Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 12:48 PM EDT

PDB ID	:	1JOJ
Title	:	CONCANAVALIN A-HEXAPEPTIDE COMPLEX
Authors	:	Jain, D.; Kaur, K.; Salunke, D.M.
Deposited on	:	2001-07-30
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:

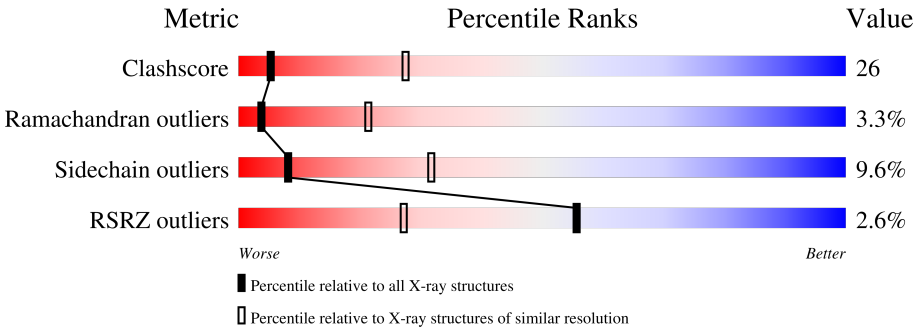
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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))
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	237	62% 31% 5%
1	B	237	% 64% 32%
1	C	237	65% 28% 7%
1	D	237	% 62% 32% 6%
2	P	8	75% 25% 12% 38% 25%
2	Q	8	62% 12% 25% 25% 38%

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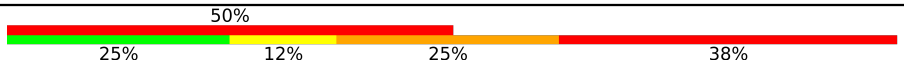
Mol	Chain	Length	Quality of chain
2	R	8	
2	S	8	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7717 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 Concanavalin-Br.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	B	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	C	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	D	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	ASP	GLY	conflict	UNP P55915
A	70	ALA	GLY	conflict	UNP P55915
A	151	ASP	GLU	conflict	UNP P55915
A	155	GLU	ARG	conflict	UNP P55915
B	58	ASP	GLY	conflict	UNP P55915
B	70	ALA	GLY	conflict	UNP P55915
B	151	ASP	GLU	conflict	UNP P55915
B	155	GLU	ARG	conflict	UNP P55915
C	58	ASP	GLY	conflict	UNP P55915
C	70	ALA	GLY	conflict	UNP P55915
C	151	ASP	GLU	conflict	UNP P55915
C	155	GLU	ARG	conflict	UNP P55915
D	58	ASP	GLY	conflict	UNP P55915
D	70	ALA	GLY	conflict	UNP P55915
D	151	ASP	GLU	conflict	UNP P55915
D	155	GLU	ARG	conflict	UNP P55915

- Molecule 2 is a protein called HEXAPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	8	Total	C	N	O	S	0	0	1
			69	50	8	10	1			
2	Q	8	Total	C	N	O	S	0	0	1
			69	50	8	10	1			
2	R	8	Total	C	N	O	S	0	0	1
			69	50	8	10	1			
2	S	8	Total	C	N	O	S	0	0	1
			69	50	8	10	1			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	54	Total	O	0	0
			54	54		
5	B	45	Total	O	0	0
			45	45		
5	C	56	Total	O	0	0
			56	56		

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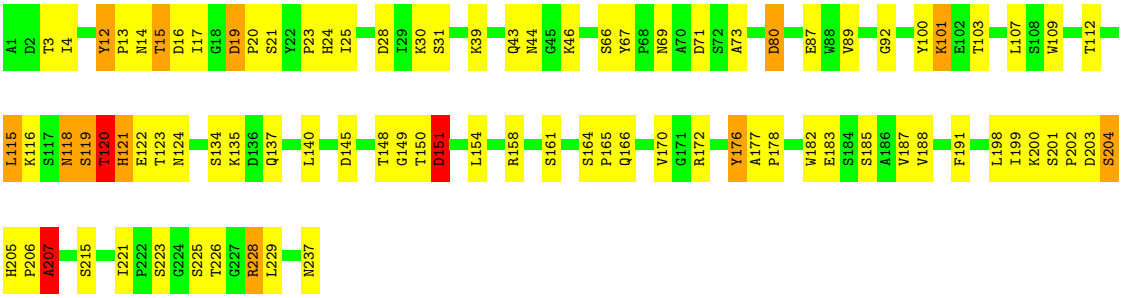
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	39	Total O 39 39	0	0
5	P	1	Total O 1 1	0	0
5	R	2	Total O 2 2	0	0

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.

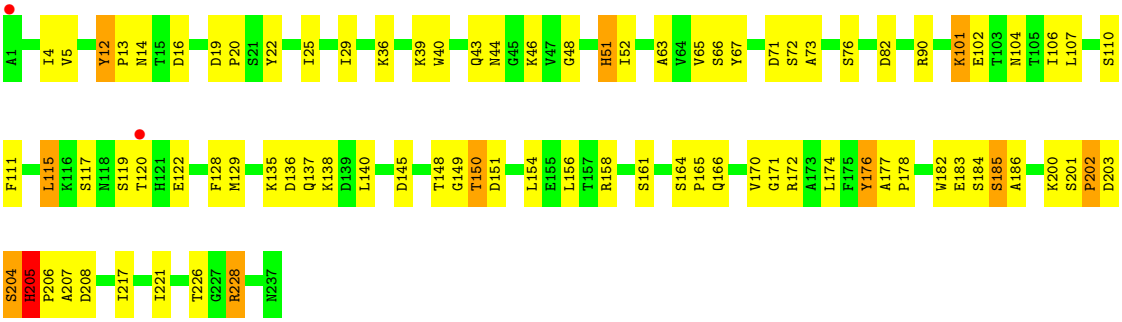
• Molecule 1: Concanavalin-Br

Chain A:



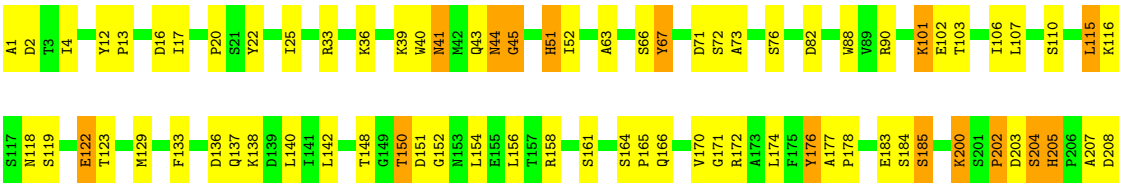
• Molecule 1: Concanavalin-Br

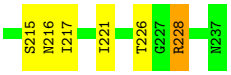
Chain B:



• Molecule 1: Concanavalin-Br

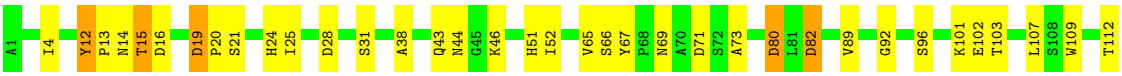
Chain C:

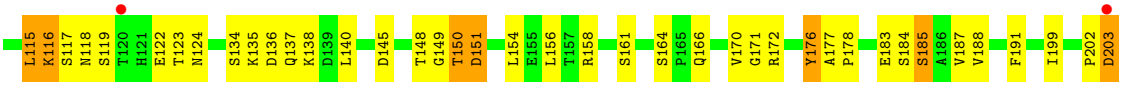




• Molecule 1: Concanavalin-Br

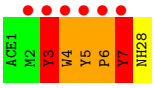
Chain D:





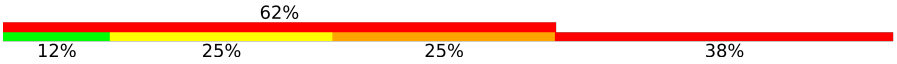
• Molecule 2: HEXAPEPTIDE

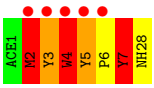
Chain P:



• Molecule 2: HEXAPEPTIDE

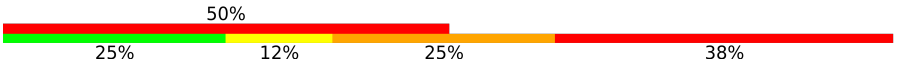
Chain Q:

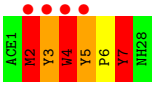




• Molecule 2: HEXAPEPTIDE

Chain R:





• Molecule 2: HEXAPEPTIDE

Chain S:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	102.69Å 118.38Å 253.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 19.67 – 3.00	Depositor EDS
% Data completeness (in resolution range)	78.1 (10.00-3.00) 75.7 (19.67-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.94 (at 2.98Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.186 , 0.231 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7717	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ACE, MN, NH2

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	0.44	0/1851	0.77	4/2522 (0.2%)
1	B	0.42	0/1851	0.74	1/2522 (0.0%)
1	C	0.83	1/1851 (0.1%)	0.77	3/2522 (0.1%)
1	D	0.47	1/1851 (0.1%)	0.72	2/2522 (0.1%)
2	P	0.77	0/71	2.34	5/98 (5.1%)
2	Q	0.83	0/71	1.93	4/98 (4.1%)
2	R	0.62	0/71	1.92	6/98 (6.1%)
2	S	0.79	0/71	1.96	3/98 (3.1%)
All	All	0.57	2/7688 (0.0%)	0.84	28/10480 (0.3%)

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
2	P	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	45	GLY	N-CA	30.81	1.92	1.46
1	D	202	PRO	C-N	-5.10	1.22	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	3	TYR	CB-CG-CD2	-11.24	114.26	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	44	ASN	C-N-CA	-10.05	101.20	122.30
2	P	5	TYR	N-CA-C	9.08	135.51	111.00
2	S	4	TRP	N-CA-C	8.50	133.95	111.00
2	P	3	TYR	CB-CG-CD1	7.56	125.54	121.00
2	R	2	MET	N-CA-C	-7.49	90.77	111.00
2	R	4	TRP	N-CA-C	7.46	131.14	111.00
2	P	3	TYR	CB-CA-C	-7.24	95.92	110.40
2	Q	2	MET	N-CA-C	-7.03	92.01	111.00
1	A	150	THR	CA-C-N	-6.96	101.89	117.20
1	B	205	HIS	N-CA-C	-6.82	92.59	111.00
2	R	4	TRP	CA-CB-CG	6.81	126.64	113.70
1	A	150	THR	C-N-CA	6.79	138.67	121.70
1	A	119	SER	N-CA-C	-6.71	92.89	111.00
2	R	5	TYR	CA-CB-CG	6.18	125.14	113.40
1	C	205	HIS	N-CA-C	-6.15	94.40	111.00
2	S	1	ACE	O-C-N	-6.12	112.91	122.70
2	Q	5	TYR	CA-CB-CG	6.01	124.82	113.40
1	A	151	ASP	CA-CB-CG	-5.79	100.66	113.40
1	D	150	THR	CA-C-N	-5.77	104.51	117.20
2	Q	5	TYR	CB-CA-C	-5.65	99.10	110.40
2	Q	4	TRP	CA-CB-CG	5.42	124.00	113.70
2	S	3	TYR	N-CA-C	-5.24	96.86	111.00
2	R	5	TYR	CB-CA-C	-5.22	99.97	110.40
2	P	3	TYR	CA-CB-CG	5.19	123.27	113.40
2	R	5	TYR	CB-CG-CD1	-5.11	117.93	121.00
1	C	67	TYR	CB-CG-CD2	5.02	124.01	121.00
1	D	203	ASP	CA-CB-CG	-5.00	102.40	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	ALA	Peptide
2	P	7	TYR	Sidechain

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	1809	0	1754	95	0
1	B	1809	0	1755	94	0
1	C	1809	0	1755	92	0
1	D	1809	0	1755	95	0
2	P	69	0	56	13	0
2	Q	69	0	56	21	0
2	R	69	0	56	22	0
2	S	69	0	56	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	54	0	0	4	0
5	B	45	0	0	3	0
5	C	56	0	0	4	0
5	D	39	0	0	5	0
5	P	1	0	0	1	0
5	R	2	0	0	0	0
All	All	7717	0	7243	391	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 26.

All (391) 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:C:45:GLY:N	1:C:45:GLY:CA	1.92	1.32
1:C:44:ASN:H	2:R:6:PRO:HD3	1.09	1.13
1:D:44:ASN:HB3	2:S:4:TRP:O	1.56	1.06
2:R:3:TYR:O	2:R:4:TRP:HB3	1.52	1.05
1:C:12:TYR:HD2	1:C:13:PRO:HD2	1.19	1.01
2:R:2:MET:HE2	2:R:2:MET:HA	1.45	0.98
1:C:116:LYS:HG2	1:C:123:THR:HG23	1.49	0.95
1:D:137:GLN:HG2	1:D:140:LEU:HD12	1.50	0.92
2:Q:2:MET:HA	2:Q:2:MET:CE	2.00	0.92
1:A:137:GLN:HG2	1:A:140:LEU:HD12	1.52	0.92
2:R:2:MET:HA	2:R:2:MET:CE	1.96	0.92
1:D:170:VAL:HG23	1:D:226:THR:HG22	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ARG:HD2	1:B:221:ILE:HG12	1.54	0.88
1:A:170:VAL:HG23	1:A:226:THR:HG22	1.56	0.88
1:C:12:TYR:CD2	1:C:13:PRO:HD2	2.09	0.86
2:Q:2:MET:HA	2:Q:2:MET:HE2	1.60	0.83
1:C:44:ASN:H	2:R:6:PRO:CD	1.90	0.83
1:C:172:ARG:HD2	1:C:221:ILE:HG12	1.61	0.83
1:B:12:TYR:HD2	1:B:13:PRO:N	1.76	0.83
1:C:43:GLN:HB2	1:C:67:TYR:CE1	2.14	0.82
2:Q:4:TRP:HZ3	2:Q:6:PRO:HA	1.45	0.81
1:C:44:ASN:C	1:C:45:GLY:CA	2.49	0.81
1:A:43:GLN:HB2	1:A:67:TYR:CE2	2.16	0.80
1:C:44:ASN:N	2:R:6:PRO:HD3	1.94	0.80
1:B:44:ASN:HB3	2:Q:4:TRP:O	1.82	0.79
1:C:43:GLN:HB2	1:C:67:TYR:HE1	1.45	0.79
1:B:119:SER:HB2	1:B:122:GLU:HG3	1.65	0.77
2:R:6:PRO:O	2:R:7:TYR:HB2	1.83	0.77
1:B:12:TYR:HD2	1:B:13:PRO:CD	1.99	0.76
1:A:200:LYS:NZ	1:A:200:LYS:HB2	2.02	0.75
1:D:43:GLN:HB2	1:D:67:TYR:CE2	2.21	0.75
2:R:4:TRP:HZ3	2:R:6:PRO:HA	1.51	0.75
1:A:203:ASP:O	1:A:205:HIS:N	2.20	0.74
1:D:203:ASP:CG	1:D:203:ASP:O	2.26	0.73
1:B:43:GLN:HB2	1:B:67:TYR:CE1	2.24	0.73
2:Q:6:PRO:O	2:Q:7:TYR:HB2	1.88	0.71
1:D:12:TYR:HD1	1:D:13:PRO:N	1.88	0.71
1:A:12:TYR:HD1	1:A:13:PRO:N	1.88	0.71
1:C:12:TYR:HD2	1:C:13:PRO:CD	2.01	0.71
1:A:43:GLN:H	1:A:67:TYR:HE2	1.39	0.71
1:C:170:VAL:CG2	1:C:226:THR:HG22	2.21	0.70
1:C:44:ASN:HB3	2:R:4:TRP:O	1.91	0.70
1:D:44:ASN:CB	2:S:4:TRP:O	2.38	0.70
1:D:187:VAL:HG12	1:D:188:VAL:HG23	1.74	0.69
1:D:25:ILE:HD11	1:D:73:ALA:HB3	1.73	0.69
1:B:44:ASN:HB3	2:Q:4:TRP:HB3	1.74	0.69
1:A:120:THR:C	1:A:122:GLU:H	1.96	0.68
1:A:120:THR:O	1:A:122:GLU:N	2.23	0.68
1:B:149:GLY:O	1:B:151:ASP:N	2.25	0.68
1:D:43:GLN:H	1:D:67:TYR:HE2	1.39	0.68
1:A:25:ILE:HD11	1:A:73:ALA:HB3	1.75	0.68
1:C:4:ILE:HD13	1:C:215:SER:HB3	1.74	0.68
1:D:148:THR:HG22	1:D:154:LEU:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:3:TYR:O	2:R:4:TRP:CB	2.36	0.68
1:B:170:VAL:CG2	1:B:226:THR:HG22	2.24	0.68
1:A:172:ARG:HD2	1:A:221:ILE:HG12	1.75	0.67
1:B:200:LYS:HD2	2:Q:3:TYR:CE2	2.30	0.67
1:D:172:ARG:NH2	5:D:339:HOH:O	2.22	0.67
1:B:12:TYR:CD2	1:B:13:PRO:HD2	2.28	0.67
2:R:4:TRP:CZ3	2:R:6:PRO:HA	2.28	0.67
2:S:6:PRO:HB3	2:S:7:TYR:HD1	1.60	0.67
2:Q:4:TRP:CZ3	2:Q:6:PRO:HA	2.29	0.66
1:A:43:GLN:HB2	1:A:67:TYR:HE2	1.59	0.66
1:B:43:GLN:HB2	1:B:67:TYR:HE1	1.59	0.66
1:B:228:ARG:HD2	5:B:326:HOH:O	1.96	0.66
1:B:102:GLU:HG2	1:B:207:ALA:O	1.96	0.65
1:D:172:ARG:HD2	1:D:221:ILE:HG12	1.79	0.65
1:B:202:PRO:HG2	1:B:203:ASP:H	1.60	0.65
1:A:148:THR:HG22	1:A:154:LEU:HD13	1.79	0.64
1:C:228:ARG:HD2	5:C:329:HOH:O	1.97	0.63
1:A:200:LYS:HE3	2:P:3:TYR:CE2	2.33	0.63
1:A:200:LYS:HB2	1:A:200:LYS:HZ2	1.61	0.63
1:A:200:LYS:HD3	2:P:3:TYR:OH	1.98	0.63
1:B:12:TYR:CD2	1:B:13:PRO:CD	2.81	0.63
1:C:204:SER:OG	2:R:4:TRP:CZ2	2.53	0.62
1:B:110:SER:HB3	1:B:129:MET:HG3	1.81	0.62
1:B:119:SER:CB	1:B:122:GLU:HG3	2.29	0.61
1:D:203:ASP:O	1:D:205:HIS:N	2.29	0.61
2:S:6:PRO:HB3	2:S:7:TYR:CD1	2.35	0.61
1:D:136:ASP:HA	5:D:330:HOH:O	1.99	0.61
1:B:205:HIS:H	1:B:206:PRO:HD3	1.65	0.61
1:B:44:ASN:HD22	2:Q:4:TRP:HB3	1.66	0.60
2:S:6:PRO:CB	2:S:7:TYR:HD1	2.14	0.60
1:A:20:PRO:HD2	1:A:24:HIS:CE1	2.35	0.60
1:B:200:LYS:NZ	1:B:200:LYS:HB3	2.15	0.60
1:D:20:PRO:HD2	1:D:24:HIS:CE1	2.36	0.60
1:D:43:GLN:HB2	1:D:67:TYR:HE2	1.64	0.60
1:C:43:GLN:CB	1:C:67:TYR:HE1	2.15	0.60
1:B:204:SER:O	1:B:205:HIS:HB2	2.01	0.60
1:A:170:VAL:CG2	1:A:226:THR:HG22	2.29	0.59
1:C:102:GLU:HG2	1:C:207:ALA:O	2.02	0.59
1:D:170:VAL:CG2	1:D:226:THR:HG22	2.27	0.59
1:B:101:LYS:HG3	1:B:165:PRO:HG2	1.85	0.59
1:C:200:LYS:HZ3	1:C:200:LYS:HB3	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:HD21	1:B:183:GLU:HB2	1.85	0.59
1:C:66:SER:O	1:C:67:TYR:HD2	1.85	0.59
1:A:228:ARG:HD2	5:A:350:HOH:O	2.03	0.58
1:C:101:LYS:HG3	1:C:165:PRO:HG2	1.85	0.58
1:D:14:ASN:OD1	1:D:228:ARG:HB3	2.03	0.58
1:C:44:ASN:O	1:C:45:GLY:CA	2.50	0.58
1:D:170:VAL:HG23	1:D:226:THR:CG2	2.30	0.58
1:B:22:TYR:CE1	1:B:39:LYS:HB3	2.39	0.58
1:C:25:ILE:CD1	1:C:73:ALA:HB3	2.34	0.58
1:C:119:SER:HB2	1:C:122:GLU:HB2	1.84	0.58
1:B:25:ILE:CD1	1:B:73:ALA:HB3	2.34	0.58
1:C:12:TYR:CD2	1:C:13:PRO:CD	2.83	0.58
1:A:43:GLN:N	1:A:67:TYR:HE2	2.02	0.57
1:C:25:ILE:HD11	1:C:73:ALA:HB3	1.86	0.57
1:A:170:VAL:HG23	1:A:226:THR:CG2	2.32	0.57
1:B:43:GLN:CD	2:Q:5:TYR:CE2	2.78	0.57
1:A:172:ARG:HD2	1:A:221:ILE:CG1	2.35	0.57
1:B:25:ILE:HD11	1:B:73:ALA:HB3	1.85	0.57
1:A:44:ASN:O	2:P:4:TRP:HA	2.04	0.56
1:D:145:ASP:HB3	1:D:158:ARG:NH1	2.20	0.56
1:B:205:HIS:H	1:B:206:PRO:CD	2.17	0.56
1:C:44:ASN:HB2	2:R:6:PRO:CG	2.35	0.56
1:C:115:LEU:HD21	1:C:183:GLU:HB2	1.87	0.56
1:D:44:ASN:O	2:S:4:TRP:O	2.22	0.56
1:D:43:GLN:N	1:D:67:TYR:HE2	2.04	0.56
1:A:187:VAL:HG12	1:A:188:VAL:HG23	1.87	0.56
1:D:116:LYS:HE3	5:D:338:HOH:O	2.06	0.56
1:A:14:ASN:OD1	1:A:228:ARG:HB3	2.06	0.56
1:A:43:GLN:CB	1:A:67:TYR:HE2	2.19	0.55
1:B:66:SER:O	1:B:67:TYR:HD2	1.90	0.55
1:C:178:PRO:CD	1:D:176:TYR:HD2	2.19	0.55
1:A:14:ASN:N	1:A:14:ASN:HD22	2.04	0.55
1:A:116:LYS:HE2	1:A:123:THR:OG1	2.07	0.54
1:A:16:ASP:OD1	1:A:16:ASP:O	2.26	0.54
1:B:12:TYR:CD2	1:B:13:PRO:N	2.67	0.54
1:A:200:LYS:HD3	5:P:135:HOH:O	2.07	0.54
1:C:176:TYR:CD2	1:D:178:PRO:HD3	2.43	0.54
1:D:149:GLY:O	1:D:151:ASP:N	2.41	0.54
2:P:6:PRO:C	2:P:7:TYR:HD1	2.11	0.53
2:S:3:TYR:O	2:S:3:TYR:HD1	1.91	0.53
1:A:23:PRO:HG2	2:P:8:NH2:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:ASN:O	1:D:19:ASP:HB2	2.08	0.53
1:C:110:SER:HB3	1:C:129:MET:HG3	1.90	0.53
1:C:119:SER:HB2	1:C:122:GLU:CB	2.38	0.53
1:B:44:ASN:HD22	2:Q:4:TRP:CB	2.22	0.53
1:C:44:ASN:O	2:R:4:TRP:O	2.26	0.53
1:D:172:ARG:HD2	1:D:221:ILE:CG1	2.38	0.53
2:P:6:PRO:O	2:P:7:TYR:HB3	2.09	0.53
1:A:205:HIS:N	1:A:206:PRO:HD3	2.22	0.53
1:B:16:ASP:N	1:B:16:ASP:OD1	2.40	0.53
1:C:178:PRO:HD2	1:D:176:TYR:HD2	1.74	0.53
1:B:36:LYS:HD3	1:B:76:SER:O	2.08	0.53
1:C:200:LYS:HB3	1:C:200:LYS:NZ	2.23	0.53
1:A:14:ASN:O	1:A:19:ASP:HB2	2.09	0.52
1:A:145:ASP:HB3	1:A:158:ARG:NH1	2.23	0.52
1:B:66:SER:HB3	1:B:72:SER:HB3	1.91	0.52
1:C:170:VAL:HG23	1:C:226:THR:HG22	1.91	0.52
1:D:43:GLN:HE21	1:D:46:LYS:HG3	1.74	0.52
1:C:106:ILE:HB	1:C:154:LEU:HB3	1.91	0.52
1:C:16:ASP:OD1	1:C:16:ASP:N	2.40	0.52
1:A:178:PRO:HD3	1:B:176:TYR:CD2	2.44	0.52
1:C:202:PRO:HG2	1:C:203:ASP:H	1.73	0.52
1:D:38:ALA:HA	5:D:337:HOH:O	2.10	0.52
2:Q:2:MET:HA	2:Q:2:MET:HE3	1.88	0.52
2:S:4:TRP:O	2:S:5:TYR:HB3	2.10	0.52
1:D:43:GLN:CB	1:D:67:TYR:HE2	2.24	0.51
2:S:7:TYR:CD1	2:S:7:TYR:N	2.76	0.51
1:B:44:ASN:OD1	1:B:200:LYS:HA	2.09	0.51
1:B:52:ILE:N	1:B:52:ILE:HD12	2.26	0.51
1:C:178:PRO:HD3	1:D:176:TYR:CD2	2.45	0.51
1:A:170:VAL:HG22	1:A:226:THR:HA	1.92	0.51
1:C:148:THR:HG22	1:C:154:LEU:HD13	1.92	0.51
1:D:89:VAL:HB	1:D:215:SER:O	2.11	0.51
1:A:43:GLN:HB2	1:A:67:TYR:CD2	2.46	0.51
1:B:174:LEU:HD12	1:B:174:LEU:N	2.26	0.51
1:B:183:GLU:O	1:B:185:SER:N	2.37	0.51
1:D:203:ASP:O	1:D:203:ASP:OD2	2.30	0.50
1:A:176:TYR:HD2	1:B:178:PRO:CD	2.25	0.50
1:D:107:LEU:N	1:D:107:LEU:HD12	2.26	0.50
1:D:16:ASP:OD1	1:D:16:ASP:O	2.29	0.50
1:A:3:THR:HA	5:A:317:HOH:O	2.12	0.50
1:B:117:SER:HA	1:B:186:ALA:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:SER:CB	2:Q:4:TRP:CZ2	2.95	0.50
1:C:156:LEU:O	1:C:171:GLY:HA3	2.11	0.50
1:D:14:ASN:C	1:D:16:ASP:H	2.15	0.50
1:A:120:THR:C	1:A:122:GLU:N	2.63	0.49
1:B:43:GLN:CB	1:B:67:TYR:HE1	2.22	0.49
1:C:203:ASP:O	1:C:203:ASP:OD2	2.29	0.49
1:D:148:THR:HG22	1:D:154:LEU:CD1	2.41	0.49
1:A:43:GLN:CB	1:A:67:TYR:CE2	2.92	0.49
1:D:115:LEU:HD21	1:D:183:GLU:HB3	1.93	0.49
1:D:12:TYR:CD1	1:D:12:TYR:C	2.86	0.49
1:D:14:ASN:C	1:D:19:ASP:HB2	2.33	0.49
1:D:44:ASN:HB3	2:S:5:TYR:HA	1.95	0.49
1:C:158:ARG:HB2	1:C:166:GLN:HB2	1.95	0.49
1:C:174:LEU:HD12	1:C:174:LEU:N	2.28	0.49
1:A:44:ASN:O	2:P:3:TYR:O	2.30	0.49
1:B:12:TYR:CD2	1:B:12:TYR:C	2.84	0.49
1:D:43:GLN:CB	1:D:67:TYR:CE2	2.96	0.49
1:B:217:ILE:HG13	5:B:319:HOH:O	2.12	0.49
1:C:150:THR:O	1:C:151:ASP:HB2	2.12	0.49
1:C:2:ASP:HB3	1:C:216:ASN:OD1	2.13	0.48
1:C:43:GLN:CB	1:C:67:TYR:CE1	2.91	0.48
1:C:178:PRO:CD	1:D:176:TYR:CD2	2.96	0.48
1:D:46:LYS:HZ3	2:S:4:TRP:HD1	1.61	0.48
1:D:119:SER:HB3	1:D:122:GLU:HG3	1.93	0.48
1:A:14:ASN:C	1:A:16:ASP:H	2.16	0.48
1:B:202:PRO:C	1:B:204:SER:H	2.16	0.48
1:C:88:TRP:CE3	1:D:138:LYS:HB2	2.48	0.48
1:A:14:ASN:C	1:A:19:ASP:HB2	2.32	0.48
1:C:44:ASN:HB2	2:R:6:PRO:HG3	1.95	0.48
2:Q:7:TYR:CD2	2:Q:8:NH2:N	2.82	0.48
1:A:12:TYR:CD1	1:A:12:TYR:C	2.86	0.48
1:C:88:TRP:CG	1:D:138:LYS:HD2	2.49	0.48
1:C:119:SER:CB	1:C:122:GLU:HB2	2.43	0.48
1:B:148:THR:HG22	1:B:154:LEU:HD13	1.95	0.48
1:B:106:ILE:HB	1:B:154:LEU:HB3	1.95	0.48
1:B:170:VAL:HG23	1:B:226:THR:HG22	1.93	0.48
1:A:176:TYR:CD2	1:B:178:PRO:HD3	2.49	0.48
1:B:200:LYS:HD2	2:Q:3:TYR:CD2	2.49	0.48
1:C:137:GLN:HG2	1:C:140:LEU:HD12	1.95	0.48
1:D:203:ASP:OD1	1:D:203:ASP:N	2.25	0.48
1:A:43:GLN:HE21	1:A:46:LYS:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:SER:O	1:A:120:THR:O	2.32	0.47
1:A:237:ASN:HD22	1:A:237:ASN:N	2.11	0.47
1:D:158:ARG:HB3	1:D:166:GLN:HG3	1.96	0.47
1:C:118:ASN:ND2	1:C:185:SER:O	2.47	0.47
1:C:183:GLU:O	1:C:185:SER:N	2.39	0.47
1:A:115:LEU:HD21	1:A:183:GLU:HB3	1.96	0.47
1:A:43:GLN:CD	1:A:67:TYR:HD2	2.18	0.47
1:A:158:ARG:HB3	1:A:166:GLN:HG3	1.96	0.47
1:B:172:ARG:HD2	1:B:221:ILE:CG1	2.36	0.47
1:A:201:SER:CB	1:A:206:PRO:HG3	2.44	0.47
1:C:4:ILE:HD13	1:C:215:SER:CB	2.44	0.47
1:C:52:ILE:HD12	1:C:52:ILE:N	2.29	0.47
1:D:25:ILE:HD11	1:D:73:ALA:CB	2.44	0.47
1:B:135:LYS:HB3	1:B:135:LYS:HE2	1.65	0.47
1:C:41:ASN:HD22	1:C:41:ASN:H	1.62	0.47
1:D:170:VAL:CG2	1:D:226:THR:CG2	2.92	0.47
1:B:200:LYS:HB3	1:B:200:LYS:HZ3	1.79	0.47
1:C:116:LYS:HG2	1:C:123:THR:CG2	2.33	0.47
2:P:6:PRO:C	2:P:7:TYR:CD1	2.88	0.47
1:B:4:ILE:HG22	1:B:5:VAL:N	2.30	0.46
1:D:237:ASN:N	1:D:237:ASN:ND2	2.63	0.46
2:S:3:TYR:O	2:S:3:TYR:CD1	2.68	0.46
1:D:237:ASN:N	1:D:237:ASN:HD22	2.10	0.46
1:A:28:ASP:HB3	1:A:31:SER:O	2.16	0.46
1:B:16:ASP:OD2	1:B:228:ARG:NH2	2.48	0.46
1:A:112:THR:O	1:A:191:PHE:HA	2.15	0.46
1:D:12:TYR:HD1	1:D:12:TYR:C	2.18	0.46
1:D:43:GLN:CD	1:D:67:TYR:HD2	2.18	0.46
1:A:170:VAL:CG2	1:A:226:THR:HA	2.45	0.46
1:D:46:LYS:NZ	2:S:4:TRP:HD1	2.14	0.46
1:D:156:LEU:O	1:D:171:GLY:HA3	2.16	0.46
2:P:5:TYR:HA	2:P:6:PRO:HD3	1.35	0.46
2:R:3:TYR:HD1	2:R:3:TYR:HA	1.61	0.46
1:D:170:VAL:CG2	1:D:226:THR:HA	2.46	0.46
1:A:107:LEU:N	1:A:107:LEU:HD12	2.31	0.46
1:D:28:ASP:HB3	1:D:31:SER:O	2.15	0.46
1:D:43:GLN:NE2	1:D:46:LYS:HG3	2.31	0.46
1:D:80:ASP:OD1	1:D:80:ASP:C	2.53	0.46
1:A:12:TYR:HD1	1:A:12:TYR:C	2.17	0.46
1:A:148:THR:HG22	1:A:154:LEU:CD1	2.44	0.46
1:B:149:GLY:O	1:B:150:THR:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:PRO:O	1:A:207:ALA:HB2	2.16	0.45
1:B:90:ARG:NH1	1:B:217:ILE:CG2	2.78	0.45
1:B:182:TRP:HB3	5:B:314:HOH:O	2.16	0.45
1:D:92:GLY:HA2	1:D:109:TRP:CH2	2.51	0.45
1:B:158:ARG:HB2	1:B:166:GLN:HB2	1.97	0.45
1:C:4:ILE:CD1	1:C:215:SER:HB3	2.42	0.45
1:C:43:GLN:NE2	1:C:67:TYR:HD1	2.14	0.45
1:D:170:VAL:HG22	1:D:226:THR:HA	1.98	0.45
1:A:237:ASN:N	1:A:237:ASN:ND2	2.65	0.45
1:B:203:ASP:O	1:B:204:SER:C	2.54	0.45
1:B:137:GLN:HG2	1:B:140:LEU:HD12	1.98	0.45
1:C:200:LYS:CG	2:R:3:TYR:HE2	2.30	0.45
1:D:224:GLY:N	5:D:336:HOH:O	2.50	0.45
1:C:36:LYS:HD3	1:C:76:SER:O	2.17	0.45
1:C:172:ARG:HD2	1:C:221:ILE:CG1	2.38	0.45
1:B:201:SER:CB	1:B:206:PRO:HB3	2.47	0.45
1:C:177:ALA:HB2	1:D:177:ALA:HB2	1.98	0.45
1:C:43:GLN:HB2	1:C:67:TYR:CD1	2.52	0.45
1:C:133:PHE:O	1:C:152:GLY:HA2	2.17	0.45
1:C:202:PRO:O	1:C:203:ASP:C	2.54	0.45
1:A:124:ASN:HA	1:B:129:MET:O	2.17	0.45
1:A:200:LYS:NZ	1:A:200:LYS:CB	2.76	0.45
1:D:52:ILE:N	1:D:52:ILE:HD12	2.31	0.44
1:A:121:HIS:O	1:A:123:THR:N	2.50	0.44
1:B:51:HIS:O	1:B:63:ALA:HA	2.17	0.44
1:D:102:GLU:HG2	1:D:207:ALA:O	2.16	0.44
1:B:90:ARG:NH1	1:B:217:ILE:HG23	2.33	0.44
1:B:207:ALA:HB1	1:B:208:ASP:CG	2.38	0.44
1:C:217:ILE:HG13	5:C:346:HOH:O	2.17	0.44
1:D:44:ASN:HB2	2:S:6:PRO:HD2	1.98	0.44
1:D:69:ASN:N	1:D:69:ASN:ND2	2.63	0.44
1:A:201:SER:HB3	1:A:206:PRO:HG3	2.00	0.44
1:B:44:ASN:CB	2:Q:4:TRP:O	2.59	0.44
1:A:14:ASN:N	1:A:14:ASN:ND2	2.65	0.44
1:A:25:ILE:HD11	1:A:73:ALA:CB	2.45	0.44
1:A:177:ALA:HB2	1:B:177:ALA:HB2	2.00	0.44
1:A:206:PRO:HD3	2:P:6:PRO:HB3	2.00	0.44
1:C:44:ASN:CB	2:R:4:TRP:O	2.63	0.44
1:D:119:SER:CB	1:D:122:GLU:HG3	2.48	0.44
1:C:1:ALA:HB1	5:C:317:HOH:O	2.17	0.44
1:D:25:ILE:HD13	1:D:65:VAL:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASP:OD1	1:A:80:ASP:C	2.56	0.44
1:B:156:LEU:O	1:B:171:GLY:HA3	2.18	0.44
1:C:16:ASP:OD2	1:C:228:ARG:NH2	2.49	0.44
1:C:66:SER:HB3	1:C:72:SER:HB3	1.99	0.44
1:D:12:TYR:HD1	1:D:13:PRO:CD	2.31	0.44
1:D:43:GLN:HB2	1:D:67:TYR:CD2	2.51	0.44
1:A:149:GLY:O	1:A:151:ASP:N	2.51	0.43
1:D:118:ASN:ND2	1:D:185:SER:O	2.51	0.43
1:B:43:GLN:NE2	1:B:67:TYR:HD1	2.16	0.43
1:B:44:ASN:N	2:Q:4:TRP:O	2.51	0.43
1:B:66:SER:CB	1:B:72:SER:HB3	2.49	0.43
1:C:51:HIS:O	1:C:63:ALA:HA	2.18	0.43
2:P:4:TRP:N	2:P:4:TRP:CD1	2.87	0.43
1:B:43:GLN:NE2	2:Q:5:TYR:CE2	2.86	0.43
1:C:44:ASN:CA	2:R:4:TRP:O	2.67	0.43
1:C:207:ALA:HA	1:C:208:ASP:HA	1.83	0.43
1:D:112:THR:O	1:D:191:PHE:HA	2.19	0.43
1:C:200:LYS:CG	2:R:3:TYR:CE2	3.02	0.43
1:C:207:ALA:HB1	1:C:208:ASP:CG	2.39	0.43
1:A:69:ASN:N	1:A:69:ASN:ND2	2.65	0.43
1:A:101:LYS:HG3	1:A:165:PRO:HG2	2.01	0.43
1:B:25:ILE:HG13	1:B:40:TRP:HB2	2.00	0.43
1:B:44:ASN:ND2	2:Q:4:TRP:HB3	2.31	0.43
1:C:44:ASN:O	1:C:45:GLY:HA3	2.18	0.43
2:P:6:PRO:O	2:P:7:TYR:CB	2.66	0.43
1:B:22:TYR:CD1	1:B:39:LYS:HB2	2.54	0.43
1:B:102:GLU:OE2	1:B:104:ASN:ND2	2.45	0.43
2:Q:5:TYR:C	2:Q:7:TYR:H	2.23	0.43
1:A:198:LEU:HD21	1:A:200:LYS:HZ1	1.84	0.42
1:D:51:HIS:C	1:D:52:ILE:HD12	2.38	0.42
1:A:12:TYR:HD1	1:A:13:PRO:CD	2.32	0.42
1:B:46:LYS:NZ	2:Q:2:MET:CE	2.82	0.42
1:A:118:ASN:HD22	1:A:118:ASN:HA	1.63	0.42
1:C:136:ASP:OD2	1:C:138:LYS:HE2	2.20	0.42
1:D:137:GLN:HG2	1:D:140:LEU:CD1	2.34	0.42
1:C:103:THR:HG21	1:C:200:LYS:HZ3	1.83	0.42
1:D:225:SER:HA	1:D:229:LEU:HD12	2.01	0.42
1:C:25:ILE:HG13	1:C:40:TRP:HB2	2.01	0.42
1:D:46:LYS:HE2	2:S:4:TRP:CD1	2.54	0.42
1:A:176:TYR:CD2	1:B:178:PRO:CD	3.03	0.42
1:B:111:PHE:HB3	1:B:128:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ASN:O	1:B:19:ASP:HB2	2.19	0.42
1:B:202:PRO:CG	1:B:203:ASP:H	2.31	0.42
2:R:5:TYR:C	2:R:7:TYR:H	2.22	0.42
1:A:103:THR:O	1:A:199:ILE:HA	2.19	0.42
1:D:14:ASN:O	1:D:16:ASP:N	2.53	0.42
1:A:12:TYR:HE2	1:A:100:TYR:CD2	2.37	0.42
1:A:176:TYR:HD2	1:B:178:PRO:HD2	1.85	0.42
1:D:14:ASN:N	1:D:14:ASN:HD22	2.18	0.42
1:A:170:VAL:CG2	1:A:226:THR:CG2	2.94	0.41
1:B:107:LEU:N	1:B:107:LEU:HD12	2.35	0.41
1:C:20:PRO:HB2	1:C:22:TYR:CZ	2.55	0.41
1:A:43:GLN:NE2	1:A:46:LYS:HG3	2.34	0.41
1:D:119:SER:HB2	1:D:122:GLU:HB2	2.02	0.41
2:S:5:TYR:HA	2:S:6:PRO:HD2	1.65	0.41
1:A:89:VAL:HB	1:A:215:SER:O	2.20	0.41
1:C:103:THR:HG21	1:C:200:LYS:NZ	2.35	0.41
1:C:142:LEU:HD11	1:C:148:THR:HG23	2.01	0.41
1:D:145:ASP:HB3	1:D:158:ARG:HG2	2.02	0.41
1:A:19:ASP:HA	1:A:20:PRO:HD3	1.91	0.41
1:B:136:ASP:OD2	1:B:138:LYS:HE2	2.21	0.41
1:D:96:SER:OG	1:D:230:LEU:HA	2.21	0.41
1:A:145:ASP:HB3	1:A:158:ARG:HG2	2.03	0.41
1:D:82:ASP:N	1:D:82:ASP:OD1	2.54	0.41
1:A:12:TYR:CE2	1:A:100:TYR:CD2	3.09	0.41
1:A:30:LYS:HG2	5:A:317:HOH:O	2.21	0.41
1:B:25:ILE:HD13	1:B:65:VAL:CG2	2.51	0.41
1:B:48:GLY:HA3	1:B:67:TYR:CE2	2.56	0.41
1:C:17:ILE:C	1:C:33:ARG:HH12	2.24	0.41
1:C:90:ARG:HG2	5:C:323:HOH:O	2.20	0.41
1:A:92:GLY:HA2	1:A:109:TRP:CH2	2.56	0.41
1:B:145:ASP:HB3	1:B:158:ARG:HE	1.86	0.41
1:D:66:SER:O	1:D:67:TYR:HD1	2.04	0.41
1:A:225:SER:HA	1:A:229:LEU:HD12	2.03	0.40
1:D:116:LYS:HE2	1:D:123:THR:OG1	2.21	0.40
1:D:118:ASN:N	1:D:118:ASN:HD22	2.19	0.40
1:A:39:LYS:N	5:A:337:HOH:O	2.49	0.40
1:A:87:GLU:HB2	1:A:182:TRP:O	2.20	0.40
1:C:107:LEU:HD12	1:C:107:LEU:N	2.36	0.40
1:A:17:ILE:HD13	1:A:228:ARG:HD3	2.04	0.40
1:A:66:SER:O	1:A:67:TYR:HD1	2.04	0.40
1:B:12:TYR:HD2	1:B:12:TYR:C	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:THR:O	1:D:199:ILE:HA	2.21	0.40
1:A:200:LYS:HB2	1:A:200:LYS:HZ3	1.86	0.40
1:A:200:LYS:CD	2:P:3:TYR:OH	2.66	0.40
1:B:5:VAL:HG13	1:B:29:ILE:HD13	2.04	0.40
1:B:14:ASN:C	1:B:19:ASP:HB2	2.41	0.40
1:C:44:ASN:N	2:R:4:TRP:O	2.55	0.40
1:C:129:MET:O	1:D:124:ASN:HA	2.22	0.40
1:D:25:ILE:CD1	1:D:73:ALA:HB3	2.46	0.40
1:D:177:ALA:HA	1:D:178:PRO:HD3	1.95	0.40
1:B:20:PRO:HB2	1:B:22:TYR:CZ	2.56	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	235/237 (99%)	207 (88%)	21 (9%)	7 (3%)	4	24
1	B	235/237 (99%)	207 (88%)	21 (9%)	7 (3%)	4	24
1	C	235/237 (99%)	210 (89%)	20 (8%)	5 (2%)	7	33
1	D	235/237 (99%)	209 (89%)	20 (8%)	6 (3%)	5	27
2	P	6/8 (75%)	3 (50%)	1 (17%)	2 (33%)	0	0
2	Q	6/8 (75%)	2 (33%)	2 (33%)	2 (33%)	0	0
2	R	6/8 (75%)	2 (33%)	2 (33%)	2 (33%)	0	0
2	S	6/8 (75%)	2 (33%)	3 (50%)	1 (17%)	0	0
All	All	964/980 (98%)	842 (87%)	90 (9%)	32 (3%)	4	21

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	THR
1	A	121	HIS
1	A	204	SER
1	B	150	THR
1	B	185	SER
1	B	205	HIS
1	C	150	THR
1	C	185	SER
1	C	202	PRO
1	C	205	HIS
1	D	204	SER
2	P	6	PRO
2	P	7	TYR
2	Q	7	TYR
2	R	7	TYR
1	A	15	THR
1	A	207	ALA
1	B	184	SER
1	C	184	SER
1	D	15	THR
1	D	150	THR
2	S	6	PRO
1	A	151	ASP
1	D	207	ALA
1	D	228	ARG
1	B	204	SER
2	R	4	TRP
1	A	228	ARG
2	Q	4	TRP
1	B	120	THR
1	D	151	ASP
1	B	202	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	203/203 (100%)	183 (90%)	20 (10%)	8 30
1	B	203/203 (100%)	192 (95%)	11 (5%)	22 57
1	C	203/203 (100%)	189 (93%)	14 (7%)	15 48
1	D	203/203 (100%)	183 (90%)	20 (10%)	8 30
2	P	6/6 (100%)	3 (50%)	3 (50%)	0 0
2	Q	6/6 (100%)	2 (33%)	4 (67%)	0 0
2	R	6/6 (100%)	3 (50%)	3 (50%)	0 0
2	S	6/6 (100%)	1 (17%)	5 (83%)	0 0
All	All	836/836 (100%)	756 (90%)	80 (10%)	8 32

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	12	TYR
1	A	15	THR
1	A	19	ASP
1	A	21	SER
1	A	71	ASP
1	A	80	ASP
1	A	101	LYS
1	A	115	LEU
1	A	118	ASN
1	A	120	THR
1	A	134	SER
1	A	135	LYS
1	A	161	SER
1	A	164	SER
1	A	176	TYR
1	A	185	SER
1	A	202	PRO
1	A	204	SER
1	A	223	SER
1	B	12	TYR
1	B	51	HIS
1	B	71	ASP
1	B	82	ASP
1	B	101	LYS
1	B	115	LEU
1	B	161	SER

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Mol	Chain	Res	Type
1	B	164	SER
1	B	176	TYR
1	B	205	HIS
1	B	228	ARG
1	C	39	LYS
1	C	41	ASN
1	C	51	HIS
1	C	71	ASP
1	C	82	ASP
1	C	101	LYS
1	C	115	LEU
1	C	122	GLU
1	C	161	SER
1	C	164	SER
1	C	176	TYR
1	C	200	LYS
1	C	204	SER
1	C	228	ARG
1	D	4	ILE
1	D	12	TYR
1	D	15	THR
1	D	19	ASP
1	D	21	SER
1	D	71	ASP
1	D	80	ASP
1	D	82	ASP
1	D	101	LYS
1	D	115	LEU
1	D	116	LYS
1	D	117	SER
1	D	134	SER
1	D	135	LYS
1	D	161	SER
1	D	164	SER
1	D	176	TYR
1	D	184	SER
1	D	185	SER
1	D	223	SER
2	P	3	TYR
2	P	4	TRP
2	P	7	TYR
2	Q	2	MET

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Mol	Chain	Res	Type
2	Q	3	TYR
2	Q	4	TRP
2	Q	7	TYR
2	R	2	MET
2	R	3	TYR
2	R	7	TYR
2	S	2	MET
2	S	3	TYR
2	S	4	TRP
2	S	5	TYR
2	S	7	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	41	ASN
1	A	43	GLN
1	A	69	ASN
1	A	118	ASN
1	A	121	HIS
1	A	166	GLN
1	A	237	ASN
1	B	41	ASN
1	B	43	GLN
1	B	51	HIS
1	B	69	ASN
1	B	83	ASN
1	B	118	ASN
1	B	121	HIS
1	B	132	GLN
1	B	237	ASN
1	C	41	ASN
1	C	43	GLN
1	C	69	ASN
1	C	83	ASN
1	C	118	ASN
1	C	132	GLN
1	C	237	ASN
1	D	43	GLN
1	D	69	ASN
1	D	83	ASN

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Mol	Chain	Res	Type
1	D	118	ASN
1	D	166	GLN
1	D	237	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	237/237 (100%)	-0.84	0 100 100	12, 18, 58, 95	0
1	B	237/237 (100%)	-0.73	2 (0%) 86 65	12, 23, 57, 89	0
1	C	237/237 (100%)	-0.82	0 100 100	12, 17, 58, 92	0
1	D	237/237 (100%)	-0.77	2 (0%) 86 65	12, 23, 60, 90	0
2	P	6/8 (75%)	3.08	6 (100%) 0 0	65, 70, 74, 97	0
2	Q	6/8 (75%)	2.87	5 (83%) 0 0	59, 73, 83, 89	0
2	R	6/8 (75%)	2.69	4 (66%) 0 0	76, 85, 92, 93	0
2	S	6/8 (75%)	3.61	6 (100%) 0 0	67, 73, 75, 83	0
All	All	972/980 (99%)	-0.70	25 (2%) 56 27	12, 21, 64, 97	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	5	TYR	5.0
2	P	4	TRP	4.6
2	S	4	TRP	3.7
2	S	6	PRO	3.6
2	R	5	TYR	3.4
2	S	7	TYR	3.3
2	Q	6	PRO	3.3
2	S	3	TYR	3.3
2	R	2	MET	3.3
2	P	7	TYR	3.3
2	Q	2	MET	3.2
2	Q	4	TRP	3.1
2	Q	5	TYR	3.1
2	R	4	TRP	3.1
1	B	120	THR	3.0
2	R	3	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	P	3	TYR	2.9
2	P	6	PRO	2.8
2	S	2	MET	2.7
2	Q	3	TYR	2.6
2	P	5	TYR	2.5
2	P	2	MET	2.5
1	D	120	THR	2.4
1	B	1	ALA	2.2
1	D	203	ASP	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	D	308	1/1	0.96	0.07	22,22,22,22	0
4	CA	A	302	1/1	0.97	0.07	22,22,22,22	0
4	CA	B	304	1/1	0.98	0.08	22,22,22,22	0
4	CA	C	306	1/1	0.98	0.14	22,22,22,22	0
3	MN	A	301	1/1	0.98	0.11	22,22,22,22	0
3	MN	C	305	1/1	0.99	0.14	22,22,22,22	0
3	MN	D	307	1/1	0.99	0.12	22,22,22,22	0
3	MN	B	303	1/1	0.99	0.10	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.