Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 11:10 AM EDT

PDB ID	:	3P2D
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 (i) 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 (1)) were used in the production of this report:

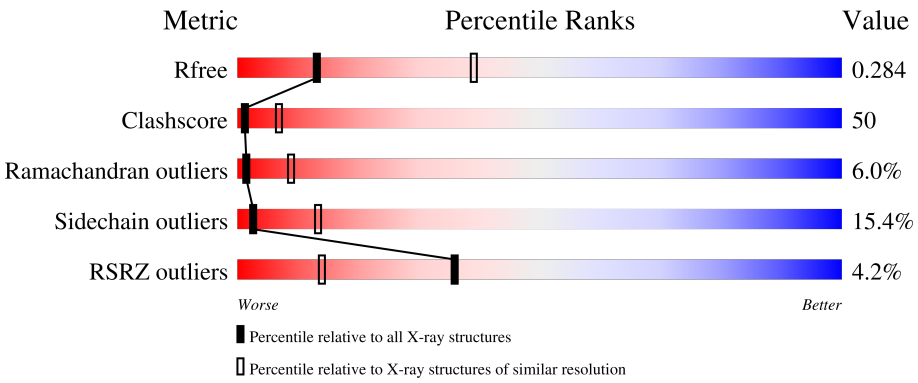
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 <=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	3%; 37%; 40%; 12%; •; 10%
1	B	393	4%; 33%; 44%; 12%; •; 10%

2 Entry composition (i)

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.

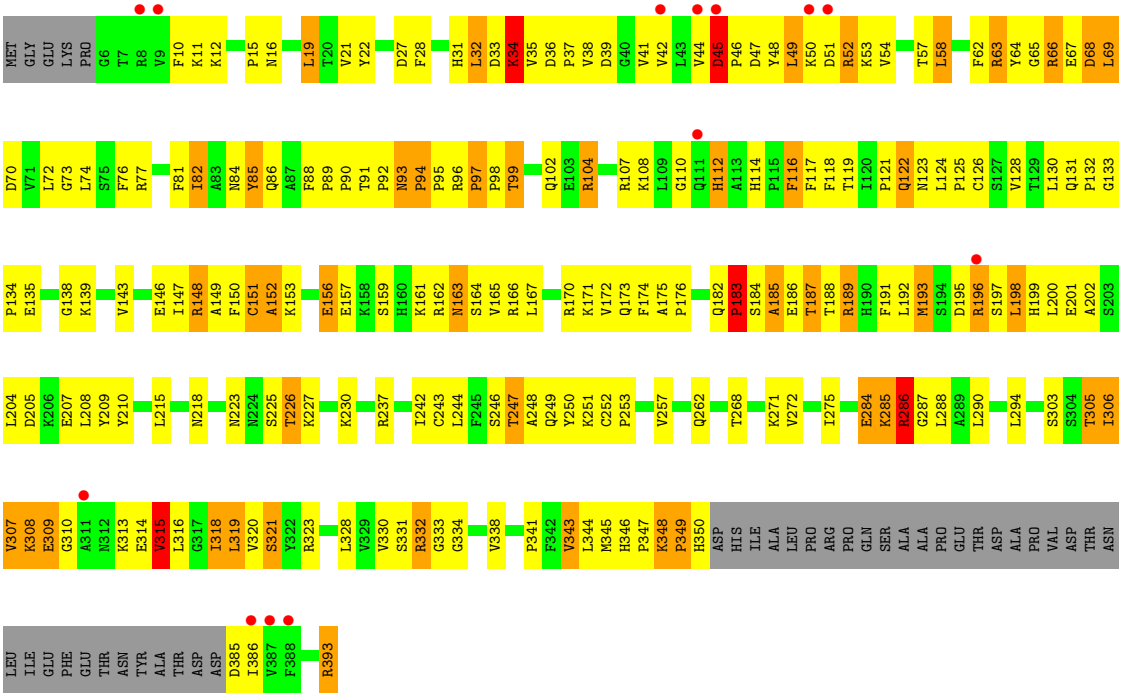
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	354	2814	1792	497	515	10	0	0	0
			Total	C	N	O	S			
1	B	352	2797	1781	493	513	10	0	0	0

3 Residue-property plots (i)

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

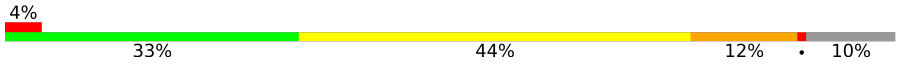
- Molecule 1: Beta-arrestin-2

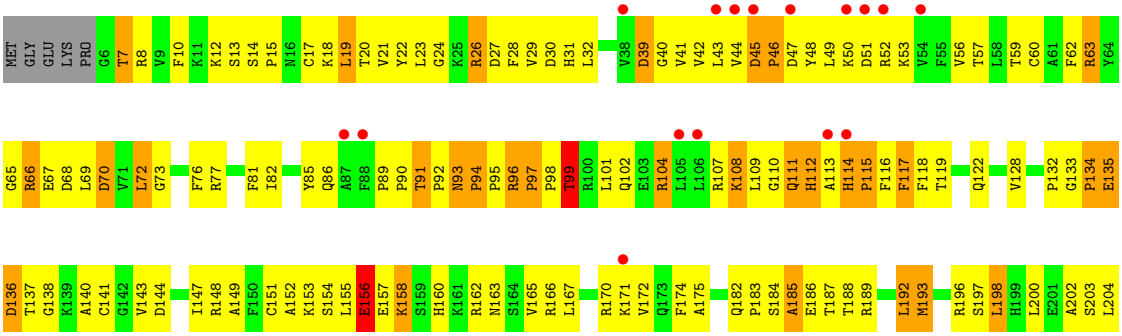
Chain A:

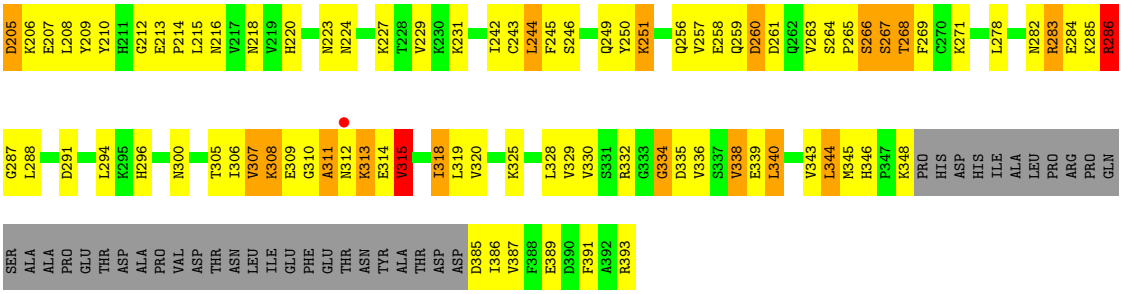


- Molecule 1: Beta-arrestin-2

Chain B:






D205 K206 E207 L208 Y209 Y210 H211 G212 E213 P214 L215 N216 V217 N218 V219 H220 N223 N224 K227 T228 V229 K230 K231 I242 C243 L244 F245 S246 Q249 Y250 K251 Q256 V257 E258 Q259 D260 D261 Q262 V263 S264 P265 S266 S267 T268 F269 C270 K271 L278 N282 R283 E284 K285 R286
G287 L288 D291 L294 K295 H296 N300 T305 I306 V307 K308 E309 G310 A311 N312 K313 E314 V315 I318 L319 V320 K325 L328 V329 V330 S331 R332 G333 G334 D335 V336 S337 V338 E339 L340 V343 L344 M345 H346 P347 K348 PRO HIS ASP HIS ILE ALA LEU PRO ARG PRO GLN
SER ALA ALA PRO GLU THR ASP ALA PRO VAL ASP THR ASN LEU ILE GLU PHE GLU THR ASN TYR ALA THR ASP ASP D385 I386 V387 F388 E389 D390 F391 A392 R393

4 Data and refinement statistics (i)

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 49.55 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.6 (35.36-3.00) 92.6 (49.55-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.219 , 0.286 0.218 , 0.284	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)	0.33 , 93.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	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.*

[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 (i)

5.1 Standard geometry (i)

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	0.56	0/2878	0.75	2/3897 (0.1%)
1	B	0.52	0/2859	0.71	0/3870
All	All	0.54	0/5737	0.73	2/7767 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	93	ASN	C-N-CD	-6.82	105.61	120.60
1	A	58	LEU	CA-CB-CG	-5.21	103.31	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2814	0	2856	284	0
1	B	2797	0	2842	289	0
All	All	5611	0	5698	569	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 50.

All (569) 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: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:311:ALA:HA	1:B:312:ASN:C	1.85	0.96
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: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:200:LEU:HD13	1:A:328:LEU:HD11	1.58	0.84
1:B:132:PRO:C	1:B:134:PRO:HD2	1.99	0.83
1:B:312:ASN:HA	1:B:313:LYS:C	1.98	0.83
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:33:ASP:HB3	1:A:34:LYS:HD2	1.68	0.75
1:A:49:LEU:HB3	1:A:52:ARG:HB3	1.67	0.75
1:B:132:PRO:O	1:B:134:PRO:HD2	1.86	0.75
1:B:117:PHE:N	1:B:117:PHE:CD2	2.54	0.75
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:185:ALA:HA	1:B:202:ALA:O	1.87	0.73
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: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:A:82:ILE:C	1:A:82:ILE:HD12	2.10	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:B:95:PRO:C	1:B:97:PRO:HD2	2.11	0.70
1:A:90:PRO:HB2	1:A:96:ARG:HH12	1.55	0.70
1:A:133:GLY:C	1:A:135:GLU:HA	2.11	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:116:PHE:CD1	1:A:116:PHE:C	2.65	0.69
1:A:218:ASN:HD21	1:B:268:THR:HG21	1.56	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:B:259:GLN:CD	1:B:271:LYS:HZ3	1.95	0.69
1:A:65:GLY:O	1:A:66:ARG:HD2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:134:PRO:HA	1:B:135:GLU:C	2.11	0.68
1:B:132:PRO:C	1:B:134:PRO:CD	2.62	0.68
1:A:308:LYS:C	1:A:309:GLU:HG2	2.13	0.68
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:A:348:LYS:C	1:A:350:HIS:H	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:313:LYS:C	1:B:313:LYS:HD2	2.17	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
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:183:PRO:O	1:A:184:SER:C	2.35	0.64
1:A:66:ARG:HB3	1:A:70:ASP:OD2	1.98	0.63
1:A:184:SER:C	1:A:185:ALA:O	2.35	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: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:A:246:SER:O	1:A:246:SER:OG	2.07	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: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: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:311:ALA:HB1	1:B:313:LYS:O	2.00	0.62
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:A:68:ASP:O	1:A:69:LEU:C	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:90:PRO:C	1:B:93:ASN:HD21	2.04	0.60
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:A:182:GLN:O	1:A:183:PRO:C	2.40	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: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:B:184:SER:O	1:B:185:ALA:C	2.41	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: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: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:331:SER:C	1:A:333:GLY:H	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: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:B:313:LYS:HA	1:B:314:GLU:C	2.24	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:B:156:GLU:CD	1:B:156:GLU:H	2.08	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: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:248:ALA:C	1:A:249:GLN:HG3	2.25	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: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: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:85:TYR:CE2	1:A:118:PHE:CZ	2.84	0.54
1:A:308:LYS:HZ2	1:A:316:LEU:HD12	1.70	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:31:HIS:O	1:B:32:LEU:HB2	2.07	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:45:ASP:C	1:B:47:ASP:H	2.08	0.54
1:A:53:LYS:HE3	1:A:88:PHE:C	2.28	0.53
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:A:308:LYS:HZ3	1:A:316:LEU:HD12	1.71	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: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:68:ASP:C	1:A:70:ASP:N	2.60	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: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:348:LYS:C	1:A:350:HIS:N	2.63	0.52
1:B:182:GLN:O	1:B:183:PRO:C	2.46	0.52
1:B:102:GLN:HE21	1:B:115:PRO:CB	2.22	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:95:PRO:C	1:A:97:PRO:HD2	2.30	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:A:303:SER:HB2	1:A:345:MET:HE2	1.92	0.52
1:A:331:SER:C	1:A:333:GLY:N	2.61	0.52
1:B:313:LYS:NZ	1:B:313:LYS:HB3	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: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: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:A:345:MET:HE2	1:A:345:MET:HA	1.92	0.51
1:B:308:LYS:O	1:B:309:GLU:HB3	2.10	0.51
1:A:11:LYS:HA	1:A:21:VAL:O	2.10	0.51
1:A:156:GLU:CD	1:A:156:GLU:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:306:ILE:O	1:A:306:ILE:CG2	2.59	0.50
1:A:198:LEU:HD23	1:A:223:ASN:HA	1.92	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:111:GLN:CD	1:B:111:GLN:C	2.70	0.50
1:B:282:ASN:ND2	1:B:283:ARG:HH21	2.08	0.50
1:A:188:THR:HG22	1:A:200:LEU:HB3	1.94	0.50
1:B:186:GLU:HB2	1:B:338:VAL:HB	1.93	0.50
1:A:95:PRO:C	1:A:97:PRO:CD	2.80	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:A:345:MET:HA	1:A:345:MET:CE	2.42	0.50
1:B:49:LEU:O	1:B:50:LYS:HB2	2.11	0.50
1:B:184:SER:C	1:B:185:ALA:O	2.50	0.50
1:A:62:PHE:O	1:A:77:ARG:HA	2.12	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: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:B:183:PRO:O	1:B:184:SER:C	2.50	0.49
1:A:53:LYS:HZ3	1:A:86:GLN:CB	2.25	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:220:HIS:HD2	1:B:269:PHE:O	1.96	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:183:PRO:HD3	1:B:206:LYS:C	2.34	0.48
1:B:249:GLN:HB3	1:B:251:LYS:HZ1	1.78	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:15:PRO:C	1:B:17:CYS:HB3	2.34	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:A:184:SER:O	1:A:185:ALA:C	2.52	0.47
1:A:307:VAL:C	1:A:308:LYS:HG3	2.35	0.47
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:167:LEU:HD12	1:A:167:LEU:C	2.34	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:B:313:LYS:HB3	1:B:313:LYS:HZ2	1.79	0.47
1:A:227:LYS:CD	1:A:332:ARG:HB3	2.45	0.47
1:A:33:ASP:C	1:A:34:LYS:HD2	2.35	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: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:A:49:LEU:HD13	1:A:51:ASP:HB2	1.97	0.46
1:A:246:SER:O	1:A:247:THR:C	2.52	0.46
1:B:192:LEU:HD13	1:B:227:LYS:CG	2.44	0.46
1:B:76:PHE:CD1	1:B:245:PHE:CD1	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:49:LEU:O	1:A:49:LEU:HD22	2.16	0.46
1:A:250:TYR:CD1	1:A:250:TYR:N	2.84	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: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: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: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:306:ILE:C	1:A:308:LYS:N	2.69	0.45
1:A:307:VAL:O	1:A:308:LYS:CB	2.64	0.45
1:A:348:LYS:C	1:A:350:HIS:HD2	2.19	0.45
1:B:22:TYR:HB2	1:B:41:VAL:HB	1.98	0.45
1:B:107:ARG:C	1:B:109:LEU:H	2.19	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:76:PHE:C	1:A:76:PHE:CD2	2.89	0.45
1:A:315:VAL:O	1:A:315:VAL:CG1	2.64	0.45
1:B:85:TYR:HH	1:B:117:PHE:HE2	1.64	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: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:53:LYS:HZ3	1:A:86:GLN:HB3	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:183:PRO:CB	1:A:204:LEU:HD12	2.47	0.45
1:A:49:LEU:N	1:A:52:ARG:HG2	2.32	0.45
1:A:88:PHE:HA	1:A:89:PRO:C	2.37	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: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: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: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:53:LYS:HZ3	1:A:86:GLN:CD	2.21	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:310:GLY:O	1:B:311:ALA:C	2.55	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:B:49:LEU:C	1:B:51:ASP:H	2.20	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:A:187:THR:O	1:A:188:THR:HB	2.18	0.43
1:B:41:VAL:CA	1:B:115:PRO:HD3	2.46	0.43
1:B:128:VAL:HG12	1:B:143:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ARG:CG	1:A:166:ARG:HH11	2.31	0.43
1:A:320:VAL:HG12	1:A:321:SER:N	2.33	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:HG23	1:A:226:THR:O	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: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:CD2	1:A:85:TYR:N	2.86	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:151:CYS:O	1:A:152:ALA:HB2	2.19	0.43
1:A:330:VAL:HB	1:A:334:GLY:O	2.19	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: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
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:268:THR:HG21	1:B:266:SER:OG	2.19	0.42
1:A:153:LYS:HG2	1:A:157:GLU:OE2	2.20	0.42
1:B:48:TYR:C	1:B:52:ARG:HB2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:312:ASN:CB	1:B:315:VAL:HB	2.49	0.42
1:A:46:PRO:HB2	1:A:48:TYR:HE1	1.83	0.42
1:A:148:ARG:NE	1:A:166:ARG:CD	2.82	0.42
1:A:230:LYS:HD3	1:A:230:LYS:C	2.41	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:53:LYS:NZ	1:A:86:GLN:CD	2.73	0.42
1:A:130:LEU:HD23	1:A:130:LEU:C	2.40	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:B:223:ASN:ND2	1:B:265:PRO:HA	2.35	0.41
1:B:348:LYS:HD3	1:B:348:LYS:C	2.41	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:93:ASN:ND2	1:B:93:ASN:N	2.68	0.41
1:B:98:PRO:O	1:B:99:THR:C	2.59	0.41
1:B:99:THR:O	1:B:102:GLN:N	2.52	0.41
1:B:188:THR:HG22	1:B:200:LEU:HB3	2.02	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:B:387:VAL:HB	2.21	0.41
1:B:7:THR:HG23	1:B:8:ARG:N	2.35	0.41
1:B:99:THR:HG22	1:B:102:GLN:OE1	2.21	0.41
1:B:313:LYS:HA	1:B:315:VAL:N	2.36	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:111:GLN:CD	1:B:112:HIS:N	2.74	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:B:250:TYR:C	1:B:251:LYS:HE2	2.40	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:B:90:PRO:C	1:B:91:THR:HG23	2.42	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:85:TYR:OH	1:B:117:PHE:HE2	2.03	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
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:391:PHE:CD2	1:B:391:PHE:C	2.94	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 9
1	B	348/393 (88%)	293 (84%)	34 (10%)	21 (6%)	1 9
All	All	698/786 (89%)	575 (82%)	81 (12%)	42 (6%)	1 9

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
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

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Mol	Chain	Res	Type
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 (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	320/353 (91%)	270 (84%)	50 (16%)	2 13
1	B	318/353 (90%)	270 (85%)	48 (15%)	3 14
All	All	638/706 (90%)	540 (85%)	98 (15%)	2 13

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	32	LEU
1	A	34	LYS
1	A	45	ASP
1	A	47	ASP
1	A	49	LEU

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Mol	Chain	Res	Type
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	93	ASN
1	A	104	ARG
1	A	112	HIS
1	A	116	PHE
1	A	119	THR
1	A	122	GLN
1	A	148	ARG
1	A	151	CYS
1	A	156	GLU
1	A	163	ASN
1	A	183	PRO
1	A	187	THR
1	A	189	ARG
1	A	193	MET
1	A	195	ASP
1	A	196	ARG
1	A	198	LEU
1	A	205	ASP
1	A	225	SER
1	A	226	THR
1	A	251	LYS
1	A	284	GLU
1	A	285	LYS
1	A	286	ARG
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	332	ARG
1	A	343	VAL
1	A	344	LEU

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Mol	Chain	Res	Type
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	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	122	GLN
1	B	135	GLU
1	B	136	ASP
1	B	147	ILE
1	B	154	SER
1	B	156	GLU
1	B	158	LYS
1	B	187	THR
1	B	192	LEU
1	B	193	MET
1	B	198	LEU
1	B	205	ASP
1	B	216	ASN
1	B	244	LEU
1	B	251	LYS
1	B	256	GLN
1	B	257	VAL
1	B	260	ASP
1	B	267	SER
1	B	268	THR
1	B	283	ARG
1	B	286	ARG
1	B	300	ASN
1	B	308	LYS

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Mol	Chain	Res	Type
1	B	313	LYS
1	B	315	VAL
1	B	318	ILE
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 (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	112	HIS
1	A	122	GLN
1	A	131	GLN
1	A	199	HIS
1	A	216	ASN
1	A	220	HIS
1	A	259	GLN
1	A	296	HIS
1	A	346	HIS
1	A	350	HIS
1	B	16	ASN
1	B	31	HIS
1	B	93	ASN
1	B	160	HIS
1	B	163	ASN
1	B	216	ASN
1	B	220	HIS
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 monosaccharides 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 (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%)	0.18	13 (3%)	41	17	60, 99, 184, 286	0
1	B	352/393 (89%)	0.22	17 (4%)	30	11	66, 116, 206, 280	0
All	All	706/786 (89%)	0.20	30 (4%)	36	14	60, 107, 198, 286	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	ASP	6.5
1	B	52	ARG	4.0
1	A	50	LYS	3.9
1	B	312	ASN	3.8
1	B	47	ASP	3.7
1	A	311	ALA	3.6
1	B	87	ALA	3.5
1	A	111	GLN	3.4
1	A	8	ARG	3.3
1	B	88	PHE	3.3
1	A	45	ASP	3.3
1	A	386	ILE	3.1
1	B	105	LEU	3.1
1	B	38	VAL	3.0
1	A	44	VAL	3.0
1	B	43	LEU	2.9
1	B	50	LYS	2.7
1	B	45	ASP	2.7
1	A	196	ARG	2.5
1	B	106	LEU	2.5
1	A	51	ASP	2.5
1	B	113	ALA	2.4
1	A	9	VAL	2.4
1	B	54	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	388	PHE	2.2
1	A	42	VAL	2.2
1	B	171	LYS	2.1
1	A	387	VAL	2.0
1	B	44	VAL	2.0
1	B	114	HIS	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 monosaccharides 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.