



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:21 PM UTC

PDB ID : 4HJ0 / pdb_00004hj0
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

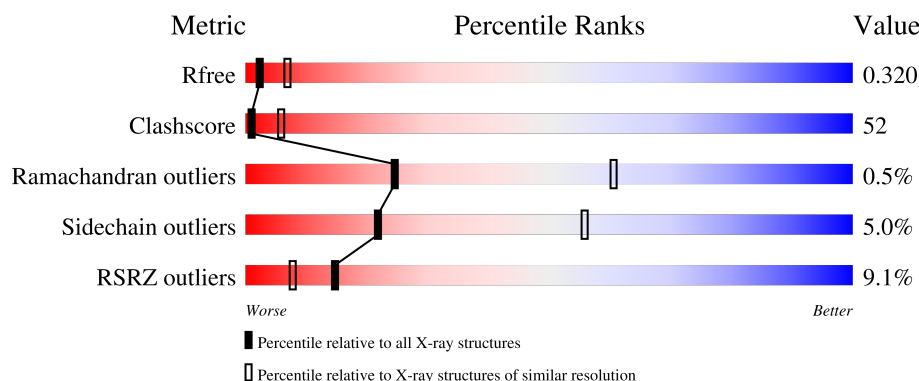
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. 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	30% 31% 6% 32%
1	B	136	24% 20% 35% 10% 33%
2	C	227	8% 37% 46% 7% 10%
2	P	227	4% 49% 37% 9%
3	D	215	10% 36% 52% 9%

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Mol	Chain	Length	Quality of chain
3	Q	215	4% 44% 45% 8%

2 Entry composition

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			

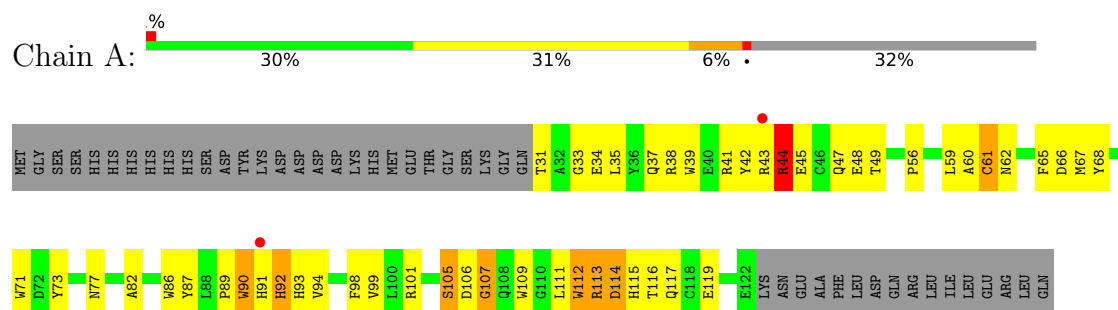
- Molecule 3 is a protein called Gipg013 Fab, Antagonizing antibody to the GIP Receptor, Light chain.

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			

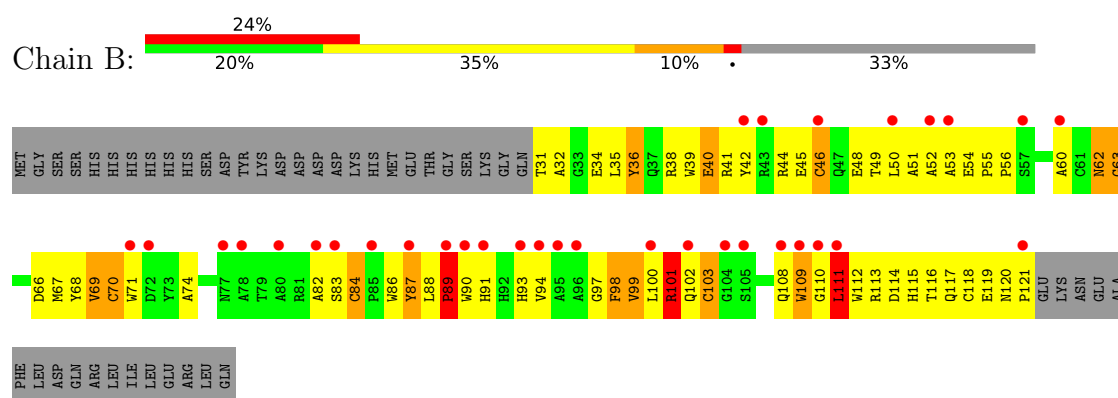
3 Residue-property plots

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.

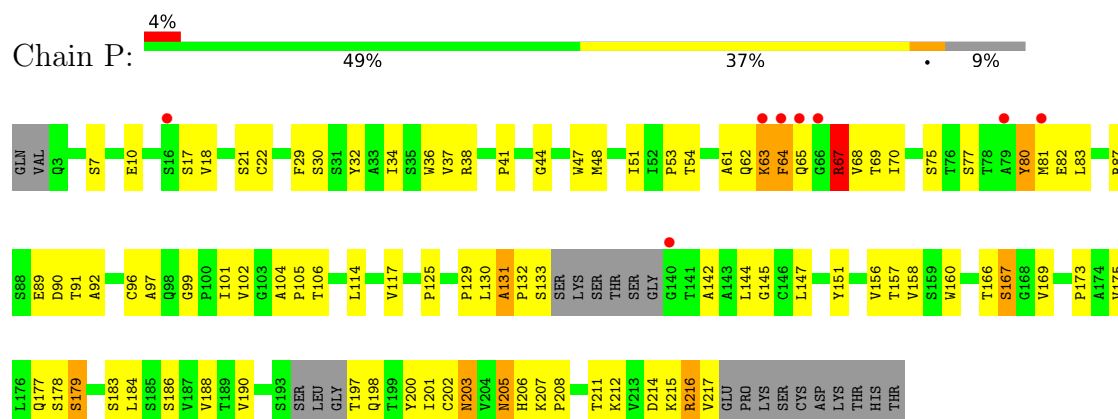
- Molecule 1: Gastric inhibitory polypeptide receptor

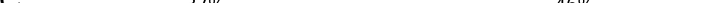


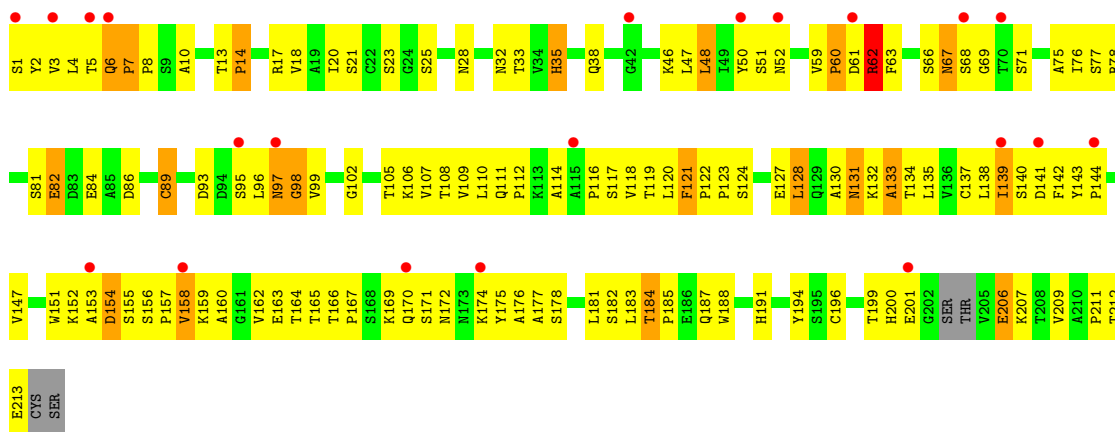
- Molecule 1: Gastric inhibitory polypeptide receptor



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



- Chain C: 



4 Data and refinement statistics

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 48.66 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.66-3.00) 99.8 (48.66-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.255 , 0.311 0.273 , 0.320	Depositor DCC
R_{free} test set	1999 reflections (9.08%)	wwPDB-VP
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 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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 ⓘ

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	0.50	1/770 (0.1%)	1.22	13/1053 (1.2%)
1	B	1.05	7/755 (0.9%)	1.54	18/1034 (1.7%)
2	C	0.39	0/1547	1.12	17/2109 (0.8%)
2	P	0.39	1/1553 (0.1%)	1.02	10/2117 (0.5%)
3	D	0.59	2/1608 (0.1%)	1.24	21/2198 (1.0%)
3	Q	0.68	3/1604 (0.2%)	1.15	16/2193 (0.7%)
All	All	0.60	14/7837 (0.2%)	1.19	95/10704 (0.9%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	51	SER	C-N	21.07	1.64	1.33
3	D	60	PRO	N-CD	-15.26	1.26	1.47
1	B	52	ALA	C-N	11.69	1.49	1.33
1	B	40	GLU	CD-OE2	10.84	1.46	1.25
1	B	48	GLU	C-N	-10.14	1.20	1.33
1	B	101	ARG	CZ-NH2	-9.21	1.21	1.33
1	B	89	PRO	N-CD	-8.77	1.35	1.47
3	Q	196	CYS	CB-SG	6.92	2.04	1.81
1	B	70	CYS	CB-SG	6.61	2.03	1.81
3	Q	156	SER	CB-OG	6.35	1.54	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	67	ARG	CZ-NH2	5.73	1.40	1.33
1	A	113	ARG	C-N	5.60	1.43	1.33
3	D	14	PRO	N-CD	-5.15	1.40	1.47
1	B	36	TYR	C-N	-5.05	1.27	1.33

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	156	SER	CA-C-N	-16.96	102.59	119.89
3	Q	156	SER	C-N-CA	-16.96	102.59	119.89
2	P	67	ARG	NE-CZ-NH2	15.47	133.12	119.20
3	D	62	ARG	CB-CA-C	-13.45	89.44	111.50
2	P	67	ARG	NE-CZ-NH1	-13.39	108.11	121.50
1	B	98	PHE	CA-C-N	-13.26	100.70	122.57
1	B	98	PHE	C-N-CA	-13.26	100.70	122.57
1	B	98	PHE	O-C-N	13.24	144.08	122.11
1	B	87	TYR	N-CA-C	11.99	125.50	111.11
2	C	4	LEU	N-CA-C	11.10	126.60	108.96
3	D	97	ASN	N-CA-C	10.81	124.75	108.31
3	D	60	PRO	CA-N-CD	10.36	126.51	112.00
3	Q	51	SER	O-C-N	-10.32	110.19	122.58
2	C	29	PHE	CB-CA-C	-10.12	95.40	111.48
2	C	102	VAL	N-CA-C	9.87	129.88	109.34
3	D	52	ASN	N-CA-C	9.87	125.24	110.64
3	D	108	THR	N-CA-C	9.86	125.92	109.76
2	C	198	GLN	N-CA-C	9.73	125.34	108.02
2	C	207	LYS	CA-C-N	-9.69	107.73	119.84
2	C	207	LYS	C-N-CA	-9.69	107.73	119.84
3	D	60	PRO	N-CA-C	9.60	132.25	112.47
1	B	62	ASN	N-CA-C	9.44	124.16	110.10
1	A	61	CYS	CA-CB-SG	9.26	135.69	114.40
3	D	60	PRO	N-CA-CB	-9.19	93.60	103.25
3	D	131	ASN	CB-CA-C	-8.63	93.25	110.42
3	Q	5	THR	N-CA-C	-8.33	98.16	110.23
1	A	90	TRP	N-CA-C	-8.29	102.74	112.86
3	Q	156	SER	CB-CA-C	8.26	126.44	110.17
1	A	73	TYR	N-CA-C	-8.06	98.35	110.28
3	Q	156	SER	CA-CB-OG	-7.96	95.18	111.10
3	D	98	GLY	N-CA-C	7.72	123.64	112.60
3	D	121	PHE	CA-C-N	7.53	128.13	120.38
3	D	121	PHE	C-N-CA	7.53	128.13	120.38
1	A	47	GLN	N-CA-C	7.53	119.12	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	67	ASN	N-CA-C	7.51	120.12	111.11
3	D	89	CYS	O-C-N	-7.46	114.34	122.85
2	P	179	SER	N-CA-C	-7.45	104.03	113.72
3	Q	174	LYS	N-CA-C	7.39	119.63	107.73
1	A	49	THR	N-CA-C	-7.30	103.25	111.14
1	A	107	GLY	N-CA-C	-7.25	104.12	116.01
3	D	62	ARG	CA-C-N	7.24	135.37	121.54
3	D	62	ARG	C-N-CA	7.24	135.37	121.54
1	A	113	ARG	N-CA-C	7.22	121.80	110.17
1	B	89	PRO	N-CA-CB	-7.02	95.88	103.25
2	C	44	GLY	N-CA-C	6.90	123.90	112.30
1	B	103	CYS	N-CA-C	6.73	118.62	111.28
2	C	54	THR	N-CA-C	6.70	118.24	111.07
1	B	109	TRP	N-CA-C	6.60	119.88	109.39
1	B	51	ALA	N-CA-C	-6.56	104.05	111.07
3	Q	3	VAL	N-CA-C	-6.53	101.14	109.30
1	A	112	TRP	N-CA-C	6.52	120.15	109.72
1	A	49	THR	N-CA-CB	6.43	119.39	110.07
1	B	111	LEU	N-CA-C	6.42	119.40	109.07
2	C	51	ILE	N-CA-C	6.41	119.20	108.81
1	B	63	GLY	N-CA-C	-6.37	102.12	111.03
1	B	49	THR	N-CA-C	6.32	119.39	111.24
2	C	171	THR	N-CA-C	6.23	119.01	107.99
2	P	216	ARG	N-CA-CB	-6.21	100.99	110.49
1	B	84	CYS	CA-C-N	6.19	126.10	119.85
1	B	84	CYS	C-N-CA	6.19	126.10	119.85
2	P	61	ALA	N-CA-C	-6.12	100.19	109.85
3	Q	97	ASN	CB-CA-C	-6.09	109.56	116.63
1	A	114	ASP	N-CA-CB	6.02	120.63	110.46
3	D	133	ALA	N-CA-CB	-5.92	101.39	111.69
1	A	44	ARG	CB-CA-C	-5.89	97.92	110.76
2	C	193	SER	N-CA-C	5.86	127.40	111.00
1	B	89	PRO	CA-N-CD	5.84	120.17	112.00
1	B	46	CYS	N-CA-C	5.83	118.13	111.02
3	Q	121	PHE	CA-C-N	5.80	126.36	120.38
3	Q	121	PHE	C-N-CA	5.80	126.36	120.38
3	D	97	ASN	CB-CA-C	-5.72	109.97	116.54
1	A	105	SER	N-CA-C	-5.69	104.98	111.07
2	C	128	PHE	CA-C-N	5.69	125.88	120.31
2	C	128	PHE	C-N-CA	5.69	125.88	120.31
1	B	48	GLU	O-C-N	-5.66	116.12	122.12
3	Q	98	GLY	N-CA-C	5.64	121.17	111.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	131	ALA	CA-C-N	-5.59	112.86	119.84
2	P	131	ALA	C-N-CA	-5.59	112.86	119.84
2	C	102	VAL	CB-CA-C	-5.57	102.16	111.29
3	Q	97	ASN	N-CA-C	5.54	117.44	108.08
2	P	177	GLN	CA-C-N	-5.52	113.50	122.34
2	P	177	GLN	C-N-CA	-5.52	113.50	122.34
2	C	30	SER	N-CA-C	-5.37	107.10	113.97
3	D	139	ILE	N-CA-C	5.36	115.76	107.78
1	A	92	HIS	N-CA-C	5.32	122.14	110.80
3	D	131	ASN	N-CA-C	5.26	122.01	110.80
2	P	167	SER	N-CA-C	-5.24	102.77	110.42
3	D	52	ASN	CB-CA-C	-5.24	103.36	109.80
1	B	51	ALA	N-CA-CB	5.19	117.53	110.01
3	Q	192	ARG	NE-CZ-NH2	5.16	123.84	119.20
2	C	152	PHE	CA-C-N	-5.15	114.64	119.89
2	C	152	PHE	C-N-CA	-5.15	114.64	119.89
3	D	67	ASN	N-CA-C	5.12	121.72	110.80
3	D	154	ASP	N-CA-C	-5.07	107.07	113.20
3	Q	110	LEU	N-CA-C	5.06	116.95	107.99

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	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	727	0	641	152	0
2	C	1512	0	1488	174	0
2	P	1518	0	1491	98	0
3	D	1570	0	1513	195	0
3	Q	1566	0	1508	153	0
All	All	7635	0	7297	774	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 52.

All (774) 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:CB	3:Q:196:CYS:SG	2.04	1.46
1:B:70:CYS:SG	1:B:70:CYS:CB	2.03	1.46
3:Q:173:ASN:O	3:Q:174:LYS:HG3	1.28	1.29
3:Q:207:LYS:NZ	3:Q:207:LYS:HB3	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
2:C:107:ASP:CG	2:C:108:TYR:HD1	1.59	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:107:ASP:CG	2:C:108:TYR:CD1	2.32	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
3:D:1:SER:HB2	3:D:2:TYR:C	1.79	1.06
2:C:33:ALA:HB2	2:C:52:ILE:HG13	1.15	1.06
2:C:207:LYS:HG3	2:C:208:PRO:HD3	1.39	1.04
2:C:146:CYS:HB2	2:C:202:CYS:SG	1.99	1.02
3:Q:207:LYS:HZ2	3:Q:207:LYS:CB	1.73	1.02
2:P:92:ALA:O	2:P:114:LEU:HD12	1.57	1.01
2:C:3:GLN:HG3	2:C:4:LEU:CD1	1.90	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:53:ASN:CG	3:Q:65:GLY:H	1.73	0.95
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
3:Q:207:LYS:HB3	3:Q:207:LYS:HZ2	0.79	0.94
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
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:156:SER:O	3:Q:157:PRO:C	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
2:P:47:TRP:CZ3	3:Q:98:GLY:HA3	2.10	0.87
3:Q:118:VAL:CG2	3:Q:207:LYS:HE2	2.04	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:A:71:TRP:HH2	1:A:99:VAL:CG1	1.89	0.86
1:B:82:ALA:O	1:B:99:VAL:HG13	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:PRO:HG3	1:B:60:ALA:HB3	1.60	0.84
3:D:67:ASN:O	3:D:68:SER:OG	1.95	0.84
2:C:146:CYS:HG	2:C:202:CYS:HG	1.14	0.84
3:D:123:PRO:HB3	3:D:133:ALA:HB1	1.57	0.84
2:C:89:GLU:N	2:C:89:GLU:OE1	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
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:A:39:TRP:CZ3	1:A:43:ARG:HD3	2.14	0.80
1:B:68:TYR:HE1	2:C:100:PRO:CA	1.94	0.80
2:C:74:GLU:N	2:C:74:GLU:OE1	2.14	0.80
2:P:91:THR:HG22	2:P:117:VAL:H	1.45	0.80
2:P:92:ALA:O	2:P:114:LEU:CD1	2.29	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:Q:173:ASN:C	3:Q:174:LYS:HG3	2.08	0.78
3:D:32:ASN:OD1	3:D:33:THR:N	2.14	0.78
3:Q:154:ASP:CG	3:Q:155:SER:H	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:102:GLN:O	1:B:111:LEU:CG	2.36	0.74
3:D:6:GLN:CB	3:D:7:PRO:CD	2.65	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:NZ	3:Q:207:LYS:CB	2.30	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:A:116:THR:HG23	1:A:117:GLN:H	1.55	0.72
1:B:71:TRP:CH2	1:B:101:ARG:NH1	2.57	0.72
3:Q:212:THR:HG22	3:Q:213:GLU:H	1.54	0.72
3:D:96:LEU:C	3:D:97:ASN:OD1	2.32	0.72
3:D:4:LEU:HD11	3:D:23:SER:OG	1.88	0.72
3:D:116:PRO:HG2	3:D:207:LYS:HE3	1.70	0.72
1:B:108:GLN:HG2	1:B:109:TRP:H	1.54	0.72
2:C:29:PHE:CD1	2:C:29:PHE:C	2.68	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:A:101:ARG:HH21	1:A:109:TRP:HB3	1.54	0.70
1:B:40:GLU:OE2	3:D:33:THR:HG21	1.91	0.70
2:P:67:ARG:NH2	2:P:90:ASP:OD2	2.25	0.70
3:D:111:GLN:HB3	3:D:112:PRO:HD2	1.71	0.70
3:D:131:ASN:HA	3:D:185:PRO:HG2	1.72	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:SG	1:B:70:CYS:CA	2.80	0.70
3:D:95:SER:OG	3:D:96:LEU:HG	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:P:131:ALA:HB2	2:P:144:LEU:HA	1.73	0.69
3:D:135:LEU:HD11	3:D:194:TYR:CD2	2.27	0.69
3:D:169:LYS:O	3:D:170:GLN:NE2	2.26	0.69
2:C:22:CYS:CB	2:C:96:CYS:SG	2.80	0.69
1:B:40:GLU:OE2	3:D:33:THR:CG2	2.41	0.69
1:B:112:TRP:HE3	1:B:113:ARG:N	1.91	0.69
2:P:145:GLY:HA2	2:P:160:TRP:HH2	1.58	0.69
3:Q:155:SER:O	3:Q:157:PRO:HD3	1.92	0.69
3:Q:162:VAL:HG23	3:Q:163:GLU:N	2.07	0.69
3:D:142:PHE:HE2	3:D:200:HIS:CE1	2.11	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
3:Q:97:ASN:CG	3:Q:98:GLY:H	2.01	0.68
1:B:115:HIS:HB2	1:B:118:CYS:HB2	1.76	0.68
1:B:112:TRP:CE3	1:B:112:TRP:C	2.72	0.68
3:D:121:PHE:CD2	2:C:130:LEU:HB3	2.28	0.68
2:C:74:GLU:H	2:C:74:GLU:CD	2.01	0.68
1:A:111:LEU:HD12	1:A:112:TRP:HB3	1.76	0.67
1:B:90:TRP:CE3	1:B:90:TRP:O	2.48	0.67
3:D:134:THR:HG21	2:C:149:LYS:HE2	1.76	0.67
3:D:142:PHE:HE1	3:D:176:ALA:HB2	1.57	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: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
1:B:102:GLN:O	1:B:111:LEU:HG	1.95	0.67
2:P:131:ALA:HB1	2:P:133:SER:OG	1.94	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
3:Q:154:ASP:CG	3:Q:155:SER:N	2.52	0.66
1:A:94:VAL:HB	1:A:117:GLN:O	1.95	0.66
1:B:38:ARG:HE	1:B:86:TRP:HH2	1.42	0.66
1:B:84:CYS:SG	1:B:97:GLY:C	2.79	0.66
2:C:3:GLN:CG	2:C:4:LEU:CD1	2.70	0.66
3:D:138:LEU:HB3	2:C:172:PHE:CZ	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:P:211:THR:C	2:P:212:LYS:HD3	2.21	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: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:110:GLY:C	1:B:111:LEU:HD22	2.22	0.64
1:B:66:ASP:OD1	1:B:69:VAL:N	2.30	0.64
2:P:91:THR:HG22	2:P:117:VAL:N	2.11	0.64
3:D:167:PRO:HA	3:D:177:ALA:HB2	1.80	0.64
3:D:143:TYR:CD1	3:D:144:PRO:HA	2.33	0.64
2:C:22:CYS:CB	2:C:96:CYS:HG	2.09	0.64
3:D:127:GLU:O	3:D:130:ALA:HB3	1.98	0.63
3:Q:169:LYS:HB2	3:Q:175:TYR:CE1	2.33	0.63
1:B:120:ASN:HB3	1:B:121:PRO:CD	2.29	0.63
3:D:184:THR:H	3:D:187:GLN:NE2	1.96	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
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:Q:3:VAL:O	3:Q:102:GLY:HA2	1.99	0.63
3:D:86:ASP:HA	3:D:105:THR:O	1.98	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
2:C:163:GLY:C	2:C:165:LEU:H	2.07	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:OE1	3:D:6:GLN:HA	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
1:B:101:ARG:HD2	1:B:113:ARG:CZ	2.30	0.62
3:Q:53:ASN:OD1	3:Q:64:SER:HA	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:134:THR:HG22	3:D:182:SER:HA	1.81	0.62
3:Q:212:THR:CG2	3:Q:213:GLU:H	2.12	0.62
2:C:107:ASP:CG	2:C:108:TYR:CE1	2.75	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:6:GLN:HE22	2:C:95:TYR:HA	1.65	0.62
2:C:59:ASN:OD1	2:C:102:VAL:HG11	1.99	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
2:C:73:ASP:HB3	2:C:76:THR:OG1	1.99	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
3:D:164:THR:HG22	3:D:165:THR:N	2.15	0.61
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:28:THR:O	2:C:30:SER:N	2.34	0.60
2:P:131:ALA:C	2:P:133:SER:N	2.56	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
3:D:154:ASP:C	3:D:156:SER:H	2.07	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
2:P:156:VAL:HG23	2:P:184:LEU:HD21	1.83	0.60
2:C:48:MET:HE1	2:C:94:TYR:HD2	1.67	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:143:TYR:O	3:D:200:HIS:NE2	2.28	0.59
3:D:162:VAL:CG2	3:D:181:LEU:HD12	2.25	0.59
1:A:116:THR:O	1:A:119:GLU:N	2.31	0.59
1:B:89:PRO:O	1:B:90:TRP:CG	2.56	0.59
3:D:130:ALA:O	3:D:131:ASN:CB	2.50	0.59
2:C:153:PRO:HD2	2:C:208:PRO:HG2	1.83	0.59
2:C:100:PRO:O	2:C:101:ILE:HG23	2.03	0.59
3:Q:6:GLN:H	3:Q:7:PRO:HD2	1.65	0.59
3:D:152:LYS:HB3	3:D:155:SER:HA	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:110:LEU:HD12	3:D:110:LEU:N	2.18	0.59
1:B:31:THR:O	1:B:35:LEU:HD13	2.02	0.59
3:Q:25:SER:H	3:Q:28:ASN:HD21	1.51	0.59
1:A:115:HIS:HD2	1:A:119:GLU:OE2	1.86	0.59
3:Q:206:GLU:OE1	3:Q:206:GLU:HA	2.02	0.59
3:D:98:GLY:HA3	2:C:47:TRP:CZ3	2.37	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
3:Q:92:TRP:CZ3	3:Q:98:GLY:HA2	2.38	0.58
2:C:3:GLN:CG	2:C:4:LEU:HD12	2.16	0.58
1:A:116:THR:HG23	1:A:117:GLN:N	2.17	0.58
2:P:101:ILE:CG2	2:P:102:VAL:N	2.66	0.58
2:C:60:TYR:HE1	2:C:70:ILE:HD12	1.66	0.58
2:P:64:PHE:HB3	2:P:68:VAL:HG23	1.84	0.58
1:A:90:TRP:HE1	1:A:119:GLU:HA	1.69	0.58
1:B:86:TRP:CE3	1:B:87:TYR:HA	2.35	0.58
3:Q:173:ASN:O	3:Q:174:LYS:HG2	1.97	0.58
3:D:4:LEU:HD12	3:D:4:LEU:C	2.29	0.58
3:D:156:SER:CB	3:D:157:PRO:HD3	2.16	0.58
2:C:64:PHE:O	2:C:65:GLN:HG2	2.04	0.58
2:C:160:TRP:HB3	2:C:165:LEU:CD2	2.34	0.58
1:B:62:ASN:OD1	1:B:63:GLY:O	2.22	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
3:Q:39:GLN:O	3:Q:85:ALA:HB1	2.04	0.57
3:Q:148:THR:OG1	3:Q:199:THR:HG23	2.04	0.57
2:C:199:THR:O	2:C:200:TYR:CD1	2.57	0.57
1:B:41:ARG:O	1:B:44:ARG:CG	2.51	0.57
1:B:109:TRP:O	1:B:109:TRP:CE3	2.57	0.57
2:P:175:VAL:HG12	2:P:183:SER:O	2.03	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
3:D:213:GLU:HA	3:D:213:GLU:OE1	2.05	0.57
2:C:28:THR:O	2:C:29:PHE:CD2	2.57	0.57
3:Q:168:SER:OG	3:Q:170:GLN:OE1	2.22	0.57
3:D:120:LEU:HD23	3:D:209:VAL:HG12	1.85	0.57
3:D:139:ILE:HG22	3:D:176:ALA:HB3	1.86	0.57
2:P:32:TYR:HB3	2:P:99:GLY:O	2.05	0.57
3:Q:168:SER:O	3:Q:175:TYR:HA	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:P:166:THR:O	2:P:167:SER:C	2.47	0.56
1:B:120:ASN:O	1:B:121:PRO:C	2.48	0.56
2:P:34:ILE:HD12	2:P:53:PRO:HG3	1.88	0.56
2:P:131:ALA:H	3:Q:121:PHE:HD2	1.53	0.56
3:D:114:ALA:HB3	3:D:142:PHE:HA	1.87	0.56
3:D:137:CYS:CB	3:D:196:CYS:HG	2.16	0.56
3:D:139:ILE:HG22	3:D:176:ALA:CB	2.36	0.56
2:C:28:THR:C	2:C:29:PHE:CD2	2.84	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
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
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:142:PHE:CD2	3:D:143:TYR:N	2.74	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:88:LEU:HD11	1:B:90:TRP:CE2	2.39	0.55
1:B:89:PRO:O	1:B:90:TRP:CD1	2.59	0.55
1:B:115:HIS:CB	1:B:118:CYS:HB2	2.37	0.55
3:Q:4:LEU:HD12	3:Q:4:LEU:O	2.06	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
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
1:B:86:TRP:CE3	1:B:86:TRP:C	2.85	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
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
2:C:125:PRO:HD2	2:C:211:THR:HG21	1.88	0.55
1:B:69:VAL:HG11	1:B:99:VAL:HG11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:Q:7:PRO:O	3:Q:105:THR:OG1	2.24	0.54
2:P:29:PHE:CZ	2:P:53:PRO:HB3	2.42	0.54
2:P:205:ASN:OD1	2:P:212:LYS:HE3	2.06	0.54
3:D:120:LEU:HD23	3:D:211:PRO:HD3	1.90	0.54
2:C:209:SER:HB3	2:C:211:THR:CG2	2.37	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:17:ARG:NH2	3:D:75:ALA:HB1	2.23	0.54
3:D:159:LYS:HD2	3:D:160:ALA:N	2.23	0.54
2:C:184:LEU:C	2:C:184:LEU:HD23	2.32	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
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
2:P:70:ILE:HG12	2:P:81:MET:SD	2.48	0.53
3:Q:92:TRP:CH2	3:Q:98:GLY:HA2	2.43	0.53
1:A:113:ARG:HD2	1:A:115:HIS:HE1	1.73	0.53
3:D:6:GLN:HB2	3:D:7:PRO:CD	2.33	0.53
2:C:190:VAL:CG2	2:C:191:PRO:HD2	2.38	0.53
2:C:28:THR:C	2:C:29:PHE:CG	2.86	0.53
3:D:14:PRO:HG3	3:D:109:VAL:HG13	1.91	0.53
1:A:92:HIS:CE1	1:A:93:HIS:CE1	2.96	0.53
3:D:154:ASP:O	3:D:155:SER:HB2	2.07	0.53
2:C:25:SER:O	2:C:29:PHE:HD2	1.90	0.53
3:Q:120:LEU:HD13	3:Q:137:CYS:HB2	1.91	0.53
3:Q:128:LEU:HD21	3:Q:188:TRP:CD1	2.44	0.53
3:D:130:ALA:O	3:D:131:ASN:HB2	2.08	0.53
2:P:87:ARG:HG2	2:P:89:GLU:H	1.73	0.53
1:B:115:HIS:HE1	2:C:32:TYR:CZ	2.27	0.53
3:Q:120:LEU:HD22	3:Q:196:CYS:HB2	1.89	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
1:B:44:ARG:O	1:B:45:GLU:C	2.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ARG:NH1	1:B:113:ARG:HE	2.06	0.52
1:B:102:GLN:H	1:B:111:LEU:HD12	1.74	0.52
3:Q:196:CYS:SG	3:Q:196:CYS:CA	2.93	0.52
3:D:23:SER:HA	3:D:71:SER:HB2	1.91	0.52
2:C:73:ASP:O	2:C:76:THR:OG1	2.27	0.52
1:B:112:TRP:HZ3	1:B:114:ASP:CG	2.17	0.52
3:Q:120:LEU:HD22	3:Q:196:CYS:CB	2.39	0.52
3:D:67:ASN:CG	3:D:69:GLY:H	2.17	0.52
2:P:205:ASN:OD1	2:P:205:ASN:C	2.52	0.52
1:B:68:TYR:CE1	2:C:100:PRO:N	2.78	0.52
2:P:104:ALA:HB1	2:P:105:PRO:HD2	1.91	0.52
3:Q:192:ARG:O	3:Q:212:THR:HG23	2.09	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:D:159:LYS:HD2	3:D:160:ALA:H	1.74	0.52
3:D:188:TRP:HE3	3:D:194:TYR:CE2	2.28	0.52
2:C:81:MET:HE3	2:C:83:LEU:HB2	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
1:B:66:ASP:CG	1:B:69:VAL:H	2.18	0.52
3:Q:13:THR:HG22	3:Q:110:LEU:HD12	1.92	0.52
3:Q:142:PHE:HE1	3:Q:176:ALA:HA	1.74	0.52
2:C:100:PRO:O	2:C:101:ILE:CG2	2.58	0.52
1:B:111:LEU:N	1:B:111:LEU:CD2	2.72	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:107:ASP:CG	2:C:108:TYR:H	2.15	0.52
2:P:184:LEU:C	2:P:184:LEU:HD12	2.35	0.51
1:B:88:LEU:HD12	1:B:88:LEU:C	2.35	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
2:P:30:SER:HB3	2:P:54:THR:OG1	2.11	0.51
3:Q:118:VAL:HG11	3:Q:198:VAL:HG21	1.92	0.51
1:B:97:GLY:CA	1:B:117:GLN:HG2	2.40	0.51
3:Q:3:VAL:HG22	3:Q:101:PHE:O	2.10	0.51
3:Q:53:ASN:HB2	3:Q:65:GLY:CA	2.41	0.51
3:D:62:ARG:O	3:D:63:PHE:CE2	2.60	0.51
3:D:143:TYR:CD1	3:D:144:PRO:CA	2.92	0.51
1:A:89:PRO:O	1:A:90:TRP:CD2	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:33:GLY:O	1:A:37:GLN:HG2	2.11	0.51
2:P:211:THR:O	2:P:212:LYS:HD3	2.10	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
1:B:100:LEU:C	1:B:100:LEU:HD12	2.36	0.50
2:P:7:SER:HB3	2:P:21:SER:H	1.75	0.50
3:D:142:PHE:CE2	3:D:200:HIS:CE1	2.95	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
3:D:163:GLU:N	3:D:163:GLU:OE1	2.44	0.50
2:C:28:THR:C	2:C:30:SER:H	2.18	0.50
2:C:64:PHE:C	2:C:65:GLN:HG2	2.36	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:38:GLN:HB2	3:D:48:LEU:HD13	1.92	0.50
3:D:138:LEU:CD1	2:C:187:VAL:HG21	2.41	0.50
1:B:66:ASP:OD1	1:B:66:ASP:C	2.53	0.50
1:B:115:HIS:HE1	2:C:32:TYR:CE1	2.29	0.50
1:B:120:ASN:ND2	2:C:54:THR:HG21	2.26	0.50
2:P:157:THR:CB	2:C:210:ASN:HD21	2.25	0.50
3:Q:162:VAL:CG2	3:Q:163:GLU:N	2.75	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: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
2:C:38:ARG:HB3	2:C:48:MET:HE2	1.93	0.50
3:Q:62:ARG:HD2	3:Q:78:ARG:O	2.12	0.49
3:D:130:ALA:O	3:D:131:ASN:OD1	2.30	0.49
1:B:34:GLU:OE1	1:B:34:GLU:N	2.40	0.49
1:B:109:TRP:O	1:B:109:TRP:HE3	1.93	0.49
2:P:47:TRP:CD2	3:Q:99:VAL:HG12	2.47	0.49
3:Q:88:TYR:CD1	3:Q:104:GLY:HA3	2.47	0.49
3:Q:155:SER:C	3:Q:157:PRO:HD3	2.37	0.49
2:C:76:THR:O	2:C:77:SER:HB2	2.11	0.49
1:A:31:THR:CG2	1:A:34:GLU:HG3	2.40	0.49
1:B:68:TYR:CE1	2:C:100:PRO:HB3	2.47	0.49
1:B:90:TRP:HH2	1:B:118:CYS:O	1.95	0.49
1:B:101:ARG:NH1	1:B:113:ARG:NE	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:3:VAL:HB	3:D:23:SER:O	2.13	0.49
2:C:100:PRO:C	2:C:101:ILE:HG23	2.37	0.49
1:A:82:ALA:O	1:A:98:PHE:HA	2.13	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:56:PRO:HG3	1:A:60:ALA:HB3	1.95	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:B:86:TRP:CE3	1:B:86:TRP:O	2.66	0.49
2:P:157:THR:HA	2:C:210:ASN:HD21	1.77	0.49
2:C:11:VAL:O	2:C:12:LYS:HD2	2.11	0.49
1:B:62:ASN:OD1	1:B:62:ASN:C	2.56	0.48
2:P:38:ARG:NH1	2:P:90:ASP:OD1	2.31	0.48
2:C:107:ASP:OD1	2:C:108:TYR:CD1	2.43	0.48
2:P:10:GLU:HG2	2:P:18:VAL:HG21	1.95	0.48
2:P:130:LEU:HB2	2:P:145:GLY:O	2.13	0.48
3:Q:80:GLN:O	3:Q:109:VAL:HG21	2.13	0.48
2:C:47:TRP:CE2	2:C:49:GLY:HA2	2.48	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:P:101:ILE:CG2	2:P:102:VAL:H	2.24	0.48
3:D:138:LEU:HD22	2:C:172:PHE:CD1	2.48	0.48
2:P:101:ILE:HG22	2:P:102:VAL:N	2.28	0.48
2:P:173:PRO:HD3	3:Q:170:GLN:OE1	2.13	0.48
2:C:67:ARG:HH21	2:C:83:LEU:HD11	1.79	0.48
2:P:62:GLN:O	2:P:63:LYS:CB	2.62	0.48
1:A:87:TYR:CD1	1:A:87:TYR:C	2.91	0.48
3:Q:143:TYR:HA	3:Q:144:PRO:C	2.39	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
3:Q:53:ASN:HB2	3:Q:65:GLY:HA3	1.94	0.48
1:B:90:TRP:O	1:B:90:TRP:HE3	1.92	0.48
1:B:101:ARG:HH11	1:B:113:ARG:CZ	2.27	0.48
3:Q:111:GLN:HB2	3:Q:112:PRO:CD	2.37	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
1:B:120:ASN:ND2	2:C:54:THR:CG2	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Q:143:TYR:CG	3:Q:144:PRO:HA	2.48	0.47
3:D:127:GLU:OE2	3:D:134:THR:N	2.47	0.47
1:B:66:ASP:OD1	1:B:68:TYR:N	2.32	0.47
2:P:175:VAL:HB	3:Q:165:THR:HG22	1.95	0.47
3:D:4:LEU:CD1	3:D:23:SER:OG	2.58	0.47
3:Q:142:PHE:O	3:Q:142:PHE:CD2	2.68	0.47
3:D:4:LEU:HD11	3:D:23:SER:HG	1.78	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:88:TYR:CE1	3:Q:104:GLY:HA3	2.49	0.47
3:Q:118:VAL:HA	3:Q:138:LEU:O	2.13	0.47
3:D:165:THR:CG2	3:D:178:SER:H	2.28	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
3:Q:172:ASN:C	3:Q:173:ASN:HD22	2.23	0.47
2:C:23:LYS:HG3	2:C:24:ALA:H	1.80	0.47
1:B:42:TYR:CD1	1:B:42:TYR:C	2.93	0.46
3:Q:109:VAL:C	3:Q:110:LEU:HD23	2.41	0.46
3:D:114:ALA:CB	3:D:174:LYS:HE3	2.35	0.46
3:D:141:ASP:OD1	3:D:141:ASP:O	2.32	0.46
1:B:117:GLN:O	1:B:117:GLN:HG3	2.14	0.46
3:Q:131:ASN:HA	3:Q:185:PRO:HG2	1.97	0.46
2:C:108:TYR:HD1	2:C:108:TYR:H	1.62	0.46
1:A:115:HIS:CE1	2:P:32:TYR:HH	2.33	0.46
1:B:50:LEU:HA	1:B:53:ALA:CB	2.46	0.46
1:B:112:TRP:CZ3	1:B:114:ASP:HB3	2.51	0.46
2:P:205:ASN:HA	2:P:212:LYS:HD2	1.98	0.46
3:D:46:LYS:HE2	3:D:48:LEU:HD12	1.96	0.46
2:C:59:ASN:OD1	2:C:102:VAL:HG21	2.15	0.46
1:A:43:ARG:CZ	3:Q:51:SER:CB	2.91	0.46
1:B:115:HIS:NE2	2:C:28:THR:HA	2.30	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
1:B:120:ASN:CB	1:B:121:PRO:CD	2.93	0.46
3:Q:118:VAL:CG2	3:Q:207:LYS:CE	2.83	0.46
3:D:130:ALA:O	3:D:131:ASN:CG	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:171:SER:C	3:D:175:TYR:HE2	2.23	0.46
3:Q:67:ASN:O	3:Q:68:SER:CB	2.64	0.46
3:Q:118:VAL:HG21	3:Q:207:LYS:HZ1	1.79	0.46
2:C:46:GLU:OE2	2:C:63:LYS:NZ	2.30	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
3:D:5:THR:HG23	3:D:5:THR:O	2.15	0.45
3:D:60:PRO:O	3:D:61:ASP:C	2.57	0.45
2:C:34:ILE:HD11	2:C:51:ILE:HG22	1.98	0.45
2:C:91:THR:HG23	2:C:116:THR:HA	1.97	0.45
1:B:112:TRP:CE3	1:B:113:ARG:C	2.94	0.45
3:D:20:ILE:HG12	3:D:105:THR:HG21	1.98	0.45
3:D:172:ASN:HB2	3:D:175:TYR:CD2	2.51	0.45
2:P:160:TRP:CZ3	2:P:202:CYS:HB3	2.51	0.45
3:Q:106:LYS:O	3:Q:106:LYS:HG3	2.16	0.45
3:D:201:GLU:H	3:D:201:GLU:CD	2.24	0.45
2:C:125:PRO:HD3	2:C:206:HIS:HD2	1.81	0.45
2:P:144:LEU:HD12	2:P:145:GLY:N	2.32	0.45
3:Q:27:SER:HB3	3:Q:95:SER:H	1.82	0.45
3:D:135:LEU:HD11	3:D:194:TYR:HD2	1.77	0.45
2:C:24:ALA:HB1	2:C:29:PHE:CB	2.46	0.45
2:P:105:PRO:HG3	3:Q:50:TYR:HB2	1.98	0.45
3:D:153:ALA:O	3:D:194:TYR:CD1	2.68	0.45
1:B:90:TRP:CE3	1:B:120:ASN:OD1	2.70	0.45
3:D:199:THR:HG23	3:D:206:GLU:OE1	2.17	0.45
2:C:29:PHE:O	2:C:53:PRO:HG2	2.17	0.45
3:Q:172:ASN:C	3:Q:173:ASN:ND2	2.75	0.45
3:D:1:SER:CB	3:D:2:TYR:C	2.70	0.45
1:B:67:MET:HE3	2:C:105:PRO:HG2	1.98	0.45
3:Q:60:PRO:HG2	3:Q:63:PHE:HE1	1.82	0.45
3:D:8:PRO:O	3:D:106:LYS:N	2.49	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:205:ASN:OD1	2:C:205:ASN:C	2.59	0.45
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
1:A:115:HIS:HB3	1:A:119:GLU:OE1	2.17	0.44
2:P:97:ALA:HB1	2:P:106:THR:HB	1.99	0.44
3:Q:52:ASN:O	3:Q:53:ASN:HB3	2.16	0.44
3:Q:79:LEU:HD12	3:Q:80:GLN:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:25:SER:O	2:C:29:PHE:CD2	2.70	0.44
1:B:90:TRP:CZ2	1:B:120:ASN:OD1	2.70	0.44
2:P:216:ARG:HG2	2:P:217:VAL:H	1.82	0.44
3:Q:13:THR:O	3:Q:16:GLN:HG2	2.17	0.44
3:D:120:LEU:HD12	3:D:121:PHE:N	2.32	0.44
2:C:3:GLN:CG	2:C:4:LEU:HD13	2.46	0.44
2:C:209:SER:C	2:C:210:ASN:OD1	2.60	0.44
2:P:44:GLY:HA2	3:Q:88:TYR:CE1	2.52	0.44
3:D:32:ASN:CG	3:D:33:THR:H	2.17	0.44
2:C:151:TYR:CE1	2:C:182:TYR:HB2	2.53	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
1:A:105:SER:OG	1:A:106:ASP:N	2.51	0.44
3:Q:49:ILE:HD12	3:Q:74:LEU:CD1	2.48	0.44
3:Q:85:ALA:O	3:Q:106:LYS:HA	2.17	0.44
3:D:142:PHE:CZ	3:D:147:VAL:HB	2.50	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:A:42:TYR:CG	1:A:87:TYR:HD2	2.36	0.44
1:B:102:GLN:O	1:B:111:LEU:HD21	2.18	0.44
1:A:89:PRO:O	1:A:90:TRP:CG	2.71	0.44
1:B:120:ASN:HD22	2:C:54:THR:CG2	2.31	0.44
3:Q:25:SER:H	3:Q:28:ASN:ND2	2.15	0.44
3:D:50:TYR:CG	3:D:51:SER:N	2.82	0.44
1:A:90:TRP:HZ2	1:A:119:GLU:CG	2.31	0.43
1:B:110:GLY:C	1:B:111:LEU:CD2	2.91	0.43
1:B:112:TRP:HE3	1:B:113:ARG:C	2.26	0.43
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: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
3:D:116:PRO:HG2	3:D:207:LYS:CE	2.43	0.43
3:D:184:THR:HG23	3:D:187:GLN:HE22	1.84	0.43
2:P:87:ARG:HE	2:P:87:ARG:HB2	1.54	0.43
2:P:125:PRO:HB3	2:P:151:TYR:HB3	2.00	0.43
2:P:130:LEU:HB3	3:Q:121:PHE:CD2	2.54	0.43
3:Q:48:LEU:HD21	3:Q:63:PHE:CD2	2.53	0.43
2:C:3:GLN:HG3	2:C:4:LEU:HD13	1.91	0.43
1:A:101:ARG:HH21	1:A:109:TRP:CB	2.25	0.43
2:P:203:ASN:CG	2:P:214:ASP:OD1	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:132:LYS:CA	3:D:185:PRO:HD3	2.48	0.43
2:C:83:LEU:HD21	2:C:90:ASP:OD2	2.19	0.43
1:A:34:GLU:O	1:A:38:ARG:HG3	2.19	0.43
1:B:112:TRP:C	1:B:112:TRP:CD2	2.95	0.43
3:Q:118:VAL:HG11	3:Q:198:VAL:CG2	2.49	0.43
3:Q:123:PRO:HD3	3:Q:135:LEU:HD12	2.01	0.43
3:Q:144:PRO:HG2	3:Q:201:GLU:OE2	2.18	0.43
1:A:101:ARG:NH2	1:A:109:TRP:HB3	2.29	0.43
1:B:82:ALA:HB3	1:B:99:VAL:HG11	2.00	0.43
2:P:75:SER:C	2:P:77:SER:N	2.73	0.43
2:C:35:SER:O	2:C:96:CYS:HA	2.18	0.43
2:C:37:VAL:HG23	2:C:46:GLU:O	2.18	0.43
2:C:127:VAL:HG22	2:C:148:VAL:HG12	2.00	0.43
2:C:155:PRO:HD2	2:C:207:LYS:HE2	2.01	0.43
1:A:35:LEU:HD12	1:A:35:LEU:H	1.84	0.43
1:A:115:HIS:CE1	2:P:32:TYR:OH	2.72	0.43
1:B:112:TRP:CE3	1:B:113:ARG:N	2.77	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
2:P:158:VAL:HG11	2:P:186:SER:OG	2.19	0.43
3:Q:13:THR:OG1	3:Q:16:GLN:OE1	2.33	0.43
3:D:38:GLN:O	3:D:46:LYS:HB3	2.19	0.43
3:D:187:GLN:H	3:D:187:GLN:CD	2.25	0.43
2:C:3:GLN:OE1	2:C:4:LEU:CD1	2.67	0.43
1:B:112:TRP:CZ3	1:B:114:ASP:CG	2.95	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
3:D:137:CYS:HB2	3:D:196:CYS:SG	2.58	0.43
1:A:71:TRP:CH2	1:A:99:VAL:HG11	2.52	0.43
1:B:98:PHE:HB3	1:B:99:VAL:H	1.28	0.43
3:Q:81:SER:O	3:Q:84:GLU:HG2	2.19	0.43
3:Q:96:LEU:O	3:Q:97:ASN:CG	2.61	0.43
3:Q:199:THR:HB	3:Q:206:GLU:CD	2.44	0.43
3:D:212:THR:O	3:D:213:GLU:HB2	2.19	0.42
2:C:13:LYS:O	2:C:16:SER:OG	2.36	0.42
1:B:68:TYR:CE1	2:C:100:PRO:CB	3.02	0.42
1:B:88:LEU:HD13	1:B:90:TRP:CD1	2.52	0.42
2:P:67:ARG:NH2	2:P:90:ASP:CG	2.76	0.42
3:D:127:GLU:HG2	3:D:133:ALA:HA	2.00	0.42
3:D:151:TRP:O	3:D:158:VAL:HG12	2.18	0.42
3:D:183:LEU:CD1	3:D:187:GLN:HE21	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:P:70:ILE:HG12	2:P:81:MET:HG3	2.01	0.42
3:D:191:HIS:ND1	3:D:194:TYR:CE1	2.88	0.42
3:D:128:LEU:O	3:D:131:ASN:N	2.51	0.42
3:D:163:GLU:O	3:D:163:GLU:HG2	2.20	0.42
3:D:206:GLU:C	3:D:207:LYS:HG2	2.45	0.42
1:B:41:ARG:HG2	1:B:44:ARG:NH1	2.35	0.42
1:B:54:GLU:HA	1:B:55:PRO:HD3	1.82	0.42
1:B:112:TRP:HZ3	1:B:114:ASP:HB3	1.83	0.42
2:C:48:MET:SD	2:C:81:MET:HE2	2.60	0.42
1:A:92:HIS:CE1	1:A:93:HIS:ND1	2.87	0.42
1:B:101:ARG:CD	1:B:113:ARG:CZ	2.97	0.42
3:Q:49:ILE:CG2	3:Q:53:ASN:HA	2.50	0.42
3:D:84:GLU:HG2	3:D:107:VAL:O	2.19	0.42
2:C:28:THR:CG2	2:C:29:PHE:N	2.49	0.42
2:C:68:VAL:HA	2:C:82:GLU:O	2.20	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
1:A:62:ASN:O	1:A:109:TRP:NE1	2.46	0.42
3:Q:153:ALA:HA	3:Q:194:TYR:CD1	2.55	0.42
3:D:6:GLN:N	3:D:7:PRO:HD2	2.35	0.42
2:C:81:MET:CE	2:C:83:LEU:HB2	2.49	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
1:B:102:GLN:O	1:B:111:LEU:CD2	2.68	0.42
2:P:41:PRO:HD3	2:P:92:ALA:HA	2.02	0.42
3:Q:92:TRP:HA	3:Q:99:VAL:HA	2.02	0.42
3:D:164:THR:CG2	3:D:165:THR:N	2.83	0.42
1:A:68:TYR:HD2	2:P:32:TYR:CE1	2.37	0.41
1:B:50:LEU:HA	1:B:53:ALA:HB3	2.01	0.41
1:B:71:TRP:CZ2	1:B:101:ARG:NH1	2.88	0.41
3:Q:60:PRO:HG2	3:Q:63:PHE:CE1	2.55	0.41
3:Q:61:ASP:C	3:Q:61:ASP:OD1	2.63	0.41
3:D:109:VAL:C	3:D:110:LEU:HD12	2.44	0.41
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
2:C:94:TYR:CE1	2:C:115:VAL:HB	2.54	0.41
3:Q:127:GLU:HG2	3:Q:132:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:TRP:CD1	1:A:86:TRP:C	2.97	0.41
1:B:68:TYR:HE1	2:C:100:PRO:CB	2.33	0.41
3:Q:3:VAL:O	3:Q:3:VAL:HG23	2.20	0.41
3:Q:66:SER:OG	3:Q:67:ASN:N	2.53	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:Q:154:ASP:HA	3:Q:193:SER:O	2.20	0.41
3:D:212:THR:OG1	3:D:213:GLU:N	2.53	0.41
2:C:203:ASN:HD22	2:C:214:ASP:CG	2.29	0.41
2:P:22:CYS:HB2	2:P:36:TRP:CH2	2.56	0.41
2:P:75:SER:C	2:P:77:SER:H	2.27	0.41
3:D:18:VAL:HG12	3:D:76:ILE:HG23	2.02	0.41
3:D:153:ALA:HA	3:D:194:TYR:CD1	2.55	0.41
2:C:28:THR:O	2:C:29:PHE:C	2.63	0.41
2:C:28:THR:C	2:C:30:SER:N	2.76	0.41
2:C:106:THR:OG1	2:C:109:TRP:NE1	2.54	0.41
2:C:206:HIS:HB3	2:C:211:THR:HG23	2.03	0.41
1:A:91:HIS:CG	1:A:92:HIS:H	2.39	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
2:C:34:ILE:CD1	2:C:51:ILE:HG22	2.50	0.41
2:C:39:GLN:C	2:C:92:ALA:HB1	2.46	0.41
1:A:111:LEU:CD1	1:A:112:TRP:HD1	2.32	0.41
1:B:101:ARG:HH11	1:B:113:ARG:NE	2.18	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
2:P:75:SER:O	2:P:77:SER:N	2.54	0.41
3:D:165:THR:OG1	3:D:166:THR:N	2.54	0.41
1:B:90:TRP:HZ3	1:B:94:VAL:CG1	2.34	0.41
3:Q:206:GLU:OE1	3:Q:206:GLU:CA	2.67	0.41
3:D:77:SER:O	3:D:78:ARG:C	2.63	0.41
2:C:24:ALA:HB1	2:C:29:PHE:CG	2.55	0.41
2:C:33:ALA:CB	2:C:101:ILE:HA	2.49	0.41
1:B:67:MET:HE2	2:C:105:PRO:O	2.20	0.40
3:D:35:HIS:CE1	2:C:105:PRO:HD3	2.56	0.40
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:P:175:VAL:HB	3:Q:165:THR:CG2	2.51	0.40
2:C:41:PRO:HD3	2:C:92:ALA:HA	2.03	0.40
1:A:90:TRP:O	1:A:90:TRP:CD1	2.73	0.40
1:A:91:HIS:CG	1:A:92:HIS:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:34:ILE:H	2:C:34:ILE:HG13	1.70	0.40
2:C:76:THR:HB	2:C:78:THR:OG1	2.21	0.40
2:P:160:TRP:CE2	2:P:188:VAL:HG13	2.57	0.40
3:D:154:ASP:HB3	3:D:157:PRO:HD3	2.03	0.40
2:C:18:VAL:CG1	2:C:86:LEU:HD11	2.45	0.40
2:P:144:LEU:HD13	2:P:217:VAL:HG11	2.04	0.40
3:Q:97:ASN:OD1	3:Q:97:ASN:C	2.61	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

5.3.1 Protein backbone

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%)	11	43
2	C	199/227 (88%)	175 (88%)	23 (12%)	1 (0%)	24	60
2	P	200/227 (88%)	187 (94%)	13 (6%)	0	100	100
3	D	207/215 (96%)	168 (81%)	38 (18%)	1 (0%)	24	60
3	Q	206/215 (96%)	185 (90%)	19 (9%)	2 (1%)	12	45
All	All	991/1156 (86%)	873 (88%)	113 (11%)	5 (0%)	24	60

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 ⓘ

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%)	70 (96%)	3 (4%)	27	61
1	B	71/113 (63%)	68 (96%)	3 (4%)	26	61
2	C	168/188 (89%)	158 (94%)	10 (6%)	17	50
2	P	169/188 (90%)	160 (95%)	9 (5%)	20	54
3	D	176/180 (98%)	166 (94%)	10 (6%)	18	52
3	Q	176/180 (98%)	169 (96%)	7 (4%)	28	62
All	All	833/962 (87%)	791 (95%)	42 (5%)	22	56

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	59	LEU
1	A	77	ASN
1	B	69	VAL
1	B	99	VAL
1	B	111	LEU
2	P	17	SER
2	P	37	VAL
2	P	51	ILE
2	P	63	LYS
2	P	80	TYR
2	P	179	SER
2	P	197	THR
2	P	203	ASN
2	P	205	ASN
3	Q	55	ARG
3	Q	70	THR
3	Q	136	VAL
3	Q	147	VAL
3	Q	162	VAL
3	Q	207	LYS
3	Q	208	THR

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Mol	Chain	Res	Type
3	D	6	GLN
3	D	35	HIS
3	D	48	LEU
3	D	82	GLU
3	D	99	VAL
3	D	119	THR
3	D	128	LEU
3	D	158	VAL
3	D	184	THR
3	D	206	GLU
2	C	37	VAL
2	C	63	LYS
2	C	68	VAL
2	C	81	MET
2	C	84	SER
2	C	88	SER
2	C	108	TYR
2	C	116	THR
2	C	184	LEU
2	C	211	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	HIS
1	A	92	HIS
1	A	115	HIS
1	B	93	HIS
1	B	115	HIS
1	B	120	ASN
2	P	98	GLN
2	P	177	GLN
3	Q	54	GLN
3	Q	173	ASN
3	Q	187	GLN
3	D	35	HIS
3	D	131	ASN
3	D	170	GLN
3	D	172	ASN
3	D	187	GLN
2	C	177	GLN
2	C	206	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Q	51:SER	C	52:ASN	N	1.63

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	92/136 (67%)	0.71	2 (2%) 62 39	28, 53, 71, 87	1 (1%)
1	B	91/136 (66%)	1.78	33 (36%) 1 1	23, 100, 129, 141	1 (1%)
2	C	205/227 (90%)	0.86	19 (9%) 14 7	33, 53, 77, 91	0
2	P	206/227 (90%)	0.31	8 (3%) 43 24	19, 30, 56, 76	0
3	D	211/215 (98%)	1.00	21 (9%) 12 7	22, 53, 67, 84	0
3	Q	210/215 (97%)	0.34	9 (4%) 40 21	16, 27, 40, 48	0
All	All	1015/1156 (87%)	0.74	92 (9%) 15 8	16, 45, 98, 141	2 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	6	GLN	5.5
3	D	5	THR	5.0
1	B	109	TRP	4.8
3	Q	6	GLN	4.5
1	B	105	SER	4.4
1	B	93	HIS	4.2
1	B	111	LEU	4.2
2	P	81	MET	4.2
1	B	96	ALA	4.2
1	B	83	SER	4.1
2	C	132	PRO	3.9
1	B	121	PRO	3.8
1	B	85	PRO	3.7
3	D	174	LYS	3.7
1	B	53	ALA	3.5
2	P	66	GLY	3.5
3	D	3	VAL	3.4
1	B	110	GLY	3.2
2	C	131	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	59	ASN	3.1
2	C	58	ALA	3.0
1	B	108	GLN	3.0
3	D	1	SER	3.0
3	D	52	ASN	3.0
2	C	197	THR	3.0
2	C	52	ILE	2.9
1	B	60	ALA	2.9
1	B	89	PRO	2.9
1	B	80	ALA	2.9
2	P	63	LYS	2.8
3	D	61	ASP	2.8
3	D	139	ILE	2.8
1	B	91	HIS	2.7
1	A	43	ARG	2.7
1	B	42	TYR	2.7
1	B	94	VAL	2.7
2	P	65	GLN	2.6
2	C	191	PRO	2.6
3	D	50	TYR	2.6
3	Q	68	SER	2.6
2	C	162	SER	2.6
2	C	55	PHE	2.6
3	D	68	SER	2.6
3	D	42	GLY	2.5
3	D	70	THR	2.5
1	B	46	CYS	2.5
3	Q	31	SER	2.5
3	D	153	ALA	2.5
1	B	77	ASN	2.5
2	C	51	ILE	2.5
2	C	43	GLN	2.5
2	C	72	ALA	2.4
2	C	104	ALA	2.4
2	C	210	ASN	2.4
3	D	97	ASN	2.3
1	B	72	ASP	2.3
1	B	102	GLN	2.3
1	B	57	SER	2.3
1	B	90	TRP	2.3
1	B	78	ALA	2.3
3	Q	67	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	P	64	PHE	2.3
3	Q	207	LYS	2.3
2	C	102	VAL	2.3
1	B	104	GLY	2.3
2	P	79	ALA	2.3
1	B	100	LEU	2.2
1	B	71	TRP	2.2
3	D	144	PRO	2.2
3	Q	212	THR	2.2
3	D	95	SER	2.2
2	C	50	GLY	2.2
3	D	170	GLN	2.2
1	B	52	ALA	2.2
2	C	152	PHE	2.2
2	C	209	SER	2.1
3	D	115	ALA	2.1
2	C	103	GLY	2.1
3	Q	97	ASN	2.1
3	Q	70	THR	2.1
1	B	87	TYR	2.1
1	B	95	ALA	2.1
3	D	158	VAL	2.1
1	B	43	ARG	2.1
1	B	82	ALA	2.1
2	P	16	SER	2.1
2	P	140	GLY	2.1
3	D	141	ASP	2.0
3	Q	69	GLY	2.0
3	D	201	GLU	2.0
1	A	91	HIS	2.0
1	B	50	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.