Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:12 PM GMT

PDB ID	:	4HJ0
Title	:	Crystal structure of the human GIPr ECD in complex with Gipg013 Fab at 3-A resolution
Authors	:	Madhurantakam, C.; Ravn, P.; Gruetter, M.G.; Jackson, R.H.
Deposited on	:	2012-10-12
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
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:

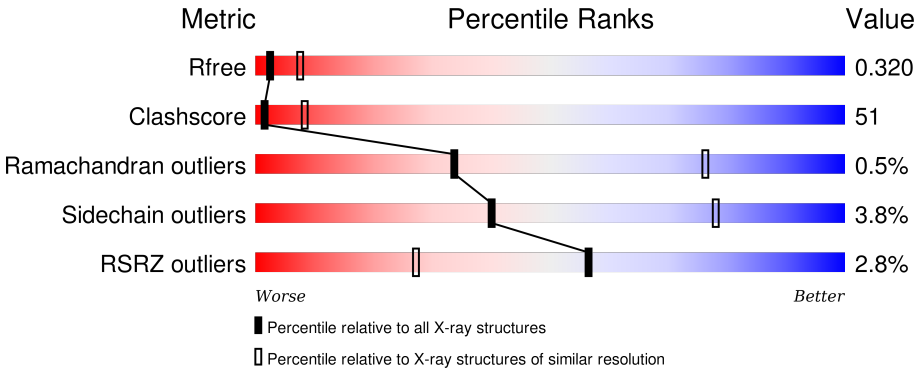
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 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	136	35% 30% 32%
1	B	136	9% 20% 41% 33%
2	C	227	3% 39% 47% 10%
2	P	227	51% 37% 9%
3	D	215	4% 35% 57% 6%

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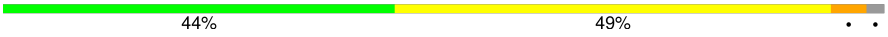
Mol	Chain	Length	Quality of chain
3	Q	215	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7635 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 Gastric inhibitory polypeptide receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	92	Total	C	N	O	S	2	0	0
			742	465	135	135	7			
1	B	91	Total	C	N	O	S	2	0	0
			727	457	131	132	7			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	EXPRESSION TAG	UNP P48546
A	4	GLY	-	EXPRESSION TAG	UNP P48546
A	5	SER	-	EXPRESSION TAG	UNP P48546
A	6	SER	-	EXPRESSION TAG	UNP P48546
A	7	HIS	-	EXPRESSION TAG	UNP P48546
A	8	HIS	-	EXPRESSION TAG	UNP P48546
A	9	HIS	-	EXPRESSION TAG	UNP P48546
A	10	HIS	-	EXPRESSION TAG	UNP P48546
A	11	HIS	-	EXPRESSION TAG	UNP P48546
A	12	HIS	-	EXPRESSION TAG	UNP P48546
A	13	SER	-	EXPRESSION TAG	UNP P48546
A	14	ASP	-	EXPRESSION TAG	UNP P48546
A	15	TYR	-	EXPRESSION TAG	UNP P48546
A	16	LYS	-	EXPRESSION TAG	UNP P48546
A	17	ASP	-	EXPRESSION TAG	UNP P48546
A	18	ASP	-	EXPRESSION TAG	UNP P48546
A	19	ASP	-	EXPRESSION TAG	UNP P48546
A	20	ASP	-	EXPRESSION TAG	UNP P48546
A	21	LYS	-	EXPRESSION TAG	UNP P48546
A	22	HIS	-	EXPRESSION TAG	UNP P48546
A	23	MET	-	EXPRESSION TAG	UNP P48546
B	3	MET	-	EXPRESSION TAG	UNP P48546
B	4	GLY	-	EXPRESSION TAG	UNP P48546
B	5	SER	-	EXPRESSION TAG	UNP P48546
B	6	SER	-	EXPRESSION TAG	UNP P48546

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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	EXPRESSION TAG	UNP P48546
B	8	HIS	-	EXPRESSION TAG	UNP P48546
B	9	HIS	-	EXPRESSION TAG	UNP P48546
B	10	HIS	-	EXPRESSION TAG	UNP P48546
B	11	HIS	-	EXPRESSION TAG	UNP P48546
B	12	HIS	-	EXPRESSION TAG	UNP P48546
B	13	SER	-	EXPRESSION TAG	UNP P48546
B	14	ASP	-	EXPRESSION TAG	UNP P48546
B	15	TYR	-	EXPRESSION TAG	UNP P48546
B	16	LYS	-	EXPRESSION TAG	UNP P48546
B	17	ASP	-	EXPRESSION TAG	UNP P48546
B	18	ASP	-	EXPRESSION TAG	UNP P48546
B	19	ASP	-	EXPRESSION TAG	UNP P48546
B	20	ASP	-	EXPRESSION TAG	UNP P48546
B	21	LYS	-	EXPRESSION TAG	UNP P48546
B	22	HIS	-	EXPRESSION TAG	UNP P48546
B	23	MET	-	EXPRESSION TAG	UNP P48546

- Molecule 2 is a protein called Gipg013 Fab, Antagonizing antibody to the GIP Receptor, Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	206	Total	C	N	O	S	0	0	0
			1518	959	252	301	6			
2	C	205	Total	C	N	O	S	0	0	0
			1512	956	251	299	6			

- Molecule 3 is a protein called Gipg013 Fab, Antagonizing antibody to the GIP Receptor, Light chain.

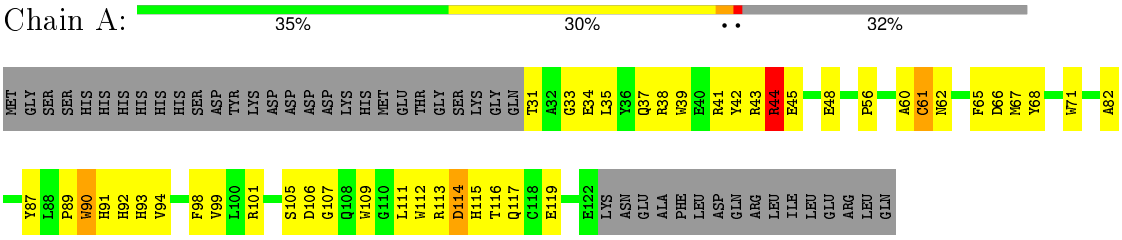
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Q	210	Total	C	N	O	S	0	0	0
			1566	976	266	320	4			
3	D	211	Total	C	N	O	S	0	0	0
			1570	978	267	321	4			

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.

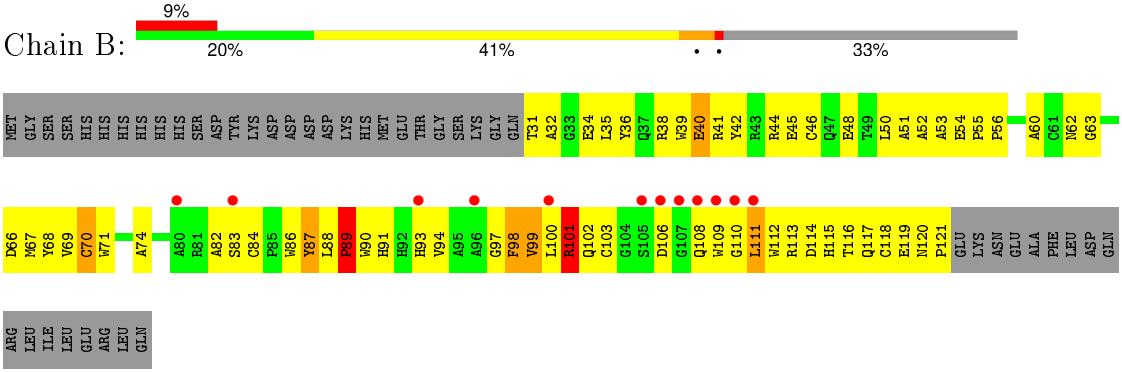
- Molecule 1: Gastric inhibitory polypeptide receptor

Chain A:



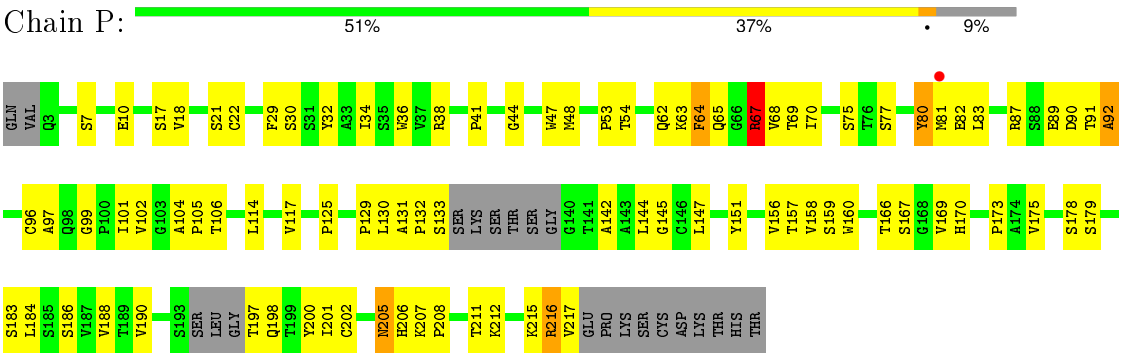
- Molecule 1: Gastric inhibitory polypeptide receptor

Chain B:



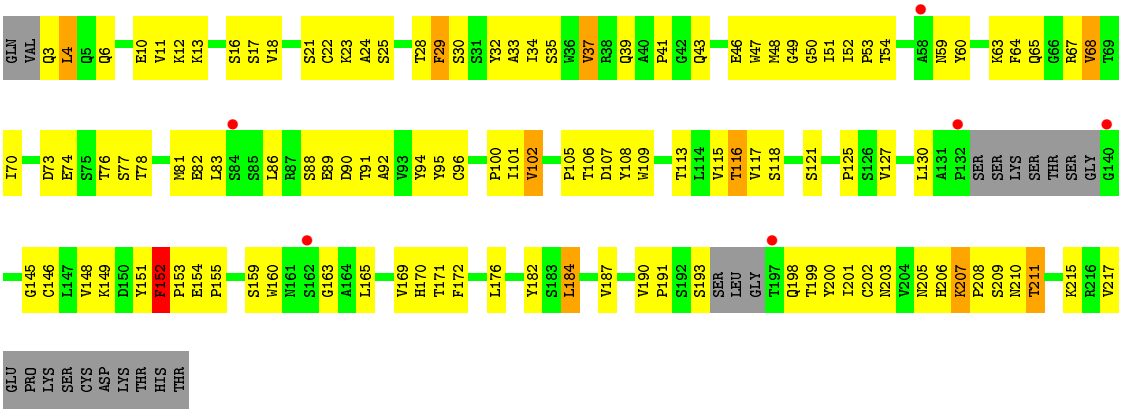
- Molecule 2: Gipg013 Fab, Antagonizing antibody to the GIP Receptor, Heavy chain

Chain P:



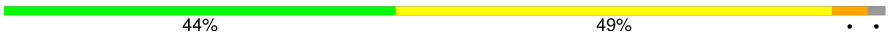
- Molecule 2: Gipg013 Fab, Antagonizing antibody to the GIP Receptor, Heavy chain

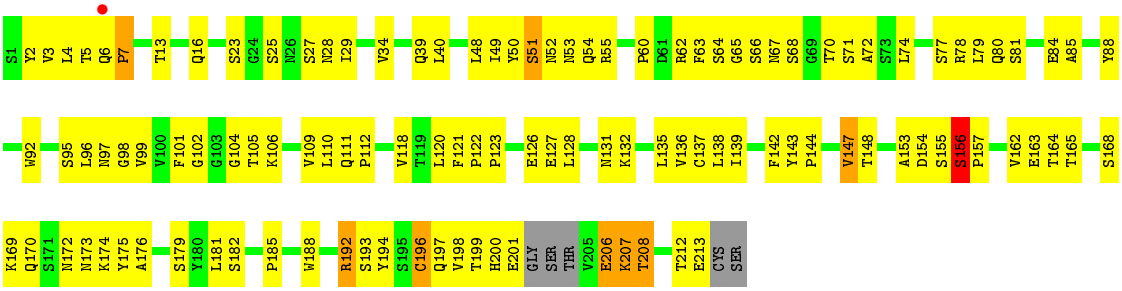
Chain C:



• Molecule 3: Gipg013 Fab, Antagonizing antibody to the GIP Receptor, Light chain

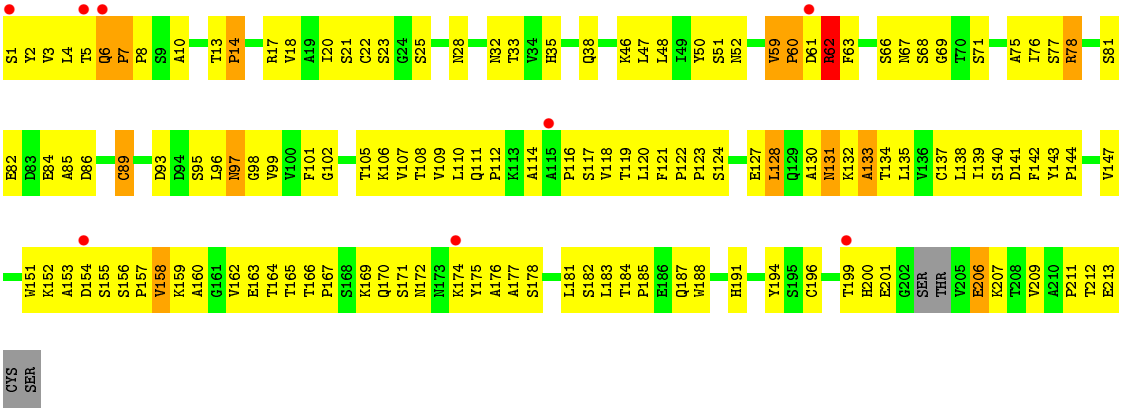
Chain Q:





• Molecule 3: Gipg013 Fab, Antagonizing antibody to the GIP Receptor, Light chain

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.27Å 109.85Å 105.94Å 90.00° 97.76° 90.00°	Depositor
Resolution (Å)	48.66 – 3.00 48.67 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.66-3.00) 100.0 (48.67-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.255 , 0.311 0.272 , 0.320	Depositor DCC
R_{free} test set	1996 reflections (9.08%)	DCC
Wilson B-factor (Å^2)	48.9	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	1 of 21996 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	7635	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.12% 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	0.53	1/770 (0.1%)	0.86	4/1053 (0.4%)
1	B	1.14	7/755 (0.9%)	1.10	10/1034 (1.0%)
2	C	0.33	0/1547	0.71	6/2109 (0.3%)
2	P	0.33	1/1553 (0.1%)	0.96	4/2117 (0.2%)
3	D	0.55	3/1608 (0.2%)	0.86	14/2198 (0.6%)
3	Q	0.59	3/1604 (0.2%)	0.68	5/2193 (0.2%)
All	All	0.57	15/7837 (0.2%)	0.85	43/10704 (0.4%)

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	B	0	1
2	C	0	1
2	P	0	3
3	D	0	2
All	All	0	7

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	40	GLU	CD-OE2	18.46	1.46	1.25
3	D	60	PRO	N-CD	-15.34	1.26	1.47
3	Q	51	SER	C-N	12.99	1.64	1.34
3	Q	196	CYS	CB-SG	12.84	2.04	1.82
1	B	70	CYS	CB-SG	12.23	2.03	1.82
1	A	61	CYS	CB-SG	-9.73	1.65	1.82
3	Q	156	SER	CB-OG	9.69	1.54	1.42
1	B	101	ARG	CZ-NH2	-8.91	1.21	1.33
1	B	89	PRO	N-CD	-8.84	1.35	1.47
3	D	22	CYS	CB-SG	8.14	1.96	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	40	GLU	CD-OE1	-7.73	1.17	1.25
1	B	52	ALA	C-N	6.63	1.49	1.34
2	P	67	ARG	CZ-NH2	6.04	1.40	1.33
1	B	48	GLU	C-N	-5.83	1.20	1.34
3	D	14	PRO	N-CD	-5.22	1.40	1.47

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	67	ARG	NE-CZ-NH2	25.64	133.12	120.30
2	P	67	ARG	NE-CZ-NH1	-24.38	108.11	120.30
1	B	98	PHE	O-C-N	13.37	144.08	122.70
1	A	61	CYS	CA-CB-SG	12.05	135.69	114.00
1	B	98	PHE	CA-C-N	-10.61	93.86	117.20
3	D	60	PRO	CA-N-CD	10.58	126.51	111.70
3	D	62	ARG	CB-CA-C	-10.48	89.44	110.40
3	Q	156	SER	CB-CA-C	8.60	126.44	110.10
3	D	131	ASN	CB-CA-C	-8.58	93.25	110.40
1	B	98	PHE	C-N-CA	-8.40	100.70	121.70
3	D	60	PRO	N-CA-CB	-8.09	93.60	103.30
3	Q	51	SER	O-C-N	-7.82	110.19	122.70
3	D	60	PRO	N-CA-C	7.75	132.25	112.10
2	C	29	PHE	CB-CA-C	-7.50	95.40	110.40
3	Q	192	ARG	NE-CZ-NH2	7.09	123.84	120.30
3	D	6	GLN	C-N-CD	-7.01	105.17	120.60
2	C	102	VAL	N-CA-C	6.99	129.88	111.00
3	Q	156	SER	C-N-CD	6.83	142.74	128.40
1	B	101	ARG	NE-CZ-NH1	-6.51	117.04	120.30
1	B	101	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	A	44	ARG	CB-CA-C	-6.24	97.92	110.40
3	D	133	ALA	N-CA-CB	-6.22	101.39	110.10
1	B	89	PRO	N-CA-CB	-6.11	95.88	102.60
2	C	193	SER	N-CA-C	6.08	127.40	111.00
1	B	89	PRO	CA-N-CD	6.05	120.17	111.70
1	B	70	CYS	CA-CB-SG	-6.03	103.15	114.00
2	P	92	ALA	CB-CA-C	5.99	119.09	110.10
3	Q	156	SER	CA-CB-OG	-5.93	95.18	111.20
2	C	4	LEU	N-CA-C	5.78	126.60	111.00
1	A	114	ASP	N-CA-CB	5.57	120.63	110.60
3	D	108	THR	N-CA-C	5.53	125.92	111.00
3	D	62	ARG	C-N-CA	5.47	135.37	121.70
1	B	87	TYR	N-CA-C	5.37	125.50	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	85	ALA	CB-CA-C	5.34	118.11	110.10
2	P	216	ARG	N-CA-CB	-5.34	100.99	110.60
2	C	207	LYS	C-N-CD	5.34	139.61	128.40
1	B	51	ALA	N-CA-CB	5.31	117.53	110.10
2	C	198	GLN	N-CA-C	5.31	125.34	111.00
3	D	52	ASN	N-CA-C	5.28	125.24	111.00
3	D	89	CYS	O-C-N	-5.22	114.34	122.70
1	A	44	ARG	N-CA-CB	5.11	119.80	110.60
3	D	97	ASN	N-CA-C	5.09	124.75	111.00
3	D	59	VAL	C-N-CD	-5.04	109.51	120.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	101	ARG	Sidechain
2	C	152	PHE	Peptide
3	D	62	ARG	Peptide
3	D	66	SER	Peptide
2	P	178	SER	Peptide
2	P	64	PHE	Peptide
2	P	67	ARG	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	742	0	656	64	0
1	B	727	0	640	148	0
2	C	1512	0	1488	169	0
2	P	1518	0	1491	95	0
3	D	1570	0	1513	189	0
3	Q	1566	0	1508	149	0
All	All	7635	0	7296	752	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 51.

All (752) 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)
3:Q:196:CYS:SG	3:Q:196:CYS:CB	2.04	1.46
1:B:70:CYS:CB	1:B:70:CYS:SG	2.03	1.46
3:Q:173:ASN:O	3:Q:174:LYS:HG3	1.28	1.29
3:Q:207:LYS:HB3	3:Q:207:LYS:NZ	1.43	1.19
3:D:1:SER:HB2	3:D:2:TYR:CA	1.72	1.18
3:Q:173:ASN:O	3:Q:174:LYS:CG	1.94	1.15
3:Q:118:VAL:HG22	3:Q:207:LYS:HE2	1.17	1.14
3:D:1:SER:HB2	3:D:2:TYR:HA	1.24	1.14
3:D:62:ARG:O	3:D:63:PHE:CD2	2.01	1.12
2:C:3:GLN:HG3	2:C:4:LEU:HD12	1.23	1.12
1:B:88:LEU:HD12	1:B:89:PRO:O	1.46	1.11
3:Q:96:LEU:O	3:Q:96:LEU:HD12	1.50	1.11
1:A:71:TRP:HH2	1:A:99:VAL:HG12	1.09	1.10
1:B:46:CYS:SG	1:B:70:CYS:CB	2.38	1.10
3:D:1:SER:CB	3:D:2:TYR:HA	1.83	1.09
3:D:156:SER:HB2	3:D:157:PRO:HD3	1.30	1.08
3:Q:6:GLN:HB3	3:Q:7:PRO:HD3	1.32	1.07
2:C:28:THR:HG22	2:C:29:PHE:H	1.19	1.07
1:A:43:ARG:HH12	3:Q:51:SER:HB3	1.18	1.07
2:C:33:ALA:HB2	2:C:52:ILE:HG13	1.15	1.06
2:C:107:ASP:CG	2:C:108:TYR:HD1	1.59	1.06
2:C:207:LYS:HG3	2:C:208:PRO:HD3	1.39	1.04
2:C:107:ASP:CG	2:C:108:TYR:CD1	2.32	1.03
2:C:146:CYS:HB2	2:C:202:CYS:SG	1.99	1.02
3:D:1:SER:HB2	3:D:2:TYR:C	1.79	1.01
2:P:92:ALA:O	2:P:114:LEU:HD12	1.57	1.01
3:Q:207:LYS:CB	3:Q:207:LYS:HZ2	1.74	1.00
2:C:3:GLN:HG3	2:C:4:LEU:CD1	1.90	1.00
2:C:28:THR:HG22	2:C:29:PHE:N	1.76	0.99
3:Q:28:ASN:OD1	3:Q:29:ILE:N	1.94	0.99
1:A:71:TRP:CH2	1:A:99:VAL:HG12	1.97	0.98
2:P:144:LEU:HD21	2:P:200:TYR:HD2	1.29	0.97
2:C:33:ALA:HB2	2:C:52:ILE:CG1	1.95	0.97
3:D:165:THR:HG23	3:D:177:ALA:HB1	1.46	0.97
3:D:162:VAL:HG22	3:D:181:LEU:HD12	1.43	0.96
3:D:171:SER:O	3:D:172:ASN:ND2	1.99	0.96
1:B:88:LEU:CD1	1:B:89:PRO:O	2.14	0.95
3:Q:207:LYS:HB3	3:Q:207:LYS:HZ2	0.80	0.94
1:A:43:ARG:NH1	3:Q:51:SER:CB	2.30	0.94
3:D:6:GLN:CB	3:D:7:PRO:HD3	1.95	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:107:ASP:OD2	2:C:108:TYR:CE1	2.21	0.94
3:Q:6:GLN:N	3:Q:7:PRO:HD2	1.82	0.93
2:C:107:ASP:OD1	2:C:108:TYR:HD1	1.50	0.92
2:C:33:ALA:CB	2:C:52:ILE:HG13	1.99	0.92
3:D:96:LEU:O	3:D:97:ASN:OD1	1.85	0.92
2:P:69:THR:HG22	2:P:82:GLU:HB3	1.49	0.92
1:B:88:LEU:HD13	1:B:90:TRP:NE1	1.86	0.91
1:B:88:LEU:HD13	1:B:90:TRP:CE2	2.05	0.91
3:Q:53:ASN:CG	3:Q:65:GLY:H	1.73	0.91
1:A:43:ARG:NH1	3:Q:51:SER:HB3	1.83	0.91
3:D:82:GLU:N	3:D:82:GLU:OE1	2.05	0.89
3:D:142:PHE:CE1	3:D:176:ALA:HB2	2.07	0.89
3:Q:67:ASN:O	3:Q:68:SER:OG	1.92	0.88
1:B:46:CYS:HB3	1:B:70:CYS:SG	2.15	0.87
3:Q:147:VAL:HG23	3:Q:200:HIS:HB2	1.53	0.87
3:Q:6:GLN:N	3:Q:7:PRO:CD	2.35	0.87
3:Q:118:VAL:CG2	3:Q:207:LYS:HE2	2.04	0.87
2:P:47:TRP:CZ3	3:Q:98:GLY:HA3	2.10	0.87
3:D:114:ALA:HB2	3:D:174:LYS:HE3	1.56	0.87
3:D:67:ASN:OD1	3:D:68:SER:N	2.07	0.86
2:C:146:CYS:CB	2:C:202:CYS:SG	2.63	0.86
3:Q:154:ASP:OD1	3:Q:192:ARG:HB3	1.74	0.86
1:B:82:ALA:O	1:B:99:VAL:HG13	1.74	0.86
1:A:71:TRP:HH2	1:A:99:VAL:CG1	1.89	0.86
3:D:6:GLN:HB2	3:D:21:SER:HB3	1.59	0.85
1:A:43:ARG:HB3	1:A:65:PHE:CZ	2.12	0.85
3:D:117:SER:HB2	3:D:140:SER:HB2	1.57	0.85
1:B:90:TRP:HB2	1:B:93:HIS:HD2	1.39	0.85
2:C:146:CYS:HG	2:C:202:CYS:HG	1.24	0.85
3:D:67:ASN:O	3:D:68:SER:OG	1.95	0.84
1:B:56:PRO:HG3	1:B:60:ALA:HB3	1.60	0.84
3:Q:156:SER:O	3:Q:157:PRO:C	2.07	0.84
3:D:123:PRO:HB3	3:D:133:ALA:HB1	1.57	0.84
2:C:89:GLU:OE1	2:C:89:GLU:N	2.11	0.84
3:Q:111:GLN:HB2	3:Q:112:PRO:HD2	1.59	0.84
3:Q:97:ASN:OD1	3:Q:98:GLY:N	2.11	0.83
1:B:46:CYS:SG	1:B:70:CYS:HB2	2.15	0.83
2:C:107:ASP:OD2	2:C:108:TYR:HE1	1.63	0.82
1:B:88:LEU:CD1	1:B:90:TRP:CE2	2.63	0.82
3:D:142:PHE:CD1	3:D:176:ALA:HB2	2.15	0.82
3:D:4:LEU:HD12	3:D:4:LEU:O	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:153:ALA:O	3:Q:157:PRO:HD2	1.80	0.81
2:P:63:LYS:HA	2:P:65:GLN:NE2	1.95	0.81
1:B:120:ASN:HB3	1:B:121:PRO:HD2	1.61	0.81
3:D:172:ASN:HB2	3:D:175:TYR:CE2	2.15	0.81
2:C:28:THR:CG2	2:C:29:PHE:H	1.93	0.80
1:B:68:TYR:HE1	2:C:100:PRO:CA	1.94	0.80
1:A:39:TRP:CZ3	1:A:43:ARG:HD3	2.14	0.80
2:C:74:GLU:N	2:C:74:GLU:OE1	2.14	0.80
2:P:92:ALA:O	2:P:114:LEU:CD1	2.29	0.80
2:P:91:THR:HG22	2:P:117:VAL:H	1.45	0.80
1:A:31:THR:HG22	1:A:34:GLU:HG3	1.63	0.79
1:B:46:CYS:SG	1:B:70:CYS:HB3	2.20	0.79
3:Q:6:GLN:CB	3:Q:7:PRO:HD3	2.07	0.79
2:C:169:VAL:O	2:C:170:HIS:ND1	2.15	0.79
3:D:13:THR:HG22	3:D:110:LEU:HD22	1.65	0.79
2:C:206:HIS:CE1	2:C:208:PRO:HD2	2.17	0.78
3:D:32:ASN:OD1	3:D:33:THR:N	2.14	0.78
2:C:29:PHE:CD1	2:C:29:PHE:O	2.36	0.78
1:B:102:GLN:O	1:B:111:LEU:HD11	1.83	0.77
3:Q:118:VAL:HG22	3:Q:207:LYS:CE	2.08	0.77
2:P:142:ALA:HB3	2:P:190:VAL:HG23	1.67	0.76
1:A:43:ARG:HH12	3:Q:51:SER:CB	1.92	0.76
1:B:88:LEU:HB2	1:B:89:PRO:HD2	1.65	0.76
1:A:71:TRP:CH2	1:A:99:VAL:CG1	2.64	0.76
2:P:144:LEU:HD21	2:P:200:TYR:CD2	2.18	0.76
3:Q:23:SER:HA	3:Q:71:SER:CB	2.15	0.76
1:A:43:ARG:NH2	3:Q:54:GLN:HG3	2.00	0.76
1:B:41:ARG:O	1:B:44:ARG:HG3	1.85	0.75
3:Q:121:PHE:HB2	3:Q:136:VAL:HG13	1.69	0.75
2:C:107:ASP:OD2	2:C:108:TYR:CD1	2.38	0.75
1:B:86:TRP:HE3	1:B:87:TYR:HA	1.52	0.75
3:Q:197:GLN:HG2	3:Q:208:THR:HB	1.69	0.75
3:Q:118:VAL:HG12	3:Q:139:ILE:HG23	1.69	0.74
2:C:29:PHE:O	2:C:29:PHE:HD1	1.70	0.74
2:C:18:VAL:HG12	2:C:86:LEU:HD11	1.67	0.74
3:D:6:GLN:CB	3:D:7:PRO:CD	2.65	0.74
1:B:102:GLN:O	1:B:111:LEU:CG	2.36	0.74
2:P:145:GLY:HA2	2:P:160:TRP:CH2	2.23	0.74
3:D:6:GLN:HB2	3:D:7:PRO:HD3	1.70	0.73
3:Q:207:LYS:CB	3:Q:207:LYS:NZ	2.30	0.73
3:Q:173:ASN:C	3:Q:174:LYS:HG3	2.08	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:154:ASP:CG	3:Q:155:SER:H	1.92	0.73
3:Q:23:SER:HA	3:Q:71:SER:HB3	1.70	0.73
3:D:194:TYR:O	3:D:211:PRO:HD2	1.88	0.73
1:B:90:TRP:CE2	1:B:120:ASN:OD1	2.41	0.73
3:Q:212:THR:HG22	3:Q:213:GLU:N	2.04	0.73
3:D:50:TYR:HB2	2:C:105:PRO:HG3	1.70	0.73
1:B:71:TRP:CH2	1:B:101:ARG:NH1	2.57	0.72
1:A:116:THR:HG23	1:A:117:GLN:H	1.55	0.72
3:Q:212:THR:HG22	3:Q:213:GLU:H	1.54	0.72
3:D:116:PRO:HG2	3:D:207:LYS:HE3	1.70	0.72
3:D:4:LEU:HD11	3:D:23:SER:OG	1.88	0.72
1:B:108:GLN:HG2	1:B:109:TRP:H	1.54	0.72
1:B:120:ASN:CB	1:B:121:PRO:HD2	2.20	0.72
1:B:90:TRP:CD2	1:B:120:ASN:OD1	2.43	0.71
3:Q:28:ASN:OD1	3:Q:29:ILE:HG13	1.90	0.71
1:A:65:PHE:CE2	1:A:67:MET:HA	2.26	0.71
3:D:156:SER:HB2	3:D:157:PRO:CD	2.17	0.71
2:C:22:CYS:HB2	2:C:96:CYS:SG	2.30	0.71
1:B:40:GLU:OE2	3:D:33:THR:HG21	1.91	0.70
1:A:101:ARG:HH21	1:A:109:TRP:HB3	1.54	0.70
2:P:67:ARG:NH2	2:P:90:ASP:OD2	2.25	0.70
3:D:131:ASN:HA	3:D:185:PRO:HG2	1.72	0.70
3:D:111:GLN:HB3	3:D:112:PRO:HD2	1.71	0.70
3:D:6:GLN:HB3	3:D:7:PRO:HD3	1.74	0.70
1:B:102:GLN:O	1:B:111:LEU:CD1	2.40	0.70
1:B:70:CYS:CA	1:B:70:CYS:SG	2.80	0.70
3:D:95:SER:OG	3:D:96:LEU:HG	1.91	0.70
3:D:50:TYR:CD1	3:D:51:SER:N	2.56	0.69
1:A:43:ARG:HH22	3:Q:54:GLN:HG3	1.53	0.69
3:D:47:LEU:HD22	2:C:106:THR:O	1.92	0.69
2:P:198:GLN:NE2	2:C:10:GLU:OE2	2.24	0.69
2:C:22:CYS:HG	2:C:96:CYS:HG	0.83	0.69
2:C:22:CYS:CB	2:C:96:CYS:SG	2.80	0.69
2:P:131:ALA:HB2	2:P:144:LEU:HA	1.73	0.69
3:D:169:LYS:O	3:D:170:GLN:NE2	2.26	0.69
3:D:135:LEU:HD11	3:D:194:TYR:CD2	2.27	0.69
1:B:40:GLU:OE2	3:D:33:THR:CG2	2.41	0.69
2:P:145:GLY:HA2	2:P:160:TRP:HH2	1.58	0.69
3:D:142:PHE:HE2	3:D:200:HIS:CE1	2.11	0.69
3:Q:155:SER:O	3:Q:157:PRO:HD3	1.92	0.69
1:B:112:TRP:HE3	1:B:113:ARG:N	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:162:VAL:HG23	3:Q:163:GLU:N	2.07	0.69
1:B:46:CYS:CB	1:B:70:CYS:SG	2.82	0.68
3:D:6:GLN:CB	3:D:21:SER:HB3	2.24	0.68
3:Q:96:LEU:O	3:Q:96:LEU:CD1	2.35	0.68
1:B:115:HIS:HB2	1:B:118:CYS:HB2	1.76	0.68
3:D:121:PHE:CD2	2:C:130:LEU:HB3	2.28	0.68
3:D:96:LEU:C	3:D:97:ASN:OD1	2.32	0.67
1:A:111:LEU:HD12	1:A:112:TRP:HB3	1.76	0.67
1:B:90:TRP:O	1:B:90:TRP:CE3	2.48	0.67
3:D:142:PHE:HE1	3:D:176:ALA:HB2	1.57	0.67
3:D:134:THR:HG21	2:C:149:LYS:HE2	1.76	0.67
3:Q:164:THR:HG23	3:Q:179:SER:HB2	1.75	0.67
2:C:60:TYR:CE1	2:C:70:ILE:HD12	2.30	0.67
2:C:29:PHE:CD1	2:C:29:PHE:C	2.68	0.67
2:P:169:VAL:HG22	2:P:188:VAL:HG12	1.75	0.67
3:D:1:SER:HB2	3:D:2:TYR:O	1.93	0.67
2:P:131:ALA:HB1	2:P:133:SER:OG	1.94	0.67
1:B:102:GLN:O	1:B:111:LEU:HG	1.95	0.67
1:A:41:ARG:O	1:A:45:GLU:HG3	1.94	0.66
2:C:68:VAL:HG23	2:C:81:MET:SD	2.36	0.66
2:C:3:GLN:CG	2:C:4:LEU:CD1	2.70	0.66
1:B:38:ARG:HE	1:B:86:TRP:HH2	1.42	0.66
1:A:94:VAL:HB	1:A:117:GLN:O	1.95	0.66
3:D:138:LEU:HB3	2:C:172:PHE:CZ	2.30	0.66
2:C:28:THR:O	2:C:29:PHE:CG	2.48	0.66
2:C:33:ALA:HB3	2:C:101:ILE:HA	1.76	0.66
2:C:200:TYR:HB2	2:C:217:VAL:HG11	1.78	0.66
1:B:108:GLN:HG2	1:B:109:TRP:N	2.11	0.65
2:P:68:VAL:HG22	2:P:83:LEU:HD13	1.79	0.65
3:D:89:CYS:O	3:D:102:GLY:N	2.29	0.65
2:C:50:GLY:H	2:C:59:ASN:ND2	1.95	0.65
2:C:48:MET:HE1	2:C:94:TYR:HD2	1.60	0.65
2:C:121:SER:O	2:C:152:PHE:CD2	2.50	0.64
1:A:39:TRP:CH2	1:A:43:ARG:HD3	2.32	0.64
3:D:165:THR:CG2	3:D:177:ALA:HB1	2.25	0.64
3:D:170:GLN:O	3:D:175:TYR:CD2	2.49	0.64
1:B:90:TRP:HB2	1:B:93:HIS:CD2	2.27	0.64
1:B:66:ASP:OD1	1:B:69:VAL:N	2.30	0.64
3:D:167:PRO:HA	3:D:177:ALA:HB2	1.80	0.64
2:P:91:THR:HG22	2:P:117:VAL:N	2.11	0.64
2:C:22:CYS:CB	2:C:96:CYS:HG	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:143:TYR:CD1	3:D:144:PRO:HA	2.33	0.64
3:D:127:GLU:O	3:D:130:ALA:HB3	1.98	0.63
1:B:112:TRP:C	1:B:112:TRP:CE3	2.72	0.63
3:Q:169:LYS:HB2	3:Q:175:TYR:CE1	2.33	0.63
2:C:74:GLU:H	2:C:74:GLU:CD	2.01	0.63
1:B:120:ASN:HB3	1:B:121:PRO:CD	2.29	0.63
2:C:107:ASP:OD1	2:C:108:TYR:N	2.27	0.63
2:C:207:LYS:HG3	2:C:208:PRO:CD	2.23	0.63
3:D:184:THR:H	3:D:187:GLN:NE2	1.96	0.63
1:B:101:ARG:HH11	1:B:113:ARG:NH2	1.97	0.63
1:B:108:GLN:CG	1:B:109:TRP:H	2.12	0.63
3:D:86:ASP:HA	3:D:105:THR:O	1.98	0.63
3:Q:3:VAL:O	3:Q:102:GLY:HA2	1.99	0.63
1:B:83:SER:HA	1:B:98:PHE:CD1	2.34	0.63
3:D:164:THR:HG22	3:D:165:THR:H	1.64	0.62
3:Q:212:THR:O	3:Q:213:GLU:HB2	1.99	0.62
3:D:153:ALA:O	3:D:194:TYR:HD1	1.81	0.62
1:B:84:CYS:SG	1:B:97:GLY:O	2.57	0.62
1:B:86:TRP:HA	1:B:91:HIS:ND1	2.13	0.62
3:D:6:GLN:HA	3:D:6:GLN:OE1	2.00	0.62
3:D:120:LEU:CD2	3:D:211:PRO:HD3	2.29	0.62
1:B:94:VAL:O	1:B:97:GLY:N	2.31	0.62
3:Q:53:ASN:OD1	3:Q:64:SER:HA	2.00	0.62
3:D:134:THR:HG22	3:D:182:SER:HA	1.81	0.62
1:B:101:ARG:HD2	1:B:113:ARG:CZ	2.30	0.62
3:Q:212:THR:CG2	3:Q:213:GLU:H	2.12	0.62
3:Q:5:THR:HG22	3:Q:7:PRO:HD2	1.82	0.62
3:D:111:GLN:HB3	3:D:112:PRO:CD	2.30	0.62
2:C:59:ASN:OD1	2:C:102:VAL:HG11	1.99	0.62
2:C:6:GLN:HE22	2:C:95:TYR:HA	1.65	0.62
2:P:62:GLN:H	3:Q:97:ASN:HD21	1.48	0.61
3:Q:153:ALA:HA	3:Q:194:TYR:CE1	2.35	0.61
3:Q:154:ASP:CG	3:Q:155:SER:N	2.52	0.61
2:C:73:ASP:HB3	2:C:76:THR:OG1	1.99	0.61
3:Q:97:ASN:CG	3:Q:98:GLY:H	2.01	0.61
1:B:84:CYS:SG	1:B:97:GLY:C	2.79	0.61
1:A:39:TRP:CH2	1:A:43:ARG:CD	2.83	0.61
3:D:124:SER:O	3:D:128:LEU:HD12	2.00	0.61
3:D:1:SER:OG	3:D:2:TYR:HA	2.00	0.61
2:P:211:THR:C	2:P:212:LYS:HD3	2.21	0.61
3:D:164:THR:HG22	3:D:165:THR:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:28:THR:O	2:C:30:SER:N	2.34	0.60
1:A:43:ARG:O	1:A:44:ARG:HB2	2.01	0.60
1:A:111:LEU:HD11	1:A:112:TRP:HD1	1.66	0.60
2:C:201:ILE:HA	2:C:215:LYS:O	2.01	0.60
3:D:62:ARG:NH2	3:D:78:ARG:O	2.33	0.60
2:C:39:GLN:NE2	2:C:43:GLN:O	2.29	0.60
2:C:127:VAL:HG13	2:C:146:CYS:SG	2.42	0.60
1:B:110:GLY:C	1:B:111:LEU:HD22	2.22	0.60
2:P:156:VAL:HG23	2:P:184:LEU:HD21	1.83	0.60
1:B:68:TYR:CD1	2:C:100:PRO:HB3	2.37	0.60
2:C:50:GLY:O	2:C:59:ASN:ND2	2.34	0.60
3:Q:7:PRO:HG2	3:Q:105:THR:OG1	2.02	0.60
2:P:62:GLN:O	2:P:63:LYS:HB2	2.01	0.59
3:D:81:SER:HA	3:D:109:VAL:HG21	1.84	0.59
3:D:162:VAL:CG2	3:D:181:LEU:HD12	2.25	0.59
3:D:143:TYR:O	3:D:200:HIS:NE2	2.28	0.59
1:B:89:PRO:O	1:B:90:TRP:CG	2.56	0.59
2:C:153:PRO:HD2	2:C:208:PRO:HG2	1.83	0.59
3:D:130:ALA:O	3:D:131:ASN:CB	2.50	0.59
1:A:116:THR:O	1:A:119:GLU:N	2.31	0.59
2:C:100:PRO:O	2:C:101:ILE:HG23	2.03	0.59
3:D:152:LYS:HB3	3:D:155:SER:HA	1.85	0.59
3:Q:6:GLN:H	3:Q:7:PRO:HD2	1.65	0.59
2:C:34:ILE:HD12	2:C:34:ILE:O	2.02	0.59
1:B:39:TRP:CD1	1:B:40:GLU:HG2	2.37	0.59
3:D:110:LEU:HD12	3:D:110:LEU:N	2.18	0.59
3:Q:25:SER:H	3:Q:28:ASN:HD21	1.51	0.59
1:B:31:THR:O	1:B:35:LEU:HD13	2.02	0.59
1:A:115:HIS:HD2	1:A:119:GLU:OE2	1.86	0.59
3:D:98:GLY:HA3	2:C:47:TRP:CZ3	2.37	0.59
3:Q:206:GLU:OE1	3:Q:206:GLU:HA	2.02	0.59
1:B:41:ARG:HA	1:B:44:ARG:HD2	1.85	0.58
1:B:68:TYR:HE1	2:C:100:PRO:HA	1.64	0.58
2:C:3:GLN:CG	2:C:4:LEU:HD12	2.16	0.58
3:Q:92:TRP:CZ3	3:Q:98:GLY:HA2	2.38	0.58
1:A:116:THR:HG23	1:A:117:GLN:N	2.17	0.58
2:C:60:TYR:HE1	2:C:70:ILE:HD12	1.66	0.58
2:P:101:ILE:CG2	2:P:102:VAL:N	2.66	0.58
2:P:64:PHE:HB3	2:P:68:VAL:HG23	1.84	0.58
1:B:86:TRP:CE3	1:B:87:TYR:HA	2.35	0.58
1:A:90:TRP:HE1	1:A:119:GLU:HA	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:131:ALA:C	2:P:133:SER:N	2.56	0.58
2:C:163:GLY:C	2:C:165:LEU:H	2.07	0.58
3:Q:173:ASN:O	3:Q:174:LYS:HG2	1.97	0.58
3:D:156:SER:CB	3:D:157:PRO:HD3	2.16	0.58
2:C:160:TRP:HB3	2:C:165:LEU:CD2	2.34	0.58
2:C:64:PHE:O	2:C:65:GLN:HG2	2.04	0.58
1:B:68:TYR:HE1	2:C:100:PRO:N	2.02	0.58
3:D:13:THR:CG2	3:D:110:LEU:HD22	2.33	0.58
1:B:62:ASN:OD1	1:B:63:GLY:O	2.22	0.58
2:C:199:THR:O	2:C:200:TYR:CD1	2.57	0.57
3:Q:148:THR:OG1	3:Q:199:THR:HG23	2.04	0.57
3:Q:39:GLN:O	3:Q:85:ALA:HB1	2.04	0.57
1:B:41:ARG:O	1:B:44:ARG:CG	2.51	0.57
1:B:109:TRP:CE3	1:B:109:TRP:O	2.57	0.57
2:P:175:VAL:HG12	2:P:183:SER:O	2.03	0.57
2:C:107:ASP:CG	2:C:108:TYR:CE1	2.75	0.57
3:D:165:THR:HG22	3:D:178:SER:O	2.05	0.57
2:C:12:LYS:HE2	2:C:17:SER:O	2.04	0.57
3:Q:172:ASN:ND2	3:Q:172:ASN:O	2.38	0.57
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.39	0.57
2:C:28:THR:O	2:C:29:PHE:CD2	2.57	0.57
3:D:213:GLU:HA	3:D:213:GLU:OE1	2.05	0.57
3:D:139:ILE:HG22	3:D:176:ALA:HB3	1.86	0.57
3:D:120:LEU:HD23	3:D:209:VAL:HG12	1.85	0.57
3:Q:168:SER:OG	3:Q:170:GLN:OE1	2.22	0.57
2:P:32:TYR:HB3	2:P:99:GLY:O	2.05	0.57
3:D:137:CYS:CB	3:D:196:CYS:SG	2.93	0.57
3:D:170:GLN:O	3:D:175:TYR:CE2	2.58	0.57
3:Q:168:SER:O	3:Q:175:TYR:HA	2.05	0.57
2:C:107:ASP:OD1	2:C:108:TYR:CD1	2.43	0.56
2:P:131:ALA:H	3:Q:121:PHE:HD2	1.53	0.56
2:P:34:ILE:HD12	2:P:53:PRO:HG3	1.88	0.56
3:D:137:CYS:CB	3:D:196:CYS:HG	2.16	0.56
3:D:114:ALA:HB3	3:D:142:PHE:HA	1.87	0.56
3:D:139:ILE:HG22	3:D:176:ALA:CB	2.36	0.56
2:C:160:TRP:HB3	2:C:165:LEU:HD22	1.85	0.56
1:B:60:ALA:HB1	1:B:74:ALA:O	2.05	0.56
3:D:154:ASP:C	3:D:156:SER:H	2.07	0.56
1:A:61:CYS:HA	1:A:107:GLY:O	2.06	0.56
3:D:25:SER:OG	3:D:28:ASN:ND2	2.39	0.56
3:D:142:PHE:CD2	3:D:143:TYR:N	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ASP:N	1:B:114:ASP:OD1	2.37	0.56
2:P:64:PHE:O	2:P:67:ARG:N	2.38	0.56
3:D:187:GLN:OE1	3:D:187:GLN:N	2.39	0.56
1:B:36:TYR:O	1:B:39:TRP:HB3	2.06	0.55
3:D:62:ARG:HA	3:D:77:SER:HB3	1.88	0.55
1:B:41:ARG:O	1:B:45:GLU:HG2	2.06	0.55
3:Q:2:TYR:HE1	3:Q:102:GLY:O	1.88	0.55
3:Q:34:VAL:HG11	3:Q:72:ALA:CB	2.36	0.55
1:B:115:HIS:CB	1:B:118:CYS:HB2	2.37	0.55
1:B:89:PRO:O	1:B:90:TRP:CD1	2.59	0.55
1:B:88:LEU:HD11	1:B:90:TRP:CE2	2.39	0.55
3:D:132:LYS:HA	3:D:185:PRO:HD3	1.87	0.55
2:C:176:LEU:HD13	2:C:182:TYR:CE1	2.41	0.55
3:Q:4:LEU:O	3:Q:4:LEU:HD12	2.06	0.55
1:A:66:ASP:O	1:A:67:MET:HB2	2.06	0.55
2:P:130:LEU:HD11	2:P:147:LEU:HB2	1.87	0.55
3:D:142:PHE:HE1	3:D:176:ALA:CB	2.20	0.55
2:C:108:TYR:CD1	2:C:108:TYR:N	2.74	0.55
1:A:65:PHE:CZ	1:A:67:MET:HA	2.41	0.55
3:Q:212:THR:CG2	3:Q:213:GLU:N	2.69	0.55
1:B:40:GLU:O	1:B:44:ARG:HG2	2.07	0.55
2:C:125:PRO:HD2	2:C:211:THR:HG21	1.88	0.55
1:B:62:ASN:OD1	1:B:63:GLY:N	2.39	0.55
3:D:10:ALA:HB3	3:D:107:VAL:HG22	1.89	0.55
1:B:69:VAL:HG11	1:B:99:VAL:HG11	1.89	0.55
2:P:156:VAL:HG12	2:P:206:HIS:HB2	1.88	0.55
2:P:47:TRP:HZ3	3:Q:98:GLY:HA3	1.71	0.54
3:D:142:PHE:HZ	3:D:147:VAL:HB	1.72	0.54
2:P:166:THR:O	2:P:169:VAL:N	2.40	0.54
2:C:209:SER:HB3	2:C:211:THR:CG2	2.37	0.54
3:D:120:LEU:HD23	3:D:211:PRO:HD3	1.90	0.54
2:P:205:ASN:OD1	2:P:212:LYS:HE3	2.06	0.54
2:P:29:PHE:CZ	2:P:53:PRO:HB3	2.42	0.54
1:B:101:ARG:HH11	1:B:113:ARG:HH21	1.54	0.54
2:C:94:TYR:HE1	2:C:115:VAL:HB	1.72	0.54
1:B:82:ALA:HB3	1:B:99:VAL:CG1	2.36	0.54
3:Q:156:SER:O	3:Q:157:PRO:O	2.26	0.54
3:D:159:LYS:HD2	3:D:160:ALA:N	2.23	0.54
3:D:17:ARG:NH2	3:D:75:ALA:HB1	2.23	0.54
2:P:80:TYR:N	2:P:80:TYR:CD1	2.76	0.54
2:C:6:GLN:OE1	2:C:113:THR:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:GLN:CG	1:B:109:TRP:N	2.70	0.54
2:C:159:SER:OG	2:C:203:ASN:HB2	2.07	0.54
3:Q:92:TRP:CH2	3:Q:98:GLY:HA2	2.43	0.53
2:P:70:ILE:HG12	2:P:81:MET:SD	2.48	0.53
3:D:6:GLN:HB2	3:D:7:PRO:CD	2.33	0.53
1:A:113:ARG:HD2	1:A:115:HIS:HE1	1.73	0.53
2:C:81:MET:HE3	2:C:83:LEU:HB2	1.89	0.53
2:C:190:VAL:CG2	2:C:191:PRO:HD2	2.38	0.53
3:D:14:PRO:HG3	3:D:109:VAL:HG13	1.91	0.53
2:C:25:SER:O	2:C:29:PHE:HD2	1.90	0.53
3:D:154:ASP:O	3:D:155:SER:HB2	2.07	0.53
1:A:92:HIS:CE1	1:A:93:HIS:CE1	2.96	0.53
3:D:4:LEU:C	3:D:4:LEU:HD12	2.29	0.53
3:Q:120:LEU:HD13	3:Q:137:CYS:HB2	1.91	0.53
3:D:130:ALA:O	3:D:131:ASN:HB2	2.08	0.53
3:Q:128:LEU:HD21	3:Q:188:TRP:CD1	2.44	0.53
2:P:87:ARG:HG2	2:P:89:GLU:H	1.73	0.53
3:Q:120:LEU:HD22	3:Q:196:CYS:HB2	1.89	0.53
1:B:115:HIS:HE1	2:C:32:TYR:CZ	2.27	0.53
3:D:170:GLN:O	3:D:175:TYR:HD2	1.92	0.53
1:B:36:TYR:CE2	3:D:32:ASN:ND2	2.77	0.53
1:B:74:ALA:HB3	1:B:103:CYS:SG	2.48	0.53
1:B:116:THR:O	1:B:119:GLU:HG2	2.09	0.53
3:Q:196:CYS:CA	3:Q:196:CYS:SG	2.93	0.52
3:D:23:SER:HA	3:D:71:SER:HB2	1.91	0.52
1:B:102:GLN:H	1:B:111:LEU:HD12	1.74	0.52
1:B:101:ARG:NH1	1:B:113:ARG:HE	2.06	0.52
2:C:73:ASP:O	2:C:76:THR:OG1	2.27	0.52
3:Q:120:LEU:HD22	3:Q:196:CYS:CB	2.39	0.52
1:B:68:TYR:CE1	2:C:100:PRO:N	2.78	0.52
3:D:67:ASN:O	3:D:68:SER:CB	2.57	0.52
3:D:141:ASP:HA	3:D:175:TYR:HA	1.90	0.52
3:Q:192:ARG:O	3:Q:212:THR:HG23	2.09	0.52
3:D:188:TRP:HE3	3:D:194:TYR:CE2	2.28	0.52
3:D:159:LYS:HD2	3:D:160:ALA:H	1.74	0.52
2:P:104:ALA:HB1	2:P:105:PRO:HD2	1.91	0.52
2:P:166:THR:O	2:P:169:VAL:HG23	2.09	0.52
3:Q:40:LEU:HD23	3:Q:85:ALA:HB2	1.91	0.52
2:C:100:PRO:O	2:C:101:ILE:CG2	2.58	0.52
3:Q:142:PHE:HE1	3:Q:176:ALA:HA	1.74	0.52
3:Q:13:THR:HG22	3:Q:110:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:7:PRO:O	3:Q:105:THR:OG1	2.24	0.52
2:P:166:THR:O	2:P:167:SER:C	2.47	0.52
1:B:111:LEU:CD2	1:B:111:LEU:N	2.72	0.52
1:B:120:ASN:O	1:B:121:PRO:C	2.48	0.52
3:Q:53:ASN:OD1	3:Q:65:GLY:N	2.36	0.52
3:D:123:PRO:HD3	3:D:135:LEU:HD23	1.92	0.52
3:D:172:ASN:ND2	3:D:175:TYR:OH	2.42	0.52
2:C:28:THR:C	2:C:29:PHE:CD2	2.84	0.51
2:P:10:GLU:HG2	2:P:18:VAL:CG2	2.40	0.51
1:A:43:ARG:NH1	3:Q:51:SER:OG	2.42	0.51
2:C:50:GLY:H	2:C:59:ASN:HD22	1.58	0.51
3:Q:118:VAL:HG11	3:Q:198:VAL:HG21	1.92	0.51
2:P:30:SER:HB3	2:P:54:THR:OG1	2.11	0.51
1:B:97:GLY:CA	1:B:117:GLN:HG2	2.40	0.51
3:D:62:ARG:O	3:D:63:PHE:CE2	2.60	0.51
3:Q:53:ASN:HB2	3:Q:65:GLY:CA	2.41	0.51
3:D:143:TYR:CD1	3:D:144:PRO:CA	2.92	0.51
3:Q:3:VAL:HG22	3:Q:101:PHE:O	2.10	0.51
1:A:89:PRO:O	1:A:90:TRP:CD2	2.63	0.51
2:P:22:CYS:CB	2:P:96:CYS:SG	2.99	0.51
3:D:142:PHE:HD1	3:D:176:ALA:HB2	1.74	0.51
2:P:211:THR:O	2:P:212:LYS:HD3	2.10	0.51
1:A:33:GLY:O	1:A:37:GLN:HG2	2.11	0.51
3:D:114:ALA:HB2	3:D:174:LYS:CE	2.33	0.50
1:B:97:GLY:HA2	1:B:117:GLN:HG2	1.93	0.50
3:D:142:PHE:CE2	3:D:200:HIS:CE1	2.95	0.50
2:P:7:SER:HB3	2:P:21:SER:H	1.75	0.50
3:D:38:GLN:CB	3:D:48:LEU:HD13	2.41	0.50
1:B:67:MET:CE	2:C:105:PRO:HG2	2.42	0.50
3:D:62:ARG:O	3:D:63:PHE:CG	2.60	0.50
1:B:86:TRP:C	1:B:86:TRP:CE3	2.85	0.50
3:D:163:GLU:OE1	3:D:163:GLU:N	2.44	0.50
3:D:38:GLN:HB2	3:D:48:LEU:HD13	1.92	0.50
3:D:4:LEU:HD11	3:D:23:SER:HG	1.76	0.50
1:B:112:TRP:HE3	1:B:113:ARG:CA	2.23	0.50
1:B:112:TRP:HZ3	1:B:114:ASP:CB	2.25	0.50
3:D:138:LEU:CD1	2:C:187:VAL:HG21	2.41	0.50
1:B:120:ASN:ND2	2:C:54:THR:HG21	2.26	0.50
1:B:115:HIS:HE1	2:C:32:TYR:CE1	2.29	0.50
3:Q:162:VAL:CG2	3:Q:163:GLU:N	2.75	0.50
2:P:157:THR:CB	2:C:210:ASN:HD21	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:184:LEU:HD23	2:C:184:LEU:C	2.32	0.50
3:Q:96:LEU:O	3:Q:97:ASN:OD1	2.30	0.50
3:Q:111:GLN:CB	3:Q:112:PRO:HD2	2.37	0.50
3:Q:23:SER:HA	3:Q:71:SER:HB2	1.93	0.50
3:Q:34:VAL:HG11	3:Q:72:ALA:HB1	1.93	0.50
3:D:130:ALA:O	3:D:131:ASN:OD1	2.30	0.49
3:Q:62:ARG:HD2	3:Q:78:ARG:O	2.12	0.49
2:P:47:TRP:CD2	3:Q:99:VAL:HG12	2.47	0.49
1:B:109:TRP:HE3	1:B:109:TRP:O	1.93	0.49
3:Q:88:TYR:CD1	3:Q:104:GLY:HA3	2.47	0.49
1:B:34:GLU:OE1	1:B:34:GLU:N	2.40	0.49
2:C:76:THR:O	2:C:77:SER:HB2	2.11	0.49
1:B:90:TRP:HH2	1:B:118:CYS:O	1.95	0.49
1:B:68:TYR:CE1	2:C:100:PRO:HB3	2.47	0.49
1:A:31:THR:CG2	1:A:34:GLU:HG3	2.40	0.49
1:B:101:ARG:NH1	1:B:113:ARG:NE	2.59	0.49
3:D:3:VAL:HB	3:D:23:SER:O	2.13	0.49
1:B:101:ARG:HG3	1:B:111:LEU:HB3	1.93	0.49
2:P:132:PRO:HG3	3:Q:122:PRO:HG3	1.95	0.49
2:P:7:SER:HB3	2:P:21:SER:OG	2.13	0.49
2:P:129:PRO:HG3	3:Q:126:GLU:OE2	2.12	0.49
1:A:82:ALA:O	1:A:98:PHE:HA	2.13	0.49
1:B:40:GLU:OE2	3:D:33:THR:HG23	2.13	0.49
2:P:101:ILE:HG23	2:P:102:VAL:H	1.77	0.49
2:C:145:GLY:HA2	2:C:160:TRP:CH2	2.48	0.49
2:C:190:VAL:HG23	2:C:191:PRO:HD2	1.94	0.49
1:A:56:PRO:HG3	1:A:60:ALA:HB3	1.95	0.49
1:B:86:TRP:O	1:B:86:TRP:CE3	2.66	0.49
2:C:11:VAL:O	2:C:12:LYS:HD2	2.11	0.49
2:P:157:THR:HA	2:C:210:ASN:HD21	1.77	0.49
2:P:38:ARG:NH1	2:P:90:ASP:OD1	2.31	0.48
2:P:130:LEU:HB2	2:P:145:GLY:O	2.13	0.48
2:C:47:TRP:CE2	2:C:49:GLY:HA2	2.48	0.48
3:Q:80:GLN:O	3:Q:109:VAL:HG21	2.13	0.48
2:P:10:GLU:HG2	2:P:18:VAL:HG21	1.95	0.48
3:D:93:ASP:OD1	3:D:95:SER:HB3	2.13	0.48
2:C:200:TYR:HB2	2:C:217:VAL:CG1	2.42	0.48
2:C:28:THR:C	2:C:29:PHE:CG	2.86	0.48
3:D:138:LEU:HD22	2:C:172:PHE:CD1	2.48	0.48
2:P:101:ILE:CG2	2:P:102:VAL:H	2.24	0.48
2:C:67:ARG:HH21	2:C:83:LEU:HD11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:173:PRO:HD3	3:Q:170:GLN:OE1	2.13	0.48
2:P:101:ILE:HG22	2:P:102:VAL:N	2.28	0.48
2:P:62:GLN:O	2:P:63:LYS:CB	2.62	0.48
3:Q:53:ASN:HB2	3:Q:65:GLY:HA3	1.94	0.48
1:A:112:TRP:HZ3	1:A:114:ASP:HB2	1.79	0.48
2:P:201:ILE:HG13	2:P:215:LYS:O	2.13	0.48
1:B:44:ARG:O	1:B:45:GLU:C	2.51	0.48
1:B:90:TRP:O	1:B:90:TRP:HE3	1.92	0.48
3:Q:121:PHE:HB2	3:Q:136:VAL:CG1	2.39	0.48
3:D:170:GLN:O	3:D:172:ASN:N	2.46	0.48
3:Q:111:GLN:HB2	3:Q:112:PRO:CD	2.37	0.48
1:B:101:ARG:HH11	1:B:113:ARG:CZ	2.27	0.48
1:B:120:ASN:ND2	2:C:54:THR:CG2	2.76	0.48
2:C:6:GLN:HA	2:C:21:SER:O	2.14	0.48
2:C:154:GLU:OE1	2:C:154:GLU:N	2.38	0.48
3:D:127:GLU:OE2	3:D:134:THR:N	2.47	0.47
2:P:205:ASN:OD1	2:P:205:ASN:C	2.52	0.47
3:Q:143:TYR:CG	3:Q:144:PRO:HA	2.48	0.47
1:B:66:ASP:OD1	1:B:68:TYR:N	2.32	0.47
3:D:4:LEU:CD1	3:D:23:SER:OG	2.58	0.47
1:B:112:TRP:HZ3	1:B:114:ASP:CG	2.17	0.47
2:P:175:VAL:HB	3:Q:165:THR:HG22	1.95	0.47
3:Q:142:PHE:CD2	3:Q:142:PHE:O	2.68	0.47
1:B:66:ASP:CG	1:B:69:VAL:H	2.18	0.47
3:D:67:ASN:CG	3:D:69:GLY:H	2.17	0.47
3:D:120:LEU:HD21	3:D:211:PRO:HD3	1.97	0.47
1:B:102:GLN:H	1:B:111:LEU:CD1	2.28	0.47
3:Q:118:VAL:HA	3:Q:138:LEU:O	2.13	0.47
2:C:107:ASP:CG	2:C:108:TYR:H	2.15	0.47
3:D:165:THR:CG2	3:D:178:SER:H	2.28	0.47
3:Q:88:TYR:CE1	3:Q:104:GLY:HA3	2.49	0.47
2:C:46:GLU:OE2	2:C:63:LYS:NZ	2.30	0.47
3:D:38:GLN:N	3:D:46:LYS:O	2.38	0.47
2:C:3:GLN:HG3	2:C:4:LEU:N	2.28	0.47
2:P:184:LEU:C	2:P:184:LEU:HD12	2.35	0.47
1:B:88:LEU:HD12	1:B:88:LEU:C	2.35	0.47
2:C:23:LYS:HG3	2:C:24:ALA:H	1.80	0.47
3:D:141:ASP:OD1	3:D:141:ASP:O	2.32	0.46
3:D:114:ALA:CB	3:D:174:LYS:HE3	2.35	0.46
3:Q:118:VAL:HG21	3:Q:207:LYS:HZ1	1.78	0.46
1:B:117:GLN:HG3	1:B:117:GLN:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:108:TYR:HD1	2:C:108:TYR:H	1.62	0.46
3:Q:131:ASN:HA	3:Q:185:PRO:HG2	1.97	0.46
1:A:115:HIS:CE1	2:P:32:TYR:HH	2.33	0.46
3:D:46:LYS:HE2	3:D:48:LEU:HD12	1.96	0.46
1:B:112:TRP:CZ3	1:B:114:ASP:HB3	2.51	0.46
2:C:59:ASN:OD1	2:C:102:VAL:HG21	2.15	0.46
2:P:205:ASN:HA	2:P:212:LYS:HD2	1.98	0.46
1:B:50:LEU:HA	1:B:53:ALA:CB	2.46	0.46
1:B:115:HIS:NE2	2:C:28:THR:HA	2.30	0.46
1:A:43:ARG:CZ	3:Q:51:SER:CB	2.91	0.46
2:P:144:LEU:HG	2:P:188:VAL:HG23	1.97	0.46
3:D:59:VAL:HA	3:D:60:PRO:HD3	1.35	0.46
1:B:82:ALA:N	1:B:99:VAL:HG22	2.30	0.46
3:D:32:ASN:O	3:D:68:SER:HB2	2.16	0.46
3:D:35:HIS:HB3	3:D:50:TYR:HA	1.96	0.46
3:Q:118:VAL:CG2	3:Q:207:LYS:CE	2.83	0.46
1:B:120:ASN:CB	1:B:121:PRO:CD	2.93	0.46
3:Q:67:ASN:O	3:Q:68:SER:CB	2.64	0.46
1:B:100:LEU:HD12	1:B:100:LEU:C	2.36	0.46
1:B:68:TYR:HD1	2:C:100:PRO:HB3	1.79	0.45
1:B:101:ARG:HE	1:B:111:LEU:HB2	1.81	0.45
2:C:34:ILE:HD11	2:C:51:ILE:HG22	1.98	0.45
3:D:5:THR:HG23	3:D:5:THR:O	2.15	0.45
2:C:91:THR:HG23	2:C:116:THR:HA	1.97	0.45
3:D:172:ASN:HB2	3:D:175:TYR:CD2	2.51	0.45
3:D:20:ILE:HG12	3:D:105:THR:HG21	1.98	0.45
1:B:66:ASP:C	1:B:66:ASP:OD1	2.53	0.45
2:C:125:PRO:HD3	2:C:206:HIS:HD2	1.81	0.45
2:P:160:TRP:CZ3	2:P:202:CYS:HB3	2.51	0.45
2:C:64:PHE:C	2:C:65:GLN:HG2	2.36	0.45
3:Q:106:LYS:O	3:Q:106:LYS:HG3	2.16	0.45
2:C:24:ALA:HB1	2:C:29:PHE:CB	2.46	0.45
2:P:144:LEU:HD12	2:P:145:GLY:N	2.32	0.45
3:D:135:LEU:HD11	3:D:194:TYR:HD2	1.77	0.45
3:Q:27:SER:HB3	3:Q:95:SER:H	1.82	0.45
3:D:153:ALA:O	3:D:194:TYR:CD1	2.68	0.45
2:P:105:PRO:HG3	3:Q:50:TYR:HB2	1.98	0.45
1:B:90:TRP:CE3	1:B:120:ASN:OD1	2.70	0.45
2:C:29:PHE:O	2:C:53:PRO:HG2	2.17	0.45
3:D:199:THR:HG23	3:D:206:GLU:OE1	2.17	0.45
2:C:28:THR:C	2:C:30:SER:H	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:155:SER:C	3:Q:157:PRO:HD3	2.37	0.45
3:D:8:PRO:O	3:D:106:LYS:N	2.49	0.45
3:Q:60:PRO:HG2	3:Q:63:PHE:HE1	1.82	0.45
3:D:7:PRO:HG2	3:D:20:ILE:HG23	1.98	0.45
3:D:114:ALA:O	3:D:142:PHE:HB2	2.17	0.45
2:C:39:GLN:O	2:C:92:ALA:HB1	2.17	0.45
2:C:25:SER:O	2:C:29:PHE:CD2	2.70	0.44
1:A:39:TRP:CH2	1:A:43:ARG:HD2	2.51	0.44
1:A:43:ARG:HD2	1:A:65:PHE:CE2	2.52	0.44
3:Q:52:ASN:O	3:Q:53:ASN:HB3	2.16	0.44
1:A:115:HIS:HB3	1:A:119:GLU:OE1	2.17	0.44
3:Q:79:LEU:HD12	3:Q:80:GLN:H	1.82	0.44
2:P:97:ALA:HB1	2:P:106:THR:HB	1.99	0.44
1:B:90:TRP:CZ2	1:B:120:ASN:OD1	2.70	0.44
2:C:3:GLN:CG	2:C:4:LEU:HD13	2.46	0.44
2:P:216:ARG:HG2	2:P:217:VAL:H	1.82	0.44
3:D:120:LEU:HD12	3:D:121:PHE:N	2.32	0.44
3:Q:13:THR:O	3:Q:16:GLN:HG2	2.17	0.44
2:C:151:TYR:CE1	2:C:182:TYR:HB2	2.53	0.44
2:P:44:GLY:HA2	3:Q:88:TYR:CE1	2.52	0.44
1:A:112:TRP:HE3	1:A:113:ARG:O	2.00	0.44
3:Q:181:LEU:HD12	3:Q:182:SER:N	2.33	0.44
3:Q:49:ILE:HD12	3:Q:74:LEU:CD1	2.48	0.44
3:D:142:PHE:CZ	3:D:147:VAL:HB	2.50	0.44
3:Q:85:ALA:O	3:Q:106:LYS:HA	2.17	0.44
1:A:105:SER:OG	1:A:106:ASP:N	2.51	0.44
2:C:171:THR:HG23	2:C:184:LEU:HD21	2.00	0.44
1:B:66:ASP:O	1:B:67:MET:HB3	2.18	0.44
1:B:97:GLY:O	1:B:98:PHE:CD1	2.70	0.44
1:B:62:ASN:OD1	1:B:62:ASN:C	2.56	0.44
1:B:102:GLN:O	1:B:111:LEU:HD21	2.18	0.44
1:A:42:TYR:CG	1:A:87:TYR:HD2	2.36	0.44
1:B:67:MET:HE3	2:C:105:PRO:HG2	2.00	0.44
1:B:120:ASN:HD22	2:C:54:THR:CG2	2.31	0.44
3:D:50:TYR:CG	3:D:51:SER:N	2.82	0.44
3:Q:25:SER:H	3:Q:28:ASN:ND2	2.15	0.44
1:A:89:PRO:O	1:A:90:TRP:CG	2.71	0.44
3:D:48:LEU:HD21	3:D:63:PHE:CE1	2.53	0.43
2:C:152:PHE:HB3	2:C:153:PRO:HD3	2.00	0.43
1:A:90:TRP:HZ2	1:A:119:GLU:CG	2.31	0.43
3:D:116:PRO:HG2	3:D:207:LYS:CE	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:GLU:O	1:A:48:GLU:HG2	2.17	0.43
1:B:31:THR:OG1	1:B:32:ALA:N	2.51	0.43
2:C:100:PRO:C	2:C:101:ILE:HG23	2.37	0.43
3:D:184:THR:HG23	3:D:187:GLN:HE22	1.84	0.43
2:C:3:GLN:HG3	2:C:4:LEU:HD13	1.91	0.43
2:P:130:LEU:HB3	3:Q:121:PHE:CD2	2.54	0.43
2:C:48:MET:HE1	2:C:94:TYR:CD2	2.47	0.43
2:P:87:ARG:HE	2:P:87:ARG:HB2	1.54	0.43
3:Q:143:TYR:HA	3:Q:144:PRO:C	2.39	0.43
3:Q:48:LEU:HD21	3:Q:63:PHE:CD2	2.53	0.43
1:A:87:TYR:CD1	1:A:87:TYR:C	2.91	0.43
2:P:125:PRO:HB3	2:P:151:TYR:HB3	2.00	0.43
3:D:132:LYS:CA	3:D:185:PRO:HD3	2.48	0.43
1:A:101:ARG:HH21	1:A:109:TRP:CB	2.25	0.43
2:C:83:LEU:HD21	2:C:90:ASP:OD2	2.19	0.43
3:Q:118:VAL:HG11	3:Q:198:VAL:CG2	2.49	0.43
1:A:34:GLU:O	1:A:38:ARG:HG3	2.19	0.43
3:Q:144:PRO:HG2	3:Q:201:GLU:OE2	2.18	0.43
3:Q:123:PRO:HD3	3:Q:135:LEU:HD12	2.01	0.43
1:B:82:ALA:HB3	1:B:99:VAL:HG11	2.00	0.43
2:C:35:SER:O	2:C:96:CYS:HA	2.18	0.43
2:C:155:PRO:HD2	2:C:207:LYS:HE2	2.01	0.43
2:C:127:VAL:HG22	2:C:148:VAL:HG12	2.00	0.43
1:A:101:ARG:NH2	1:A:109:TRP:HB3	2.29	0.43
2:C:37:VAL:HG23	2:C:46:GLU:O	2.18	0.43
3:D:38:GLN:O	3:D:46:LYS:HB3	2.19	0.43
2:C:3:GLN:OE1	2:C:4:LEU:CD1	2.67	0.43
1:B:112:TRP:CE3	1:B:113:ARG:N	2.77	0.43
1:A:115:HIS:CE1	2:P:32:TYR:OH	2.72	0.43
2:P:64:PHE:O	2:P:67:ARG:HB2	2.19	0.43
2:P:156:VAL:CG2	2:P:184:LEU:HD21	2.47	0.43
3:Q:13:THR:OG1	3:Q:16:GLN:OE1	2.33	0.43
2:P:158:VAL:HG11	2:P:186:SER:OG	2.19	0.43
1:A:35:LEU:H	1:A:35:LEU:HD12	1.84	0.43
3:D:137:CYS:HB2	3:D:196:CYS:SG	2.58	0.43
2:P:175:VAL:CB	3:Q:165:THR:HG22	2.48	0.43
2:P:207:LYS:N	2:P:208:PRO:CD	2.81	0.43
1:B:98:PHE:HB3	1:B:99:VAL:H	1.28	0.43
1:A:71:TRP:CH2	1:A:99:VAL:HG11	2.52	0.43
3:Q:81:SER:O	3:Q:84:GLU:HG2	2.19	0.43
3:D:212:THR:O	3:D:213:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:13:LYS:O	2:C:16:SER:OG	2.36	0.42
1:B:88:LEU:HD13	1:B:90:TRP:CD1	2.52	0.42
1:B:68:TYR:CE1	2:C:100:PRO:CB	3.02	0.42
3:D:127:GLU:HG2	3:D:133:ALA:HA	2.00	0.42
3:D:183:LEU:CD1	3:D:187:GLN:HE21	2.33	0.42
3:D:151:TRP:O	3:D:158:VAL:HG12	2.18	0.42
3:D:6:GLN:N	3:D:7:PRO:CD	2.78	0.42
3:D:114:ALA:CB	3:D:174:LYS:CE	2.96	0.42
3:D:121:PHE:HD2	2:C:130:LEU:HB3	1.81	0.42
3:D:191:HIS:ND1	3:D:194:TYR:CE1	2.88	0.42
2:P:70:ILE:HG12	2:P:81:MET:HG3	2.01	0.42
3:D:128:LEU:O	3:D:131:ASN:N	2.51	0.42
3:D:163:GLU:HG2	3:D:163:GLU:O	2.20	0.42
1:B:41:ARG:HG2	1:B:44:ARG:NH1	2.35	0.42
1:B:112:TRP:HZ3	1:B:114:ASP:HB3	1.83	0.42
1:B:54:GLU:HA	1:B:55:PRO:HD3	1.82	0.42
2:P:75:SER:C	2:P:77:SER:N	2.73	0.42
3:Q:172:ASN:C	3:Q:173:ASN:HD22	2.23	0.42
2:C:28:THR:CG2	2:C:29:PHE:N	2.49	0.42
3:Q:49:ILE:CG2	3:Q:53:ASN:HA	2.50	0.42
1:B:101:ARG:CD	1:B:113:ARG:CZ	2.97	0.42
2:C:68:VAL:HA	2:C:82:GLU:O	2.20	0.42
3:D:84:GLU:HG2	3:D:107:VAL:O	2.19	0.42
1:A:92:HIS:CE1	1:A:93:HIS:ND1	2.87	0.42
1:B:88:LEU:CB	1:B:89:PRO:HD2	2.37	0.42
3:D:116:PRO:HD3	3:D:200:HIS:HD2	1.84	0.42
3:D:132:LYS:HA	3:D:184:THR:HA	2.02	0.42
3:D:6:GLN:N	3:D:7:PRO:HD2	2.35	0.42
3:Q:153:ALA:HA	3:Q:194:TYR:CD1	2.55	0.42
1:A:62:ASN:O	1:A:109:TRP:NE1	2.46	0.42
3:Q:109:VAL:C	3:Q:110:LEU:HD23	2.41	0.42
1:B:42:TYR:CD1	1:B:42:TYR:C	2.93	0.42
1:B:44:ARG:HG3	1:B:45:GLU:H	1.84	0.42
1:B:68:TYR:CE1	2:C:100:PRO:CA	2.86	0.42
3:Q:92:TRP:HA	3:Q:99:VAL:HA	2.02	0.42
2:P:41:PRO:HD3	2:P:92:ALA:HA	2.02	0.42
3:D:164:THR:CG2	3:D:165:THR:N	2.83	0.42
1:B:102:GLN:O	1:B:111:LEU:CD2	2.68	0.42
3:D:121:PHE:HA	3:D:122:PRO:HD3	1.66	0.41
3:D:188:TRP:CZ3	3:D:194:TYR:CD2	3.08	0.41
1:B:71:TRP:CZ2	1:B:101:ARG:NH1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:TYR:HD2	2:P:32:TYR:CE1	2.37	0.41
2:C:94:TYR:CE1	2:C:115:VAL:HB	2.54	0.41
1:B:50:LEU:HA	1:B:53:ALA:HB3	2.01	0.41
3:Q:60:PRO:HG2	3:Q:63:PHE:CE1	2.55	0.41
3:Q:127:GLU:HG2	3:Q:132:LYS:O	2.20	0.41
1:B:68:TYR:HE1	2:C:100:PRO:CB	2.33	0.41
3:Q:66:SER:OG	3:Q:67:ASN:N	2.53	0.41
3:Q:3:VAL:O	3:Q:3:VAL:HG23	2.20	0.41
2:C:163:GLY:C	2:C:165:LEU:N	2.72	0.41
2:P:157:THR:HB	2:C:210:ASN:HD21	1.85	0.41
2:C:117:VAL:O	2:C:118:SER:HB3	2.21	0.41
3:D:171:SER:C	3:D:175:TYR:HE2	2.23	0.41
3:Q:154:ASP:HA	3:Q:193:SER:O	2.20	0.41
3:D:130:ALA:O	3:D:131:ASN:CG	2.59	0.41
2:C:48:MET:SD	2:C:81:MET:HE2	2.61	0.41
3:D:212:THR:OG1	3:D:213:GLU:N	2.53	0.41
2:C:206:HIS:HB3	2:C:211:THR:HG23	2.03	0.41
2:P:22:CYS:HB2	2:P:36:TRP:CH2	2.56	0.41
3:D:153:ALA:HA	3:D:194:TYR:CD1	2.55	0.41
2:C:81:MET:CE	2:C:83:LEU:HB2	2.49	0.41
3:D:18:VAL:HG12	3:D:76:ILE:HG23	2.02	0.41
1:B:36:TYR:OH	3:D:35:HIS:CE1	2.73	0.41
3:D:118:VAL:HG22	3:D:139:ILE:CG1	2.51	0.41
1:B:111:LEU:HD22	1:B:111:LEU:N	2.35	0.41
1:B:112:TRP:CE3	1:B:113:ARG:C	2.94	0.41
2:C:34:ILE:CD1	2:C:51:ILE:HG22	2.50	0.41
1:A:91:HIS:CG	1:A:92:HIS:H	2.39	0.41
3:D:165:THR:OG1	3:D:166:THR:N	2.54	0.41
1:B:101:ARG:HH11	1:B:113:ARG:NE	2.18	0.41
1:A:111:LEU:CD1	1:A:112:TRP:HD1	2.32	0.41
2:P:48:MET:HG2	2:P:64:PHE:CE2	2.56	0.41
2:P:70:ILE:HG12	2:P:81:MET:CG	2.50	0.41
3:D:60:PRO:O	3:D:61:ASP:C	2.57	0.41
2:P:75:SER:O	2:P:77:SER:N	2.54	0.41
3:Q:172:ASN:C	3:Q:173:ASN:ND2	2.75	0.41
1:B:90:TRP:HZ3	1:B:94:VAL:CG1	2.34	0.41
2:C:33:ALA:CB	2:C:101:ILE:HA	2.49	0.41
2:C:24:ALA:HB1	2:C:29:PHE:CG	2.55	0.41
3:Q:206:GLU:OE1	3:Q:206:GLU:CA	2.67	0.41
3:D:201:GLU:CD	3:D:201:GLU:H	2.24	0.41
3:D:35:HIS:CE1	2:C:105:PRO:HD3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:142:PHE:CD2	3:D:200:HIS:CD2	3.08	0.40
2:C:10:GLU:OE1	2:C:18:VAL:HG23	2.21	0.40
2:C:106:THR:OG1	2:C:109:TRP:NE1	2.54	0.40
2:C:41:PRO:HD3	2:C:92:ALA:HA	2.03	0.40
2:P:175:VAL:HB	3:Q:165:THR:CG2	2.51	0.40
1:A:90:TRP:O	1:A:90:TRP:CD1	2.73	0.40
2:C:76:THR:HB	2:C:78:THR:OG1	2.21	0.40
2:C:34:ILE:H	2:C:34:ILE:HG13	1.70	0.40
1:A:91:HIS:CG	1:A:92:HIS:N	2.89	0.40
3:D:154:ASP:HB3	3:D:157:PRO:HD3	2.03	0.40
2:P:160:TRP:CE2	2:P:188:VAL:HG13	2.57	0.40
2:C:18:VAL:CG1	2:C:86:LEU:HD11	2.45	0.40
2:C:205:ASN:C	2:C:205:ASN:OD1	2.59	0.40
2:P:144:LEU:HD13	2:P:217:VAL:HG11	2.04	0.40
3:D:14:PRO:HG3	3:D:109:VAL:CG1	2.51	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	90/136 (66%)	82 (91%)	8 (9%)	0	100	100
1	B	89/136 (65%)	76 (85%)	12 (14%)	1 (1%)	17	58
2	C	199/227 (88%)	175 (88%)	23 (12%)	1 (0%)	34	76
2	P	200/227 (88%)	187 (94%)	13 (6%)	0	100	100
3	D	207/215 (96%)	168 (81%)	38 (18%)	1 (0%)	34	76
3	Q	206/215 (96%)	185 (90%)	19 (9%)	2 (1%)	19	61
All	All	991/1156 (86%)	873 (88%)	113 (11%)	5 (0%)	34	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Q	156	SER
3	D	7	PRO
1	B	89	PRO
2	C	152	PHE
3	Q	7	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	73/113 (65%)	71 (97%)	2 (3%)	52	85
1	B	71/113 (63%)	68 (96%)	3 (4%)	36	76
2	C	168/188 (89%)	162 (96%)	6 (4%)	42	79
2	P	169/188 (90%)	162 (96%)	7 (4%)	37	76
3	D	176/180 (98%)	169 (96%)	7 (4%)	38	77
3	Q	176/180 (98%)	169 (96%)	7 (4%)	38	77
All	All	833/962 (87%)	801 (96%)	32 (4%)	40	78

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	90	TRP
1	B	99	VAL
1	B	106	ASP
1	B	111	LEU
2	P	17	SER
2	P	80	TYR
2	P	159	SER
2	P	170	HIS
2	P	179	SER
2	P	197	THR
2	P	205	ASN
3	Q	55	ARG
3	Q	70	THR

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Mol	Chain	Res	Type
3	Q	77	SER
3	Q	147	VAL
3	Q	206	GLU
3	Q	207	LYS
3	Q	208	THR
3	D	78	ARG
3	D	99	VAL
3	D	101	PHE
3	D	119	THR
3	D	128	LEU
3	D	158	VAL
3	D	206	GLU
2	C	37	VAL
2	C	68	VAL
2	C	88	SER
2	C	116	THR
2	C	184	LEU
2	C	211	THR

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	92	HIS
1	A	115	HIS
1	B	93	HIS
1	B	115	HIS
2	P	98	GLN
3	Q	54	GLN
3	Q	173	ASN
3	D	35	HIS
3	D	131	ASN
3	D	170	GLN
3	D	172	ASN
3	D	187	GLN
2	C	206	HIS

5.3.3 RNA

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

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	92/136 (67%)	0.02	0 100 100	29, 53, 71, 87	1 (1%)
1	B	91/136 (66%)	0.89	12 (13%) 4 2	23, 100, 129, 141	1 (1%)
2	C	205/227 (90%)	0.17	6 (2%) 55 26	33, 53, 77, 91	0
2	P	206/227 (90%)	-0.24	1 (0%) 91 76	19, 30, 56, 76	0
3	D	211/215 (98%)	0.28	8 (3%) 44 18	22, 53, 67, 84	0
3	Q	210/215 (97%)	-0.14	1 (0%) 91 76	16, 27, 40, 48	0
All	All	1015/1156 (87%)	0.10	28 (2%) 56 27	16, 45, 98, 141	2 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	105	SER	6.2
1	B	93	HIS	6.0
1	B	110	GLY	4.3
3	D	61	ASP	3.7
1	B	107	GLY	3.6
3	D	6	GLN	3.5
1	B	109	TRP	3.5
1	B	108	GLN	3.5
1	B	111	LEU	3.2
2	C	162	SER	3.2
2	C	132	PRO	3.1
1	B	96	ALA	2.8
3	D	1	SER	2.7
2	C	140	GLY	2.7
1	B	83	SER	2.5
1	B	80	ALA	2.4
3	D	174	LYS	2.3
2	C	84	SER	2.3
2	C	58	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
3	Q	6	GLN	2.2
3	D	5	THR	2.2
3	D	115	ALA	2.2
2	P	81	MET	2.1
2	C	197	THR	2.1
1	B	106	ASP	2.0
3	D	199	THR	2.0
1	B	100	LEU	2.0
3	D	154	ASP	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.