Full wwPDB X-ray Structure Validation Report (i)

PDB ID	:	1YM7
Title	:	G Protein-Coupled Receptor Kinase 2 (GRK2)
Authors	:	Lodowski, D.T.; Barnhill, J.F.; Pyskadlo, R.M.; Ghirlando, R.; Sterne-Marr, R.; Tesmer, J.J.G.
Deposited on	:	2005-01-20
Resolution	:	4.50 Å(reported)

The following versions of software and data (see references (i)) 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 4.50 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.
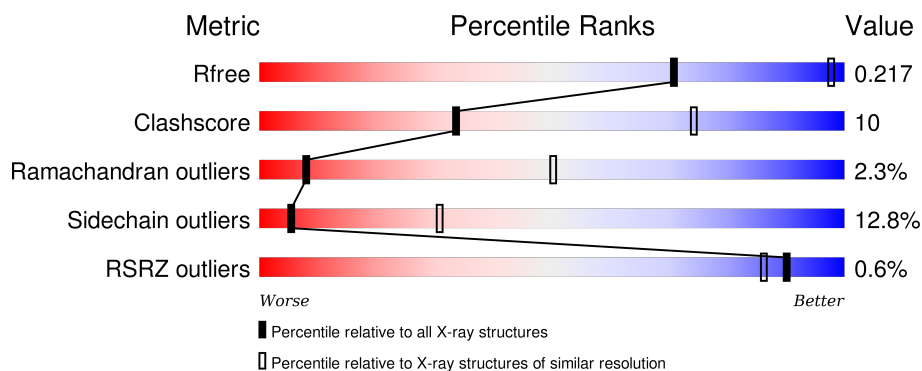
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	689	59% 24% 5% 12%
1	B	689	58% 25% • 12%
1	C	689	60% 24% • 12%
1	D	689	61% 21% • 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 19846 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-adrenergic receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	608	Total	C	N	O	S	0	0	0
			4982	3177	865	905	35			
1	B	608	Total	C	N	O	S	0	0	0
			4982	3177	865	905	35			
1	C	607	Total	C	N	O	S	0	0	0
			4975	3173	864	903	35			
1	D	599	Total	C	N	O	S	0	0	0
			4907	3132	850	890	35			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	670	ALA	SER	ENGINEERED	UNP P21146
B	670	ALA	SER	ENGINEERED	UNP P21146
C	670	ALA	SER	ENGINEERED	UNP P21146
D	670	ALA	SER	ENGINEERED	UNP P21146

3 Residue-property plots ⓘ

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

- Molecule 1: Beta-adrenergic receptor kinase 1
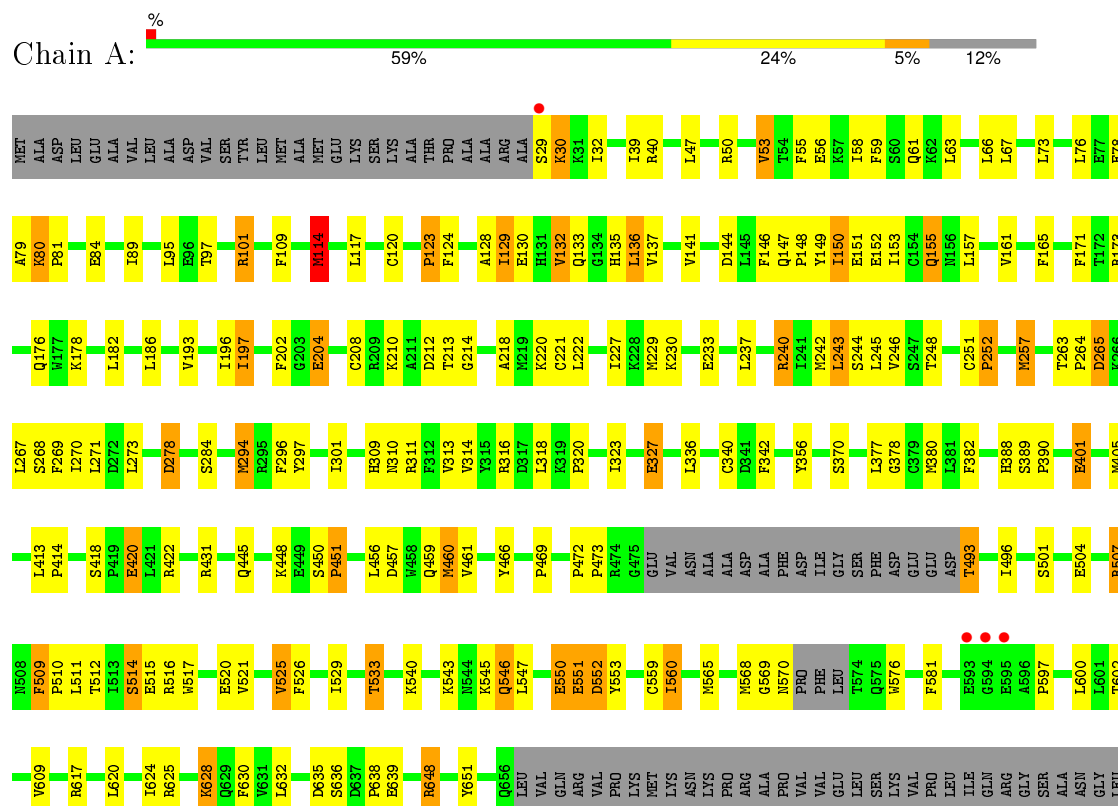
%

Chain A:

59% 24% 5% 12%

- Molecule 1: Beta-adrenergic receptor kinase 1

%

Chain B:

58% 25% · 12%
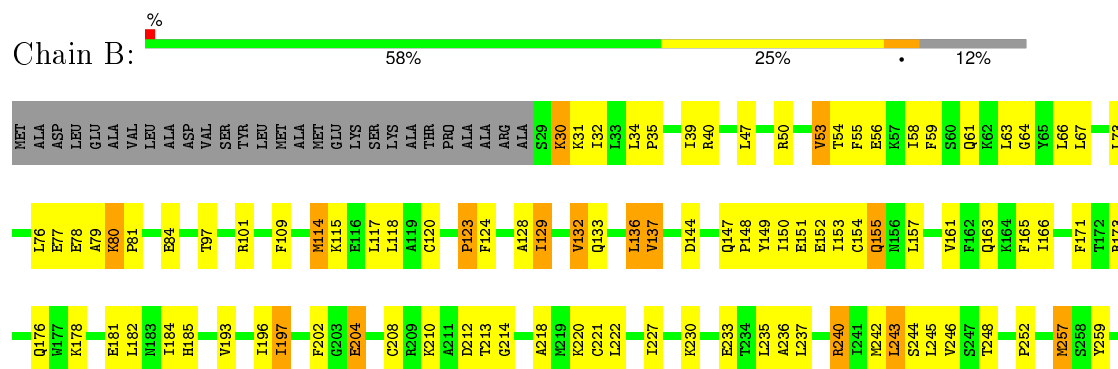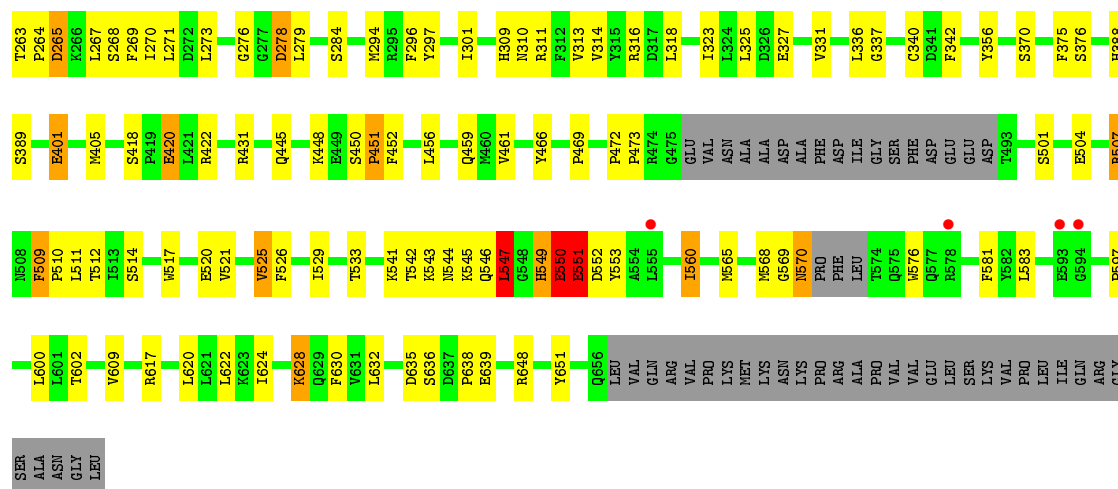
• Molecule 1: Beta-adrenergic receptor kinase 1
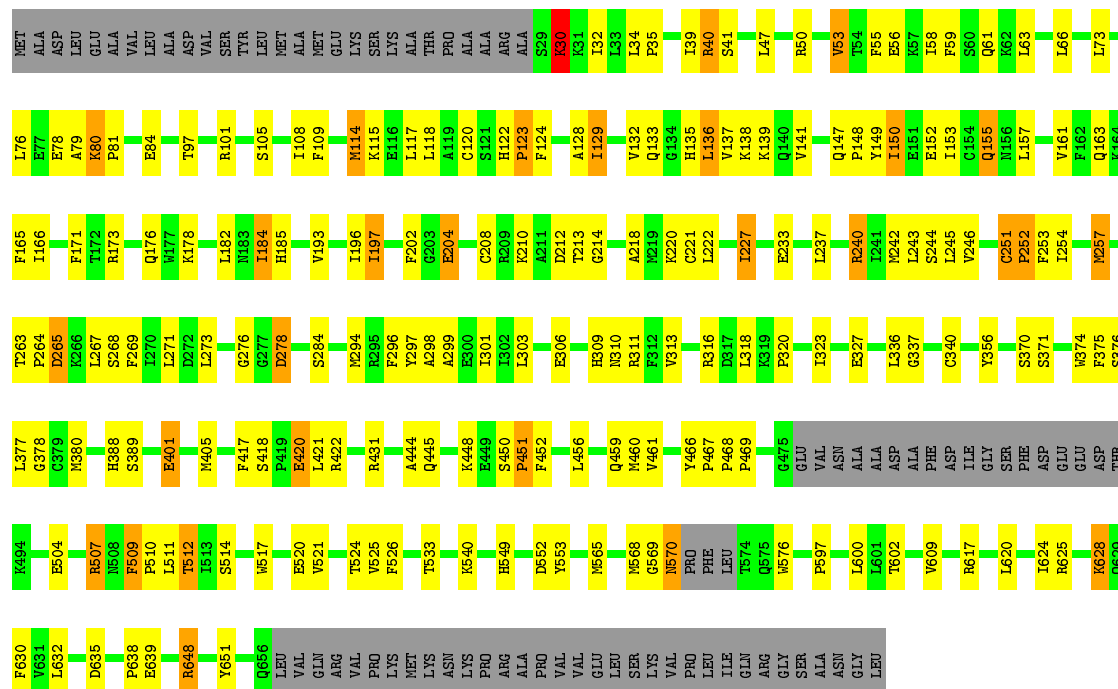
Chain C:

• Molecule 1: Beta-adrenergic receptor kinase 1

Chain D:
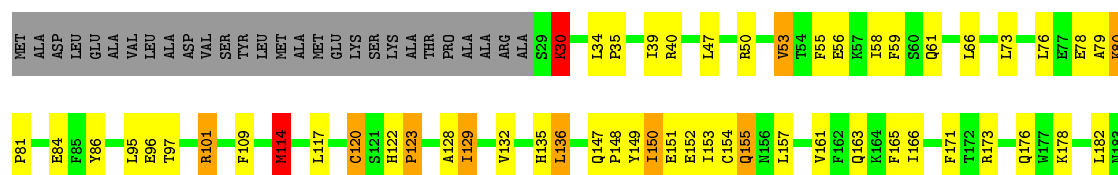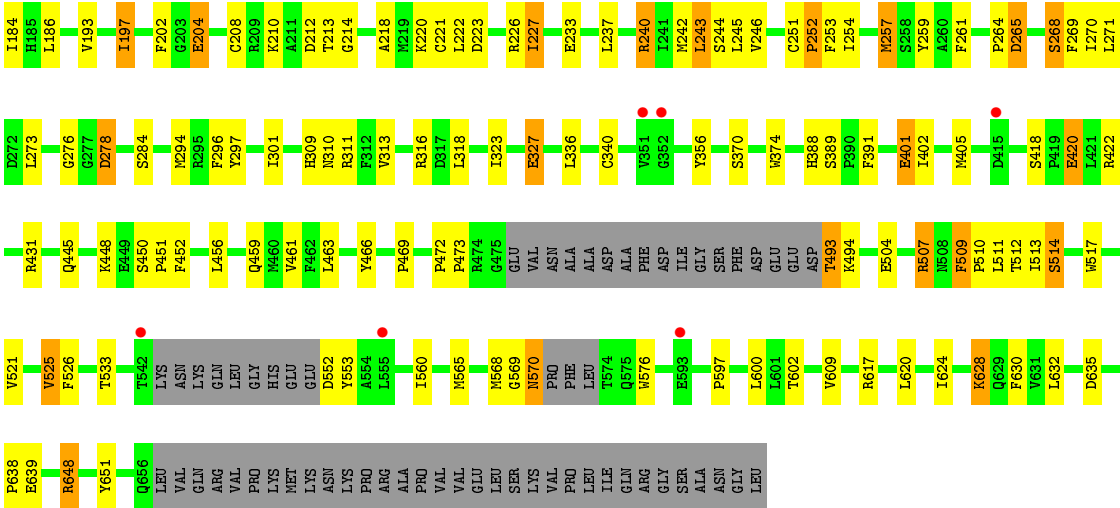
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants	115.16Å 82.16Å 218.79Å	Depositor
a, b, c, α, β, γ	90.00° 95.57° 90.00°	
Resolution (Å)	14.98 – 4.50	Depositor
	19.99 – 3.98	EDS
% Data completeness	99.9 (14.98-4.50)	Depositor
(in resolution range)	97.9 (19.99-3.98)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 3.94Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.224 , 0.279	Depositor
	0.212 , 0.217	DCC
R_{free} test set	1210 reflections (4.98%)	DCC
Wilson B-factor (Å^2)	206.3	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 30.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Outliers	1 of 34472 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19846	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (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	0.79	4/5093 (0.1%)	0.76	0/6842
1	B	0.88	8/5093 (0.2%)	0.79	1/6842 (0.0%)
1	C	0.68	0/5086	0.76	0/6832
1	D	0.57	0/5016	0.71	0/6739
All	All	0.74	12/20288 (0.1%)	0.75	1/27255 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	546	GLN	CD-OE1	25.76	1.80	1.24
1	B	550	GLU	CD-OE2	20.09	1.47	1.25
1	B	546	GLN	CD-OE1	13.80	1.54	1.24
1	B	547	LEU	C-N	10.28	1.51	1.33
1	B	551	GLU	CD-OE2	9.34	1.35	1.25
1	B	551	GLU	CD-OE1	8.52	1.35	1.25
1	B	547	LEU	C-O	-8.44	1.07	1.23
1	B	550	GLU	CD-OE1	8.32	1.34	1.25
1	A	546	GLN	CD-NE2	7.19	1.50	1.32
1	A	545	LYS	CE-NZ	6.33	1.64	1.49
1	B	543	LYS	CE-NZ	-6.25	1.33	1.49
1	A	545	LYS	CG-CD	5.35	1.70	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	551	GLU	OE1-CD-OE2	5.76	130.21	123.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	493	THR	Peptide
1	B	547	LEU	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4982	0	4968	106	0
1	B	4982	0	4968	106	0
1	C	4975	0	4961	108	0
1	D	4907	0	4894	89	0
All	All	19846	0	19791	404	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 10.

All (404) 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:546:GLN:CD	1:A:546:GLN:OE1	1.80	1.18
1:D:493:THR:HG22	1:D:494:LYS:HG2	1.55	0.88
1:B:173:ARG:HA	1:B:176:GLN:OE1	1.82	0.79
1:C:297:TYR:O	1:C:301:ILE:HG12	1.81	0.79
1:A:130:GLU:OE2	1:C:115:LYS:HE2	1.82	0.78
1:B:243:LEU:HG	1:B:336:LEU:HD13	1.67	0.77
1:B:309:HIS:CE1	1:B:370:SER:HB2	2.21	0.75
1:A:240:ARG:HG3	1:A:509:PHE:CD1	2.23	0.73
1:A:173:ARG:HA	1:A:176:GLN:OE1	1.89	0.72
1:C:240:ARG:NH1	1:C:511:LEU:HD22	2.05	0.71
1:A:309:HIS:CE1	1:A:370:SER:HB2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:TYR:O	1:A:301:ILE:HG12	1.93	0.69
1:B:227:ILE:HG22	1:B:233:GLU:HG3	1.74	0.69
1:A:152:GLU:HA	1:A:155:GLN:HB2	1.75	0.69
1:D:240:ARG:NH1	1:D:511:LEU:HD22	2.09	0.68
1:B:265:ASP:OD1	1:B:265:ASP:N	2.27	0.67
1:A:147:GLN:HB3	1:A:148:PRO:HD3	1.77	0.67
1:C:152:GLU:HA	1:C:155:GLN:HB2	1.74	0.67
1:B:210:LYS:HD3	1:B:520:GLU:OE2	1.95	0.67
1:A:509:PHE:H	1:A:510:PRO:CD	2.07	0.67
1:A:61:GLN:HE22	1:A:178:LYS:HE2	1.61	0.66
1:D:265:ASP:N	1:D:265:ASP:OD1	2.28	0.66
1:A:243:LEU:HG	1:A:336:LEU:HD13	1.77	0.66
1:B:227:ILE:CG2	1:B:233:GLU:HG3	2.25	0.66
1:B:204:GLU:CD	1:B:204:GLU:H	1.99	0.66
1:C:204:GLU:H	1:C:204:GLU:CD	1.99	0.65
1:D:204:GLU:H	1:D:204:GLU:CD	1.99	0.65
1:C:210:LYS:HD3	1:C:520:GLU:OE2	1.96	0.65
1:B:152:GLU:HA	1:B:155:GLN:HB2	1.79	0.65
1:B:509:PHE:H	1:B:510:PRO:CD	2.10	0.64
1:D:173:ARG:HA	1:D:176:GLN:OE1	1.96	0.64
1:C:509:PHE:H	1:C:510:PRO:HD2	1.62	0.64
1:C:509:PHE:H	1:C:510:PRO:CD	2.10	0.64
1:C:184:ILE:HG21	1:C:512:THR:HG21	1.79	0.64
1:D:152:GLU:HA	1:D:155:GLN:HB2	1.79	0.64
1:D:61:GLN:HE22	1:D:178:LYS:HE2	1.62	0.63
1:D:297:TYR:O	1:D:301:ILE:HG12	1.99	0.63
1:B:240:ARG:HG3	1:B:509:PHE:CD1	2.33	0.63
1:B:297:TYR:O	1:B:301:ILE:HG12	1.97	0.63
1:A:227:ILE:HG22	1:A:233:GLU:HG3	1.80	0.63
1:A:204:GLU:H	1:A:204:GLU:CD	2.01	0.63
1:B:509:PHE:H	1:B:510:PRO:HD2	1.64	0.63
1:C:76:LEU:HD23	1:C:79:ALA:HB2	1.81	0.63
1:D:240:ARG:HG3	1:D:509:PHE:CD1	2.34	0.62
1:C:401:GLU:O	1:C:405:MET:HG2	1.98	0.62
1:A:265:ASP:OD1	1:A:265:ASP:N	2.32	0.62
1:D:309:HIS:CE1	1:D:370:SER:HB2	2.35	0.62
1:A:336:LEU:HD12	1:A:336:LEU:H	1.65	0.62
1:D:147:GLN:HB3	1:D:148:PRO:HD3	1.82	0.62
1:D:227:ILE:CG2	1:D:233:GLU:HG3	2.29	0.62
1:C:184:ILE:CG2	1:C:512:THR:HG21	2.29	0.62
1:B:517:TRP:O	1:B:521:VAL:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ARG:NH1	1:A:511:LEU:HD22	2.15	0.61
1:A:157:LEU:HD23	1:A:161:VAL:HG11	1.82	0.61
1:C:210:LYS:HG2	1:C:212:ASP:HB2	1.82	0.61
1:B:213:THR:OG1	1:B:214:GLY:N	2.34	0.61
1:A:509:PHE:H	1:A:510:PRO:HD2	1.65	0.61
1:D:243:LEU:HG	1:D:336:LEU:HD13	1.82	0.60
1:A:210:LYS:HG2	1:A:212:ASP:HB2	1.81	0.60
1:B:541:LYS:O	1:B:545:LYS:N	2.34	0.60
1:B:61:GLN:HE22	1:B:178:LYS:HE2	1.66	0.60
1:C:240:ARG:HG3	1:C:509:PHE:CD1	2.36	0.60
1:C:265:ASP:N	1:C:265:ASP:OD1	2.33	0.60
1:D:227:ILE:HG22	1:D:233:GLU:HG3	1.83	0.60
1:D:210:LYS:HG2	1:D:212:ASP:HB2	1.85	0.59
1:D:509:PHE:H	1:D:510:PRO:HD2	1.68	0.59
1:C:157:LEU:HD23	1:C:161:VAL:HG11	1.85	0.59
1:C:227:ILE:CG2	1:C:233:GLU:HG3	2.32	0.59
1:D:509:PHE:H	1:D:510:PRO:CD	2.16	0.58
1:D:157:LEU:HD23	1:D:161:VAL:HG11	1.85	0.58
1:C:316:ARG:NH2	1:C:340:CYS:HB2	2.19	0.58
1:A:213:THR:OG1	1:A:214:GLY:N	2.36	0.58
1:D:517:TRP:O	1:D:521:VAL:HG23	2.04	0.58
1:B:76:LEU:HD23	1:B:79:ALA:HB2	1.86	0.58
1:B:210:LYS:HG2	1:B:212:ASP:HB2	1.84	0.57
1:D:76:LEU:HD23	1:D:79:ALA:HB2	1.86	0.57
1:D:202:PHE:HB2	1:D:222:LEU:HD22	1.86	0.57
1:D:213:THR:OG1	1:D:214:GLY:N	2.38	0.57
1:B:173:ARG:NE	1:B:176:GLN:OE1	2.32	0.57
1:B:638:PRO:O	1:B:639:GLU:C	2.43	0.57
1:C:301:ILE:HD12	1:C:323:ILE:HD13	1.87	0.57
1:C:336:LEU:H	1:C:336:LEU:HD12	1.67	0.57
1:C:173:ARG:NE	1:C:176:GLN:OE1	2.32	0.57
1:C:61:GLN:HE22	1:C:178:LYS:HE2	1.69	0.57
1:C:456:LEU:HD22	1:C:466:TYR:CE2	2.40	0.57
1:B:296:PHE:CD2	1:B:469:PRO:HD2	2.38	0.57
1:A:76:LEU:HD23	1:A:79:ALA:HB2	1.87	0.57
1:C:193:VAL:HA	1:C:208:CYS:HB3	1.87	0.57
1:C:242:MET:O	1:C:246:VAL:HG23	2.05	0.56
1:A:227:ILE:CG2	1:A:233:GLU:HG3	2.34	0.56
1:D:193:VAL:HA	1:D:208:CYS:HB3	1.88	0.56
1:B:157:LEU:HD23	1:B:161:VAL:HG11	1.87	0.56
1:C:243:LEU:HB3	1:C:257:MET:HE3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ILE:HG22	1:C:233:GLU:HG3	1.87	0.56
1:D:173:ARG:NE	1:D:176:GLN:OE1	2.31	0.56
1:A:30:LYS:H	1:A:30:LYS:HD2	1.71	0.55
1:B:132:VAL:HG21	1:B:149:TYR:CE1	2.41	0.55
1:C:149:TYR:O	1:C:150:ILE:C	2.45	0.55
1:A:173:ARG:NE	1:A:176:GLN:OE1	2.34	0.55
1:A:63:LEU:HD22	1:A:526:PHE:CE1	2.42	0.55
1:B:240:ARG:NH1	1:B:511:LEU:HD22	2.22	0.55
1:D:149:TYR:O	1:D:150:ILE:C	2.44	0.54
1:D:445:GLN:HG3	1:D:448:LYS:HE3	1.89	0.54
1:D:128:ALA:O	1:D:129:ILE:C	2.45	0.54
1:B:128:ALA:O	1:B:129:ILE:C	2.41	0.54
1:C:309:HIS:CE1	1:C:370:SER:HB2	2.42	0.54
1:B:445:GLN:HG3	1:B:448:LYS:HE3	1.90	0.54
1:A:123:PRO:HD2	1:A:124:PHE:CE2	2.43	0.54
1:A:620:LEU:HB2	1:A:632:LEU:HB2	1.89	0.54
1:C:213:THR:OG1	1:C:214:GLY:N	2.40	0.54
1:D:336:LEU:HD12	1:D:336:LEU:H	1.73	0.53
1:D:132:VAL:HG21	1:D:149:TYR:CE1	2.43	0.53
1:C:243:LEU:HG	1:C:336:LEU:HD13	1.89	0.53
1:A:257:MET:HA	1:A:271:LEU:HD23	1.89	0.53
1:A:130:GLU:OE2	1:C:115:LYS:CE	2.55	0.53
1:C:123:PRO:HD2	1:C:124:PHE:CE2	2.44	0.53
1:B:147:GLN:HB3	1:B:148:PRO:HD3	1.89	0.53
1:B:316:ARG:NH2	1:B:340:CYS:HB2	2.24	0.53
1:A:210:LYS:HD3	1:A:520:GLU:OE2	2.09	0.53
1:D:86:TYR:HD1	1:D:153:ILE:HD12	1.73	0.53
1:A:193:VAL:HA	1:A:208:CYS:HB3	1.91	0.53
1:A:202:PHE:HE1	1:A:230:LYS:HB2	1.74	0.52
1:C:418:SER:HB2	1:C:420:GLU:HG3	1.91	0.52
1:A:550:GLU:O	1:A:552:ASP:N	2.42	0.52
1:B:197:ILE:HG23	1:B:197:ILE:O	2.09	0.52
1:D:568:MET:HB2	1:D:576:TRP:CZ3	2.44	0.52
1:A:202:PHE:HB2	1:A:222:LEU:HD22	1.91	0.52
1:A:638:PRO:O	1:A:639:GLU:C	2.46	0.52
1:B:263:THR:O	1:B:265:ASP:N	2.43	0.52
1:B:181:GLU:O	1:B:184:ILE:HG22	2.10	0.52
1:A:137:VAL:HG13	1:C:136:LEU:HB3	1.92	0.52
1:B:257:MET:HA	1:B:271:LEU:HD23	1.92	0.52
1:B:109:PHE:CD1	1:B:136:LEU:HD12	2.44	0.52
1:C:173:ARG:HA	1:C:176:GLN:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:GLN:HG3	1:A:448:LYS:HE3	1.92	0.51
1:B:202:PHE:HB2	1:B:222:LEU:HD22	1.91	0.51
1:A:132:VAL:HG21	1:A:149:TYR:CE1	2.46	0.51
1:B:149:TYR:O	1:B:150:ILE:C	2.46	0.51
1:C:638:PRO:O	1:C:639:GLU:C	2.49	0.51
1:D:278:ASP:N	1:D:278:ASP:OD1	2.43	0.51
1:A:240:ARG:HG3	1:A:509:PHE:HD1	1.74	0.51
1:C:417:PHE:HB3	1:C:421:LEU:HD23	1.93	0.51
1:D:257:MET:HA	1:D:271:LEU:HD23	1.93	0.51
1:B:504:GLU:HG2	1:B:507:ARG:HH11	1.75	0.51
1:A:301:ILE:HD12	1:A:323:ILE:HD13	1.93	0.51
1:D:197:ILE:HG23	1:D:197:ILE:O	2.10	0.51
1:B:55:PHE:CZ	1:B:59:PHE:CD2	3.00	0.50
1:C:568:MET:HB2	1:C:576:TRP:CZ3	2.46	0.50
1:B:456:LEU:HD22	1:B:466:TYR:CE2	2.47	0.50
1:C:374:TRP:CE3	1:C:374:TRP:HA	2.47	0.50
1:A:504:GLU:HG2	1:A:507:ARG:HH11	1.77	0.49
1:A:514:SER:O	1:A:515:GLU:C	2.51	0.49
1:D:218:ALA:HB2	1:D:273:LEU:HA	1.93	0.49
1:C:375:PHE:O	1:C:376:SER:C	2.49	0.49
1:B:63:LEU:HD22	1:B:526:PHE:CE1	2.47	0.49
1:C:445:GLN:HG3	1:C:448:LYS:HE3	1.95	0.49
1:C:620:LEU:HB2	1:C:632:LEU:HB2	1.93	0.49
1:B:80:LYS:HB2	1:B:81:PRO:HD3	1.94	0.49
1:C:202:PHE:HB2	1:C:222:LEU:HD22	1.93	0.49
1:A:568:MET:HB2	1:A:576:TRP:CZ3	2.46	0.49
1:C:147:GLN:O	1:C:150:ILE:HB	2.13	0.49
1:B:568:MET:HB2	1:B:576:TRP:CZ3	2.47	0.49
1:D:242:MET:O	1:D:246:VAL:HG23	2.12	0.49
1:C:257:MET:HA	1:C:271:LEU:HD23	1.94	0.49
1:B:609:VAL:HG13	1:B:622:LEU:CD2	2.42	0.49
1:A:278:ASP:OD1	1:A:278:ASP:N	2.45	0.49
1:B:114:MET:O	1:B:117:LEU:N	2.46	0.49
1:B:336:LEU:O	1:B:337:GLY:C	2.49	0.48
1:C:109:PHE:CD1	1:C:136:LEU:HD12	2.48	0.48
1:B:624:ILE:HB	1:B:628:LYS:HB3	1.95	0.48
1:C:570:ASN:OD1	1:C:570:ASN:N	2.46	0.48
1:B:418:SER:HB2	1:B:420:GLU:HG3	1.94	0.48
1:D:296:PHE:CD2	1:D:469:PRO:HD2	2.48	0.48
1:A:336:LEU:HD12	1:A:336:LEU:N	2.29	0.48
1:C:609:VAL:HB	1:C:648:ARG:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLN:NE2	1:A:178:LYS:HE2	2.26	0.48
1:D:624:ILE:HB	1:D:628:LYS:HB3	1.94	0.48
1:B:132:VAL:HG21	1:B:149:TYR:HE1	1.78	0.48
1:A:517:TRP:O	1:A:521:VAL:HG23	2.14	0.48
1:D:257:MET:O	1:D:513:ILE:HD12	2.12	0.48
1:A:624:ILE:HB	1:A:628:LYS:HB3	1.94	0.48
1:D:301:ILE:HD12	1:D:323:ILE:HD13	1.95	0.47
1:A:456:LEU:HD22	1:A:466:TYR:CE2	2.48	0.47
1:C:114:MET:O	1:C:117:LEU:N	2.46	0.47
1:A:316:ARG:NH2	1:A:340:CYS:HB2	2.29	0.47
1:C:147:GLN:HB3	1:C:148:PRO:HD3	1.96	0.47
1:B:218:ALA:HB2	1:B:273:LEU:HD12	1.96	0.47
1:B:401:GLU:O	1:B:405:MET:HG2	2.13	0.47
1:C:251:CYS:SG	1:C:252:PRO:HD2	2.53	0.47
1:B:609:VAL:HB	1:B:648:ARG:HD3	1.97	0.47
1:A:144:ASP:O	1:A:147:GLN:HB2	2.14	0.47
1:D:73:LEU:HD21	1:D:84:GLU:HG3	1.95	0.47
1:C:624:ILE:HB	1:C:628:LYS:HB3	1.96	0.47
1:C:30:LYS:H	1:C:30:LYS:HD2	1.79	0.47
1:D:34:LEU:HA	1:D:35:PRO:HD3	1.81	0.47
1:A:242:MET:O	1:A:246:VAL:HG23	2.15	0.47
1:A:153:ILE:O	1:A:157:LEU:HD12	2.15	0.47
1:D:401:GLU:O	1:D:405:MET:HG2	2.14	0.47
1:B:450:SER:O	1:B:452:PHE:N	2.48	0.47
1:C:165:PHE:O	1:C:171:PHE:HB2	2.14	0.47
1:A:109:PHE:CD1	1:A:136:LEU:HD12	2.50	0.47
1:B:278:ASP:OD1	1:B:278:ASP:N	2.47	0.47
1:A:418:SER:HB2	1:A:420:GLU:HG3	1.97	0.47
1:B:193:VAL:HA	1:B:208:CYS:HB3	1.97	0.47
1:A:197:ILE:O	1:A:197:ILE:HG23	2.15	0.47
1:C:80:LYS:HB2	1:C:81:PRO:HD3	1.97	0.47
1:D:638:PRO:O	1:D:639:GLU:C	2.53	0.47
1:C:320:PRO:HD3	1:C:380:MET:HG3	1.96	0.47
1:D:109:PHE:CD1	1:D:136:LEU:HD12	2.50	0.47
1:A:149:TYR:O	1:A:150:ILE:C	2.54	0.46
1:C:263:THR:O	1:C:265:ASP:N	2.47	0.46
1:D:251:CYS:HA	1:D:252:PRO:HD3	1.75	0.46
1:C:336:LEU:N	1:C:336:LEU:HD12	2.30	0.46
1:A:136:LEU:HA	1:A:136:LEU:HD23	1.52	0.46
1:D:418:SER:HB2	1:D:420:GLU:HG3	1.97	0.46
1:D:151:GLU:O	1:D:154:CYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:570:ASN:N	1:D:570:ASN:OD1	2.49	0.46
1:A:251:CYS:HA	1:A:252:PRO:HD3	1.77	0.46
1:D:30:LYS:HD2	1:D:30:LYS:H	1.81	0.46
1:B:133:GLN:O	1:B:137:VAL:HG23	2.15	0.46
1:B:144:ASP:O	1:B:147:GLN:HB2	2.16	0.46
1:A:457:ASP:O	1:A:460:MET:HB2	2.15	0.46
1:C:132:VAL:HG21	1:C:149:TYR:CE1	2.51	0.46
1:C:504:GLU:HG2	1:C:507:ARG:HH11	1.80	0.46
1:B:620:LEU:HB2	1:B:632:LEU:HB2	1.97	0.46
1:B:235:LEU:O	1:B:236:ALA:C	2.54	0.46
1:B:30:LYS:HD2	1:B:30:LYS:H	1.80	0.46
1:D:259:TYR:HD1	1:D:270:ILE:HG21	1.80	0.45
1:B:279:LEU:HA	1:B:279:LEU:HD23	1.83	0.45
1:C:517:TRP:O	1:C:521:VAL:HG23	2.15	0.45
1:A:296:PHE:CD2	1:A:469:PRO:HD2	2.51	0.45
1:C:213:THR:HB	1:C:524:THR:OG1	2.17	0.45
1:D:136:LEU:HD23	1:D:136:LEU:HA	1.50	0.45
1:C:133:GLN:O	1:C:137:VAL:HG23	2.16	0.45
1:B:375:PHE:O	1:B:376:SER:C	2.54	0.45
1:C:445:GLN:HA	1:C:448:LYS:HG3	1.98	0.45
1:A:128:ALA:O	1:A:129:ILE:C	2.54	0.45
1:B:123:PRO:HD2	1:B:124:PHE:CE2	2.52	0.45
1:B:620:LEU:HD23	1:B:620:LEU:HA	1.72	0.45
1:A:472:PRO:HA	1:A:473:PRO:HD3	1.83	0.45
1:C:63:LEU:HD22	1:C:526:PHE:CE1	2.52	0.45
1:A:222:LEU:HB2	1:A:267:LEU:HB2	1.98	0.45
1:D:271:LEU:HD23	1:D:271:LEU:HA	1.72	0.45
1:D:445:GLN:HA	1:D:448:LYS:HG3	1.99	0.45
1:C:128:ALA:O	1:C:129:ILE:C	2.53	0.45
1:B:53:VAL:HA	1:B:58:ILE:HD11	1.99	0.45
1:B:570:ASN:N	1:B:570:ASN:OD1	2.50	0.45
1:C:123:PRO:HD2	1:C:124:PHE:CD2	2.52	0.45
1:A:504:GLU:OE2	1:A:507:ARG:NH1	2.50	0.45
1:C:138:LYS:O	1:C:139:LYS:HB2	2.17	0.45
1:D:163:GLN:O	1:D:166:ILE:HB	2.17	0.45
1:D:261:PHE:CE1	1:D:268:SER:HB3	2.51	0.45
1:B:314:VAL:HG23	1:B:342:PHE:CD1	2.52	0.45
1:C:218:ALA:HB2	1:C:273:LEU:HA	1.98	0.45
1:B:218:ALA:HB2	1:B:273:LEU:HA	1.99	0.44
1:C:220:LYS:HB3	1:C:269:PHE:HB2	1.98	0.44
1:D:61:GLN:NE2	1:D:178:LYS:HE2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:VAL:HA	1:D:58:ILE:HD11	1.98	0.44
1:B:504:GLU:OE2	1:B:507:ARG:NH1	2.51	0.44
1:B:542:THR:C	1:B:544:ASN:H	2.20	0.44
1:A:413:LEU:HA	1:A:414:PRO:HD3	1.90	0.44
1:B:202:PHE:HE1	1:B:230:LYS:HB2	1.81	0.44
1:A:609:VAL:HB	1:A:648:ARG:HD3	1.99	0.44
1:A:401:GLU:O	1:A:405:MET:HG2	2.17	0.44
1:D:153:ILE:O	1:D:157:LEU:HD12	2.17	0.44
1:D:513:ILE:O	1:D:514:SER:C	2.56	0.44
1:C:34:LEU:HA	1:C:35:PRO:HD3	1.81	0.44
1:A:314:VAL:HG23	1:A:342:PHE:CD1	2.53	0.44
1:C:620:LEU:HD23	1:C:620:LEU:HA	1.69	0.44
1:C:243:LEU:HB3	1:C:257:MET:CE	2.47	0.44
1:C:568:MET:HG3	1:C:569:GLY:N	2.32	0.44
1:A:457:ASP:HB3	1:A:460:MET:HG3	2.00	0.44
1:A:636:SER:O	1:A:639:GLU:HB2	2.18	0.44
1:A:445:GLN:HA	1:A:448:LYS:HG3	2.00	0.43
1:B:163:GLN:O	1:B:166:ILE:HB	2.18	0.43
1:A:55:PHE:CZ	1:A:59:PHE:CD2	3.06	0.43
1:C:53:VAL:HA	1:C:58:ILE:HD11	2.00	0.43
1:C:271:LEU:HD23	1:C:271:LEU:HA	1.67	0.43
1:D:96:GLU:OE2	1:D:463:LEU:HD12	2.17	0.43
1:C:253:PHE:O	1:C:254:ILE:HG13	2.18	0.43
1:C:197:ILE:O	1:C:197:ILE:HG23	2.18	0.43
1:A:80:LYS:HB2	1:A:81:PRO:HD3	2.00	0.43
1:A:95:LEU:HB2	1:A:101:ARG:HG3	1.99	0.43
1:B:636:SER:O	1:B:639:GLU:HB2	2.18	0.43
1:C:61:GLN:NE2	1:C:178:LYS:HE2	2.32	0.43
1:D:609:VAL:HB	1:D:648:ARG:HD3	2.00	0.43
1:D:620:LEU:HB2	1:D:632:LEU:HB2	2.00	0.43
1:B:67:LEU:HA	1:B:67:LEU:HD23	1.80	0.43
1:D:147:GLN:O	1:D:150:ILE:HB	2.18	0.43
1:A:568:MET:HG3	1:A:569:GLY:N	2.33	0.43
1:C:218:ALA:HB2	1:C:273:LEU:HD12	2.00	0.43
1:D:80:LYS:HB2	1:D:81:PRO:HD3	1.99	0.43
1:D:525:VAL:O	1:D:526:PHE:C	2.56	0.43
1:C:450:SER:HA	1:C:451:PRO:HD3	1.89	0.43
1:B:581:PHE:CD1	1:B:581:PHE:N	2.87	0.43
1:B:56:GLU:HG3	1:B:56:GLU:H	1.59	0.43
1:C:55:PHE:CZ	1:C:59:PHE:CD2	3.07	0.43
1:B:151:GLU:O	1:B:154:CYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:PRO:HD3	1:A:380:MET:HG3	2.00	0.43
1:C:298:ALA:O	1:C:299:ALA:C	2.57	0.43
1:D:122:HIS:HA	1:D:123:PRO:HD3	1.72	0.43
1:B:549:HIS:O	1:B:551:GLU:N	2.50	0.43
1:B:115:LYS:O	1:B:118:LEU:HB2	2.19	0.43
1:B:147:GLN:O	1:B:150:ILE:N	2.52	0.43
1:A:263:THR:O	1:A:265:ASP:N	2.51	0.43
1:A:150:ILE:HG22	1:A:151:GLU:N	2.34	0.43
1:B:450:SER:HA	1:B:451:PRO:HD3	1.89	0.43
1:A:529:ILE:O	1:A:533:THR:OG1	2.37	0.43
1:C:40:ARG:O	1:C:41:SER:C	2.56	0.43
1:D:456:LEU:HD22	1:D:466:TYR:CE2	2.53	0.43
1:D:132:VAL:HG21	1:D:149:TYR:HE1	1.83	0.42
1:A:133:GLN:OE1	1:C:114:MET:HG2	2.19	0.42
1:B:118:LEU:HA	1:B:118:LEU:HD23	1.83	0.42
1:B:242:MET:O	1:B:246:VAL:HG23	2.19	0.42
1:B:31:LYS:HE2	1:B:529:ILE:HD11	2.01	0.42
1:C:306:GLU:HG3	1:C:444:ALA:CB	2.49	0.42
1:D:253:PHE:O	1:D:254:ILE:HG13	2.19	0.42
1:D:327:GLU:HG3	1:D:327:GLU:H	1.63	0.42
1:C:278:ASP:N	1:C:278:ASP:OD1	2.53	0.42
1:B:155:GLN:HA	1:B:155:GLN:OE1	2.18	0.42
1:D:184:ILE:HD11	1:D:212:ASP:OD2	2.19	0.42
1:C:450:SER:O	1:C:452:PHE:N	2.52	0.42
1:D:165:PHE:O	1:D:171:PHE:HB2	2.19	0.42
1:B:73:LEU:HD21	1:B:84:GLU:HG3	2.01	0.42
1:D:472:PRO:HA	1:D:473:PRO:HD3	1.89	0.42
1:C:222:LEU:HB2	1:C:267:LEU:HB2	2.01	0.42
1:D:55:PHE:CZ	1:D:59:PHE:CD2	3.08	0.42
1:C:377:LEU:O	1:C:378:GLY:C	2.56	0.42
1:A:559:CYS:SG	1:A:560:ILE:N	2.92	0.42
1:A:294:MET:HE2	1:A:294:MET:HB3	1.94	0.42
1:B:336:LEU:HD12	1:B:336:LEU:H	1.85	0.42
1:B:79:ALA:O	1:B:80:LYS:C	2.58	0.42
1:C:336:LEU:O	1:C:337:GLY:C	2.57	0.42
1:A:63:LEU:HD22	1:A:526:PHE:CD1	2.55	0.42
1:C:163:GLN:O	1:C:166:ILE:HB	2.20	0.42
1:D:316:ARG:NH2	1:D:340:CYS:HB2	2.35	0.42
1:C:153:ILE:H	1:C:153:ILE:HG13	1.73	0.42
1:B:525:VAL:O	1:B:526:PHE:C	2.58	0.42
1:D:223:ASP:HB3	1:D:226:ARG:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:MET:O	1:A:117:LEU:N	2.49	0.42
1:A:624:ILE:CG2	1:A:625:ARG:H	2.33	0.42
1:D:504:GLU:HG2	1:D:507:ARG:HH11	1.84	0.42
1:C:467:PRO:HA	1:C:468:PRO:HD3	1.87	0.42
1:A:220:LYS:HB3	1:A:269:PHE:HB2	2.01	0.41
1:A:450:SER:HA	1:A:451:PRO:HD3	1.90	0.41
1:A:270:ILE:HA	1:A:270:ILE:HD13	1.63	0.41
1:B:259:TYR:OH	1:B:520:GLU:OE1	2.25	0.41
1:C:136:LEU:HD23	1:C:136:LEU:HA	1.65	0.41
1:B:271:LEU:HA	1:B:271:LEU:HD23	1.67	0.41
1:B:58:ILE:O	1:B:64:GLY:HA3	2.19	0.41
1:D:450:SER:O	1:D:452:PHE:N	2.53	0.41
1:B:34:LEU:HA	1:B:35:PRO:HD3	1.79	0.41
1:A:53:VAL:HA	1:A:58:ILE:HD11	2.02	0.41
1:C:153:ILE:O	1:C:157:LEU:HD12	2.21	0.41
1:A:624:ILE:HG22	1:A:625:ARG:N	2.35	0.41
1:D:620:LEU:HD23	1:D:620:LEU:HA	1.71	0.41
1:D:56:GLU:H	1:D:56:GLU:HG3	1.62	0.41
1:A:73:LEU:HD21	1:A:84:GLU:HG3	2.03	0.41
1:D:114:MET:O	1:D:117:LEU:N	2.49	0.41
1:A:382:PHE:CE1	1:A:390:PRO:HA	2.56	0.41
1:B:560:ILE:HG22	1:B:583:LEU:HD23	2.03	0.41
1:B:325:LEU:HG	1:B:331:VAL:HG12	2.02	0.41
1:B:165:PHE:O	1:B:171:PHE:HB2	2.21	0.41
1:A:327:GLU:H	1:A:327:GLU:HG3	1.61	0.41
1:B:270:ILE:HA	1:B:270:ILE:HD13	1.68	0.41
1:B:309:HIS:ND1	1:B:370:SER:HB2	2.36	0.41
1:B:301:ILE:HD12	1:B:323:ILE:HD13	2.02	0.41
1:A:149:TYR:O	1:A:153:ILE:HG13	2.21	0.41
1:B:61:GLN:NE2	1:B:178:LYS:HE2	2.33	0.41
1:B:220:LYS:HB3	1:B:269:PHE:HB2	2.03	0.41
1:A:581:PHE:N	1:A:581:PHE:CD1	2.88	0.41
1:D:184:ILE:HG23	1:D:184:ILE:O	2.20	0.41
1:A:123:PRO:HD2	1:A:124:PHE:CD2	2.55	0.41
1:C:251:CYS:SG	1:C:252:PRO:CD	3.08	0.41
1:C:56:GLU:H	1:C:56:GLU:HG3	1.68	0.41
1:D:220:LYS:HB3	1:D:269:PHE:HB2	2.03	0.41
1:C:624:ILE:CG2	1:C:625:ARG:H	2.34	0.41
1:C:296:PHE:CD2	1:C:469:PRO:HD2	2.56	0.41
1:B:77:GLU:HA	1:B:77:GLU:OE2	2.20	0.41
1:A:218:ALA:HB2	1:A:273:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:TRP:HA	1:D:374:TRP:CE3	2.54	0.41
1:A:165:PHE:O	1:A:171:PHE:HB2	2.20	0.41
1:D:336:LEU:N	1:D:336:LEU:HD12	2.35	0.41
1:B:153:ILE:O	1:B:157:LEU:HD12	2.21	0.41
1:A:525:VAL:O	1:A:526:PHE:C	2.59	0.41
1:C:624:ILE:HG22	1:C:625:ARG:N	2.36	0.41
1:C:73:LEU:HD21	1:C:84:GLU:HG3	2.03	0.41
1:C:79:ALA:O	1:C:80:LYS:C	2.59	0.40
1:A:67:LEU:HA	1:A:67:LEU:HD23	1.86	0.40
1:A:89:ILE:HD13	1:A:146:PHE:HB3	2.04	0.40
1:B:568:MET:HG3	1:B:569:GLY:N	2.36	0.40
1:A:377:LEU:O	1:A:378:GLY:C	2.60	0.40
1:B:222:LEU:HB2	1:B:267:LEU:HB2	2.04	0.40
1:A:56:GLU:H	1:A:56:GLU:HG3	1.63	0.40
1:C:105:SER:HA	1:C:108:ILE:HD12	2.03	0.40
1:D:568:MET:HG3	1:D:569:GLY:N	2.35	0.40
1:A:137:VAL:HG11	1:C:136:LEU:HD13	2.04	0.40
1:B:54:THR:O	1:B:55:PHE:C	2.59	0.40
1:D:95:LEU:HB2	1:D:101:ARG:HG3	2.02	0.40
1:B:472:PRO:HA	1:B:473:PRO:HD3	1.77	0.40
1:C:118:LEU:HD23	1:C:118:LEU:HA	1.92	0.40
1:C:122:HIS:HA	1:C:123:PRO:HD3	1.72	0.40
1:A:114:MET:HA	1:A:114:MET:HE3	2.04	0.40
1:D:391:PHE:HB2	1:D:402:ILE:HG23	2.04	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	602/689 (87%)	521 (86%)	68 (11%)	13 (2%)	8	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	602/689 (87%)	513 (85%)	75 (12%)	14 (2%)	8	50
1	C	601/689 (87%)	515 (86%)	72 (12%)	14 (2%)	8	50
1	D	591/689 (86%)	513 (87%)	64 (11%)	14 (2%)	7	49
All	All	2396/2756 (87%)	2062 (86%)	279 (12%)	55 (2%)	8	50

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	551	GLU
1	B	549	HIS
1	B	550	GLU
1	A	40	ARG
1	A	120	CYS
1	A	514	SER
1	B	120	CYS
1	B	264	PRO
1	B	451	PRO
1	C	40	ARG
1	C	264	PRO
1	C	276	GLY
1	C	514	SER
1	D	40	ARG
1	D	264	PRO
1	D	514	SER
1	A	264	PRO
1	A	451	PRO
1	B	40	ARG
1	B	551	GLU
1	C	120	CYS
1	C	371	SER
1	D	30	LYS
1	D	451	PRO
1	A	509	PHE
1	B	509	PHE
1	B	514	SER
1	D	120	CYS
1	D	276	GLY
1	A	123	PRO
1	B	597	PRO
1	C	30	LYS
1	C	80	LYS

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Mol	Chain	Res	Type
1	C	451	PRO
1	C	509	PHE
1	D	114	MET
1	D	123	PRO
1	D	509	PHE
1	A	80	LYS
1	A	114	MET
1	A	252	PRO
1	A	597	PRO
1	B	80	LYS
1	B	123	PRO
1	B	252	PRO
1	C	123	PRO
1	D	80	LYS
1	A	150	ILE
1	C	597	PRO
1	D	597	PRO
1	C	150	ILE
1	D	150	ILE
1	C	252	PRO
1	D	252	PRO
1	B	276	GLY

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	546/611 (89%)	468 (86%)	78 (14%)	4	27
1	B	546/611 (89%)	479 (88%)	67 (12%)	6	32
1	C	545/611 (89%)	476 (87%)	69 (13%)	5	31
1	D	538/611 (88%)	474 (88%)	64 (12%)	6	34
All	All	2175/2444 (89%)	1897 (87%)	278 (13%)	5	31

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	30	LYS
1	A	32	ILE
1	A	39	ILE
1	A	47	LEU
1	A	50	ARG
1	A	53	VAL
1	A	66	LEU
1	A	78	GLU
1	A	97	THR
1	A	101	ARG
1	A	114	MET
1	A	129	ILE
1	A	132	VAL
1	A	135	HIS
1	A	136	LEU
1	A	141	VAL
1	A	155	GLN
1	A	182	LEU
1	A	186	LEU
1	A	196	ILE
1	A	197	ILE
1	A	204	GLU
1	A	221	CYS
1	A	229	MET
1	A	237	LEU
1	A	240	ARG
1	A	243	LEU
1	A	244	SER
1	A	245	LEU
1	A	248	THR
1	A	257	MET
1	A	265	ASP
1	A	268	SER
1	A	278	ASP
1	A	284	SER
1	A	294	MET
1	A	310	ASN
1	A	311	ARG
1	A	313	VAL
1	A	318	LEU
1	A	327	GLU
1	A	356	TYR

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Mol	Chain	Res	Type
1	A	388	HIS
1	A	389	SER
1	A	401	GLU
1	A	420	GLU
1	A	422	ARG
1	A	431	ARG
1	A	459	GLN
1	A	460	MET
1	A	461	VAL
1	A	493	THR
1	A	496	ILE
1	A	501	SER
1	A	507	ARG
1	A	512	THR
1	A	516	ARG
1	A	525	VAL
1	A	533	THR
1	A	540	LYS
1	A	543	LYS
1	A	547	LEU
1	A	550	GLU
1	A	551	GLU
1	A	552	ASP
1	A	553	TYR
1	A	560	ILE
1	A	565	MET
1	A	570	ASN
1	A	600	LEU
1	A	602	THR
1	A	617	ARG
1	A	628	LYS
1	A	630	PHE
1	A	635	ASP
1	A	648	ARG
1	A	651	TYR
1	B	30	LYS
1	B	32	ILE
1	B	39	ILE
1	B	47	LEU
1	B	50	ARG
1	B	53	VAL
1	B	66	LEU

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Mol	Chain	Res	Type
1	B	78	GLU
1	B	97	THR
1	B	101	ARG
1	B	114	MET
1	B	129	ILE
1	B	132	VAL
1	B	136	LEU
1	B	137	VAL
1	B	155	GLN
1	B	182	LEU
1	B	185	HIS
1	B	196	ILE
1	B	197	ILE
1	B	204	GLU
1	B	221	CYS
1	B	237	LEU
1	B	240	ARG
1	B	243	LEU
1	B	244	SER
1	B	245	LEU
1	B	248	THR
1	B	257	MET
1	B	265	ASP
1	B	268	SER
1	B	278	ASP
1	B	284	SER
1	B	294	MET
1	B	310	ASN
1	B	311	ARG
1	B	313	VAL
1	B	318	LEU
1	B	327	GLU
1	B	356	TYR
1	B	388	HIS
1	B	389	SER
1	B	401	GLU
1	B	420	GLU
1	B	422	ARG
1	B	431	ARG
1	B	459	GLN
1	B	461	VAL
1	B	501	SER

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Mol	Chain	Res	Type
1	B	507	ARG
1	B	512	THR
1	B	525	VAL
1	B	533	THR
1	B	547	LEU
1	B	550	GLU
1	B	552	ASP
1	B	553	TYR
1	B	560	ILE
1	B	565	MET
1	B	570	ASN
1	B	600	LEU
1	B	602	THR
1	B	617	ARG
1	B	628	LYS
1	B	630	PHE
1	B	635	ASP
1	B	651	TYR
1	C	30	LYS
1	C	32	ILE
1	C	39	ILE
1	C	47	LEU
1	C	50	ARG
1	C	53	VAL
1	C	66	LEU
1	C	78	GLU
1	C	97	THR
1	C	101	ARG
1	C	114	MET
1	C	129	ILE
1	C	135	HIS
1	C	136	LEU
1	C	141	VAL
1	C	155	GLN
1	C	182	LEU
1	C	184	ILE
1	C	185	HIS
1	C	196	ILE
1	C	197	ILE
1	C	204	GLU
1	C	221	CYS
1	C	227	ILE

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Mol	Chain	Res	Type
1	C	237	LEU
1	C	240	ARG
1	C	244	SER
1	C	245	LEU
1	C	251	CYS
1	C	257	MET
1	C	265	ASP
1	C	268	SER
1	C	278	ASP
1	C	284	SER
1	C	294	MET
1	C	303	LEU
1	C	310	ASN
1	C	311	ARG
1	C	313	VAL
1	C	318	LEU
1	C	327	GLU
1	C	356	TYR
1	C	388	HIS
1	C	389	SER
1	C	401	GLU
1	C	420	GLU
1	C	422	ARG
1	C	431	ARG
1	C	459	GLN
1	C	460	MET
1	C	461	VAL
1	C	507	ARG
1	C	512	THR
1	C	525	VAL
1	C	533	THR
1	C	540	LYS
1	C	549	HIS
1	C	552	ASP
1	C	553	TYR
1	C	565	MET
1	C	570	ASN
1	C	600	LEU
1	C	602	THR
1	C	617	ARG
1	C	628	LYS
1	C	630	PHE

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Mol	Chain	Res	Type
1	C	635	ASP
1	C	648	ARG
1	C	651	TYR
1	D	30	LYS
1	D	39	ILE
1	D	47	LEU
1	D	50	ARG
1	D	53	VAL
1	D	66	LEU
1	D	78	GLU
1	D	97	THR
1	D	101	ARG
1	D	114	MET
1	D	120	CYS
1	D	129	ILE
1	D	135	HIS
1	D	136	LEU
1	D	155	GLN
1	D	182	LEU
1	D	186	LEU
1	D	197	ILE
1	D	204	GLU
1	D	221	CYS
1	D	227	ILE
1	D	237	LEU
1	D	240	ARG
1	D	243	LEU
1	D	244	SER
1	D	245	LEU
1	D	257	MET
1	D	265	ASP
1	D	268	SER
1	D	278	ASP
1	D	284	SER
1	D	294	MET
1	D	310	ASN
1	D	311	ARG
1	D	313	VAL
1	D	318	LEU
1	D	327	GLU
1	D	356	TYR
1	D	388	HIS

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Mol	Chain	Res	Type
1	D	389	SER
1	D	401	GLU
1	D	420	GLU
1	D	422	ARG
1	D	431	ARG
1	D	459	GLN
1	D	461	VAL
1	D	493	THR
1	D	507	ARG
1	D	512	THR
1	D	525	VAL
1	D	533	THR
1	D	552	ASP
1	D	553	TYR
1	D	560	ILE
1	D	565	MET
1	D	570	ASN
1	D	600	LEU
1	D	602	THR
1	D	617	ARG
1	D	628	LYS
1	D	630	PHE
1	D	635	ASP
1	D	648	ARG
1	D	651	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	ASN
1	A	434	ASN
1	A	459	GLN
1	A	607	GLN
1	B	309	HIS
1	B	459	GLN
1	B	607	GLN
1	C	310	ASN
1	C	459	GLN
1	C	607	GLN
1	D	434	ASN
1	D	459	GLN
1	D	607	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 (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(Å²)	Q<0.9
1	A	608/689 (88%)	-0.59	4 (0%)	89	84	40, 40, 40, 40	0
1	B	608/689 (88%)	-0.56	4 (0%)	89	84	40, 40, 40, 40	0
1	C	607/689 (88%)	-0.51	0	100	100	40, 40, 40, 40	0
1	D	599/689 (86%)	-0.41	6 (1%)	84	78	40, 40, 40, 40	0
All	All	2422/2756 (87%)	-0.52	14 (0%)	90	86	40, 40, 40, 40	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	593	GLU	6.7
1	A	593	GLU	3.8
1	D	351	VAL	3.4
1	A	595	GLU	3.2
1	D	593	GLU	3.2
1	A	594	GLY	3.0
1	B	594	GLY	2.8
1	D	542	THR	2.6
1	A	29	SER	2.5
1	D	415	ASP	2.4
1	D	555	LEU	2.4
1	D	352	GLY	2.1
1	B	555	LEU	2.1
1	B	578	ARG	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.