Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:39 PM GMT

PDB ID	:	4J23
Title	:	Low resolution crystal structure of the FGFR2D2D3/FGF1/SR128545 complex
Authors	:	Kudlinzki, D.; Saxena, K.; Sreeramulu, S.; Schieborr, U.; Dreyer, M.; Schreuder, H.; Schwalbe, H.
Deposited on	:	2013-02-04
Resolution	:	3.88 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

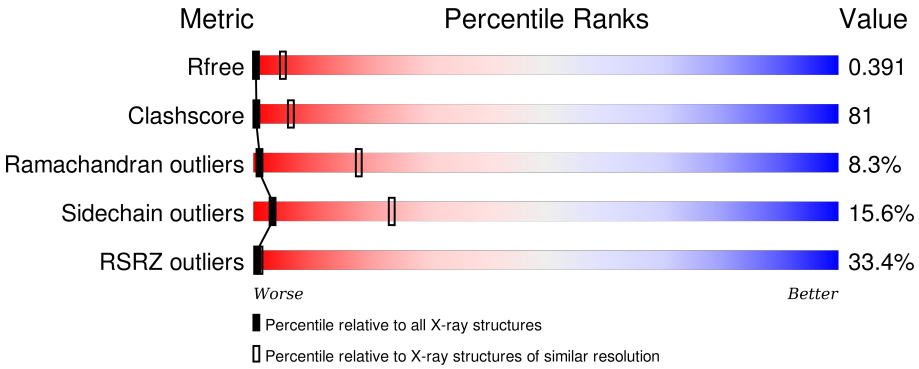
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.88 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1005 (4.24-3.52)
Clashscore	102246	1026 (4.20-3.56)
Ramachandran outliers	100387	1003 (4.22-3.54)
Sidechain outliers	100360	1043 (4.24-3.52)
RSRZ outliers	91569	1009 (4.24-3.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	223	29%, 16%, 49%, 20%, ·, 11%
2	B	138	34%, 24%, 55%, 14%, ·, ·

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2642 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 Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1571	1001	276	286	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	MET	-	EXPRESSION TAG	UNP P21802
A	367	LEU	-	EXPRESSION TAG	UNP P21802
A	368	GLU	-	EXPRESSION TAG	UNP P21802

- Molecule 2 is a protein called Fibroblast growth factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	134	Total	C	N	O	S	0	0	0
			1071	675	187	205	4			

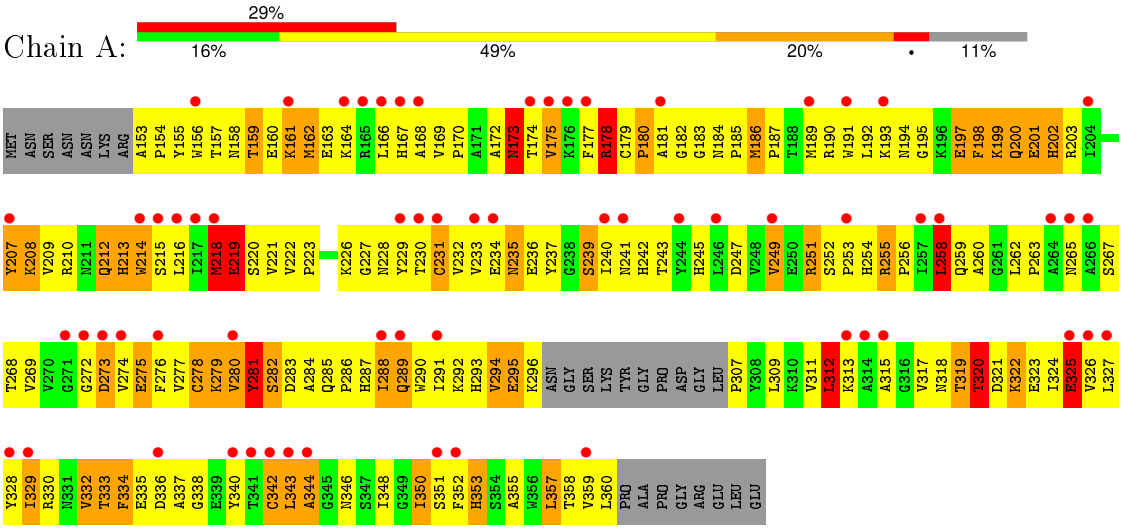
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	18	GLY	-	EXPRESSION TAG	UNP P05230
B	19	HIS	-	EXPRESSION TAG	UNP P05230
B	20	MET	-	EXPRESSION TAG	UNP P05230

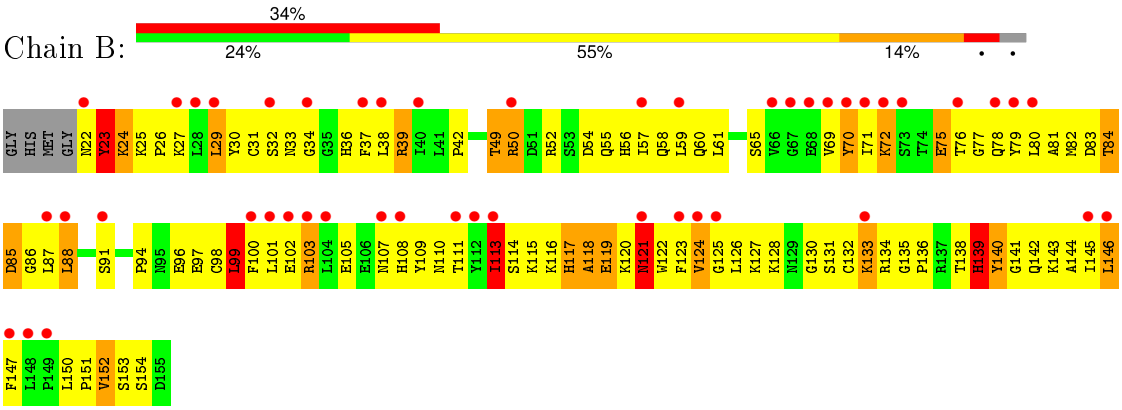
3 Residue-property plots (i)

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

- Molecule 1: Fibroblast growth factor receptor 2



- Molecule 2: Fibroblast growth factor 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α, β, γ	210.67Å 210.67Å 72.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.81 – 3.88 182.45 – 3.88	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.81-3.88) 100.0 (182.45-3.88)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 3.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.321 , 0.384 0.329 , 0.391	Depositor DCC
R_{free} test set	435 reflections (4.74%)	DCC
Wilson B-factor (Å^2)	175.0	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 363.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 9200 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	2642	wwPDB-VP
Average B, all atoms (Å^2)	284.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.98	4/1613 (0.2%)	1.38	17/2191 (0.8%)
2	B	0.87	1/1095 (0.1%)	1.19	5/1477 (0.3%)
All	All	0.94	5/2708 (0.2%)	1.31	22/3668 (0.6%)

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	6
2	B	0	4
All	All	0	10

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	CYS	CB-SG	7.16	1.94	1.82
1	A	231	CYS	CB-SG	-6.13	1.71	1.82
1	A	344	ALA	CA-CB	-5.34	1.41	1.52
1	A	178	ARG	CG-CD	5.21	1.65	1.51
2	B	75	GLU	CG-CD	-5.03	1.44	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	342	CYS	CA-CB-SG	16.34	143.42	114.00
1	A	312	LEU	CA-CB-CG	8.02	133.75	115.30
2	B	121	ASN	N-CA-CB	-6.84	98.28	110.60
1	A	207	TYR	CA-CB-CG	6.59	125.92	113.40
1	A	251	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	281	TYR	CB-CG-CD1	6.30	124.78	121.00
2	B	99	LEU	CA-CB-CG	6.07	129.25	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	357	LEU	CA-CB-CG	6.00	129.09	115.30
1	A	320	THR	N-CA-C	5.96	127.10	111.00
1	A	343	LEU	CB-CG-CD2	5.96	121.12	111.00
1	A	258	LEU	CA-CB-CG	-5.96	101.60	115.30
1	A	251	ARG	NE-CZ-NH2	-5.92	117.34	120.30
2	B	113	ILE	CG1-CB-CG2	-5.82	98.60	111.40
1	A	325	GLU	C-N-CA	5.78	136.15	121.70
2	B	29	LEU	CA-CB-CG	-5.60	102.42	115.30
2	B	139	HIS	N-CA-C	-5.57	95.95	111.00
1	A	288	ILE	CG1-CB-CG2	-5.55	99.19	111.40
1	A	218	MET	CB-CG-SD	-5.43	96.12	112.40
1	A	281	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	A	255	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	342	CYS	N-CA-C	5.13	124.85	111.00
1	A	219	GLU	N-CA-CB	5.02	119.64	110.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	ASN	Peptide
1	A	197	GLU	Peptide
1	A	198	PHE	Peptide
1	A	199	LYS	Peptide
1	A	218	MET	Peptide
1	A	334	PHE	Peptide
2	B	117	HIS	Peptide
2	B	121	ASN	Peptide
2	B	23	TYR	Peptide
2	B	84	THR	Peptide

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	1571	0	1541	266	0
2	B	1071	0	1049	176	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2642	0	2590	425	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 81.

All (425) 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:156:TRP:CH2	1:A:233:VAL:HG21	1.20	1.62
1:A:156:TRP:CD1	1:A:240:ILE:CG2	1.77	1.58
1:A:156:TRP:NE1	1:A:240:ILE:CG2	1.71	1.49
1:A:156:TRP:CD1	1:A:240:ILE:HG21	0.94	1.46
1:A:156:TRP:CZ2	1:A:233:VAL:HG21	1.50	1.46
1:A:156:TRP:CZ2	1:A:233:VAL:CG2	2.06	1.39
1:A:156:TRP:HE1	1:A:240:ILE:CB	1.35	1.38
1:A:156:TRP:CH2	1:A:233:VAL:CG2	2.13	1.31
1:A:156:TRP:CE3	1:A:181:ALA:HB2	1.65	1.30
1:A:156:TRP:HE1	1:A:240:ILE:HB	1.07	1.15
1:A:156:TRP:NE1	1:A:240:ILE:CB	2.01	1.13
2:B:113:ILE:HG22	2:B:123:PHE:HB3	1.31	1.11
2:B:96:GLU:HA	2:B:115:LYS:HZ3	1.11	1.10
1:A:156:TRP:HE1	1:A:240:ILE:CG2	1.43	1.09
1:A:156:TRP:NE1	1:A:240:ILE:HB	1.65	1.09
1:A:320:THR:O	1:A:324:ILE:HD11	1.50	1.08
1:A:280:VAL:HG11	2:B:23:TYR:CD2	1.88	1.08
2:B:128:LYS:H	2:B:128:LYS:HD2	1.22	1.05
1:A:156:TRP:NE1	1:A:240:ILE:HG21	1.51	1.03
1:A:180:PRO:O	1:A:214:TRP:NE1	1.91	1.03
1:A:156:TRP:NE1	1:A:240:ILE:HG22	1.72	1.00
1:A:337:ALA:HA	1:A:357:LEU:HD11	1.42	1.00
1:A:273:ASP:HB2	1:A:329:ILE:HD13	1.44	0.98
1:A:322:LYS:HG2	1:A:323:GLU:H	1.28	0.97
1:A:156:TRP:HZ2	1:A:233:VAL:CG2	1.64	0.96
2:B:99:LEU:H	2:B:115:LYS:HD2	1.31	0.95
1:A:158:ASN:O	1:A:160:GLU:N	2.00	0.95
1:A:156:TRP:CD1	1:A:240:ILE:HG22	2.01	0.94
2:B:39:ARG:HH22	2:B:57:ILE:HG12	1.33	0.94
2:B:96:GLU:HA	2:B:115:LYS:NZ	1.83	0.94
1:A:167:HIS:HD1	1:A:177:PHE:HE1	1.17	0.92
1:A:156:TRP:CD2	1:A:181:ALA:HB2	2.04	0.91
1:A:200:GLN:HG2	1:A:207:TYR:HB2	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:SER:O	2:B:22:ASN:HA	1.70	0.91
1:A:290:TRP:HB2	1:A:312:LEU:HG	1.53	0.91
2:B:25:LYS:HZ1	2:B:152:VAL:HG22	1.35	0.90
1:A:295:GLU:OE2	1:A:296:LYS:HE2	1.73	0.89
1:A:156:TRP:CZ2	1:A:233:VAL:HG23	2.08	0.87
1:A:259:GLN:HB2	1:A:279:LYS:HD3	1.57	0.85
2:B:117:HIS:HB2	2:B:119:GLU:HB3	1.59	0.84
1:A:156:TRP:HZ2	1:A:233:VAL:HG23	1.39	0.84
1:A:156:TRP:CE3	1:A:181:ALA:CB	2.56	0.84
1:A:251:ARG:NH1	2:B:110:ASN:OD1	2.10	0.83
1:A:207:TYR:HA	1:A:218:MET:SD	2.19	0.83
1:A:156:TRP:HH2	1:A:233:VAL:HG21	1.02	0.83
1:A:280:VAL:HG11	2:B:23:TYR:CG	2.15	0.81
1:A:329:ILE:HD12	1:A:329:ILE:H	1.46	0.81
2:B:83:ASP:OD1	2:B:84:THR:N	2.14	0.81
2:B:25:LYS:NZ	2:B:152:VAL:HG22	1.95	0.80
1:A:322:LYS:HG2	1:A:323:GLU:N	1.95	0.80
1:A:320:THR:O	1:A:324:ILE:CD1	2.30	0.80
1:A:234:GLU:HB3	1:A:239:SER:HB2	1.64	0.79
2:B:86:GLY:HA2	2:B:122:TRP:HZ3	1.48	0.79
2:B:39:ARG:NH2	2:B:57:ILE:HG12	1.96	0.79
1:A:263:PRO:HB2	1:A:276:PHE:HB3	1.65	0.78
2:B:123:PHE:CE1	2:B:138:THR:HB	2.19	0.78
1:A:279:LYS:NZ	1:A:281:TYR:CD2	2.52	0.78
1:A:170:PRO:HB3	2:B:108:HIS:CG	2.19	0.78
2:B:127:LYS:HD2	2:B:128:LYS:HZ2	1.48	0.78
2:B:85:ASP:HB3	2:B:87:LEU:HG	1.67	0.77
2:B:99:LEU:HD13	2:B:115:LYS:HZ1	1.50	0.76
2:B:39:ARG:NH2	2:B:57:ILE:H	1.83	0.76
1:A:290:TRP:H	1:A:312:LEU:HD11	1.49	0.76
1:A:156:TRP:CZ2	1:A:233:VAL:CB	2.68	0.75
1:A:210:ARG:CZ	1:A:215:SER:HB2	2.17	0.75
2:B:39:ARG:NH1	2:B:54:ASP:HB3	2.01	0.75
2:B:39:ARG:CZ	2:B:54:ASP:HB3	2.17	0.74
1:A:231:CYS:O	1:A:241:ASN:HB2	1.87	0.74
1:A:191:TRP:O	1:A:192:LEU:HD23	1.88	0.73
1:A:200:GLN:CG	1:A:207:TYR:HB2	2.18	0.73
2:B:39:ARG:CZ	2:B:57:ILE:HG23	2.19	0.73
1:A:235:ASN:N	1:A:235:ASN:OD1	2.18	0.72
2:B:36:HIS:HD2	2:B:49:THR:HA	1.53	0.72
1:A:156:TRP:HH2	1:A:233:VAL:CG2	1.76	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:ARG:NE	2:B:111:THR:OG1	2.24	0.71
1:A:262:LEU:HD13	1:A:277:VAL:O	1.91	0.71
1:A:291:ILE:HG13	1:A:309:LEU:HD22	1.74	0.70
1:A:290:TRP:H	1:A:312:LEU:CD1	2.05	0.70
2:B:123:PHE:HB2	2:B:145:ILE:HD13	1.74	0.70
2:B:36:HIS:ND1	2:B:126:LEU:HD11	2.06	0.70
2:B:39:ARG:HH21	2:B:56:HIS:N	1.90	0.69
2:B:99:LEU:O	2:B:115:LYS:HB3	1.93	0.69
1:A:218:MET:HA	1:A:219:GLU:HB3	1.75	0.69
1:A:210:ARG:O	1:A:214:TRP:HA	1.93	0.69
1:A:160:GLU:OE2	1:A:178:ARG:HD3	1.94	0.68
2:B:37:PHE:HE2	2:B:52:ARG:HB3	1.59	0.68
1:A:255:ARG:HA	1:A:346:ASN:HD21	1.59	0.68
1:A:284:ALA:HB3	1:A:346:ASN:HD22	1.57	0.68
2:B:105:GLU:O	2:B:108:HIS:N	2.26	0.68
2:B:113:ILE:CG2	2:B:123:PHE:HB3	2.16	0.67
1:A:272:GLY:O	1:A:332:VAL:HG12	1.95	0.66
1:A:156:TRP:HE1	1:A:240:ILE:HG22	1.41	0.66
2:B:70:TYR:CE1	2:B:99:LEU:HG	2.31	0.66
1:A:161:LYS:HB3	1:A:164:LYS:HD3	1.78	0.66
2:B:61:LEU:HD11	2:B:71:ILE:HG23	1.76	0.66
1:A:156:TRP:HD1	1:A:240:ILE:CG2	1.55	0.66
1:A:192:LEU:O	1:A:230:THR:N	2.28	0.66
1:A:262:LEU:HD21	1:A:279:LYS:HG2	1.78	0.66
2:B:22:ASN:N	2:B:27:LYS:HE2	2.11	0.66
1:A:333:THR:OG1	1:A:334:PHE:N	2.28	0.65
2:B:39:ARG:NH1	2:B:57:ILE:HG23	2.11	0.65
1:A:160:GLU:OE2	1:A:178:ARG:NH1	2.22	0.65
2:B:116:LYS:NZ	2:B:117:HIS:HB3	2.10	0.65
1:A:342:CYS:SG	1:A:352:PHE:HD2	2.20	0.65
1:A:289:GLN:CD	1:A:343:LEU:HD22	2.16	0.65
2:B:122:TRP:CE3	2:B:135:GLY:HA3	2.32	0.64
1:A:265:ASN:HD21	1:A:355:ALA:HA	1.61	0.64
1:A:190:ARG:O	1:A:191:TRP:CD1	2.50	0.64
2:B:142:GLN:HB3	2:B:144:ALA:H	1.62	0.64
2:B:52:ARG:NH2	2:B:153:SER:O	2.30	0.64
2:B:81:ALA:HB1	2:B:97:GLU:CB	2.27	0.64
2:B:25:LYS:HG2	2:B:26:PRO:O	1.98	0.64
1:A:230:THR:OG1	1:A:243:THR:HG22	1.97	0.64
1:A:256:PRO:HD3	1:A:346:ASN:ND2	2.13	0.64
2:B:110:ASN:O	2:B:111:THR:HG23	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:HB2	1:A:212:GLN:HG3	1.80	0.63
2:B:34:GLY:H	2:B:126:LEU:HD21	1.63	0.63
1:A:340:TYR:O	1:A:355:ALA:N	2.30	0.63
2:B:39:ARG:HH21	2:B:56:HIS:H	1.46	0.63
2:B:96:GLU:CA	2:B:115:LYS:NZ	2.60	0.63
2:B:52:ARG:HH12	2:B:154:SER:HA	1.64	0.62
1:A:222:VAL:HB	1:A:223:PRO:HD2	1.81	0.62
1:A:281:TYR:HA	1:A:282:SER:HB3	1.81	0.62
1:A:258:LEU:HG	1:A:352:PHE:CE2	2.33	0.62
1:A:265:ASN:HA	1:A:276:PHE:CE2	2.35	0.62
2:B:36:HIS:CD2	2:B:49:THR:HA	2.33	0.61
1:A:251:ARG:HH22	2:B:110:ASN:ND2	1.98	0.61
2:B:103:ARG:HB3	2:B:111:THR:OG1	2.00	0.61
1:A:324:ILE:HG22	1:A:324:ILE:O	2.01	0.61
2:B:111:THR:HG22	2:B:145:ILE:O	2.01	0.61
1:A:322:LYS:HG2	1:A:323:GLU:HG3	1.83	0.60
1:A:262:LEU:HD13	1:A:278:CYS:HA	1.83	0.60
1:A:200:GLN:OE1	1:A:201:GLU:N	2.35	0.59
1:A:170:PRO:HA	1:A:249:VAL:HG23	1.82	0.59
1:A:156:TRP:CZ2	1:A:233:VAL:HB	2.37	0.59
1:A:251:ARG:HE	1:A:283:ASP:CG	2.06	0.59
1:A:154:PRO:HA	1:A:183:GLY:HA3	1.83	0.59
1:A:292:LYS:HZ1	1:A:338:GLY:HA3	1.67	0.59
1:A:337:ALA:HA	1:A:357:LEU:CD1	2.27	0.59
2:B:55:GLN:HB3	2:B:75:GLU:OE1	2.04	0.58
1:A:193:LYS:HD3	1:A:198:PHE:HB3	1.84	0.58
1:A:251:ARG:HH22	2:B:110:ASN:HD21	1.51	0.58
1:A:193:LYS:HA	1:A:228:ASN:O	2.03	0.58
2:B:117:HIS:CG	2:B:118:ALA:N	2.71	0.58
1:A:320:THR:HG22	1:A:321:ASP:H	1.69	0.58
1:A:319:THR:OG1	1:A:323:GLU:OE1	2.22	0.58
1:A:156:TRP:HA	1:A:181:ALA:CB	2.33	0.58
2:B:23:TYR:CD2	2:B:24:LYS:HA	2.39	0.58
2:B:82:MET:O	2:B:83:ASP:HB3	2.04	0.58
1:A:290:TRP:HB2	1:A:312:LEU:CG	2.32	0.58
1:A:344:ALA:N	1:A:350:ILE:HD11	2.18	0.58
2:B:31:CYS:HB2	2:B:147:PHE:CZ	2.39	0.57
1:A:342:CYS:O	1:A:352:PHE:CD2	2.55	0.57
2:B:132:CYS:SG	2:B:133:LYS:N	2.69	0.57
2:B:30:TYR:CE1	2:B:32:SER:HA	2.39	0.57
2:B:80:LEU:O	2:B:98:CYS:HA	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:GLU:CD	2:B:105:GLU:N	2.57	0.57
1:A:317:VAL:HG13	1:A:319:THR:HB	1.87	0.57
1:A:255:ARG:HD3	1:A:350:ILE:N	2.19	0.57
1:A:340:TYR:N	1:A:355:ALA:O	2.29	0.57
2:B:123:PHE:HB2	2:B:145:ILE:CD1	2.35	0.57
2:B:103:ARG:HE	2:B:105:GLU:CD	2.08	0.57
1:A:160:GLU:CD	1:A:178:ARG:HD3	2.25	0.57
2:B:143:LYS:HD2	2:B:146:LEU:HD21	1.87	0.56
2:B:39:ARG:NH2	2:B:57:ILE:N	2.53	0.56
1:A:290:TRP:CD1	1:A:342:CYS:HB2	2.41	0.56
1:A:157:THR:HG22	1:A:181:ALA:H	1.70	0.56
1:A:156:TRP:HD1	1:A:240:ILE:HG21	0.76	0.56
2:B:36:HIS:CD2	2:B:50:ARG:HD2	2.40	0.56
1:A:276:PHE:CD1	1:A:327:LEU:HD21	2.41	0.56
2:B:105:GLU:OE1	2:B:105:GLU:N	2.38	0.56
1:A:290:TRP:NE1	1:A:342:CYS:HB2	2.21	0.56
1:A:251:ARG:HG2	2:B:108:HIS:CE1	2.40	0.55
2:B:81:ALA:HB1	2:B:97:GLU:HB2	1.87	0.55
1:A:280:VAL:HG13	1:A:281:TYR:N	2.21	0.55
1:A:291:ILE:HG22	1:A:311:VAL:HA	1.88	0.55
2:B:131:SER:HB3	2:B:133:LYS:NZ	2.22	0.55
2:B:119:GLU:HG2	2:B:120:LYS:HB3	1.89	0.55
1:A:351:SER:C	1:A:352:PHE:HD1	2.10	0.55
1:A:203:ARG:NH2	1:A:219:GLU:O	2.39	0.55
2:B:84:THR:O	2:B:122:TRP:CH2	2.60	0.54
1:A:279:LYS:HE3	1:A:280:VAL:O	2.06	0.54
1:A:325:GLU:N	1:A:326:VAL:HG22	2.21	0.54
1:A:290:TRP:HZ3	1:A:327:LEU:H	1.54	0.54
1:A:262:LEU:HD12	1:A:262:LEU:C	2.27	0.54
1:A:174:THR:HG22	1:A:219:GLU:HA	1.89	0.54
1:A:292:LYS:HZ1	1:A:338:GLY:CA	2.21	0.54
1:A:288:ILE:HG22	1:A:344:ALA:CB	2.38	0.54
1:A:275:GLU:OE2	1:A:327:LEU:O	2.26	0.54
2:B:99:LEU:HD13	2:B:115:LYS:NZ	2.22	0.53
1:A:288:ILE:HG22	1:A:344:ALA:HB1	1.89	0.53
2:B:117:HIS:C	2:B:119:GLU:H	2.11	0.53
2:B:85:ASP:CB	2:B:87:LEU:HG	2.37	0.53
1:A:239:SER:O	1:A:240:ILE:HD13	2.09	0.53
2:B:31:CYS:HB2	2:B:147:PHE:CE2	2.43	0.53
1:A:172:ALA:O	1:A:220:SER:HA	2.09	0.53
1:A:295:GLU:OE2	1:A:307:PRO:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:SER:OG	2:B:154:SER:N	2.41	0.53
2:B:99:LEU:CD1	2:B:115:LYS:HZ1	2.19	0.53
1:A:160:GLU:OE2	1:A:178:ARG:CD	2.57	0.53
1:A:170:PRO:HB3	2:B:108:HIS:CD2	2.42	0.53
2:B:39:ARG:HH21	2:B:57:ILE:H	1.55	0.53
2:B:36:HIS:HB2	2:B:126:LEU:HD13	1.90	0.53
1:A:170:PRO:HB3	2:B:108:HIS:ND1	2.23	0.52
1:A:279:LYS:O	1:A:279:LYS:HG3	2.09	0.52
1:A:200:GLN:HE21	1:A:207:TYR:HB2	1.74	0.52
1:A:290:TRP:HE1	1:A:342:CYS:HB2	1.74	0.52
1:A:210:ARG:CZ	1:A:213:HIS:CD2	2.93	0.52
1:A:192:LEU:HA	1:A:198:PHE:CD2	2.45	0.52
1:A:265:ASN:HA	1:A:276:PHE:HE2	1.73	0.52
1:A:284:ALA:HB3	1:A:346:ASN:ND2	2.23	0.52
1:A:344:ALA:C	1:A:350:ILE:HD12	2.30	0.52
1:A:156:TRP:CZ3	1:A:181:ALA:HB2	2.37	0.52
1:A:207:TYR:CD1	1:A:209:VAL:HG22	2.45	0.52
1:A:292:LYS:HD2	1:A:340:TYR:CZ	2.45	0.52
1:A:344:ALA:HB3	1:A:352:PHE:CZ	2.44	0.52
2:B:116:LYS:HZ3	2:B:117:HIS:HB3	1.74	0.52
1:A:281:TYR:HE1	2:B:24:LYS:HE2	1.74	0.52
1:A:336:ASP:O	1:A:340:TYR:OH	2.21	0.52
2:B:117:HIS:HD2	2:B:120:LYS:H	1.57	0.52
1:A:236:GLU:OE2	1:A:237:TYR:CE1	2.62	0.52
1:A:207:TYR:CZ	1:A:216:LEU:HD13	2.44	0.51
2:B:127:LYS:NZ	2:B:128:LYS:HZ2	2.08	0.51
1:A:288:ILE:HG13	1:A:315:ALA:HB2	1.91	0.51
1:A:292:LYS:NZ	1:A:338:GLY:HA3	2.24	0.51
2:B:60:GLN:HG3	2:B:61:LEU:N	2.26	0.51
1:A:168:ALA:O	1:A:169:VAL:HG23	2.11	0.51
1:A:207:TYR:HD1	1:A:209:VAL:HG22	1.75	0.51
1:A:210:ARG:HE	1:A:213:HIS:C	2.13	0.51
1:A:289:GLN:HG2	1:A:343:LEU:HB3	1.92	0.51
1:A:230:THR:HG22	1:A:231:CYS:O	2.10	0.51
2:B:126:LEU:N	2:B:144:ALA:O	2.44	0.51
1:A:174:THR:OG1	1:A:175:VAL:N	2.43	0.51
2:B:107:ASN:O	2:B:108:HIS:HB3	2.10	0.51
2:B:127:LYS:CD	2:B:128:LYS:HZ2	2.21	0.51
1:A:252:SER:O	1:A:254:HIS:N	2.41	0.50
1:A:240:ILE:O	1:A:241:ASN:HB3	2.11	0.50
2:B:99:LEU:C	2:B:100:PHE:HD1	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:PHE:CZ	2:B:139:HIS:N	2.79	0.50
1:A:259:GLN:HG3	1:A:260:ALA:O	2.10	0.50
2:B:120:LYS:O	2:B:122:TRP:CD1	2.65	0.50
2:B:124:VAL:O	2:B:145:ILE:HD13	2.11	0.50
2:B:85:ASP:HB3	2:B:87:LEU:H	1.77	0.50
2:B:99:LEU:HD22	2:B:115:LYS:HZ1	1.77	0.50
2:B:117:HIS:HB2	2:B:119:GLU:CB	2.38	0.50
2:B:116:LYS:HZ2	2:B:117:HIS:HB3	1.76	0.50
1:A:208:LYS:H	1:A:218:MET:CE	2.25	0.50
1:A:153:ALA:N	1:A:237:TYR:HD2	2.09	0.50
1:A:156:TRP:CE2	1:A:240:ILE:HB	2.43	0.50
2:B:81:ALA:HB1	2:B:97:GLU:HB3	1.92	0.50
1:A:280:VAL:HG21	2:B:23:TYR:CD1	2.47	0.50
2:B:113:ILE:HG22	2:B:123:PHE:CB	2.21	0.50
2:B:115:LYS:C	2:B:117:HIS:H	2.15	0.50
2:B:83:ASP:HA	2:B:97:GLU:OE1	2.12	0.50
1:A:343:LEU:HA	1:A:350:ILE:HD11	1.93	0.50
2:B:25:LYS:HZ1	2:B:151:PRO:HB2	1.77	0.49
1:A:269:VAL:HA	1:A:360:LEU:CD1	2.41	0.49
1:A:174:THR:HB	1:A:219:GLU:HA	1.93	0.49
1:A:269:VAL:HA	1:A:360:LEU:HD11	1.94	0.49
2:B:72:LYS:HD2	2:B:77:GLY:C	2.33	0.49
2:B:69:VAL:C	2:B:70:TYR:HD1	2.16	0.49
1:A:193:LYS:HG2	1:A:193:LYS:O	2.12	0.49
2:B:29:LEU:HB3	2:B:147:PHE:HD2	1.76	0.49
1:A:210:ARG:NH1	1:A:215:SER:HB2	2.27	0.49
1:A:197:GLU:CD	1:A:198:PHE:H	2.16	0.49
2:B:145:ILE:O	2:B:147:PHE:HD1	1.96	0.49
1:A:208:LYS:H	1:A:218:MET:HE1	1.78	0.49
1:A:329:ILE:CD1	1:A:329:ILE:H	2.12	0.49
1:A:291:ILE:HD12	1:A:309:LEU:HB2	1.94	0.49
2:B:72:LYS:HB2	2:B:79:TYR:HD1	1.78	0.49
1:A:267:SER:HB3	1:A:358:THR:OG1	2.12	0.49
1:A:252:SER:C	1:A:254:HIS:H	2.15	0.48
1:A:200:GLN:HE21	1:A:207:TYR:HD2	1.61	0.48
1:A:169:VAL:HG22	2:B:109:TYR:OH	2.13	0.48
2:B:37:PHE:CE2	2:B:52:ARG:HB3	2.46	0.48
1:A:159:THR:HG22	1:A:163:GLU:OE2	2.14	0.48
1:A:156:TRP:CH2	1:A:231:CYS:SG	3.07	0.48
1:A:157:THR:N	1:A:181:ALA:HA	2.29	0.48
2:B:114:SER:O	2:B:117:HIS:ND1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:LYS:NZ	2:B:151:PRO:HB2	2.28	0.48
1:A:194:ASN:OD1	1:A:228:ASN:HB2	2.13	0.48
1:A:194:ASN:OD1	1:A:228:ASN:O	2.31	0.48
1:A:200:GLN:HG2	1:A:207:TYR:CB	2.33	0.48
1:A:174:THR:CB	1:A:219:GLU:HA	2.44	0.48
1:A:169:VAL:HA	1:A:170:PRO:HD3	1.58	0.48
2:B:29:LEU:HA	2:B:29:LEU:HD23	1.63	0.47
2:B:81:ALA:HB3	2:B:91:SER:OG	2.14	0.47
2:B:127:LYS:NZ	2:B:128:LYS:NZ	2.62	0.47
1:A:157:THR:HG22	1:A:181:ALA:N	2.29	0.47
1:A:268:THR:C	1:A:360:LEU:HD21	2.34	0.47
1:A:192:LEU:O	1:A:229:TYR:HA	2.14	0.47
2:B:75:GLU:HG3	2:B:76:THR:HG23	1.96	0.47
1:A:156:TRP:CZ3	1:A:179:CYS:HB3	2.50	0.47
2:B:99:LEU:HD22	2:B:115:LYS:NZ	2.30	0.47
1:A:174:THR:CG2	1:A:219:GLU:HA	2.45	0.47
1:A:210:ARG:HG2	1:A:215:SER:H	1.78	0.47
1:A:195:GLY:CA	1:A:198:PHE:HZ	2.27	0.47
2:B:86:GLY:HA2	2:B:122:TRP:CZ3	2.39	0.47
1:A:320:THR:HG22	1:A:321:ASP:N	2.29	0.47
1:A:201:GLU:HG2	1:A:202:HIS:N	2.30	0.47
1:A:154:PRO:HD3	1:A:235:ASN:HD21	1.79	0.47
1:A:164:LYS:HE3	1:A:167:HIS:HE1	1.80	0.46
1:A:268:THR:HG21	1:A:274:VAL:HG23	1.97	0.46
2:B:120:LYS:HE2	2:B:139:HIS:CG	2.50	0.46
2:B:111:THR:CG2	2:B:145:ILE:HG13	2.44	0.46
1:A:280:VAL:HG11	2:B:23:TYR:CB	2.45	0.46
2:B:31:CYS:HB3	2:B:126:LEU:HD22	1.97	0.46
1:A:275:GLU:HG3	1:A:327:LEU:O	2.15	0.46
1:A:289:GLN:OE1	1:A:343:LEU:HD22	2.15	0.46
1:A:232:VAL:O	1:A:232:VAL:HG13	2.15	0.46
2:B:141:GLY:HA3	2:B:142:GLN:HA	1.59	0.46
2:B:34:GLY:H	2:B:126:LEU:CD2	2.27	0.46
1:A:290:TRP:CZ2	1:A:325:GLU:O	2.69	0.46
2:B:97:GLU:CA	2:B:115:LYS:HD3	2.46	0.46
2:B:120:LYS:O	2:B:122:TRP:HD1	1.99	0.46
1:A:207:TYR:CE1	1:A:216:LEU:HD13	2.51	0.46
2:B:109:TYR:CD2	2:B:146:LEU:HD13	2.51	0.45
1:A:321:ASP:OD1	1:A:321:ASP:O	2.34	0.45
2:B:33:ASN:HB3	2:B:126:LEU:HD23	1.98	0.45
1:A:253:PRO:O	1:A:348:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:LYS:C	2:B:117:HIS:N	2.67	0.45
2:B:126:LEU:H	2:B:144:ALA:HB1	1.81	0.45
1:A:255:ARG:HA	1:A:346:ASN:ND2	2.30	0.45
2:B:39:ARG:HB2	2:B:57:ILE:HG23	1.99	0.45
2:B:56:HIS:CD2	2:B:56:HIS:N	2.84	0.45
1:A:186:MET:HA	1:A:187:PRO:HD3	1.43	0.45
1:A:292:LYS:HE3	1:A:294:VAL:HG13	1.99	0.45
1:A:251:ARG:NE	1:A:283:ASP:OD2	2.48	0.45
2:B:42:PRO:HG3	2:B:56:HIS:HE1	1.82	0.45
2:B:61:LEU:HG	2:B:71:ILE:HG12	1.99	0.45
1:A:262:LEU:CD1	1:A:278:CYS:HA	2.47	0.45
2:B:23:TYR:CG	2:B:24:LYS:N	2.84	0.44
2:B:72:LYS:HD3	2:B:79:TYR:CD1	2.51	0.44
1:A:156:TRP:CH2	1:A:179:CYS:HB3	2.52	0.44
2:B:115:LYS:HG3	2:B:116:LYS:N	2.32	0.44
2:B:97:GLU:N	2:B:115:LYS:HZ2	2.15	0.44
1:A:201:GLU:O	1:A:203:ARG:N	2.51	0.44
1:A:258:LEU:HD22	1:A:258:LEU:HA	1.67	0.44
1:A:290:TRP:CH2	1:A:325:GLU:C	2.91	0.44
1:A:281:TYR:HA	1:A:282:SER:CB	2.45	0.44
1:A:201:GLU:C	1:A:203:ARG:H	2.21	0.44
1:A:210:ARG:NE	1:A:215:SER:HB2	2.32	0.44
2:B:38:LEU:HA	2:B:38:LEU:HD12	1.66	0.44
2:B:36:HIS:CE1	2:B:130:GLY:CA	3.00	0.44
1:A:190:ARG:C	1:A:191:TRP:CD1	2.91	0.44
2:B:103:ARG:O	2:B:110:ASN:HA	2.18	0.44
2:B:84:THR:O	2:B:86:GLY:N	2.51	0.44
1:A:344:ALA:N	1:A:350:ILE:CD1	2.80	0.44
1:A:265:ASN:ND2	1:A:355:ALA:HA	2.31	0.44
2:B:58:GLN:OE1	2:B:58:GLN:N	2.51	0.44
2:B:96:GLU:C	2:B:115:LYS:NZ	2.72	0.43
1:A:259:GLN:HB2	1:A:279:LYS:CD	2.38	0.43
2:B:72:LYS:HB2	2:B:79:TYR:CD1	2.53	0.43
2:B:125:GLY:HA3	2:B:132:CYS:SG	2.59	0.43
2:B:83:ASP:HB3	2:B:85:ASP:OD2	2.19	0.43
1:A:285:GLN:HG2	1:A:286:PRO:HD2	2.00	0.43
1:A:319:THR:O	1:A:319:THR:HG23	2.18	0.43
2:B:79:TYR:HE2	2:B:94:PRO:HD3	1.82	0.43
1:A:290:TRP:CB	1:A:312:LEU:HG	2.35	0.43
1:A:287:HIS:ND1	2:B:65:SER:HA	2.33	0.43
2:B:117:HIS:HD2	2:B:120:LYS:N	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:GLY:CA	2:B:122:TRP:HZ3	2.25	0.43
2:B:86:GLY:O	2:B:88:LEU:HD12	2.18	0.43
2:B:99:LEU:HD22	2:B:115:LYS:HE3	2.00	0.43
2:B:72:LYS:HD2	2:B:78:GLN:N	2.33	0.43
1:A:287:HIS:CG	2:B:65:SER:HA	2.53	0.43
1:A:292:LYS:HD2	1:A:340:TYR:CE2	2.54	0.43
1:A:161:LYS:HB3	1:A:164:LYS:CD	2.46	0.43
1:A:223:PRO:O	1:A:226:LYS:HB2	2.19	0.43
1:A:192:LEU:HD22	1:A:198:PHE:HE2	1.83	0.43
1:A:156:TRP:HA	1:A:181:ALA:HA	2.01	0.42
1:A:343:LEU:CA	1:A:350:ILE:HD11	2.49	0.42
1:A:267:SER:HB3	1:A:358:THR:HG1	1.83	0.42
1:A:227:GLY:O	1:A:245:HIS:HA	2.18	0.42
1:A:156:TRP:CZ3	1:A:181:ALA:CB	2.99	0.42
2:B:126:LEU:HA	2:B:132:CYS:HB2	2.01	0.42
1:A:322:LYS:CG	1:A:323:GLU:HG3	2.50	0.42
1:A:263:PRO:CB	1:A:276:PHE:HB3	2.41	0.42
1:A:230:THR:HG23	1:A:242:HIS:O	2.20	0.42
1:A:168:ALA:HA	1:A:247:ASP:O	2.20	0.42
1:A:166:LEU:HG	1:A:167:HIS:N	2.35	0.42
1:A:360:LEU:HG	1:A:360:LEU:H	1.50	0.42
2:B:101:LEU:O	2:B:103:ARG:N	2.53	0.42
2:B:119:GLU:HG2	2:B:120:LYS:N	2.34	0.42
1:A:200:GLN:NE2	1:A:207:TYR:HB2	2.34	0.42
2:B:140:TYR:OH	2:B:142:GLN:NE2	2.53	0.41
2:B:30:TYR:HD2	2:B:37:PHE:HE1	1.67	0.41
1:A:353:HIS:ND1	1:A:353:HIS:N	2.68	0.41
2:B:115:LYS:CG	2:B:116:LYS:N	2.82	0.41
1:A:154:PRO:HD3	1:A:235:ASN:OD1	2.20	0.41
1:A:157:THR:H	1:A:181:ALA:HA	1.84	0.41
2:B:96:GLU:C	2:B:115:LYS:HZ2	2.24	0.41
1:A:183:GLY:O	1:A:185:PRO:O	2.38	0.41
2:B:70:TYR:N	2:B:70:TYR:CD1	2.88	0.41
1:A:173:ASN:O	1:A:220:SER:N	2.53	0.41
1:A:164:LYS:HD2	1:A:167:HIS:NE2	2.35	0.41
1:A:235:ASN:HB2	1:A:236:GLU:H	1.61	0.41
1:A:327:LEU:HD13	1:A:329:ILE:HG13	2.03	0.41
1:A:343:LEU:HG	1:A:350:ILE:HD13	2.03	0.41
1:A:317:VAL:O	1:A:318:ASN:HB3	2.20	0.41
1:A:184:ASN:HA	1:A:185:PRO:HA	1.73	0.41
1:A:162:MET:HB3	1:A:242:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:GLU:HG3	2:B:102:GLU:O	2.21	0.41
2:B:111:THR:HG22	2:B:145:ILE:HG13	2.03	0.41
1:A:231:CYS:HB3	1:A:242:HIS:H	1.85	0.41
2:B:82:MET:HE3	2:B:100:PHE:HZ	1.85	0.41
2:B:116:LYS:HG3	2:B:117:HIS:HB3	2.02	0.41
2:B:131:SER:HB3	2:B:133:LYS:HZ1	1.85	0.41
1:A:168:ALA:CB	2:B:150:LEU:HD11	2.51	0.41
2:B:50:ARG:HA	2:B:50:ARG:NE	2.36	0.41
1:A:219:GLU:O	1:A:220:SER:OG	2.36	0.41
1:A:175:VAL:HG13	1:A:175:VAL:O	2.21	0.41
1:A:155:TYR:O	1:A:182:GLY:N	2.53	0.41
2:B:115:LYS:O	2:B:117:HIS:N	2.54	0.41
1:A:209:VAL:HG12	1:A:210:ARG:H	1.85	0.41
1:A:258:LEU:HD12	1:A:352:PHE:CD2	2.56	0.41
1:A:290:TRP:CD1	1:A:342:CYS:CB	3.03	0.40
1:A:273:ASP:OD2	1:A:328:TYR:CE1	2.74	0.40
2:B:122:TRP:CH2	2:B:136:PRO:HD3	2.57	0.40
1:A:194:ASN:HD21	1:A:228:ASN:H	1.69	0.40
1:A:324:ILE:HD12	1:A:324:ILE:HG23	1.69	0.40
1:A:344:ALA:H	1:A:350:ILE:HD11	1.86	0.40
1:A:156:TRP:HA	1:A:181:ALA:HB2	2.02	0.40
1:A:251:ARG:HD2	1:A:283:ASP:OD2	2.22	0.40
2:B:61:LEU:CG	2:B:71:ILE:HG12	2.52	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	194/223 (87%)	134 (69%)	43 (22%)	17 (9%)	1 17
2	B	132/138 (96%)	102 (77%)	20 (15%)	10 (8%)	1 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	326/361 (90%)	236 (72%)	63 (19%)	27 (8%)	1 18

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	THR
1	A	175	VAL
1	A	214	TRP
1	A	280	VAL
1	A	313	LYS
2	B	85	ASP
2	B	121	ASN
2	B	133	LYS
2	B	139	HIS
2	B	140	TYR
2	B	152	VAL
1	A	173	ASN
1	A	180	PRO
1	A	219	GLU
1	A	273	ASP
1	A	281	TYR
2	B	118	ALA
2	B	119	GLU
1	A	282	SER
1	A	295	GLU
1	A	350	ILE
2	B	88	LEU
1	A	221	VAL
1	A	332	VAL
1	A	202	HIS
1	A	335	GLU
2	B	124	VAL

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	170/190 (90%)	138 (81%)	32 (19%)	2 15
2	B	118/120 (98%)	105 (89%)	13 (11%)	8 37
All	All	288/310 (93%)	243 (84%)	45 (16%)	3 23

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	LYS
1	A	162	MET
1	A	178	ARG
1	A	186	MET
1	A	189	MET
1	A	199	LYS
1	A	200	GLN
1	A	201	GLU
1	A	208	LYS
1	A	212	GLN
1	A	213	HIS
1	A	218	MET
1	A	219	GLU
1	A	235	ASN
1	A	239	SER
1	A	249	VAL
1	A	258	LEU
1	A	275	GLU
1	A	279	LYS
1	A	289	GLN
1	A	293	HIS
1	A	294	VAL
1	A	312	LEU
1	A	319	THR
1	A	320	THR
1	A	322	LYS
1	A	325	GLU
1	A	329	ILE
1	A	330	ARG
1	A	333	THR
1	A	353	HIS
1	A	359	VAL
2	B	23	TYR
2	B	24	LYS
2	B	39	ARG

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Mol	Chain	Res	Type
2	B	49	THR
2	B	50	ARG
2	B	59	LEU
2	B	70	TYR
2	B	72	LYS
2	B	99	LEU
2	B	103	ARG
2	B	113	ILE
2	B	134	ARG
2	B	146	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	A	173	ASN
1	A	213	HIS
1	A	242	HIS
1	A	265	ASN
2	B	36	HIS
2	B	56	HIS
2	B	142	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	198/223 (88%)	1.59	64 (32%) 1 1	134, 278, 416, 527	0
2	B	134/138 (97%)	1.64	47 (35%) 0 1	162, 281, 425, 455	0
All	All	332/361 (91%)	1.61	111 (33%) 0 1	134, 279, 424, 527	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	VAL	9.3
1	A	352	PHE	7.5
2	B	22	ASN	7.2
2	B	38	LEU	7.0
2	B	68	GLU	6.9
1	A	351	SER	6.9
2	B	71	ILE	6.3
1	A	342	CYS	6.1
1	A	233	VAL	6.0
1	A	156	TRP	6.0
1	A	289	GLN	5.9
2	B	27	LYS	5.9
2	B	124	VAL	5.8
2	B	100	PHE	5.8
1	A	325	GLU	5.8
1	A	273	ASP	5.7
1	A	264	ALA	5.6
1	A	343	LEU	5.5
1	A	291	ILE	5.2
1	A	314	ALA	5.1
2	B	121	ASN	5.0
2	B	123	PHE	5.0
2	B	70	TYR	4.8
2	B	29	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	125	GLY	4.6
2	B	37	PHE	4.6
1	A	229	TYR	4.5
1	A	328	TYR	4.4
1	A	207	TYR	4.4
2	B	28	LEU	4.3
1	A	340	TYR	4.3
2	B	80	LEU	4.3
2	B	59	LEU	4.2
2	B	133	LYS	4.2
1	A	244	TYR	4.1
1	A	177	PHE	4.0
1	A	327	LEU	4.0
1	A	288	ILE	4.0
2	B	87	LEU	4.0
1	A	164	LYS	4.0
1	A	249	VAL	3.9
2	B	148	LEU	3.9
2	B	112	TYR	3.9
1	A	191	TRP	3.9
2	B	88	LEU	3.7
1	A	176	LYS	3.7
1	A	276	PHE	3.7
2	B	103	ARG	3.7
2	B	40	ILE	3.7
1	A	341	THR	3.6
2	B	104	LEU	3.6
1	A	329	ILE	3.6
1	A	359	VAL	3.5
1	A	313	LYS	3.5
1	A	326	VAL	3.4
1	A	240	ILE	3.4
2	B	73	SER	3.4
1	A	272	GLY	3.4
1	A	216	LEU	3.4
1	A	175	VAL	3.3
2	B	78	GLN	3.3
2	B	69	VAL	3.3
1	A	215	SER	3.2
1	A	166	LEU	3.1
2	B	146	LEU	3.0
1	A	231	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	315	ALA	3.0
2	B	107	ASN	2.9
2	B	67	GLY	2.9
1	A	336	ASP	2.9
1	A	266	ALA	2.9
1	A	257	ILE	2.9
2	B	113	ILE	2.9
1	A	271	GLY	2.8
1	A	258	LEU	2.8
2	B	79	TYR	2.8
2	B	91	SER	2.8
2	B	149	PRO	2.7
1	A	214	TRP	2.7
1	A	246	LEU	2.7
1	A	265	ASN	2.7
1	A	234	GLU	2.7
1	A	168	ALA	2.6
1	A	280	VAL	2.6
2	B	147	PHE	2.6
1	A	189	MET	2.5
2	B	76	THR	2.5
2	B	145	ILE	2.5
2	B	32	SER	2.5
2	B	111	THR	2.5
1	A	218	MET	2.5
1	A	217	ILE	2.5
1	A	161	LYS	2.5
1	A	165	ARG	2.4
2	B	108	HIS	2.3
1	A	344	ALA	2.3
1	A	174	THR	2.3
2	B	72	LYS	2.2
2	B	50	ARG	2.2
1	A	253	PRO	2.2
1	A	167	HIS	2.2
1	A	193	LYS	2.2
1	A	230	THR	2.1
2	B	66	VAL	2.1
2	B	34	GLY	2.1
2	B	102	GLU	2.1
1	A	241	ASN	2.1
1	A	181	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	204	ILE	2.0
2	B	57	ILE	2.0
2	B	101	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.