL:HB	2.00	0.43
1:A:148:ARG:CG	1:A:166:ARG:HH11	2.31	0.43
1:B:186:GLU:HA	1:B:186:GLU:OE1	2.18	0.43
1:A:146:GLU:OE1	1:A:166:ARG:NH1	2.52	0.43
1:A:309:GLU:HB2	1:A:310:GLY:H	1.69	0.43
1:A:348:LYS:O	1:A:348:LYS:HG2	2.18	0.43
1:B:134:PRO:CB	1:B:135:GLU:HA	2.48	0.43
1:B:172:VAL:HG21	1:B:346:HIS:CD2	2.53	0.43
1:B:203:SER:HA	1:B:340:LEU:CD2	2.48	0.43
1:B:244:LEU:O	1:B:246:SER:N	2.50	0.43
1:B:152:ALA:HB1	1:B:157:GLU:HB3	1.99	0.43
1:B:132:PRO:HB2	1:B:134:PRO:HD3	2.01	0.43
1:B:148:ARG:HE	1:B:166:ARG:NH1	2.16	0.43
1:A:94:PRO:HG2	1:A:117:PHE:HE1	1.84	0.43
1:A:134:PRO:N	1:A:135:GLU:HA	2.33	0.43
1:A:226:THR:O	1:A:226:THR:HG23	2.18	0.43
1:A:308:LYS:HG2	1:A:316:LEU:CD1	2.45	0.43
1:B:174:PHE:CE1	1:B:210:TYR:CE2	3.06	0.43
1:A:147:ILE:O	1:A:147:ILE:HG22	2.19	0.43
1:A:174:PHE:CD2	1:A:174:PHE:C	2.94	0.43
1:B:136:ASP:O	1:B:138:GLY:N	2.51	0.43
1:B:152:ALA:HB2	1:B:157:GLU:HG2	1.99	0.43
1:A:85:TYR:CD1	1:A:85:TYR:C	2.96	0.43
1:A:85:TYR:CD2	1:A:85:TYR:N	2.86	0.43
1:B:90:PRO:C	1:B:93:ASN:ND2	2.73	0.43
1:B:155:LEU:O	1:B:157:GLU:N	2.51	0.43
1:B:215:LEU:N	1:B:215:LEU:HD12	2.33	0.43
1:A:167:LEU:HD12	1:A:167:LEU:O	2.19	0.43
1:A:305:THR:CG2	1:A:320:VAL:N	2.82	0.43
1:B:200:LEU:CD2	1:B:338:VAL:HG22	2.49	0.43
1:A:49:LEU:CD1	1:A:51:ASP:HB2	2.49	0.43
1:A:53:LYS:HZ3	1:A:86:GLN:HB3	1.83	0.43
1:A:187:THR:O	1:A:188:THR:HB	2.18	0.43
1:A:330:VAL:HB	1:A:334:GLY:O	2.19	0.43
1:B:93:ASN:O	1:B:94:PRO:C	2.62	0.43
1:B:148:ARG:CG	1:B:166:ARG:HD2	2.42	0.43
1:B:229:VAL:HB	1:B:263:VAL:H	1.83	0.43
1:B:249:GLN:HB3	1:B:251:LYS:HZ1	1.83	0.43
1:A:46:PRO:HD2	1:A:48:TYR:HE1	1.84	0.42
1:A:186:GLU:OE1	1:A:186:GLU:HA	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASN:HD21	1:B:268:THR:CG2	2.27	0.42
1:B:10:PHE:HE1	1:B:24:GLY:O	2.03	0.42
1:A:53:LYS:HE3	1:A:88:PHE:O	2.19	0.42
1:A:126:CYS:SG	1:A:173:GLN:HB2	2.59	0.42
1:A:303:SER:O	1:A:304:SER:C	2.62	0.42
1:A:268:THR:HG21	1:B:266:SER:OG	2.19	0.42
1:A:320:VAL:HG12	1:A:321:SER:N	2.33	0.42
1:A:153:LYS:HG2	1:A:157:GLU:OE2	2.20	0.42
1:A:125:PRO:HG2	1:A:143:VAL:HG11	2.02	0.42
1:A:150:PHE:HB3	1:A:164:SER:HB2	2.01	0.42
1:B:27:ASP:OD1	1:B:170:ARG:HB2	2.18	0.42
1:B:309:GLU:O	1:B:309:GLU:CG	2.68	0.42
1:A:45:ASP:CB	1:A:46:PRO:HD3	2.43	0.42
1:A:53:LYS:CE	1:A:89:PRO:HD2	2.49	0.42
1:A:67:GLU:C	1:A:68:ASP:CG	2.87	0.42
1:A:209:TYR:CD2	1:A:215:LEU:HG	2.54	0.42
1:B:207:GLU:HG2	1:B:208:LEU:N	2.34	0.42
1:B:265:PRO:O	1:B:266:SER:C	2.63	0.42
1:B:312:ASN:CB	1:B:315:VAL:HB	2.49	0.42
1:B:47:ASP:O	1:B:47:ASP:CG	2.63	0.42
1:A:46:PRO:HB2	1:A:48:TYR:HE1	1.83	0.42
1:A:99:THR:O	1:A:100:ARG:C	2.63	0.42
1:A:148:ARG:NE	1:A:166:ARG:CD	2.82	0.42
1:A:151:CYS:O	1:A:152:ALA:HB2	2.19	0.42
1:B:67:GLU:O	1:B:67:GLU:HG2	2.20	0.42
1:B:209:TYR:O	1:B:344:LEU:HD23	2.20	0.42
1:A:148:ARG:HE	1:A:166:ARG:HH11	1.68	0.42
1:A:175:ALA:HA	1:A:176:PRO:HD3	1.82	0.42
1:A:208:LEU:HG	1:A:343:VAL:HG22	2.01	0.42
1:B:149:ALA:HB3	1:B:165:VAL:HG13	2.01	0.42
1:B:213:GLU:HA	1:B:214:PRO:HD3	1.84	0.42
1:B:325:LYS:HG3	1:B:339:GLU:HG2	2.01	0.42
1:A:208:LEU:HD23	1:A:208:LEU:C	2.44	0.41
1:B:223:ASN:ND2	1:B:265:PRO:HA	2.35	0.41
1:A:107:ARG:HG2	1:A:107:ARG:NH1	2.35	0.41
1:B:56:VAL:HG22	1:B:149:ALA:CB	2.51	0.41
1:B:285:LYS:O	1:B:286:ARG:O	2.36	0.41
1:A:314:GLU:HG2	1:A:315:VAL:H	1.85	0.41
1:B:56:VAL:HG22	1:B:149:ALA:HB2	2.02	0.41
1:B:90:PRO:O	1:B:91:THR:OG1	2.30	0.41
1:B:99:THR:O	1:B:102:GLN:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:THR:HG22	1:B:200:LEU:HB3	2.02	0.41
1:A:96:ARG:O	1:A:97:PRO:C	2.63	0.41
1:A:124:LEU:O	1:A:171:LYS:NZ	2.53	0.41
1:B:15:PRO:HG2	1:B:162:ARG:HA	2.02	0.41
1:A:33:ASP:O	1:A:122:GLN:NE2	2.53	0.41
1:A:66:ARG:CG	1:A:66:ARG:NH1	2.79	0.41
1:A:96:ARG:O	1:A:98:PRO:HD3	2.21	0.41
1:A:98:PRO:O	1:A:99:THR:C	2.64	0.41
1:A:250:TYR:CD2	1:A:287:GLY:HA3	2.55	0.41
1:A:319:LEU:HA	1:A:319:LEU:HD13	1.84	0.41
1:B:170:ARG:HD3	1:B:291:ASP:O	2.20	0.41
1:B:200:LEU:HD22	1:B:328:LEU:CD1	2.49	0.41
1:B:200:LEU:HD21	1:B:338:VAL:HG22	2.02	0.41
1:A:36:ASP:HA	1:A:37:PRO:HD3	1.94	0.41
1:A:306:ILE:O	1:A:308:LYS:CG	2.69	0.41
1:B:7:THR:HG23	1:B:8:ARG:N	2.35	0.41
1:B:7:THR:O	1:B:387:VAL:HB	2.21	0.41
1:B:99:THR:HG22	1:B:102:GLN:OE1	2.21	0.41
1:A:41:VAL:CG1	1:A:42:VAL:N	2.84	0.41
1:B:66:ARG:HD3	1:B:72:LEU:O	2.21	0.41
1:B:313:LYS:HA	1:B:315:VAL:N	2.36	0.41
1:A:148:ARG:NE	1:A:166:ARG:NH1	2.68	0.41
1:A:209:TYR:CE2	1:A:215:LEU:HG	2.56	0.41
1:A:252:CYS:HA	1:A:253:PRO:HD2	1.92	0.41
1:A:308:LYS:HZ1	1:A:319:LEU:HD21	1.86	0.41
1:B:85:TYR:OH	1:B:117:PHE:HE2	2.03	0.41
1:A:64:TYR:CD2	1:A:64:TYR:C	2.99	0.41
1:A:174:PHE:CG	1:A:175:ALA:N	2.88	0.41
1:B:28:PHE:CD1	1:B:28:PHE:N	2.89	0.41
1:A:46:PRO:CB	1:A:48:TYR:HE1	2.34	0.40
1:B:19:LEU:HD11	1:B:42:VAL:HG22	2.01	0.40
1:A:150:PHE:HB3	1:A:164:SER:CB	2.51	0.40
1:A:346:HIS:HA	1:A:347:PRO:HD3	1.94	0.40
1:B:45:ASP:HB3	1:B:46:PRO:HD3	2.02	0.40
1:B:93:ASN:O	1:B:96:ARG:HG3	2.21	0.40
1:A:44:VAL:O	1:A:44:VAL:HG13	2.21	0.40
1:A:65:GLY:HA2	1:A:139:LYS:HD3	2.03	0.40
1:A:244:LEU:HD23	1:A:244:LEU:HA	1.81	0.40
1:B:22:TYR:O	1:B:23:LEU:HG	2.22	0.40
1:B:65:GLY:HA3	1:B:73:GLY:O	2.21	0.40
1:A:54:VAL:HG22	1:A:151:CYS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:THR:HG21	1:A:319:LEU:HA	2.04	0.40
1:B:109:LEU:HD23	1:B:109:LEU:HA	1.93	0.40
1:B:133:GLY:HA3	1:B:286:ARG:HA	2.04	0.40
1:B:279:LEU:O	1:B:280:SER:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	350/393 (89%)	282 (81%)	47 (13%)	21 (6%)	1	7
1	B	348/393 (88%)	293 (84%)	34 (10%)	21 (6%)	1	7
All	All	698/786 (89%)	575 (82%)	81 (12%)	42 (6%)	1	7

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	PRO
1	A	185	ALA
1	A	307	VAL
1	A	308	LYS
1	A	348	LYS
1	B	46	PRO
1	B	70	ASP
1	B	91	THR
1	B	94	PRO
1	B	115	PRO
1	B	134	PRO
1	B	286	ARG
1	B	334	GLY
1	A	99	THR

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Mol	Chain	Res	Type
1	A	193	MET
1	A	247	THR
1	A	315	VAL
1	B	99	THR
1	B	137	THR
1	A	34	LYS
1	A	69	LEU
1	A	313	LYS
1	B	97	PRO
1	B	156	GLU
1	B	266	SER
1	B	307	VAL
1	A	85	TYR
1	A	152	ALA
1	A	183	PRO
1	A	286	ARG
1	B	45	ASP
1	B	108	LYS
1	B	193	MET
1	A	45	ASP
1	B	114	HIS
1	B	185	ALA
1	B	311	ALA
1	B	315	VAL
1	A	81	PHE
1	A	110	GLY
1	A	349	PRO
1	A	97	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/353 (91%)	260 (81%)	60 (19%)	1	9
1	B	318/353 (90%)	264 (83%)	54 (17%)	2	11
All	All	638/706 (90%)	524 (82%)	114 (18%)	2	10

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	19	LEU
1	A	32	LEU
1	A	34	LYS
1	A	45	ASP
1	A	47	ASP
1	A	49	LEU
1	A	52	ARG
1	A	57	THR
1	A	63	ARG
1	A	66	ARG
1	A	68	ASP
1	A	72	LEU
1	A	82	ILE
1	A	84	ASN
1	A	104	ARG
1	A	108	LYS
1	A	112	HIS
1	A	116	PHE
1	A	119	THR
1	A	122	GLN
1	A	129	THR
1	A	147	ILE
1	A	148	ARG
1	A	151	CYS
1	A	156	GLU
1	A	163	ASN
1	A	166	ARG
1	A	178	LYS
1	A	183	PRO
1	A	187	THR
1	A	192	LEU
1	A	193	MET
1	A	195	ASP
1	A	196	ARG
1	A	198	LEU
1	A	203	SER
1	A	205	ASP
1	A	225	SER
1	A	226	THR
1	A	230	LYS
1	A	251	LYS

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Mol	Chain	Res	Type
1	A	275	ILE
1	A	276	THR
1	A	285	LYS
1	A	286	ARG
1	A	288	LEU
1	A	305	THR
1	A	306	ILE
1	A	309	GLU
1	A	315	VAL
1	A	318	ILE
1	A	319	LEU
1	A	321	SER
1	A	323	ARG
1	A	332	ARG
1	A	343	VAL
1	A	344	LEU
1	A	385	ASP
1	A	393	ARG
1	B	7	THR
1	B	19	LEU
1	B	26	ARG
1	B	39	ASP
1	B	57	THR
1	B	63	ARG
1	B	66	ARG
1	B	72	LEU
1	B	82	ILE
1	B	93	ASN
1	B	96	ARG
1	B	99	THR
1	B	104	ARG
1	B	111	GLN
1	B	112	HIS
1	B	117	PHE
1	B	119	THR
1	B	120	ILE
1	B	122	GLN
1	B	135	GLU
1	B	136	ASP
1	B	147	ILE
1	B	154	SER
1	B	156	GLU

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Mol	Chain	Res	Type
1	B	158	LYS
1	B	182	GLN
1	B	187	THR
1	B	192	LEU
1	B	193	MET
1	B	198	LEU
1	B	205	ASP
1	B	244	LEU
1	B	251	LYS
1	B	256	GLN
1	B	257	VAL
1	B	260	ASP
1	B	263	VAL
1	B	267	SER
1	B	268	THR
1	B	283	ARG
1	B	286	ARG
1	B	294	LEU
1	B	300	ASN
1	B	308	LYS
1	B	313	LYS
1	B	315	VAL
1	B	318	ILE
1	B	319	LEU
1	B	323	ARG
1	B	332	ARG
1	B	338	VAL
1	B	340	LEU
1	B	343	VAL
1	B	344	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	122	GLN
1	A	131	GLN
1	A	199	HIS
1	A	216	ASN
1	A	259	GLN
1	A	296	HIS
1	A	346	HIS

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Mol	Chain	Res	Type
1	A	350	HIS
1	B	16	ASN
1	B	31	HIS
1	B	93	ASN
1	B	114	HIS
1	B	122	GLN
1	B	160	HIS
1	B	163	ASN
1	B	182	GLN
1	B	211	HIS
1	B	216	ASN
1	B	218	ASN
1	B	220	HIS
1	B	223	ASN
1	B	282	ASN
1	B	312	ASN
1	B	346	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	354/393 (90%)	-0.36	3 (0%) 82 64	60, 99, 184, 286	0
1	B	352/393 (89%)	-0.34	0 100 100	66, 116, 206, 280	0
All	All	706/786 (89%)	-0.35	3 (0%) 88 76	60, 107, 198, 286	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	LYS	4.5
1	A	85	TYR	2.3
1	A	45	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.