



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:55 AM UTC

PDB ID : 2A6K / pdb_00002a6k
Title : Crystal Structure Analysis of the germline antibody 36-65 Fab in complex with the dodecapeptide SLGDNLTNHNLRL
Authors : Sethi, D.K.; Agarwal, A.; Manivel, V.; Rao, K.V.; Salunke, D.M.
Deposited on : 2005-07-03
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

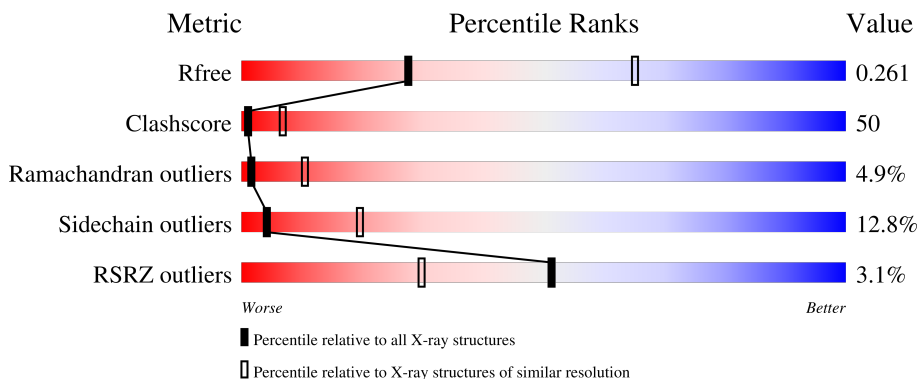
1 Overall quality at a glance

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	214	2% 34% 53% 14%
1	L	214	4% 40% 46% 13%
2	B	222	3% 36% 50% 11%
2	H	222	3% 36% 48% 12%
3	P	12	8% 25% 33% 25% 17%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6764 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 Germline antibody 36-65 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1651	1021	283	340	7			
1	L	214	Total	C	N	O	S	0	0	0
			1658	1024	283	344	7			

- Molecule 2 is a protein called Germline antibody 36-65 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1634	1036	267	324	7			
2	H	216	Total	C	N	O	S	0	0	0
			1637	1039	267	324	7			

- Molecule 3 is a protein called DODECAPEPTIDE: SLGDNLTNHNLR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	0	0	0
			81	46	18	17			

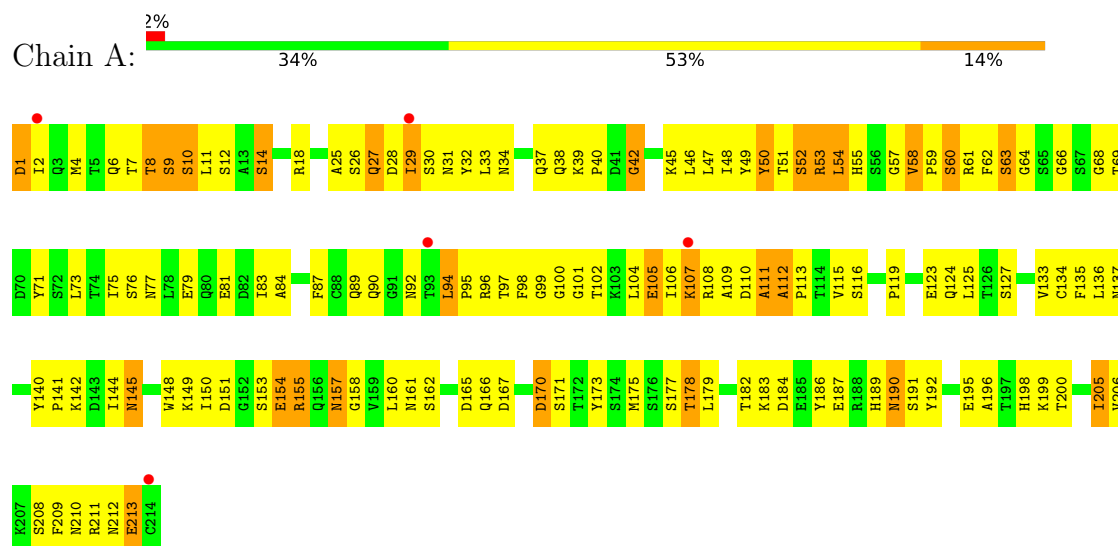
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		
4	B	21	Total	O	0	0
			21	21		
4	L	20	Total	O	0	0
			20	20		
4	H	26	Total	O	0	0
			26	26		
4	P	3	Total	O	0	0
			3	3		

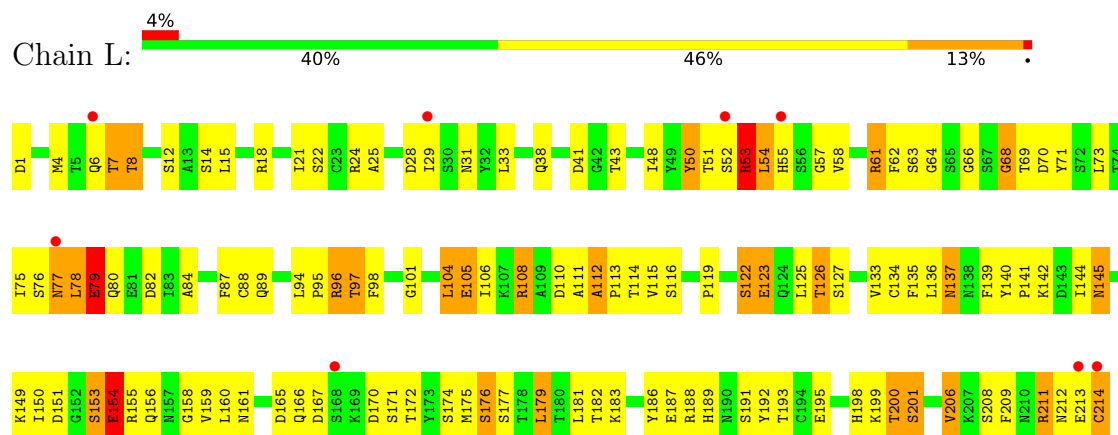
3 Residue-property plots

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.

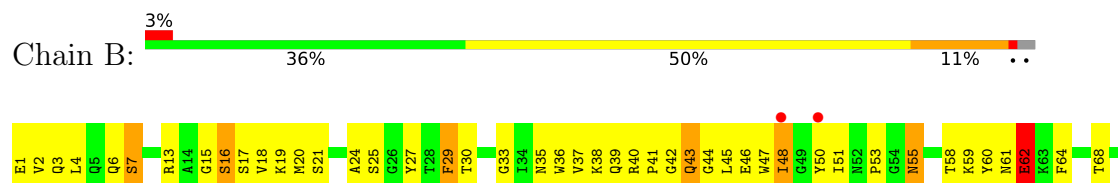
• Molecule 1: Germline antibody 36-65 Fab light chain

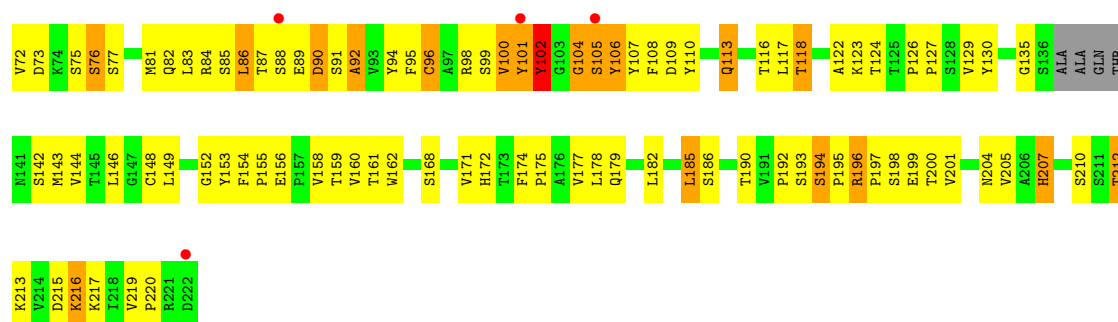


• Molecule 1: Germline antibody 36-65 Fab light chain

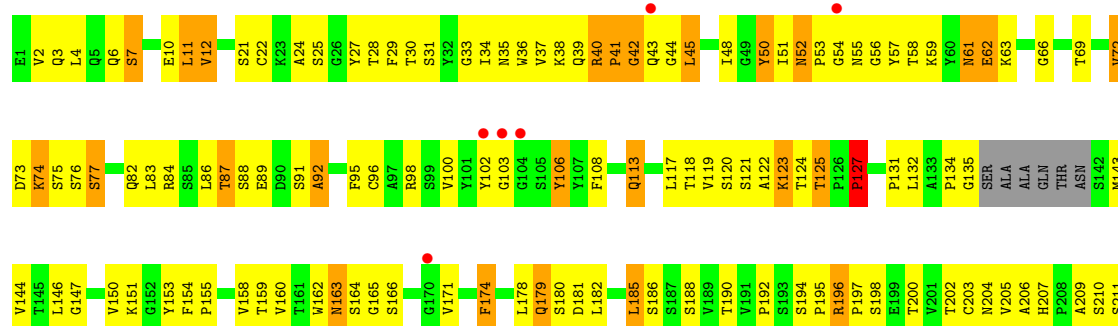


• Molecule 2: Germline antibody 36-65 Fab heavy chain

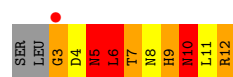
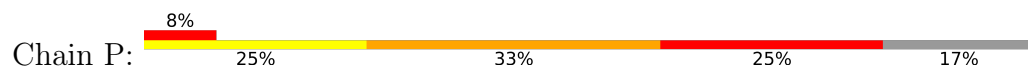




• Molecule 2: Germline antibody 36-65 Fab heavy chain



• Molecule 3: DODECAPEPTIDE: SLGDNLTNHNLRL



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.13Å 144.92Å 70.99Å 90.00° 104.35° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.6 (50.00-3.00) 88.6 (50.00-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.43 (at 2.87Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.245 , 0.264 0.244 , 0.261	Depositor DCC
R_{free} test set	1813 reflections (8.24%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6764	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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	0.56	0/1684	1.07	10/2284 (0.4%)
1	L	0.62	0/1691	1.14	12/2293 (0.5%)
2	B	0.74	5/1677 (0.3%)	1.17	14/2289 (0.6%)
2	H	0.58	0/1680	1.09	12/2290 (0.5%)
3	P	1.66	1/81 (1.2%)	2.52	7/107 (6.5%)
All	All	0.65	6/6813 (0.1%)	1.14	55/9263 (0.6%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	101	TYR	CA-C	11.31	1.67	1.53
2	B	102	TYR	N-CA	8.73	1.57	1.46
3	P	5	ASN	CA-C	-6.19	1.44	1.52
2	B	100	VAL	CA-C	5.68	1.58	1.52
2	B	101	TYR	N-CA	5.40	1.53	1.46
2	B	102	TYR	CB-CG	5.05	1.62	1.51

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	101	TYR	N-CA-C	16.27	135.46	112.04
3	P	11	LEU	N-CA-C	-9.86	100.74	113.17
1	A	111	ALA	N-CA-C	8.46	124.09	113.43
1	A	170	ASP	N-CA-C	-8.06	97.64	110.14
2	H	222	ASP	N-CA-C	7.58	132.23	111.00
3	P	9	HIS	CA-CB-CG	7.47	121.27	113.80
1	A	190	ASN	N-CA-C	7.45	122.33	112.13
1	L	154	GLU	N-CA-CB	-7.43	97.94	110.49
1	L	206	VAL	N-CA-C	7.27	118.36	107.75
2	B	76	SER	N-CA-C	-7.13	104.59	112.72
2	B	207	HIS	CA-C-N	6.97	128.56	119.84
2	B	207	HIS	C-N-CA	6.97	128.56	119.84
2	B	101	TYR	CA-CB-CG	6.89	126.30	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	6	LEU	N-CA-C	6.76	125.21	110.80
2	B	90	ASP	N-CA-C	-6.74	105.21	113.50
1	L	153	SER	CA-C-N	6.39	133.75	121.54
1	L	153	SER	C-N-CA	6.39	133.75	121.54
1	A	18	ARG	N-CA-C	-6.27	99.79	109.76
2	B	135	GLY	N-CA-C	6.18	122.67	112.66
1	L	54	LEU	N-CA-C	6.12	118.58	109.59
1	L	191	SER	N-CA-C	5.94	118.41	108.96
2	H	163	ASN	N-CA-C	-5.89	103.32	111.28
2	H	221	ARG	N-CA-C	-5.89	98.25	110.80
2	H	56	GLY	N-CA-C	-5.88	106.65	114.95
2	B	102	TYR	N-CA-C	5.82	123.20	110.80
1	A	153	SER	N-CA-C	5.76	117.86	108.76
1	L	122	SER	N-CA-C	-5.71	104.95	111.07
1	A	137	ASN	N-CA-C	5.65	118.93	109.95
1	L	18	ARG	N-CA-C	-5.61	100.67	109.25
2	H	103	GLY	N-CA-C	-5.60	99.91	113.18
2	H	12	VAL	N-CA-C	5.60	116.74	108.45
2	B	122	ALA	N-CA-C	-5.57	103.29	110.19
1	L	22	SER	N-CA-C	5.50	118.94	110.42
1	A	9	SER	N-CA-C	-5.48	104.72	111.40
1	A	165	ASP	N-CA-C	-5.46	103.69	110.41
3	P	7	THR	N-CA-C	5.45	118.40	110.17
1	L	79	GLU	N-CA-C	5.45	117.47	109.24
2	B	29	PHE	N-CA-C	5.43	117.63	111.11
2	B	152	GLY	N-CA-C	5.42	122.29	114.10
3	P	3	GLY	CA-C-N	-5.36	113.27	121.74
3	P	3	GLY	C-N-CA	-5.36	113.27	121.74
1	A	54	LEU	N-CA-C	5.36	116.98	108.67
1	L	137	ASN	N-CA-C	5.36	118.29	109.72
2	B	86	LEU	N-CA-C	5.34	117.77	110.24
1	L	78	LEU	N-CA-C	5.25	117.90	110.50
2	H	125	THR	CA-C-N	5.23	125.77	120.38
2	H	125	THR	C-N-CA	5.23	125.77	120.38
2	B	96	CYS	N-CA-C	-5.23	99.92	108.76
1	A	42	GLY	N-CA-C	5.13	120.92	114.25
2	H	119	VAL	N-CA-C	5.11	114.55	106.32
3	P	5	ASN	O-C-N	5.08	129.34	122.59
2	H	160	VAL	N-CA-C	5.07	115.33	107.78
2	H	151	LYS	N-CA-C	5.06	117.65	109.40
2	B	100	VAL	N-CA-C	5.05	115.98	108.65
2	H	174	PHE	N-CA-C	5.03	116.17	109.93

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1651	0	1569	173	1
1	L	1658	0	1581	158	2
2	B	1634	0	1565	150	1
2	H	1637	0	1589	168	0
3	P	81	0	73	42	0
4	A	33	0	0	13	0
4	B	21	0	0	6	0
4	H	26	0	0	1	0
4	L	20	0	0	5	0
4	P	3	0	0	2	0
All	All	6764	0	6377	647	2

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 50.

All (647) 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:P:4:ASP:OD1	3:P:5:ASN:N	1.76	1.16
1:L:31:ASN:HD22	1:L:51:THR:HG21	1.10	1.10
2:H:220:PRO:O	2:H:221:ARG:C	1.92	1.10
2:H:192:PRO:HD2	2:H:195:PRO:HG2	1.35	1.07
1:L:136:LEU:HD23	1:L:144:ILE:HD13	1.34	1.06
2:H:106:TYR:OH	3:P:9:HIS:HA	1.55	1.05
1:A:133:VAL:HG22	1:A:178:THR:HG23	1.38	1.04
3:P:12:ARG:HG3	3:P:12:ARG:NH1	1.63	1.04
1:L:25:ALA:HB2	1:L:29:ILE:HD11	1.41	1.03
1:L:112:ALA:HB2	1:L:200:THR:HG21	1.41	1.02
2:B:6:GLN:H	2:B:113:GLN:HE22	1.08	1.01
1:L:166:GLN:HE21	1:L:171:SER:HB3	1.22	1.00
3:P:12:ARG:HG3	3:P:12:ARG:HH11	0.85	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:4:ASP:O	3:P:5:ASN:CG	2.05	0.99
2:H:143:MET:HE2	2:H:190:THR:HG22	1.45	0.99
2:B:1:GLU:CD	2:B:3:GLN:HE21	1.70	0.98
1:L:166:GLN:NE2	1:L:171:SER:HB3	1.78	0.98
3:P:12:ARG:HH11	3:P:12:ARG:CG	1.76	0.98
1:A:46:LEU:HD13	2:B:108:PHE:O	1.65	0.96
2:B:64:PHE:O	2:B:68:THR:HG22	1.65	0.96
1:A:150:ILE:HD12	1:A:155:ARG:HD3	1.49	0.95
2:H:106:TYR:OH	3:P:9:HIS:CA	2.16	0.94
2:H:59:LYS:HZ3	3:P:5:ASN:HA	1.31	0.93
1:L:108:ARG:NH1	1:L:172:THR:HG23	1.83	0.92
1:A:14:SER:HA	1:A:107:LYS:HD2	1.50	0.91
1:L:108:ARG:HH11	1:L:172:THR:HG23	1.34	0.91
1:L:112:ALA:CB	1:L:200:THR:HG21	2.02	0.90
2:B:127:PRO:HB3	2:B:153:TYR:HB3	1.52	0.90
2:H:6:GLN:HE22	2:H:95:PHE:HA	1.36	0.88
1:L:31:ASN:HD22	1:L:51:THR:CG2	1.86	0.88
2:B:192:PRO:O	2:B:195:PRO:HD2	1.75	0.86
2:B:82:GLN:HE21	2:B:84:ARG:HH11	1.21	0.86
2:H:127:PRO:HB3	2:H:153:TYR:HB3	1.56	0.86
1:L:31:ASN:ND2	1:L:51:THR:HG21	1.90	0.86
1:A:29:ILE:HG22	1:A:32:TYR:H	1.39	0.86
1:L:108:ARG:NH1	1:L:172:THR:CG2	2.39	0.85
1:A:4:MET:HE3	1:A:4:MET:HA	1.59	0.85
2:B:33:GLY:HA3	2:B:50:TYR:HE1	1.41	0.85
2:H:192:PRO:O	2:H:195:PRO:HD2	1.76	0.85
3:P:4:ASP:O	3:P:5:ASN:ND2	2.10	0.84
3:P:4:ASP:CG	3:P:5:ASN:H	1.85	0.83
2:B:35:ASN:CG	2:B:108:PHE:HE1	1.87	0.83
3:P:4:ASP:O	3:P:5:ASN:CB	2.25	0.83
2:H:40:ARG:HG3	2:H:92:ALA:HB2	1.59	0.83
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.59	0.82
1:L:53:ARG:HD3	1:L:53:ARG:C	2.04	0.82
2:B:6:GLN:H	2:B:113:GLN:NE2	1.75	0.82
1:A:6:GLN:NE2	1:A:101:GLY:H	1.78	0.82
2:H:113:GLN:H	2:H:113:GLN:HE21	1.26	0.82
2:B:86:LEU:HD23	2:B:90:ASP:OD2	1.78	0.81
2:H:220:PRO:O	2:H:222:ASP:N	2.12	0.81
2:H:52:ASN:HB2	3:P:8:ASN:HD21	1.43	0.81
2:H:194:SER:O	2:H:198:SER:HB3	1.81	0.81
2:H:143:MET:CE	2:H:190:THR:HG22	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ASN:ND2	1:A:51:THR:HG21	1.97	0.80
2:H:143:MET:HE2	2:H:190:THR:CG2	2.12	0.79
1:A:31:ASN:CA	1:A:51:THR:OG1	2.30	0.79
1:A:151:ASP:OD2	1:A:189:HIS:HB3	1.82	0.79
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.65	0.79
2:B:37:VAL:CG1	2:B:45:LEU:HB3	2.13	0.79
2:B:37:VAL:HG11	2:B:45:LEU:HB3	1.64	0.78
1:A:14:SER:CA	1:A:107:LYS:HD2	2.13	0.78
2:B:161:THR:OG1	2:B:204:ASN:HB2	1.83	0.78
1:A:107:LYS:H	1:A:107:LYS:HD3	1.48	0.77
1:L:31:ASN:O	1:L:51:THR:HB	1.85	0.77
1:A:115:VAL:HG22	1:A:136:LEU:HD23	1.65	0.77
1:A:100:GLY:HA2	4:A:225:HOH:O	1.84	0.77
2:H:131:PRO:HD3	2:H:216:LYS:HD3	1.66	0.76
2:H:192:PRO:C	2:H:195:PRO:HD2	2.11	0.76
1:L:123:GLU:O	1:L:126:THR:HG23	1.86	0.76
2:H:29:PHE:CD2	2:H:77:SER:HA	2.21	0.76
1:L:53:ARG:HD2	1:L:54:LEU:HD23	1.66	0.76
1:L:136:LEU:HD23	1:L:144:ILE:CD1	2.15	0.76
2:H:6:GLN:H	2:H:113:GLN:NE2	1.83	0.76
1:L:189:HIS:O	1:L:211:ARG:NH1	2.19	0.76
1:A:48:ILE:CG2	1:A:52:SER:HA	2.16	0.76
1:L:66:GLY:HA3	1:L:71:TYR:HA	1.66	0.76
2:B:192:PRO:C	2:B:195:PRO:HD2	2.10	0.75
1:A:105:GLU:OE2	1:A:173:TYR:OH	2.04	0.75
2:B:88:SER:C	2:B:90:ASP:H	1.94	0.75
1:L:6:GLN:HE22	1:L:87:PHE:HA	1.51	0.75
2:H:124:THR:HG21	2:H:209:ALA:O	1.87	0.74
1:L:48:ILE:HG21	1:L:52:SER:HA	1.69	0.74
1:A:51:THR:HG22	1:A:51:THR:O	1.86	0.74
2:B:106:TYR:HD2	2:B:106:TYR:H	1.35	0.74
2:B:35:ASN:ND2	2:B:108:PHE:CE1	2.56	0.74
1:A:198:HIS:ND1	1:A:200:THR:HB	2.02	0.74
2:B:100:VAL:HB	2:B:107:TYR:CE1	2.22	0.74
1:A:190:ASN:HD21	1:A:212:ASN:H	1.36	0.73
1:L:12:SER:OG	1:L:105:GLU:OE1	2.05	0.73
1:A:150:ILE:CD1	1:A:155:ARG:HD3	2.17	0.73
2:B:196:ARG:HG3	2:B:201:VAL:CG2	2.18	0.73
1:L:41:ASP:OD1	1:L:43:THR:HG23	1.89	0.73
1:A:192:TYR:O	1:A:208:SER:HB2	1.89	0.73
1:A:52:SER:O	1:A:53:ARG:HB3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:ASN:CB	2:B:108:PHE:HE1	2.02	0.72
1:L:119:PRO:HB3	1:L:209:PHE:CZ	2.25	0.72
1:A:94:LEU:HD12	2:B:59:LYS:HE3	1.70	0.72
2:B:7:SER:OG	2:B:21:SER:N	2.22	0.71
2:B:100:VAL:O	2:B:106:TYR:HA	1.91	0.70
1:A:27:GLN:O	1:A:69:THR:HG22	1.89	0.70
2:H:6:GLN:H	2:H:113:GLN:HE22	1.38	0.70
1:A:31:ASN:CB	1:A:51:THR:OG1	2.40	0.70
2:B:86:LEU:CD2	2:B:90:ASP:OD2	2.40	0.70
2:H:24:ALA:HB1	2:H:27:TYR:CE2	2.27	0.70
2:H:212:THR:C	2:H:213:LYS:HD2	2.16	0.70
2:H:30:THR:HG23	2:H:54:GLY:HA2	1.72	0.69
1:L:31:ASN:CB	1:L:51:THR:HB	2.22	0.69
1:L:161:ASN:HB3	1:L:175:MET:HE3	1.74	0.69
1:L:31:ASN:HB3	1:L:51:THR:HB	1.74	0.69
1:L:111:ALA:O	1:L:112:ALA:HB3	1.92	0.69
1:A:190:ASN:ND2	1:A:212:ASN:H	1.91	0.69
1:A:48:ILE:HG21	1:A:52:SER:HA	1.74	0.69
1:L:108:ARG:HH11	1:L:172:THR:CG2	2.04	0.68
1:A:161:ASN:HD22	1:A:177:SER:HA	1.59	0.68
2:B:15:GLY:O	2:B:85:SER:HA	1.93	0.68
1:A:39:LYS:NZ	1:A:81:GLU:O	2.26	0.68
1:A:157:ASN:N	1:A:157:ASN:HD22	1.92	0.68
1:L:167:ASP:HB3	1:L:170:ASP:OD1	1.93	0.68
1:A:29:ILE:HA	1:A:92:ASN:HD22	1.58	0.68
2:H:220:PRO:C	2:H:222:ASP:N	2.48	0.68
2:H:11:LEU:HD21	2:H:154:PHE:CZ	2.29	0.68
2:B:20:MET:HE1	2:B:94:TYR:CD1	2.29	0.67
1:A:111:ALA:O	1:A:112:ALA:HB3	1.93	0.67
2:B:35:ASN:HB2	2:B:108:PHE:CE1	2.30	0.67
2:B:58:THR:HG1	2:B:60:TYR:HE1	1.41	0.67
2:B:82:GLN:HE21	2:B:84:ARG:NH1	1.92	0.67
2:H:202:THR:HG23	2:H:216:LYS:O	1.95	0.67
1:L:198:HIS:ND1	1:L:200:THR:HB	2.11	0.66
2:H:12:VAL:HG22	2:H:117:LEU:HD11	1.77	0.66
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.76	0.66
2:H:52:ASN:HB2	3:P:8:ASN:ND2	2.10	0.66
2:H:73:ASP:C	2:H:75:SER:H	2.03	0.66
2:H:51:ILE:HD11	2:H:72:VAL:HG12	1.76	0.66
1:A:167:ASP:HB3	1:A:170:ASP:O	1.96	0.66
1:A:30:SER:HA	4:A:222:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:52:SER:HB3	1:L:64:GLY:C	2.21	0.65
2:B:42:GLY:O	2:B:43:GLN:O	2.14	0.65
1:A:14:SER:CB	1:A:107:LYS:HD2	2.26	0.65
2:B:87:THR:O	2:B:90:ASP:HB2	1.96	0.65
1:L:29:ILE:HB	1:L:71:TYR:OH	1.96	0.65
2:H:52:ASN:ND2	2:H:54:GLY:H	1.93	0.65
1:A:31:ASN:C	1:A:51:THR:HG1	2.03	0.65
2:B:55:ASN:OD1	2:B:55:ASN:N	2.29	0.65
1:L:78:LEU:HG	1:L:79:GLU:N	2.10	0.65
1:L:25:ALA:CB	1:L:29:ILE:HD11	2.23	0.65
1:A:52:SER:HB3	1:A:64:GLY:HA3	1.78	0.65
2:B:13:ARG:HG2	2:B:13:ARG:HH11	1.61	0.65
1:A:31:ASN:C	1:A:51:THR:OG1	2.40	0.64
2:B:113:GLN:NE2	2:B:113:GLN:H	1.95	0.64
2:B:113:GLN:H	2:B:113:GLN:HE21	1.45	0.64
1:A:7:THR:O	1:A:8:THR:HB	1.96	0.64
2:B:6:GLN:N	2:B:113:GLN:HE22	1.88	0.64
2:B:16:SER:O	2:B:85:SER:N	2.30	0.64
1:L:112:ALA:HB2	1:L:200:THR:CG2	2.24	0.64
1:A:49:TYR:CE2	1:A:54:LEU:HD12	2.33	0.64
2:B:1:GLU:OE2	2:B:3:GLN:NE2	2.30	0.64
2:B:7:SER:HG	2:B:21:SER:H	1.43	0.64
2:B:33:GLY:HA3	2:B:50:TYR:CE1	2.29	0.64
2:H:219:VAL:HG23	2:H:222:ASP:HA	1.77	0.64
1:L:108:ARG:NH1	1:L:170:ASP:HB2	2.13	0.64
1:L:160:LEU:C	1:L:161:ASN:HD22	2.06	0.64
1:L:48:ILE:CG2	1:L:52:SER:HA	2.27	0.63
2:H:113:GLN:H	2:H:113:GLN:NE2	1.96	0.63
1:A:69:THR:HG23	4:A:231:HOH:O	1.99	0.63
1:A:6:GLN:HE22	1:A:87:PHE:HA	1.64	0.63
1:L:94:LEU:HD13	3:P:6:LEU:CD1	2.28	0.63
2:H:53:PRO:O	2:H:74:LYS:HD2	1.99	0.63
2:B:106:TYR:N	2:B:106:TYR:CD2	2.66	0.63
1:L:119:PRO:HB3	1:L:209:PHE:CE1	2.34	0.63
2:H:7:SER:HB3	2:H:21:SER:H	1.64	0.62
2:B:87:THR:HG22	2:B:88:SER:N	2.13	0.62
2:B:51:ILE:HD11	2:B:72:VAL:HG12	1.80	0.62
1:A:95:PRO:HB3	2:B:61:ASN:HD22	1.64	0.62
4:A:225:HOH:O	2:B:44:GLY:HA2	1.99	0.62
1:L:4:MET:HE1	1:L:25:ALA:HB2	1.81	0.62
2:H:6:GLN:HB2	2:H:113:GLN:HE22	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:75:ILE:O	1:L:77:ASN:N	2.33	0.62
3:P:9:HIS:CD2	3:P:10:ASN:H	2.17	0.62
2:B:64:PHE:C	2:B:68:THR:HG22	2.24	0.62
1:L:153:SER:HB2	1:L:154:GLU:HG2	1.81	0.62
2:B:192:PRO:HD2	2:B:195:PRO:HG2	1.82	0.62
1:L:115:VAL:HA	1:L:135:PHE:O	2.00	0.62
3:P:6:LEU:HG	3:P:7:THR:H	1.64	0.62
1:A:151:ASP:OD2	1:A:189:HIS:CB	2.48	0.62
2:B:196:ARG:HG3	2:B:201:VAL:HG23	1.81	0.62
2:H:11:LEU:HD21	2:H:154:PHE:HZ	1.65	0.61
1:A:6:GLN:NE2	1:A:101:GLY:N	2.48	0.61
2:B:58:THR:OG1	2:B:60:TYR:HE1	1.83	0.61
1:A:61:ARG:HD2	1:A:77:ASN:O	2.01	0.61
2:B:123:LYS:O	2:B:124:THR:C	2.43	0.61
2:H:220:PRO:O	2:H:221:ARG:O	2.16	0.61
1:A:148:TRP:O	1:A:154:GLU:O	2.19	0.61
1:L:31:ASN:ND2	1:L:51:THR:OG1	2.34	0.61
2:H:30:THR:HG23	2:H:54:GLY:CA	2.30	0.61
2:H:206:ALA:HB1	2:H:213:LYS:HE3	1.82	0.61
2:H:222:ASP:OXT	2:H:222:ASP:CG	2.39	0.61
1:A:166:GLN:NE2	1:A:171:SER:HB3	2.16	0.61
1:A:31:ASN:HA	1:A:51:THR:OG1	2.01	0.61
2:B:35:ASN:ND2	2:B:108:PHE:HE1	1.93	0.61
2:B:88:SER:O	2:B:90:ASP:N	2.32	0.61
1:L:111:ALA:O	1:L:112:ALA:CB	2.48	0.61
2:H:106:TYR:CZ	3:P:9:HIS:HA	2.35	0.60
1:L:31:ASN:ND2	1:L:51:THR:CB	2.64	0.60
1:L:151:ASP:OD2	1:L:189:HIS:HB3	2.02	0.60
1:L:192:TYR:O	1:L:208:SER:HB2	2.01	0.60
1:L:200:THR:HG23	1:L:200:THR:O	2.00	0.60
1:A:107:LYS:HD3	1:A:107:LYS:N	2.12	0.60
2:H:12:VAL:HG21	2:H:86:LEU:CD1	2.31	0.60
2:H:59:LYS:NZ	3:P:5:ASN:HA	2.13	0.60
2:H:132:LEU:HD12	2:H:147:GLY:HA3	1.84	0.60
1:A:48:ILE:HG22	1:A:52:SER:HA	1.83	0.59
2:B:35:ASN:CB	2:B:108:PHE:CE1	2.82	0.59
2:B:200:THR:HG23	2:B:217:LYS:HD2	1.83	0.59
2:B:213:LYS:N	4:B:224:HOH:O	2.35	0.59
1:A:52:SER:O	1:A:53:ARG:CB	2.50	0.59
1:L:33:LEU:HD11	1:L:88:CYS:HB2	1.84	0.59
2:H:52:ASN:ND2	2:H:54:GLY:N	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:25:ALA:HB2	1:L:29:ILE:CD1	2.25	0.59
1:L:211:ARG:O	1:L:214:CYS:HB2	2.03	0.59
2:H:24:ALA:HB1	2:H:27:TYR:HE2	1.66	0.59
1:L:51:THR:O	1:L:52:SER:HB2	2.02	0.59
1:A:55:HIS:HE1	1:A:62:PHE:O	1.86	0.59
1:L:21:ILE:HD11	1:L:104:LEU:HD21	1.85	0.58
2:H:106:TYR:OH	3:P:8:ASN:C	2.45	0.58
1:A:158:GLY:O	1:A:179:LEU:HA	2.04	0.58
2:H:210:SER:O	2:H:211:SER:OG	2.16	0.58
1:A:96:ARG:NH1	2:B:35:ASN:HD21	2.00	0.58
1:L:179:LEU:HD11	1:L:181:LEU:HD21	1.85	0.58
2:H:37:VAL:CG1	2:H:45:LEU:HB3	2.34	0.58
2:H:52:ASN:CB	3:P:8:ASN:HD21	2.15	0.58
2:H:73:ASP:O	2:H:75:SER:N	2.36	0.58
1:A:94:LEU:CD1	2:B:59:LYS:HE3	2.33	0.58
1:L:31:ASN:ND2	1:L:51:THR:CG2	2.59	0.58
1:L:38:GLN:O	1:L:84:ALA:HB1	2.04	0.58
1:L:75:ILE:O	1:L:75:ILE:HG22	2.02	0.58
2:H:113:GLN:HE21	2:H:113:GLN:N	1.99	0.58
2:H:194:SER:O	2:H:198:SER:CB	2.52	0.58
2:H:212:THR:O	2:H:213:LYS:HD2	2.03	0.58
1:A:195:GLU:HG2	1:A:206:VAL:HG13	1.85	0.58
2:B:212:THR:HG23	4:B:224:HOH:O	2.03	0.58
2:H:53:PRO:O	2:H:74:LYS:CD	2.52	0.58
3:P:10:ASN:ND2	4:P:87:HOH:O	2.36	0.57
1:A:29:ILE:CG2	1:A:32:TYR:H	2.15	0.57
4:A:225:HOH:O	2:B:44:GLY:CA	2.51	0.57
1:L:137:ASN:OD1	1:L:174:SER:HB3	2.03	0.57
1:A:186:TYR:CE2	1:A:211:ARG:HD2	2.40	0.57
2:B:1:GLU:CD	2:B:3:GLN:NE2	2.53	0.57
1:A:29:ILE:HD12	1:A:92:ASN:HB3	1.86	0.57
1:L:200:THR:CG2	1:L:200:THR:O	2.52	0.57
1:A:79:GLU:HG3	4:A:216:HOH:O	2.03	0.56
1:A:31:ASN:O	1:A:50:TYR:CD1	2.58	0.56
1:A:160:LEU:HD13	2:B:177:VAL:HG21	1.87	0.56
2:B:196:ARG:HG3	2:B:201:VAL:HG21	1.87	0.56
1:L:53:ARG:HH11	1:L:54:LEU:CD2	2.18	0.56
2:B:35:ASN:ND2	2:B:108:PHE:CZ	2.73	0.56
1:L:110:ASP:OD1	1:L:141:PRO:HD3	2.05	0.56
2:H:28:THR:HG21	2:H:31:SER:OG	2.05	0.56
1:L:29:ILE:HG22	1:L:29:ILE:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:28:THR:HG22	2:H:31:SER:H	1.69	0.56
1:A:161:ASN:ND2	1:A:177:SER:OG	2.38	0.56
2:B:35:ASN:OD1	2:B:50:TYR:HD1	1.88	0.56
1:L:61:ARG:HH21	1:L:82:ASP:CG	2.14	0.56
1:A:55:HIS:CE1	1:A:62:PHE:O	2.60	0.55
2:B:204:ASN:ND2	2:B:215:ASP:OD1	2.36	0.55
1:A:37:GLN:HB2	1:A:47:LEU:CD1	2.36	0.55
1:A:108:ARG:HB2	1:A:171:SER:HB2	1.89	0.55
1:L:108:ARG:HB2	1:L:171:SER:HB2	1.88	0.55
1:L:112:ALA:CA	1:L:200:THR:HG21	2.37	0.55
1:L:135:PHE:CE1	1:L:176:SER:HB2	2.40	0.55
1:L:50:TYR:O	1:L:52:SER:O	2.24	0.55
2:H:150:VAL:HG12	2:H:153:TYR:CD1	2.41	0.55
1:L:159:VAL:O	1:L:160:LEU:HD23	2.06	0.55
2:H:40:ARG:HD2	2:H:89:GLU:O	2.06	0.55
2:B:185:LEU:HD12	2:B:185:LEU:C	2.31	0.55
1:L:135:PHE:CE1	2:H:174:PHE:CE2	2.94	0.55
2:H:207:HIS:HD1	2:H:210:SER:HB3	1.71	0.55
1:L:55:HIS:CE1	1:L:62:PHE:O	2.60	0.55
2:H:106:TYR:OH	3:P:9:HIS:N	2.39	0.55
2:B:51:ILE:O	2:B:53:PRO:HD3	2.07	0.55
2:H:4:LEU:HD23	2:H:24:ALA:HA	1.89	0.55
2:H:61:ASN:C	2:H:61:ASN:HD22	2.15	0.55
2:B:194:SER:O	2:B:198:SER:HB3	2.07	0.54
1:L:136:LEU:CD2	1:L:144:ILE:HD13	2.22	0.54
1:L:199:LYS:C	1:L:201:SER:H	2.14	0.54
1:A:66:GLY:HA3	1:A:71:TYR:CD2	2.42	0.54
2:H:6:GLN:CB	2:H:113:GLN:HE22	2.21	0.54
1:A:113:PRO:HG2	1:A:205:ILE:HD12	1.88	0.54
1:A:151:ASP:OD2	1:A:189:HIS:CD2	2.60	0.54
1:A:161:ASN:HB3	1:A:175:MET:HE3	1.89	0.54
2:B:72:VAL:CG2	2:B:73:ASP:N	2.71	0.54
1:A:28:ASP:OD2	1:A:30:SER:N	2.38	0.54
2:B:192:PRO:HB2	2:B:195:PRO:CD	2.37	0.54
1:L:89:GLN:HG2	1:L:97:THR:O	2.07	0.54
2:B:24:ALA:HB1	2:B:27:TYR:CE2	2.42	0.54
2:H:29:PHE:CG	2:H:77:SER:HB3	2.43	0.54
1:A:50:TYR:O	1:A:52:SER:O	2.25	0.54
2:B:13:ARG:HG2	2:B:13:ARG:NH1	2.22	0.54
2:H:38:LYS:CB	2:H:48:ILE:HD11	2.34	0.54
2:H:61:ASN:O	2:H:63:LYS:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:106:TYR:CZ	3:P:8:ASN:O	2.61	0.54
2:H:219:VAL:CG2	2:H:222:ASP:HA	2.38	0.54
1:A:111:ALA:O	1:A:112:ALA:CB	2.56	0.53
1:L:94:LEU:HD13	3:P:6:LEU:HD11	1.88	0.53
2:H:123:LYS:O	2:H:124:THR:C	2.51	0.53
2:H:135:GLY:HA2	2:H:221:ARG:CD	2.38	0.53
3:P:4:ASP:O	3:P:5:ASN:HB2	2.07	0.53
1:A:4:MET:CE	1:A:25:ALA:HA	2.39	0.53
2:B:72:VAL:HG22	2:B:73:ASP:N	2.23	0.53
1:A:108:ARG:HG3	1:A:108:ARG:HH11	1.74	0.53
1:L:160:LEU:CD1	2:H:179:GLN:HG2	2.39	0.53
1:A:33:LEU:H	1:A:51:THR:H	1.57	0.53
1:A:108:ARG:NH2	4:A:237:HOH:O	2.39	0.53
2:B:46:GLU:OE1	2:B:64:PHE:CZ	2.61	0.53
1:A:8:THR:HG22	1:A:102:THR:HG23	1.90	0.53
2:B:46:GLU:OE1	2:B:64:PHE:HZ	1.92	0.53
2:H:59:LYS:NZ	3:P:5:ASN:HD22	2.07	0.53
1:A:157:ASN:N	1:A:157:ASN:ND2	2.55	0.53
1:L:1:ASP:OD1	1:L:95:PRO:HD2	2.08	0.53
2:H:106:TYR:OH	3:P:9:HIS:CB	2.57	0.53
2:H:87:THR:OG1	2:H:88:SER:N	2.37	0.53
1:A:124:GLN:O	1:A:127:SER:OG	2.20	0.52
2:H:51:ILE:HD11	2:H:72:VAL:CG1	2.39	0.52
2:H:83:LEU:HB3	2:H:86:LEU:HD21	1.91	0.52
1:A:133:VAL:HG12	1:A:134:CYS:N	2.23	0.52
1:A:140:TYR:HD2	1:A:173:TYR:HE1	1.56	0.52
2:H:29:PHE:CE2	2:H:77:SER:HA	2.44	0.52
2:H:82:GLN:OE1	2:H:84:ARG:NH1	2.42	0.52
1:L:182:THR:HB	4:L:219:HOH:O	2.09	0.52
2:H:178:LEU:HD12	2:H:182:LEU:C	2.34	0.52
2:B:126:PRO:HG3	2:B:210:SER:HB2	1.92	0.52
1:A:45:LYS:HG2	1:A:46:LEU:N	2.25	0.52
1:L:6:GLN:NE2	1:L:101:GLY:H	2.07	0.52
1:L:48:ILE:HD12	1:L:73:LEU:HD12	1.92	0.52
2:H:150:VAL:HG12	2:H:153:TYR:HD1	1.75	0.52
1:A:107:LYS:HG2	1:A:107:LYS:O	2.10	0.52
1:A:2:ILE:HG21	1:A:29:ILE:HD11	1.92	0.52
1:A:31:ASN:HB3	1:A:51:THR:OG1	2.09	0.52
1:A:51:THR:HG23	1:A:71:TYR:CE2	2.45	0.52
1:A:51:THR:HG23	1:A:71:TYR:CD2	2.45	0.51
2:B:127:PRO:CB	2:B:153:TYR:HB3	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:106:TYR:CE1	3:P:8:ASN:O	2.64	0.51
1:L:4:MET:HG2	1:L:97:THR:HB	1.92	0.51
1:L:79:GLU:O	1:L:80:GLN:C	2.54	0.51
1:A:46:LEU:HD22	2:B:109:ASP:HA	1.91	0.51
1:A:112:ALA:HA	1:A:200:THR:HG21	1.92	0.51
2:H:83:LEU:CB	2:H:86:LEU:HD21	2.41	0.51
3:P:9:HIS:O	3:P:10:ASN:HB2	2.10	0.51
1:A:31:ASN:O	1:A:50:TYR:CE1	2.64	0.51
1:A:123:GLU:OE2	2:B:216:LYS:HE2	2.10	0.51
1:A:170:ASP:OD1	1:A:170:ASP:C	2.53	0.51
1:A:191:SER:HB2	4:A:240:HOH:O	2.09	0.51
2:H:106:TYR:OH	3:P:9:HIS:HB3	2.10	0.51
1:L:52:SER:O	1:L:53:ARG:CB	2.58	0.51
2:H:194:SER:HB2	2:H:195:PRO:HD3	1.92	0.51
1:A:8:THR:HG23	1:A:10:SER:O	2.11	0.51
2:B:143:MET:HE3	2:B:190:THR:HG22	1.92	0.51
2:H:192:PRO:HB2	2:H:195:PRO:CD	2.41	0.51
1:L:77:ASN:C	1:L:77:ASN:OD1	2.53	0.51
2:H:202:THR:HG23	2:H:216:LYS:C	2.36	0.51
1:A:115:VAL:CG2	1:A:136:LEU:HD23	2.38	0.51
1:A:140:TYR:CD2	1:A:173:TYR:HE1	2.28	0.51
2:H:159:THR:HB	2:H:206:ALA:HB3	1.91	0.51
1:L:167:ASP:HB3	1:L:170:ASP:O	2.11	0.51
2:H:106:TYR:N	2:H:106:TYR:CD2	2.79	0.51
1:L:108:ARG:HH12	1:L:170:ASP:HB2	1.76	0.50
2:H:154:PHE:CE2	2:H:155:PRO:HB3	2.46	0.50
2:H:178:LEU:HD12	2:H:182:LEU:O	2.10	0.50
1:A:4:MET:HE1	1:A:25:ALA:CA	2.41	0.50
1:L:113:PRO:HB3	1:L:139:PHE:HB3	1.94	0.50
2:H:196:ARG:HD2	2:H:197:PRO:HA	1.91	0.50
1:A:7:THR:O	1:A:8:THR:CB	2.59	0.50
2:B:35:ASN:O	2:B:96:CYS:HA	2.11	0.50
1:L:51:THR:O	1:L:52:SER:CB	2.60	0.50
2:H:84:ARG:HG3	2:H:84:ARG:HH11	1.77	0.50
2:B:154:PHE:CE2	2:B:155:PRO:HB3	2.47	0.50
1:L:135:PHE:HE1	1:L:176:SER:HB2	1.76	0.50
2:H:66:GLY:O	2:H:84:ARG:NH2	2.45	0.50
2:B:158:VAL:HG23	2:B:207:HIS:HD2	1.76	0.50
1:L:29:ILE:HD12	1:L:71:TYR:CE1	2.47	0.50
2:H:131:PRO:HD3	2:H:216:LYS:CD	2.39	0.50
1:A:6:GLN:HE21	1:A:99:GLY:C	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:9:HIS:O	4:P:87:HOH:O	2.19	0.50
2:H:6:GLN:N	2:H:113:GLN:HE22	2.08	0.49
1:A:63:SER:O	1:A:73:LEU:HD12	2.12	0.49
2:B:35:ASN:HB2	2:B:108:PHE:HE1	1.66	0.49
2:H:29:PHE:HB2	2:H:77:SER:HB3	1.92	0.49
1:L:38:GLN:HA	1:L:43:THR:O	2.12	0.49
1:L:52:SER:O	1:L:53:ARG:HB3	2.12	0.49
1:L:105:GLU:HB2	1:L:166:GLN:OE1	2.11	0.49
1:L:31:ASN:C	1:L:51:THR:HB	2.37	0.49
2:H:40:ARG:O	2:H:42:GLY:N	2.45	0.49
2:H:51:ILE:HB	2:H:58:THR:HG22	1.94	0.49
1:L:170:ASP:OD1	1:L:170:ASP:C	2.55	0.49
2:B:35:ASN:HD22	2:B:47:TRP:HE1	1.60	0.49
2:B:61:ASN:O	2:B:62:GLU:C	2.55	0.49
2:H:162:TRP:O	2:H:163:ASN:HB2	2.13	0.49
1:L:50:TYR:O	1:L:51:THR:HG22	2.13	0.48
1:A:4:MET:HE1	1:A:25:ALA:HB2	1.96	0.48
1:L:153:SER:CA	1:L:154:GLU:HG2	2.40	0.48
1:A:183:LYS:O	1:A:187:GLU:HG3	2.13	0.48
2:B:76:SER:O	2:B:77:SER:C	2.57	0.48
2:B:161:THR:HG1	2:B:204:ASN:HB2	1.75	0.48
2:B:215:ASP:HB2	4:B:236:HOH:O	2.13	0.48
2:B:91:SER:O	2:B:92:ALA:HB2	2.14	0.48
2:B:148:CYS:HB2	2:B:162:TRP:CH2	2.48	0.48
1:L:94:LEU:HD13	3:P:6:LEU:HD12	1.94	0.48
2:H:37:VAL:HG11	2:H:45:LEU:HB3	1.94	0.48
2:H:185:LEU:HD12	2:H:186:SER:N	2.29	0.48
2:H:207:HIS:ND1	2:H:210:SER:HB3	2.28	0.48
1:A:107:LYS:O	1:A:107:LYS:CG	2.60	0.48
2:B:146:LEU:HD12	2:B:201:VAL:HG11	1.95	0.48
1:A:38:GLN:O	1:A:84:ALA:HB1	2.14	0.48
1:A:123:GLU:OE2	2:B:216:LYS:CE	2.62	0.48
1:A:210:ASN:HB2	1:A:213:GLU:HB2	1.95	0.48
1:L:52:SER:HB3	1:L:64:GLY:HA3	1.96	0.48
1:L:79:GLU:HG2	4:L:229:HOH:O	2.13	0.48
2:H:27:TYR:CE1	2:H:98:ARG:HD2	2.49	0.48
2:H:59:LYS:HZ3	3:P:5:ASN:HD22	1.58	0.48
1:A:48:ILE:HD12	1:A:73:LEU:HD13	1.95	0.48
1:L:96:ARG:H	1:L:96:ARG:HG2	1.41	0.48
1:A:32:TYR:CZ	2:B:104:GLY:O	2.67	0.47
1:L:31:ASN:CA	1:L:51:THR:HB	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:123:GLU:H	1:L:123:GLU:HG2	1.38	0.47
2:H:73:ASP:C	2:H:75:SER:N	2.70	0.47
1:L:31:ASN:HD22	1:L:51:THR:CB	2.25	0.47
1:A:27:GLN:C	1:A:69:THR:HG22	2.38	0.47
1:A:108:ARG:HG2	1:A:109:ALA:N	2.28	0.47
3:P:3:GLY:C	3:P:4:ASP:O	2.54	0.47
2:B:98:ARG:O	2:B:108:PHE:HA	2.14	0.47
1:L:4:MET:O	4:L:220:HOH:O	2.20	0.47
1:L:94:LEU:HD12	4:L:233:HOH:O	2.14	0.47
1:A:48:ILE:HG22	1:A:49:TYR:N	2.29	0.47
1:A:48:ILE:HD12	1:A:73:LEU:CD1	2.45	0.47
2:H:35:ASN:O	2:H:96:CYS:HA	2.15	0.47
1:A:96:ARG:NH1	2:B:35:ASN:ND2	2.62	0.47
1:A:144:ILE:HG12	1:A:145:ASN:H	1.80	0.47
2:B:81:MET:HE3	2:B:83:LEU:HD11	1.97	0.47
2:B:130:TYR:HB2	2:B:149:LEU:HB3	1.96	0.47
1:L:161:ASN:HB3	1:L:175:MET:CE	2.42	0.47
3:P:8:ASN:O	3:P:8:ASN:OD1	2.32	0.47
1:A:50:TYR:CD2	2:B:102:TYR:HE2	2.33	0.47
2:H:40:ARG:O	2:H:41:PRO:C	2.58	0.47
2:H:153:TYR:CD2	2:H:153:TYR:C	2.92	0.47
2:B:107:TYR:CD1	2:B:107:TYR:C	2.92	0.47
1:L:183:LYS:O	1:L:187:GLU:HG3	2.14	0.47
1:L:186:TYR:CE2	1:L:211:ARG:HD2	2.50	0.47
1:L:4:MET:HA	1:L:4:MET:HE3	1.97	0.46
1:L:24:ARG:HG3	1:L:70:ASP:OD2	2.16	0.46
1:L:153:SER:CB	1:L:154:GLU:HG2	2.44	0.46
2:B:88:SER:C	2:B:90:ASP:N	2.60	0.46
2:B:148:CYS:HB2	2:B:162:TRP:HH2	1.79	0.46
2:H:40:ARG:C	2:H:42:GLY:N	2.73	0.46
2:H:51:ILE:HG23	2:H:51:ILE:O	2.14	0.46
1:A:4:MET:SD	1:A:90:GLN:HG2	2.55	0.46
1:A:83:ILE:HD11	1:A:106:ILE:HD11	1.97	0.46
1:L:52:SER:HB3	1:L:64:GLY:CA	2.45	0.46
2:H:134:PRO:HD3	2:H:146:LEU:HD23	1.97	0.46
1:A:29:ILE:CG2	1:A:29:ILE:O	2.64	0.46
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.98	0.46
2:H:12:VAL:HG21	2:H:86:LEU:HD13	1.98	0.46
2:H:143:MET:CE	2:H:190:THR:CG2	2.84	0.46
1:A:11:LEU:HD12	1:A:12:SER:N	2.31	0.46
1:A:115:VAL:HA	1:A:135:PHE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:SER:OG	2:B:21:SER:HB2	2.16	0.46
2:B:87:THR:HG22	2:B:88:SER:H	1.79	0.46
2:H:52:ASN:CB	3:P:8:ASN:ND2	2.77	0.46
2:H:106:TYR:OH	3:P:8:ASN:O	2.34	0.46
2:B:160:VAL:HG22	2:B:205:VAL:HG22	1.98	0.46
1:L:150:ILE:HD12	1:L:155:ARG:HD3	1.97	0.46
1:A:1:ASP:HB3	1:A:95:PRO:HD2	1.98	0.46
1:A:136:LEU:CD2	1:A:196:ALA:HB2	2.46	0.46
1:A:144:ILE:HG12	1:A:145:ASN:N	2.30	0.46
2:B:38:LYS:HB2	2:B:48:ILE:HD11	1.97	0.46
2:H:11:LEU:HD21	2:H:154:PHE:CE2	2.51	0.46
2:B:15:GLY:C	2:B:85:SER:HA	2.41	0.46
2:H:153:TYR:OH	2:H:185:LEU:HD23	2.16	0.46
2:B:194:SER:N	2:B:195:PRO:CD	2.79	0.46
1:L:212:ASN:OD1	1:L:213:GLU:N	2.49	0.46
1:L:15:LEU:HD21	1:L:106:ILE:HD11	1.98	0.45
1:L:108:ARG:O	1:L:140:TYR:CE2	2.69	0.45
1:L:160:LEU:HD12	2:H:179:GLN:HG2	1.98	0.45
1:A:33:LEU:HD12	1:A:89:GLN:C	2.41	0.45
1:L:193:THR:HA	1:L:208:SER:HB3	1.99	0.45
1:A:110:ASP:HA	1:A:140:TYR:O	2.17	0.45
2:B:3:GLN:HB2	2:B:25:SER:OG	2.16	0.45
1:L:200:THR:O	1:L:201:SER:HB3	2.17	0.45
2:H:61:ASN:C	2:H:63:LYS:H	2.24	0.45
1:A:51:THR:C	1:A:52:SER:O	2.59	0.45
1:A:109:ALA:O	1:A:110:ASP:C	2.58	0.45
2:H:76:SER:O	2:H:77:SER:C	2.59	0.45
1:L:7:THR:O	1:L:8:THR:OG1	2.30	0.45
2:B:73:ASP:CG	2:B:75:SER:HG	2.18	0.45
1:L:195:GLU:HG2	1:L:206:VAL:HG22	1.98	0.45
1:A:100:GLY:C	4:A:228:HOH:O	2.60	0.45
1:A:162:SER:OG	2:B:175:PRO:HD2	2.16	0.45
2:H:91:SER:O	2:H:92:ALA:HB2	2.15	0.45
2:H:192:PRO:CD	2:H:195:PRO:HG2	2.26	0.45
1:A:107:LYS:O	1:A:107:LYS:NZ	2.29	0.45
2:B:171:VAL:HG12	2:B:172:HIS:N	2.31	0.45
1:L:158:GLY:O	1:L:179:LEU:HA	2.16	0.45
1:A:31:ASN:ND2	1:A:51:THR:CG2	2.76	0.45
2:B:100:VAL:HG21	2:B:109:ASP:OD2	2.17	0.45
1:L:79:GLU:CG	4:L:229:HOH:O	2.65	0.45
1:L:144:ILE:HG23	1:L:145:ASN:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:TRP:HB2	2:H:48:ILE:HB	1.98	0.45
2:H:120:SER:OG	2:H:121:SER:N	2.50	0.45
2:H:185:LEU:HD12	2:H:185:LEU:C	2.43	0.44
2:B:99:SER:C	2:B:100:VAL:HG23	2.42	0.44
1:A:39:LYS:HG2	4:A:242:HOH:O	2.17	0.44
1:A:149:LYS:HD2	1:A:195:GLU:OE1	2.17	0.44
1:A:186:TYR:CZ	1:A:211:ARG:HD2	2.52	0.44
2:B:87:THR:CG2	2:B:88:SER:N	2.79	0.44
1:L:28:ASP:OD2	1:L:68:GLY:HA2	2.18	0.44
2:H:33:GLY:O	2:H:34:ILE:HD13	2.17	0.44
2:H:162:TRP:HA	2:H:202:THR:O	2.18	0.44
1:L:155:ARG:O	1:L:156:GLN:HG2	2.17	0.44
1:A:8:THR:HG21	1:A:11:LEU:HB2	1.99	0.44
1:A:119:PRO:HG3	1:A:209:PHE:CE2	2.52	0.44
2:B:2:VAL:HG11	2:B:110:TYR:CD1	2.53	0.44
1:L:53:ARG:HD3	1:L:53:ARG:O	2.17	0.44
1:A:11:LEU:HD12	1:A:12:SER:H	1.83	0.44
1:A:89:GLN:HE21	1:A:90:GLN:C	2.26	0.44
2:B:20:MET:HB2	4:B:235:HOH:O	2.17	0.44
2:H:50:TYR:CD2	2:H:59:LYS:HB3	2.53	0.44
2:H:125:THR:HG22	2:H:154:PHE:HB3	1.99	0.44
2:H:220:PRO:O	2:H:222:ASP:CA	2.64	0.44
1:A:140:TYR:HD2	1:A:173:TYR:CE1	2.36	0.44
2:H:2:VAL:HG12	2:H:3:GLN:N	2.33	0.44
2:H:100:VAL:O	2:H:106:TYR:HA	2.18	0.44
1:L:53:ARG:C	1:L:53:ARG:CD	2.85	0.43
2:H:143:MET:HE2	2:H:143:MET:HB3	1.89	0.43
2:B:4:LEU:HD23	2:B:24:ALA:HA	2.01	0.43
2:B:43:GLN:N	4:B:227:HOH:O	2.50	0.43
2:H:179:GLN:HB3	2:H:180:SER:H	1.54	0.43
1:A:54:LEU:HD11	2:B:102:TYR:CE2	2.54	0.43
2:B:100:VAL:HG12	2:B:101:TYR:N	2.32	0.43
2:B:129:VAL:HG13	2:B:148:CYS:SG	2.59	0.43
2:B:178:LEU:HA	2:B:182:LEU:O	2.18	0.43
2:B:196:ARG:HE	2:B:196:ARG:HB3	1.29	0.43
2:H:72:VAL:CG2	2:H:73:ASP:N	2.81	0.43
3:P:9:HIS:O	3:P:10:ASN:CB	2.66	0.43
2:B:40:ARG:O	2:B:41:PRO:C	2.61	0.43
2:B:171:VAL:CG1	2:B:172:HIS:N	2.82	0.43
2:H:127:PRO:HB3	2:H:153:TYR:CB	2.38	0.43
2:H:154:PHE:HA	2:H:155:PRO:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ASN:OD1	1:A:49:TYR:HB2	2.18	0.43
1:A:90:GLN:HG3	1:A:97:THR:OG1	2.19	0.43
2:H:171:VAL:HA	2:H:188:SER:O	2.18	0.43
1:L:41:ASP:OD1	1:L:41:ASP:C	2.62	0.43
1:L:139:PHE:HE1	1:L:142:LYS:O	2.01	0.43
1:L:31:ASN:O	1:L:51:THR:N	2.52	0.43
2:H:29:PHE:CB	2:H:77:SER:HB3	2.49	0.43
1:L:133:VAL:HG12	1:L:134:CYS:N	2.34	0.43
1:L:161:ASN:N	1:L:161:ASN:ND2	2.67	0.43
2:H:124:THR:HG21	2:H:209:ALA:C	2.42	0.43
2:B:212:THR:HA	4:B:234:HOH:O	2.19	0.42
1:L:161:ASN:HD22	1:L:161:ASN:N	2.14	0.42
1:A:106:ILE:HG22	1:A:107:LYS:N	2.34	0.42
1:A:133:VAL:CG1	1:A:134:CYS:N	2.82	0.42
1:L:114:THR:O	1:L:136:LEU:HA	2.19	0.42
1:A:89:GLN:HG3	1:A:98:PHE:CE1	2.54	0.42
2:B:29:PHE:CD2	2:B:77:SER:HA	2.54	0.42
2:B:35:ASN:HD22	2:B:108:PHE:HZ	1.67	0.42
1:L:125:LEU:O	1:L:183:LYS:HD2	2.18	0.42
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.82	0.42
2:B:153:TYR:OH	2:B:156:GLU:OE1	2.23	0.42
1:L:153:SER:HB2	1:L:154:GLU:CG	2.48	0.42
2:H:57:TYR:CE2	3:P:6:LEU:O	2.73	0.42
2:H:202:THR:HG22	2:H:203:CYS:N	2.34	0.42
2:B:36:TRP:HA	2:B:95:PHE:O	2.20	0.42
1:L:4:MET:HB2	1:L:98:PHE:O	2.19	0.42
2:H:28:THR:CG2	2:H:31:SER:OG	2.67	0.42
2:H:61:ASN:HD22	2:H:62:GLU:N	2.18	0.42
2:H:127:PRO:CB	2:H:153:TYR:HB3	2.40	0.42
2:B:16:SER:HB3	2:B:17:SER:H	1.41	0.42
2:B:35:ASN:OD1	2:B:50:TYR:CD1	2.71	0.42
2:B:158:VAL:CG2	2:B:207:HIS:HD2	2.33	0.42
1:L:55:HIS:NE2	1:L:62:PHE:O	2.52	0.42
1:L:77:ASN:OD1	1:L:77:ASN:O	2.37	0.42
1:A:50:TYR:CD2	2:B:102:TYR:CE2	3.08	0.42
1:A:116:SER:O	1:A:134:CYS:HA	2.20	0.42
2:B:35:ASN:CG	2:B:108:PHE:CE1	2.77	0.42
1:A:40:PRO:C	1:A:42:GLY:H	2.28	0.42
2:H:163:ASN:O	2:H:165:GLY:N	2.53	0.42
2:H:181:ASP:O	2:H:182:LEU:HG	2.20	0.42
1:A:31:ASN:HB3	1:A:51:THR:HG1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLY:HA3	4:A:228:HOH:O	2.19	0.42
1:L:54:LEU:HD11	2:H:102:TYR:OH	2.20	0.42
2:H:39:GLN:O	2:H:92:ALA:HB1	2.19	0.42
2:H:61:ASN:C	2:H:61:ASN:ND2	2.78	0.42
1:A:198:HIS:CE1	1:A:200:THR:HB	2.55	0.41
1:A:211:ARG:HB2	4:A:234:HOH:O	2.20	0.41
1:A:40:PRO:C	1:A:42:GLY:N	2.78	0.41
1:A:182:THR:O	1:A:183:LYS:C	2.63	0.41
2:B:39:GLN:O	2:B:92:ALA:HB1	2.20	0.41
3:P:12:ARG:NH1	3:P:12:ARG:CG	2.47	0.41
1:A:58:VAL:HA	1:A:59:PRO:HD3	1.94	0.41
1:L:150:ILE:O	1:L:151:ASP:C	2.64	0.41
2:H:10:GLU:OE1	2:H:10:GLU:HA	2.20	0.41
2:H:35:ASN:ND2	2:H:108:PHE:CE1	2.89	0.41
2:H:50:TYR:CD1	2:H:50:TYR:C	2.98	0.41
2:H:61:ASN:HA	4:H:240:HOH:O	2.21	0.41
2:H:135:GLY:HA2	2:H:221:ARG:HD3	2.01	0.41
1:A:140:TYR:HA	1:A:141:PRO:C	2.44	0.41
1:L:199:LYS:C	1:L:201:SER:N	2.78	0.41
2:H:57:TYR:HE2	3:P:6:LEU:O	2.03	0.41
1:A:184:ASP:HA	4:A:215:HOH:O	2.21	0.41
2:B:104:GLY:O	2:B:105:SER:HB2	2.20	0.41
1:A:28:ASP:OD2	1:A:28:ASP:C	2.64	0.41
2:B:19:LYS:HA	2:B:81:MET:O	2.20	0.41
1:L:144:ILE:HG13	1:L:198:HIS:HD2	1.86	0.41
1:L:161:ASN:ND2	1:L:177:SER:OG	2.53	0.41
2:B:194:SER:O	2:B:198:SER:CB	2.69	0.41
1:L:116:SER:O	1:L:134:CYS:HA	2.20	0.41
2:H:182:LEU:HA	2:H:182:LEU:HD23	1.87	0.41
1:A:9:SER:O	1:A:102:THR:HA	2.21	0.41
2:B:144:VAL:O	2:B:144:VAL:HG13	2.21	0.41
1:L:80:GLN:C	1:L:82:ASP:N	2.78	0.41
1:L:112:ALA:HA	1:L:200:THR:HG21	2.02	0.41
2:H:41:PRO:O	2:H:42:GLY:O	2.39	0.41
2:B:104:GLY:O	2:B:105:SER:CB	2.69	0.41
2:B:117:LEU:HD12	2:B:118:THR:N	2.36	0.41
1:L:4:MET:HE1	1:L:29:ILE:HD11	2.03	0.41
1:L:79:GLU:O	1:L:82:ASP:HB2	2.21	0.41
1:A:2:ILE:O	1:A:97:THR:HG21	2.20	0.40
2:B:6:GLN:OE1	2:B:95:PHE:HA	2.21	0.40
2:B:30:THR:HA	2:B:53:PRO:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:PHE:HA	2:B:175:PRO:HD3	1.89	0.40
1:L:122:SER:O	1:L:126:THR:HG22	2.21	0.40
2:H:59:LYS:HZ3	3:P:5:ASN:CA	2.17	0.40
1:A:75:ILE:O	1:A:77:ASN:N	2.55	0.40
1:A:89:GLN:HG2	1:A:97:THR:O	2.20	0.40
1:A:133:VAL:HG22	1:A:178:THR:CG2	2.29	0.40
2:B:100:VAL:HG21	2:B:109:ASP:CG	2.46	0.40
1:L:149:LYS:HB2	1:L:193:THR:HB	2.04	0.40
2:H:53:PRO:O	2:H:74:LYS:HD3	2.21	0.40
1:A:11:LEU:O	1:A:104:LEU:HA	2.21	0.40
1:A:95:PRO:HB3	2:B:61:ASN:ND2	2.34	0.40
1:A:198:HIS:C	1:A:200:THR:N	2.78	0.40
2:B:197:PRO:HB3	2:B:220:PRO:HG3	2.03	0.40
1:L:33:LEU:HD22	1:L:71:TYR:CB	2.51	0.40
1:L:50:TYR:C	1:L:51:THR:HG22	2.46	0.40
2:H:30:THR:HA	2:H:53:PRO:HB2	2.03	0.40
1:A:26:SER:C	1:A:27:GLN:CG	2.95	0.40
1:A:140:TYR:CD2	1:A:141:PRO:HA	2.56	0.40
1:L:52:SER:CB	1:L:64:GLY:C	2.93	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:GLU:OE2	1:L:188:ARG:NH1[1_465]	2.09	0.11
1:A:60:SER:OG	1:L:79:GLU:OE1[2_555]	2.17	0.03

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	212/214 (99%)	185 (87%)	18 (8%)	9 (4%)	2 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	212/214 (99%)	182 (86%)	22 (10%)	8 (4%)	2	15
2	B	214/222 (96%)	184 (86%)	19 (9%)	11 (5%)	1	10
2	H	212/222 (96%)	184 (87%)	16 (8%)	12 (6%)	1	8
3	P	8/12 (67%)	3 (38%)	3 (38%)	2 (25%)	0	0
All	All	858/884 (97%)	738 (86%)	78 (9%)	42 (5%)	1	10

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	GLU
2	B	43	GLN
2	B	89	GLU
2	B	105	SER
1	L	8	THR
1	L	76	SER
2	H	22	CYS
2	H	44	GLY
2	H	62	GLU
2	H	74	LYS
2	H	164	SER
2	H	221	ARG
3	P	5	ASN
3	P	10	ASN
1	A	8	THR
1	A	53	ARG
1	A	76	SER
2	B	16	SER
2	B	102	TYR
1	L	68	GLY
2	H	42	GLY
2	H	43	GLN
1	A	57	GLY
2	B	62	GLU
2	B	104	GLY
1	L	50	TYR
1	L	53	ARG
1	L	112	ALA
1	A	50	TYR
1	A	112	ALA
1	A	155	ARG
2	B	92	ALA

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Mol	Chain	Res	Type
2	B	179	GLN
1	L	57	GLY
2	H	92	ALA
2	H	122	ALA
1	L	154	GLU
2	H	41	PRO
2	H	127	PRO
2	B	18	VAL
2	B	48	ILE
1	A	68	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/192 (97%)	168 (90%)	19 (10%)	7	29
1	L	190/192 (99%)	164 (86%)	26 (14%)	3	17
2	B	181/190 (95%)	163 (90%)	18 (10%)	7	30
2	H	184/190 (97%)	154 (84%)	30 (16%)	2	12
3	P	9/11 (82%)	6 (67%)	3 (33%)	0	1
All	All	751/775 (97%)	655 (87%)	96 (13%)	4	19

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	10	SER
1	A	14	SER
1	A	27	GLN
1	A	29	ILE
1	A	52	SER
1	A	58	VAL
1	A	60	SER
1	A	63	SER

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Mol	Chain	Res	Type
1	A	94	LEU
1	A	105	GLU
1	A	107	LYS
1	A	142	LYS
1	A	145	ASN
1	A	157	ASN
1	A	178	THR
1	A	199	LYS
1	A	205	ILE
1	A	213	GLU
2	B	7	SER
2	B	55	ASN
2	B	62	GLU
2	B	106	TYR
2	B	113	GLN
2	B	116	THR
2	B	118	THR
2	B	142	SER
2	B	159	THR
2	B	168	SER
2	B	185	LEU
2	B	186	SER
2	B	193	SER
2	B	194	SER
2	B	196	ARG
2	B	212	THR
2	B	216	LYS
2	B	219	VAL
1	L	7	THR
1	L	14	SER
1	L	53	ARG
1	L	58	VAL
1	L	61	ARG
1	L	63	SER
1	L	69	THR
1	L	77	ASN
1	L	79	GLU
1	L	96	ARG
1	L	97	THR
1	L	104	LEU
1	L	105	GLU
1	L	108	ARG

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Mol	Chain	Res	Type
1	L	123	GLU
1	L	126	THR
1	L	127	SER
1	L	145	ASN
1	L	154	GLU
1	L	165	ASP
1	L	176	SER
1	L	179	LEU
1	L	200	THR
1	L	201	SER
1	L	211	ARG
1	L	214	CYS
2	H	7	SER
2	H	11	LEU
2	H	25	SER
2	H	40	ARG
2	H	45	LEU
2	H	50	TYR
2	H	52	ASN
2	H	55	ASN
2	H	61	ASN
2	H	69	THR
2	H	72	VAL
2	H	77	SER
2	H	87	THR
2	H	106	TYR
2	H	113	GLN
2	H	118	THR
2	H	123	LYS
2	H	127	PRO
2	H	144	VAL
2	H	158	VAL
2	H	166	SER
2	H	179	GLN
2	H	185	LEU
2	H	196	ARG
2	H	200	THR
2	H	204	ASN
2	H	205	VAL
2	H	216	LYS
2	H	221	ARG
2	H	222	ASP

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Mol	Chain	Res	Type
3	P	6	LEU
3	P	10	ASN
3	P	12	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	31	ASN
1	A	37	GLN
1	A	55	HIS
1	A	77	ASN
1	A	92	ASN
1	A	157	ASN
1	A	161	ASN
1	A	190	ASN
2	B	3	GLN
2	B	35	ASN
2	B	52	ASN
2	B	61	ASN
2	B	82	GLN
2	B	113	GLN
1	L	6	GLN
1	L	31	ASN
1	L	161	ASN
1	L	189	HIS
2	H	6	GLN
2	H	52	ASN
2	H	55	ASN
2	H	61	ASN
2	H	113	GLN
2	H	172	HIS
3	P	5	ASN
3	P	8	ASN
3	P	9	HIS
3	P	10	ASN

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 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](#)

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, 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	214/214 (100%)	0.37	5 (2%) 61 38	12, 32, 56, 63	0
1	L	214/214 (100%)	0.29	8 (3%) 45 25	10, 30, 48, 60	0
2	B	218/222 (98%)	0.45	6 (2%) 55 32	8, 38, 58, 68	0
2	H	216/222 (97%)	0.31	7 (3%) 50 29	1, 31, 54, 65	0
3	P	10/12 (83%)	1.33	1 (10%) 12 7	35, 44, 51, 58	0
All	All	872/884 (98%)	0.37	27 (3%) 51 30	1, 33, 56, 68	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	222	ASP	4.4
1	L	52	SER	3.4
1	L	213	GLU	3.1
2	B	222	ASP	2.9
2	H	170	GLY	2.8
2	H	43	GLN	2.7
3	P	3	GLY	2.6
1	A	2	ILE	2.5
2	B	50	TYR	2.5
1	L	6	GLN	2.4
1	A	93	THR	2.4
1	L	77	ASN	2.4
2	B	88	SER	2.4
1	L	214	CYS	2.4
1	A	29	ILE	2.3
2	H	54	GLY	2.2
1	A	107	LYS	2.2
2	H	103	GLY	2.2
1	L	168	SER	2.1
2	B	105	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	55	HIS	2.1
2	B	101	TYR	2.1
1	L	29	ILE	2.1
1	A	214	CYS	2.1
2	H	102	TYR	2.1
2	H	104	GLY	2.1
2	B	48	ILE	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.