



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:01 PM UTC

PDB ID : 2A6D / pdb_00002a6d
Title : Crystal structure analysis of the anti-arsonate germline antibody 36-65 in complex with a phage display derived dodecapeptide RLLIADPPSPRE
Authors : Sethi, D.K.; Agarwal, A.; Manivel, V.; Rao, K.V.; Salunke, D.M.
Deposited on : 2005-07-02
Resolution : 2.90 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

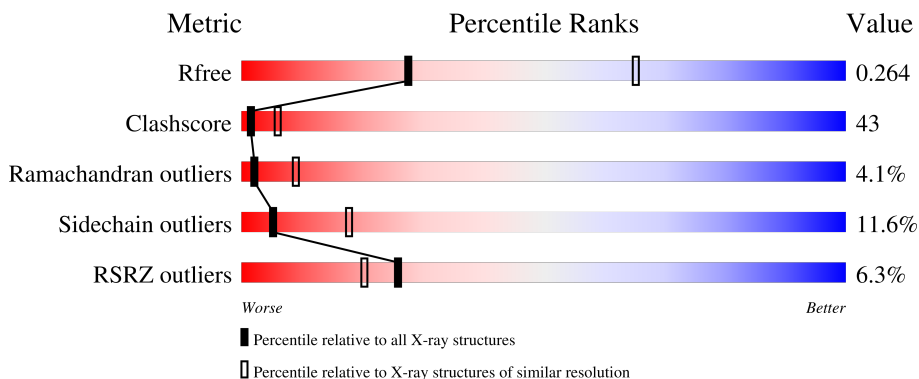
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	7% 42% 47% 11% .
1	L	214	7% 43% 46% 10% .
2	B	222	4% 49% 37% 12% .
2	H	222	9% 39% 49% 10% .
3	P	12	67% 33% 33% 33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6792 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	L	214	Total	C	N	O	S	0	0	0
			1659	1025	284	343	7			
1	A	214	Total	C	N	O	S	0	0	0
			1660	1025	284	344	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1648	1046	270	325	7			
2	B	219	Total	C	N	O	S	0	0	0
			1651	1047	270	327	7			

- Molecule 3 is a protein called Dodecapeptide, RLLIADPPSPRE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	12	Total	C	N	O	0	0	0
			96	60	18	18			

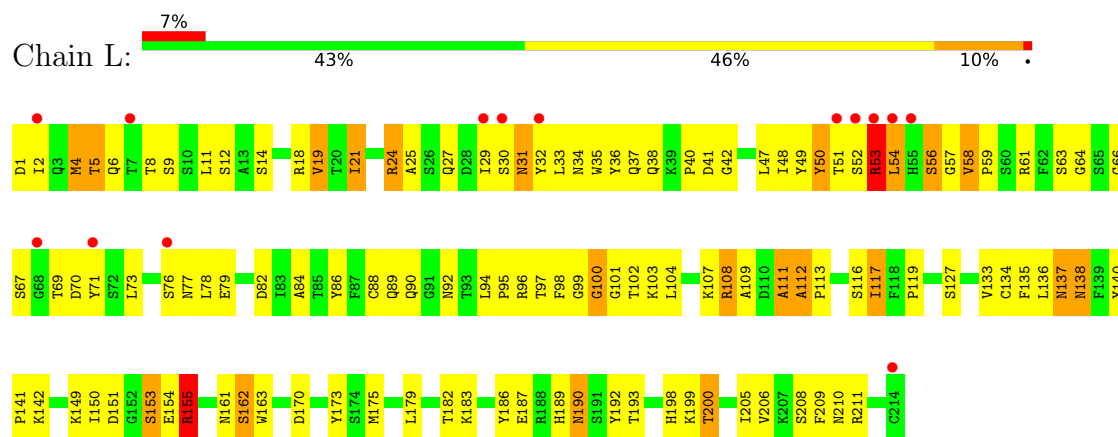
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	24	Total	O	0	0
			24	24		
4	H	20	Total	O	0	0
			20	20		
4	A	19	Total	O	0	0
			19	19		
4	B	15	Total	O	0	0
			15	15		

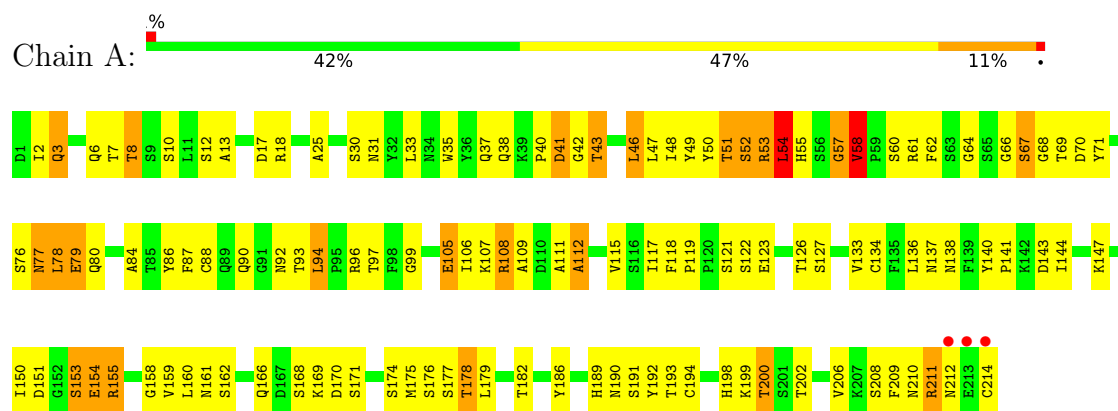
3 Residue-property plots

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.

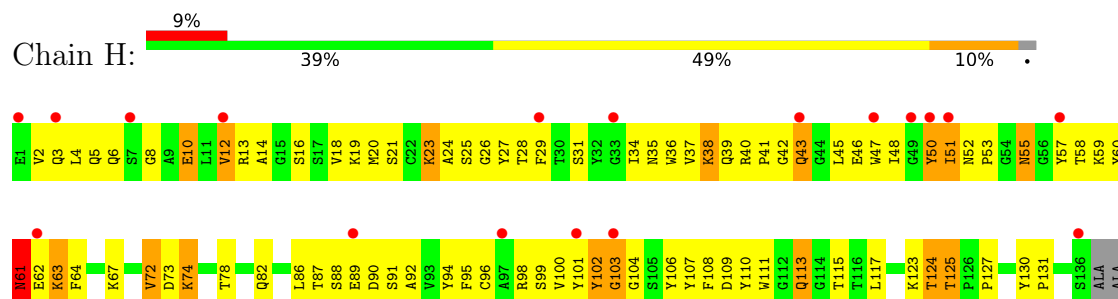
• Molecule 1: Germline antibody 36-65 Fab light chain

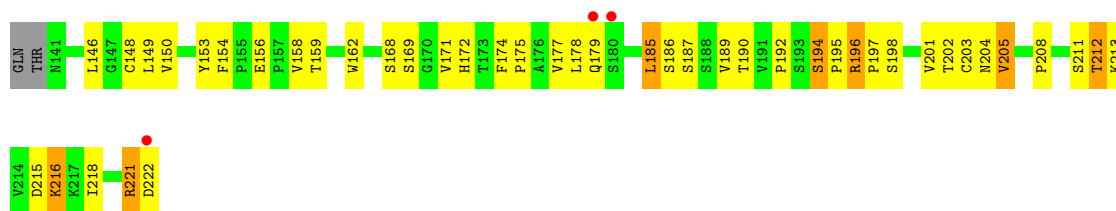


• Molecule 1: Germline antibody 36-65 Fab light chain

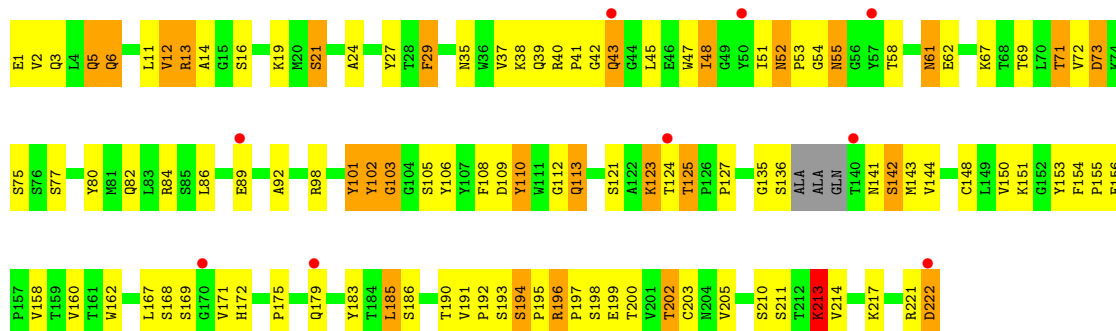


• Molecule 2: Germline antibody 36-65 Fab Heavy chain

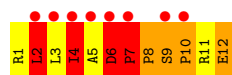




● Molecule 2: Germline antibody 36-65 Fab Heavy chain



● Molecule 3: Dodecapeptide, RLLIADPPSPRE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.30Å 145.67Å 71.35Å 90.00° 104.43° 90.00°	Depositor
Resolution (Å)	100.00 – 2.90 72.83 – 2.90	Depositor EDS
% Data completeness (in resolution range)	77.4 (100.00-2.90) 77.4 (72.83-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.62 (at 2.91Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.230 , 0.264 0.230 , 0.264	Depositor DCC
R_{free} test set	1787 reflections (9.21%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6792	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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 [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.70	0/1693	1.18	16/2295 (0.7%)
1	L	0.71	0/1692	1.18	15/2294 (0.7%)
2	B	0.70	0/1694	1.15	13/2310 (0.6%)
2	H	0.72	2/1691 (0.1%)	1.11	13/2304 (0.6%)
3	P	1.98	4/98 (4.1%)	3.21	6/132 (4.5%)
All	All	0.74	6/6868 (0.1%)	1.21	63/9335 (0.7%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	7	PRO	CA-C	7.62	1.59	1.52
2	H	20	MET	SD-CE	-7.12	1.61	1.79
3	P	6	ASP	C-O	-6.68	1.19	1.25
3	P	4	ILE	CA-CB	6.06	1.62	1.54
2	H	28	THR	CA-CB	5.73	1.59	1.52
3	P	7	PRO	C-N	5.59	1.41	1.34

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	7	PRO	N-CA-C	27.69	144.48	110.70
3	P	4	ILE	N-CA-C	11.27	132.79	109.34
2	H	91	SER	N-CA-C	-8.77	94.43	108.73
1	A	137	ASN	N-CA-C	8.01	123.06	110.17
1	A	17	ASP	N-CA-C	-7.63	97.47	109.07
1	L	153	SER	N-CA-C	7.45	119.02	108.74
1	L	190	ASN	N-CA-C	7.30	122.25	111.96
2	B	213	LYS	N-CA-C	-7.24	97.16	109.24
1	A	115	VAL	N-CA-C	7.09	119.08	108.23
1	L	5	THR	N-CA-C	6.51	119.02	108.41
2	B	156	GLU	N-CA-C	-6.46	100.63	110.07
1	A	94	LEU	N-CA-C	-6.42	101.98	110.07
1	A	127	SER	N-CA-C	-6.42	105.49	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	67	LYS	N-CA-C	-6.41	104.50	112.90
2	B	125	THR	CA-C-N	6.19	124.12	119.66
2	B	125	THR	C-N-CA	6.19	124.12	119.66
1	A	18	ARG	N-CA-C	-6.14	99.19	108.96
1	L	111	ALA	N-CA-C	6.14	120.58	112.72
2	B	151	LYS	N-CA-C	6.10	119.64	109.95
1	A	170	ASP	N-CA-C	-6.06	101.81	110.59
1	L	170	ASP	N-CA-C	-6.06	100.43	109.94
1	L	19	VAL	N-CA-C	6.03	116.98	108.36
2	H	194	SER	CA-C-N	6.00	125.55	119.19
2	H	194	SER	C-N-CA	6.00	125.55	119.19
1	A	206	VAL	N-CA-C	5.93	116.42	108.11
3	P	2	LEU	N-CA-C	-5.90	98.23	110.80
1	L	21	ILE	N-CA-C	-5.89	99.85	108.97
2	H	10	GLU	N-CA-C	5.87	118.78	109.50
1	L	127	SER	N-CA-C	-5.85	105.64	112.89
2	B	135	GLY	N-CA-C	-5.83	105.60	113.24
2	H	12	VAL	N-CA-C	5.81	116.66	108.17
1	L	137	ASN	N-CA-C	5.80	119.71	109.96
3	P	8	PRO	N-CA-C	-5.80	106.12	114.18
1	A	190	ASN	N-CA-C	5.76	120.08	111.96
1	A	54	LEU	N-CA-C	5.74	118.58	109.96
1	A	178	THR	N-CA-C	5.74	117.59	107.61
1	L	54	LEU	N-CA-C	5.71	118.53	109.96
1	L	31	ASN	N-CA-C	5.70	119.54	112.58
1	A	182	THR	N-CA-C	-5.67	101.63	110.42
2	H	88	SER	N-CA-C	-5.66	106.33	113.18
1	A	76	SER	N-CA-C	5.63	117.41	111.28
1	L	155	ARG	N-CA-C	5.59	122.71	110.80
2	H	61	ASN	N-CA-C	-5.57	98.68	108.20
2	B	110	TYR	N-CA-C	5.52	117.40	108.34
3	P	7	PRO	CB-CA-C	-5.48	104.23	110.92
2	B	12	VAL	N-CA-C	5.47	116.16	108.17
2	H	103	GLY	N-CA-C	5.46	126.13	113.18
2	B	101	TYR	N-CA-C	5.46	122.44	110.80
2	B	103	GLY	N-CA-C	5.37	125.91	113.18
1	A	78	LEU	N-CA-C	5.34	118.18	110.28
2	H	31	SER	N-CA-C	5.30	119.59	113.18
1	A	58	VAL	CA-C-N	5.29	125.58	119.92
1	A	58	VAL	C-N-CA	5.29	125.58	119.92
3	P	6	ASP	N-CA-C	-5.29	97.31	108.73
1	L	206	VAL	N-CA-C	5.27	115.45	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	202	THR	N-CA-C	5.23	117.77	109.50
1	L	27	GLN	N-CA-C	5.19	114.99	108.45
2	H	23	LYS	N-CA-C	5.17	117.15	108.73
2	B	112	GLY	N-CA-C	-5.11	104.18	112.31
2	B	29	PHE	N-CA-C	5.09	117.49	111.33
2	H	156	GLU	N-CA-C	-5.07	101.65	109.87
1	L	24	ARG	N-CA-C	5.01	117.07	108.90
2	B	55	ASN	N-CA-C	5.01	121.12	113.61

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	1660	0	1582	119	0
1	L	1659	0	1579	164	0
2	B	1651	0	1599	105	0
2	H	1648	0	1603	145	0
3	P	96	0	102	53	0
4	A	19	0	0	7	0
4	B	15	0	0	4	0
4	H	20	0	0	4	0
4	L	24	0	0	6	0
All	All	6792	0	6465	561	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 43.

All (561) 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:ILE:HD11	3:P:8:PRO:CD	1.78	1.13
3:P:4:ILE:HD11	3:P:8:PRO:HD3	1.25	1.12
3:P:4:ILE:CD1	3:P:8:PRO:HD3	1.81	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:38:LYS:HD2	2:H:94:TYR:CE2	1.90	1.06
2:H:51:ILE:HD11	2:H:72:VAL:CG2	1.87	1.05
3:P:2:LEU:HD22	3:P:9:SER:O	1.58	1.03
1:A:96:ARG:HH22	3:P:7:PRO:HD2	1.24	1.03
2:H:146:LEU:HD23	2:H:218:ILE:HG21	1.39	1.03
2:H:51:ILE:HD11	2:H:72:VAL:HG22	1.37	1.02
3:P:4:ILE:CG2	3:P:5:ALA:H	1.69	1.02
3:P:4:ILE:HG22	3:P:5:ALA:N	1.73	0.99
2:H:6:GLN:H	2:H:113:GLN:NE2	1.59	0.99
2:B:6:GLN:H	2:B:113:GLN:HE22	1.10	0.99
2:H:24:ALA:HB1	2:H:27:TYR:HE2	1.28	0.99
3:P:4:ILE:CD1	3:P:8:PRO:CD	2.40	0.97
1:L:138:ASN:N	1:L:138:ASN:HD22	1.61	0.97
1:L:112:ALA:HB2	1:L:200:THR:HG21	1.45	0.96
3:P:2:LEU:CD2	3:P:9:SER:O	2.13	0.96
2:B:6:GLN:H	2:B:113:GLN:NE2	1.63	0.96
2:H:6:GLN:H	2:H:113:GLN:HE22	1.00	0.95
2:H:35:ASN:HD22	2:H:47:TRP:HE1	1.14	0.95
3:P:4:ILE:CG2	3:P:5:ALA:N	2.23	0.95
1:L:56:SER:HB3	4:L:215:HOH:O	1.68	0.93
2:H:192:PRO:O	2:H:195:PRO:HD2	1.68	0.92
1:L:5:THR:HG21	1:L:24:ARG:HH21	1.35	0.91
3:P:4:ILE:HG23	3:P:5:ALA:H	1.36	0.91
1:L:154:GLU:HG3	1:L:155:ARG:N	1.85	0.90
2:B:192:PRO:HD2	2:B:195:PRO:HG2	1.54	0.90
2:H:53:PRO:O	2:H:74:LYS:HD3	1.72	0.88
2:H:6:GLN:N	2:H:113:GLN:HE22	1.70	0.88
2:H:192:PRO:HD2	2:H:195:PRO:HG2	1.55	0.88
1:A:52:SER:HB3	1:A:64:GLY:C	1.98	0.88
2:H:90:ASP:O	2:H:117:LEU:HD23	1.75	0.87
1:L:112:ALA:CB	1:L:200:THR:HG21	2.05	0.87
1:L:140:TYR:CD2	1:L:141:PRO:HA	2.10	0.86
2:B:61:ASN:HD22	2:B:62:GLU:N	1.72	0.86
1:A:159:VAL:O	1:A:160:LEU:HD23	1.78	0.84
1:L:57:GLY:HA3	4:L:235:HOH:O	1.77	0.84
1:L:29:ILE:HA	1:L:92:ASN:HD22	1.40	0.84
2:B:13:ARG:HH21	2:B:14:ALA:HB3	1.42	0.83
2:H:51:ILE:CD1	2:H:72:VAL:HG22	2.09	0.82
1:L:31:ASN:HB3	1:L:51:THR:HB	1.61	0.82
1:L:53:ARG:HH11	1:L:54:LEU:HD23	1.44	0.82
1:L:37:GLN:HG3	1:L:86:TYR:CE2	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:LYS:HG2	4:B:227:HOH:O	1.82	0.79
2:H:38:LYS:HD2	2:H:94:TYR:HE2	1.48	0.79
1:A:51:THR:O	1:A:52:SER:HB2	1.83	0.79
2:H:55:ASN:HD22	2:H:57:TYR:CB	1.95	0.78
2:B:192:PRO:O	2:B:195:PRO:HD2	1.83	0.78
3:P:4:ILE:HD12	3:P:7:PRO:CA	2.12	0.78
2:B:3:GLN:HG3	2:B:5:GLN:HE21	1.46	0.78
2:H:107:TYR:HE1	2:H:109:ASP:HB3	1.49	0.78
1:L:89:GLN:HB2	1:L:98:PHE:CD1	2.19	0.78
2:H:24:ALA:HB1	2:H:27:TYR:CE2	2.16	0.77
2:B:6:GLN:N	2:B:113:GLN:HE22	1.83	0.77
1:A:94:LEU:HG	3:P:7:PRO:O	1.84	0.77
3:P:4:ILE:HD11	3:P:8:PRO:HD2	1.63	0.77
2:H:38:LYS:CD	2:H:94:TYR:CE2	2.68	0.76
1:L:136:LEU:N	1:L:136:LEU:HD12	2.00	0.76
2:B:196:ARG:HD2	2:B:197:PRO:HA	1.66	0.76
1:A:94:LEU:H	3:P:8:PRO:HA	1.52	0.75
1:A:6:GLN:HE21	1:A:99:GLY:HA3	1.50	0.74
1:A:154:GLU:O	1:A:155:ARG:CB	2.35	0.74
2:B:202:THR:HB	2:B:217:LYS:HA	1.68	0.74
2:H:40:ARG:NH2	2:H:89:GLU:HA	2.02	0.74
3:P:2:LEU:HB3	3:P:10:PRO:HB3	1.69	0.74
2:H:35:ASN:ND2	2:H:47:TRP:HE1	1.85	0.73
1:L:29:ILE:HG22	1:L:32:TYR:H	1.54	0.73
2:H:192:PRO:C	2:H:195:PRO:HD2	2.12	0.73
2:B:192:PRO:C	2:B:195:PRO:HD2	2.13	0.73
2:H:46:GLU:OE1	2:H:64:PHE:HZ	1.72	0.72
2:H:146:LEU:HD23	2:H:218:ILE:CG2	2.16	0.72
2:B:127:PRO:HB3	2:B:153:TYR:HB3	1.72	0.72
2:B:61:ASN:HD22	2:B:61:ASN:C	1.95	0.72
1:A:57:GLY:HA3	4:A:225:HOH:O	1.89	0.72
2:B:52:ASN:HD22	2:B:54:GLY:H	1.37	0.72
1:L:31:ASN:CB	1:L:51:THR:HB	2.18	0.72
1:A:47:LEU:HA	1:A:58:VAL:HG11	1.71	0.71
1:L:6:GLN:HE21	1:L:99:GLY:C	1.99	0.71
2:B:185:LEU:HD12	2:B:186:SER:N	2.05	0.71
3:P:4:ILE:HD12	3:P:7:PRO:CB	2.21	0.71
2:H:55:ASN:ND2	2:H:57:TYR:HB3	2.05	0.70
3:P:2:LEU:HD23	3:P:9:SER:C	2.15	0.70
1:L:49:TYR:CE2	1:L:54:LEU:HD13	2.26	0.70
2:H:2:VAL:HG21	2:H:110:TYR:HE1	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:55:ASN:HD22	2:H:57:TYR:HB2	1.57	0.69
1:L:25:ALA:O	1:L:69:THR:HG23	1.92	0.69
2:H:89:GLU:HB2	4:H:233:HOH:O	1.92	0.69
1:L:67:SER:HA	1:L:71:TYR:HE2	1.57	0.69
2:B:39:GLN:O	2:B:92:ALA:HB1	1.91	0.69
3:P:4:ILE:HG21	3:P:6:ASP:C	2.18	0.69
3:P:4:ILE:HG21	3:P:7:PRO:N	2.08	0.69
1:L:6:GLN:HE21	1:L:99:GLY:HA3	1.57	0.69
2:H:185:LEU:C	2:H:185:LEU:HD12	2.17	0.69
2:H:72:VAL:HG12	2:H:73:ASP:H	1.58	0.68
2:B:35:ASN:HD22	2:B:47:TRP:HE1	1.39	0.68
1:A:41:ASP:OD1	1:A:43:THR:HG23	1.93	0.68
1:A:50:TYR:O	1:A:52:SER:O	2.10	0.68
1:L:5:THR:CG2	1:L:24:ARG:HH21	2.04	0.68
1:L:142:LYS:HB3	1:L:173:TYR:CZ	2.28	0.68
3:P:3:LEU:O	3:P:4:ILE:HB	1.94	0.68
2:B:42:GLY:O	2:B:43:GLN:O	2.11	0.68
2:B:12:VAL:HG21	2:B:86:LEU:CD1	2.23	0.68
1:L:31:ASN:HD22	1:L:51:THR:HG21	1.59	0.67
2:B:29:PHE:CD2	2:B:77:SER:HA	2.30	0.67
1:L:53:ARG:NH1	1:L:54:LEU:HD23	2.10	0.67
1:A:199:LYS:NZ	4:A:232:HOH:O	2.27	0.67
1:L:48:ILE:CG2	1:L:52:SER:HA	2.25	0.67
1:L:198:HIS:ND1	1:L:200:THR:HB	2.09	0.66
2:H:38:LYS:HD2	2:H:94:TYR:CZ	2.30	0.66
2:B:106:TYR:HE2	3:P:5:ALA:O	1.78	0.66
1:A:111:ALA:O	1:A:112:ALA:HB3	1.96	0.66
2:H:194:SER:OG	2:H:195:PRO:HD3	1.95	0.66
1:L:5:THR:HG21	1:L:24:ARG:NH2	2.08	0.66
1:L:138:ASN:HD22	1:L:138:ASN:H	1.41	0.66
1:L:6:GLN:HE21	1:L:99:GLY:CA	2.09	0.65
1:L:151:ASP:OD2	1:L:189:HIS:HB3	1.97	0.65
1:L:94:LEU:HD13	2:H:59:LYS:HE2	1.79	0.64
1:L:94:LEU:HB3	4:L:220:HOH:O	1.97	0.64
1:L:150:ILE:HD12	1:L:155:ARG:HD3	1.79	0.64
1:L:12:SER:HB3	1:L:107:LYS:CD	2.28	0.64
2:H:39:GLN:O	2:H:92:ALA:HB1	1.97	0.64
1:L:50:TYR:O	1:L:52:SER:O	2.16	0.64
1:L:138:ASN:N	1:L:138:ASN:ND2	2.35	0.64
3:P:2:LEU:HD23	3:P:9:SER:O	1.97	0.64
1:L:52:SER:O	1:L:53:ARG:HB3	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:50:TYR:CD1	2:H:51:ILE:N	2.67	0.63
1:L:154:GLU:HG3	1:L:155:ARG:H	1.63	0.63
2:B:13:ARG:NH2	2:B:14:ALA:HB3	2.12	0.63
1:L:48:ILE:HG21	1:L:52:SER:HA	1.80	0.63
2:H:63:LYS:HE2	2:H:64:PHE:CE2	2.34	0.63
1:L:52:SER:O	1:L:53:ARG:CB	2.46	0.63
2:H:58:THR:HG1	2:H:60:TYR:HE1	1.45	0.63
1:A:31:ASN:O	1:A:51:THR:HB	1.98	0.63
2:B:51:ILE:O	2:B:53:PRO:HD3	1.98	0.63
2:H:19:LYS:HG2	2:H:82:GLN:HG3	1.81	0.62
2:H:52:ASN:ND2	4:H:235:HOH:O	2.30	0.62
1:A:31:ASN:ND2	1:A:51:THR:HG21	2.13	0.62
2:B:3:GLN:CG	2:B:5:GLN:HE21	2.11	0.62
1:L:142:LYS:HB3	1:L:173:TYR:CE2	2.33	0.62
1:L:117:ILE:H	1:L:117:ILE:HD12	1.63	0.62
1:A:153:SER:O	1:A:154:GLU:O	2.18	0.62
3:P:3:LEU:O	3:P:4:ILE:CB	2.48	0.62
2:H:2:VAL:HG21	2:H:110:TYR:CE1	2.33	0.62
2:H:55:ASN:HD22	2:H:57:TYR:HB3	1.59	0.62
1:L:108:ARG:HB3	1:L:140:TYR:CD1	2.35	0.62
2:B:24:ALA:HB1	2:B:27:TYR:HE2	1.64	0.62
1:L:135:PHE:C	1:L:136:LEU:HD12	2.25	0.62
1:L:111:ALA:O	1:L:112:ALA:HB3	1.99	0.62
2:B:123:LYS:O	2:B:125:THR:HG23	2.00	0.62
1:L:49:TYR:CE1	1:L:54:LEU:HB3	2.35	0.61
1:A:51:THR:O	1:A:52:SER:CB	2.48	0.61
1:A:92:ASN:O	3:P:9:SER:HA	2.00	0.61
2:B:51:ILE:HD12	2:B:58:THR:HG22	1.82	0.61
2:B:192:PRO:HB2	2:B:195:PRO:HD3	1.81	0.61
1:L:149:LYS:HB2	1:L:193:THR:HB	1.80	0.61
2:H:101:TYR:HD1	2:H:106:TYR:CE1	2.17	0.61
3:P:4:ILE:CG2	3:P:6:ASP:N	2.64	0.61
2:H:46:GLU:OE1	2:H:64:PHE:CZ	2.53	0.61
3:P:2:LEU:CD2	3:P:9:SER:C	2.72	0.61
1:L:49:TYR:CD2	2:H:107:TYR:CE2	2.89	0.61
2:B:38:LYS:HB2	2:B:48:ILE:HD11	1.83	0.61
1:A:6:GLN:HE22	1:A:87:PHE:HA	1.65	0.61
3:P:11:ARG:O	3:P:12:GLU:C	2.44	0.61
1:L:67:SER:CA	1:L:71:TYR:CE2	2.83	0.61
2:B:148:CYS:HB2	2:B:162:TRP:HH2	1.64	0.60
2:H:146:LEU:CD2	2:H:218:ILE:HG21	2.23	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:50:TYR:HB3	1:L:54:LEU:HD12	1.81	0.60
2:H:86:LEU:HD23	2:H:90:ASP:OD2	2.01	0.60
2:B:24:ALA:HB1	2:B:27:TYR:CE2	2.36	0.60
3:P:4:ILE:HD12	3:P:8:PRO:CD	2.29	0.60
1:L:67:SER:CA	1:L:71:TYR:HE2	2.13	0.59
1:L:119:PRO:HG3	1:L:209:PHE:CE2	2.38	0.59
3:P:8:PRO:O	3:P:9:SER:HB3	2.02	0.59
1:L:61:ARG:HH11	1:L:82:ASP:CG	2.10	0.59
2:B:62:GLU:OE1	4:B:237:HOH:O	2.16	0.59
2:H:37:VAL:HG13	2:H:46:GLU:O	2.03	0.59
2:H:127:PRO:HB3	2:H:153:TYR:HB3	1.85	0.59
1:L:51:THR:O	1:L:52:SER:HB2	2.01	0.59
2:B:61:ASN:C	2:B:61:ASN:ND2	2.60	0.59
2:B:3:GLN:CG	2:B:5:GLN:NE2	2.66	0.59
1:L:67:SER:N	1:L:71:TYR:CE2	2.71	0.58
1:L:112:ALA:HB2	1:L:200:THR:CG2	2.29	0.58
2:H:89:GLU:O	2:H:89:GLU:HG2	2.01	0.58
1:L:32:TYR:OH	2:H:104:GLY:HA3	2.02	0.58
2:H:38:LYS:CD	2:H:94:TYR:HE2	2.11	0.58
1:A:31:ASN:O	1:A:51:THR:N	2.37	0.58
1:L:6:GLN:NE2	1:L:101:GLY:H	2.02	0.58
2:H:192:PRO:HB2	2:H:195:PRO:CD	2.34	0.58
1:A:93:THR:CB	3:P:9:SER:HB3	2.34	0.58
2:B:150:VAL:HB	2:B:185:LEU:HG	1.84	0.58
3:P:4:ILE:CD1	3:P:8:PRO:HD2	2.22	0.58
1:L:31:ASN:CA	1:L:51:THR:HB	2.34	0.58
3:P:4:ILE:CD1	3:P:7:PRO:CA	2.81	0.58
1:A:13:ALA:HA	1:A:107:LYS:HE3	1.86	0.57
1:L:4:MET:SD	1:L:90:GLN:HB3	2.45	0.57
1:L:21:ILE:HG23	1:L:102:THR:HG21	1.86	0.57
1:A:93:THR:CB	3:P:8:PRO:O	2.51	0.57
1:A:143:ASP:HA	4:A:226:HOH:O	2.03	0.57
1:L:154:GLU:CG	1:L:155:ARG:H	2.13	0.57
2:H:171:VAL:HG22	2:H:189:VAL:HG23	1.86	0.57
2:B:113:GLN:NE2	2:B:113:GLN:H	2.03	0.57
2:B:148:CYS:HB2	2:B:162:TRP:CH2	2.39	0.57
2:H:172:HIS:O	2:H:187:SER:HA	2.03	0.57
2:H:50:TYR:OH	2:H:52:ASN:HB2	2.04	0.57
1:L:89:GLN:HB2	1:L:98:PHE:CE1	2.38	0.57
2:B:192:PRO:HB2	2:B:195:PRO:CD	2.34	0.57
1:A:96:ARG:NH2	3:P:7:PRO:HD2	2.08	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:30:SER:HA	4:L:216:HOH:O	2.03	0.56
2:B:6:GLN:CB	2:B:113:GLN:HE22	2.18	0.56
1:A:140:TYR:HA	1:A:141:PRO:O	2.05	0.56
2:B:82:GLN:HE21	2:B:84:ARG:HH11	1.53	0.56
1:L:4:MET:HE3	1:L:25:ALA:HA	1.88	0.56
1:L:78:LEU:CD1	1:L:82:ASP:HB2	2.35	0.56
2:B:102:TYR:C	2:B:102:TYR:CD2	2.83	0.56
3:P:4:ILE:CG2	3:P:6:ASP:C	2.79	0.56
2:B:40:ARG:NH1	2:B:89:GLU:HA	2.21	0.56
1:A:90:GLN:HE21	1:A:97:THR:H	1.54	0.56
2:B:194:SER:N	2:B:195:PRO:CD	2.69	0.56
2:B:12:VAL:CG2	2:B:86:LEU:CD1	2.84	0.55
2:H:37:VAL:HG11	2:H:45:LEU:HB3	1.88	0.55
1:A:53:ARG:CZ	1:A:54:LEU:HD22	2.36	0.55
1:A:159:VAL:C	1:A:160:LEU:HD23	2.31	0.55
1:A:93:THR:HA	3:P:8:PRO:C	2.32	0.55
1:A:33:LEU:HD22	1:A:71:TYR:CB	2.37	0.55
2:B:52:ASN:ND2	4:B:230:HOH:O	2.26	0.55
1:A:147:LYS:HE2	1:A:154:GLU:OE1	2.06	0.55
1:A:154:GLU:O	1:A:155:ARG:HB2	2.06	0.55
1:L:190:ASN:HD21	1:L:210:ASN:HB3	1.72	0.55
1:L:31:ASN:HB3	1:L:51:THR:CB	2.35	0.55
2:H:14:ALA:C	2:H:16:SER:H	2.13	0.55
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.72	0.55
1:A:151:ASP:OD2	1:A:189:HIS:HB3	2.07	0.55
1:L:49:TYR:CE2	1:L:54:LEU:CD1	2.90	0.54
2:H:12:VAL:HG11	2:H:18:VAL:CG2	2.37	0.54
2:H:196:ARG:HD2	2:H:197:PRO:HA	1.88	0.54
1:A:140:TYR:HA	1:A:141:PRO:C	2.32	0.54
1:L:33:LEU:HD22	1:L:71:TYR:CD1	2.42	0.54
1:L:49:TYR:CZ	1:L:54:LEU:HD13	2.43	0.54
1:L:2:ILE:HG21	1:L:29:ILE:HD11	1.90	0.54
1:L:67:SER:HA	1:L:71:TYR:CE2	2.42	0.54
1:L:199:LYS:HB3	4:L:233:HOH:O	2.07	0.54
2:H:90:ASP:O	2:H:117:LEU:CD2	2.53	0.54
1:A:161:ASN:ND2	1:A:177:SER:OG	2.41	0.54
1:L:161:ASN:HD22	1:L:175:MET:HE2	1.72	0.54
2:H:23:LYS:HG3	2:H:78:THR:OG1	2.07	0.54
1:A:202:THR:HB	4:A:229:HOH:O	2.08	0.54
1:L:78:LEU:HD12	1:L:79:GLU:H	1.71	0.54
2:B:6:GLN:HG3	2:B:113:GLN:NE2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TRP:CZ3	1:A:88:CYS:HB3	2.43	0.54
2:H:12:VAL:HG11	2:H:18:VAL:HG22	1.88	0.53
1:L:90:GLN:HE21	1:L:97:THR:H	1.55	0.53
2:B:40:ARG:HH12	2:B:89:GLU:HA	1.73	0.53
3:P:8:PRO:O	3:P:9:SER:CB	2.56	0.53
2:B:12:VAL:CG2	2:B:86:LEU:HD13	2.39	0.53
1:L:61:ARG:NH1	1:L:82:ASP:OD1	2.42	0.53
2:B:195:PRO:O	2:B:199:GLU:HB2	2.08	0.53
1:L:31:ASN:O	1:L:51:THR:HB	2.09	0.53
1:A:140:TYR:C	1:A:140:TYR:CD1	2.87	0.53
1:A:154:GLU:O	1:A:155:ARG:HB3	2.07	0.53
2:H:34:ILE:HB	2:H:51:ILE:HG23	1.90	0.53
1:L:40:PRO:C	1:L:42:GLY:H	2.16	0.53
1:L:153:SER:O	1:L:154:GLU:HG2	2.08	0.53
1:L:113:PRO:HG2	1:L:205:ILE:HD12	1.91	0.53
1:L:136:LEU:N	1:L:136:LEU:CD1	2.71	0.53
1:L:189:HIS:O	1:L:211:ARG:HD3	2.08	0.53
1:L:200:THR:HG23	4:L:237:HOH:O	2.09	0.53
1:L:6:GLN:NE2	1:L:99:GLY:HA3	2.21	0.52
1:A:94:LEU:N	3:P:7:PRO:O	2.42	0.52
3:P:4:ILE:CD1	3:P:7:PRO:HA	2.39	0.52
2:B:13:ARG:HG2	2:B:121:SER:HB2	1.90	0.52
2:B:221:ARG:O	2:B:222:ASP:HB2	2.09	0.52
1:L:61:ARG:NH1	1:L:82:ASP:CG	2.67	0.52
1:L:63:SER:O	1:L:73:LEU:HD12	2.09	0.52
1:L:190:ASN:ND2	1:L:210:ASN:HB3	2.24	0.52
1:L:6:GLN:NE2	1:L:99:GLY:C	2.68	0.52
2:H:58:THR:OG1	2:H:60:TYR:HE1	1.93	0.52
1:A:49:TYR:CE2	1:A:54:LEU:HD12	2.44	0.52
1:A:162:SER:HB3	2:B:175:PRO:HD2	1.91	0.52
1:A:198:HIS:ND1	1:A:200:THR:HB	2.25	0.52
2:H:87:THR:OG1	2:H:89:GLU:HB3	2.09	0.52
1:A:166:GLN:NE2	1:A:171:SER:HB3	2.25	0.52
2:H:18:VAL:O	2:H:82:GLN:HA	2.10	0.51
1:A:48:ILE:CG2	1:A:52:SER:HA	2.41	0.51
1:L:162:SER:HB3	2:H:174:PHE:HB3	1.93	0.51
2:H:41:PRO:C	2:H:43:GLN:H	2.18	0.51
2:B:1:GLU:HA	2:B:1:GLU:OE1	2.08	0.51
1:L:98:PHE:HD2	2:H:45:LEU:O	1.93	0.51
1:L:1:ASP:CG	1:L:95:PRO:HD2	2.36	0.51
1:L:49:TYR:O	1:L:54:LEU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:51:ILE:O	2:H:53:PRO:HD3	2.10	0.51
2:B:19:LYS:HG3	2:B:82:GLN:HB2	1.92	0.51
3:P:4:ILE:HD12	3:P:7:PRO:HB3	1.91	0.51
2:B:35:ASN:HD22	2:B:47:TRP:NE1	2.08	0.51
1:L:99:GLY:O	1:L:101:GLY:N	2.44	0.51
2:H:123:LYS:O	2:H:125:THR:HG22	2.11	0.51
1:A:12:SER:HA	1:A:105:GLU:HG3	1.93	0.51
1:A:33:LEU:H	1:A:51:THR:H	1.59	0.51
1:L:29:ILE:HD12	1:L:90:GLN:HB2	1.92	0.50
2:H:18:VAL:HG23	2:H:86:LEU:HD11	1.93	0.50
2:H:201:VAL:O	2:H:218:ILE:HG12	2.10	0.50
1:A:161:ASN:HB3	1:A:175:MET:HE3	1.93	0.50
1:A:31:ASN:CB	1:A:51:THR:HB	2.42	0.50
1:A:78:LEU:HG	1:A:79:GLU:N	2.25	0.50
2:B:113:GLN:H	2:B:113:GLN:HE21	1.58	0.50
2:H:107:TYR:CE1	2:H:109:ASP:HB3	2.37	0.50
2:H:2:VAL:CG2	2:H:110:TYR:CE1	2.94	0.50
2:H:123:LYS:O	2:H:124:THR:C	2.54	0.50
2:H:37:VAL:CG1	2:H:45:LEU:HB3	2.42	0.50
1:L:24:ARG:HG3	1:L:69:THR:CG2	2.42	0.50
2:H:6:GLN:N	2:H:113:GLN:NE2	2.40	0.50
2:H:40:ARG:HG2	2:H:92:ALA:HB2	1.93	0.50
2:B:67:LYS:HD2	2:B:67:LYS:N	2.27	0.50
3:P:4:ILE:HG22	3:P:5:ALA:C	2.37	0.49
2:H:113:GLN:NE2	2:H:113:GLN:H	2.10	0.49
2:B:21:SER:HB3	2:B:80:TYR:CE2	2.47	0.49
2:B:150:VAL:HG11	2:B:158:VAL:HG11	1.94	0.49
1:L:90:GLN:CD	1:L:90:GLN:O	2.55	0.49
2:H:6:GLN:HA	2:H:21:SER:O	2.12	0.49
1:A:186:TYR:O	1:A:192:TYR:OH	2.27	0.49
1:L:24:ARG:HG3	1:L:69:THR:HG22	1.94	0.49
1:L:161:ASN:HB2	1:L:163:TRP:CH2	2.48	0.49
1:A:50:TYR:C	1:A:52:SER:N	2.68	0.49
1:A:90:GLN:HG3	1:A:97:THR:OG1	2.13	0.49
1:A:174:SER:OG	2:B:172:HIS:CE1	2.65	0.49
1:L:35:TRP:CZ3	1:L:88:CYS:HB3	2.47	0.49
1:L:77:ASN:C	1:L:77:ASN:OD1	2.56	0.49
1:L:12:SER:HB3	1:L:107:LYS:HD3	1.94	0.48
1:L:58:VAL:HG23	1:L:59:PRO:HD2	1.94	0.48
1:L:78:LEU:HD12	1:L:79:GLU:N	2.28	0.48
2:H:171:VAL:HG12	2:H:172:HIS:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:ASN:O	2:B:142:SER:C	2.56	0.48
2:H:100:VAL:HG12	2:H:101:TYR:N	2.28	0.48
1:A:41:ASP:CG	1:A:43:THR:HG23	2.37	0.48
1:A:55:HIS:CE1	1:A:62:PHE:O	2.66	0.48
1:L:182:THR:O	1:L:183:LYS:C	2.56	0.48
1:L:18:ARG:HG2	1:L:18:ARG:HH11	1.79	0.48
1:L:133:VAL:HG12	1:L:134:CYS:N	2.29	0.48
1:A:111:ALA:O	1:A:112:ALA:CB	2.61	0.48
1:L:48:ILE:HA	1:L:54:LEU:O	2.14	0.48
2:B:37:VAL:CG1	2:B:45:LEU:HB3	2.43	0.48
1:L:192:TYR:O	1:L:208:SER:HB2	2.13	0.48
2:H:185:LEU:HD12	2:H:186:SER:N	2.29	0.48
1:A:52:SER:CB	1:A:64:GLY:C	2.80	0.48
1:L:61:ARG:NH1	1:L:82:ASP:OD2	2.37	0.48
2:H:158:VAL:CG2	2:H:185:LEU:CD2	2.92	0.48
1:L:4:MET:HB2	1:L:98:PHE:O	2.13	0.48
2:H:194:SER:N	2:H:195:PRO:CD	2.77	0.48
1:L:11:LEU:HB3	1:L:104:LEU:HD23	1.96	0.47
1:A:94:LEU:H	3:P:8:PRO:CA	2.21	0.47
2:B:40:ARG:O	2:B:41:PRO:C	2.57	0.47
2:B:124:THR:HG22	2:B:155:PRO:HD3	1.95	0.47
2:H:63:LYS:HE2	2:H:64:PHE:HE2	1.79	0.47
2:H:130:TYR:HB2	2:H:149:LEU:HB3	1.95	0.47
1:A:133:VAL:HG22	1:A:178:THR:HG23	1.95	0.47
2:B:69:THR:HG22	2:B:71:THR:HG22	1.96	0.47
2:B:210:SER:O	2:B:211:SER:C	2.57	0.47
1:L:161:ASN:HB3	1:L:175:MET:HE3	1.96	0.47
2:H:2:VAL:HB	2:H:110:TYR:CE1	2.50	0.47
2:H:124:THR:HG23	4:H:230:HOH:O	2.13	0.47
2:H:221:ARG:HG2	2:H:222:ASP:H	1.79	0.47
1:A:158:GLY:O	1:A:179:LEU:HA	2.14	0.47
2:B:12:VAL:HG21	2:B:86:LEU:HD13	1.96	0.47
1:A:3:GLN:H	1:A:3:GLN:NE2	2.12	0.47
2:B:124:THR:HG22	2:B:155:PRO:CD	2.44	0.47
2:B:160:VAL:HG22	2:B:205:VAL:HG22	1.96	0.47
1:L:4:MET:HA	1:L:4:MET:CE	2.44	0.47
1:A:50:TYR:O	1:A:52:SER:N	2.47	0.47
1:A:94:LEU:HG	3:P:7:PRO:C	2.37	0.47
2:B:109:ASP:OD1	2:B:110:TYR:N	2.47	0.47
3:P:3:LEU:O	3:P:4:ILE:HG13	2.14	0.47
1:L:54:LEU:HD11	2:H:102:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:108:ARG:O	1:L:140:TYR:HE1	1.98	0.47
1:A:192:TYR:O	1:A:208:SER:HB2	2.14	0.47
2:B:73:ASP:OD1	2:B:73:ASP:O	2.33	0.47
2:H:194:SER:O	2:H:198:SER:HB3	2.15	0.47
1:A:133:VAL:HG12	1:A:134:CYS:N	2.30	0.47
2:H:146:LEU:HD23	2:H:218:ILE:CB	2.45	0.47
1:A:79:GLU:O	1:A:80:GLN:C	2.57	0.47
1:A:193:THR:HG23	1:A:208:SER:HB3	1.97	0.47
2:B:3:GLN:HG2	2:B:5:GLN:NE2	2.29	0.47
1:L:51:THR:O	1:L:52:SER:CB	2.61	0.47
1:L:66:GLY:HA3	1:L:71:TYR:HD2	1.79	0.47
2:H:3:GLN:O	2:H:4:LEU:HG	2.15	0.46
2:H:36:TRP:O	2:H:48:ILE:HB	2.15	0.46
1:A:40:PRO:C	1:A:42:GLY:H	2.22	0.46
2:B:21:SER:HB3	2:B:80:TYR:HE2	1.79	0.46
2:B:153:TYR:CE2	2:B:183:TYR:HB2	2.51	0.46
1:L:161:ASN:ND2	1:L:175:MET:HE2	2.30	0.46
2:H:158:VAL:CG2	2:H:185:LEU:HD21	2.44	0.46
1:A:46:LEU:HD13	2:B:108:PHE:O	2.15	0.46
1:L:111:ALA:O	1:L:112:ALA:CB	2.63	0.46
1:L:154:GLU:CG	1:L:155:ARG:N	2.51	0.46
2:H:109:ASP:O	2:H:110:TYR:CD2	2.68	0.46
2:B:12:VAL:HG23	2:B:12:VAL:O	2.15	0.46
2:H:124:THR:HA	2:H:154:PHE:O	2.15	0.46
2:B:142:SER:O	2:B:192:PRO:HA	2.16	0.46
2:H:101:TYR:O	2:H:102:TYR:O	2.33	0.46
1:A:61:ARG:HG2	1:A:61:ARG:NH1	2.31	0.46
1:A:138:ASN:OD1	2:B:172:HIS:CE1	2.69	0.46
2:H:131:PRO:HD3	2:H:216:LYS:HG2	1.97	0.46
2:H:212:THR:CG2	2:H:213:LYS:N	2.78	0.46
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.96	0.46
2:H:10:GLU:OE2	2:H:18:VAL:CG1	2.64	0.46
1:A:121:SER:HB2	1:A:123:GLU:OE1	2.15	0.46
2:B:213:LYS:HD2	2:B:214:VAL:N	2.31	0.46
1:L:18:ARG:HG2	1:L:18:ARG:NH1	2.31	0.46
1:L:31:ASN:ND2	1:L:51:THR:OG1	2.49	0.46
2:H:158:VAL:HG23	2:H:185:LEU:HD21	1.98	0.46
2:B:73:ASP:C	2:B:75:SER:H	2.24	0.46
2:B:221:ARG:O	2:B:222:ASP:CB	2.63	0.45
1:L:33:LEU:HD12	1:L:89:GLN:O	2.16	0.45
2:H:63:LYS:CE	2:H:64:PHE:CE2	2.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:185:LEU:C	2:H:185:LEU:CD1	2.86	0.45
2:B:3:GLN:HG3	2:B:5:GLN:NE2	2.20	0.45
2:B:67:LYS:CG	4:B:227:HOH:O	2.55	0.45
2:B:154:PHE:CD1	2:B:155:PRO:HA	2.52	0.45
1:L:31:ASN:C	1:L:51:THR:HB	2.42	0.45
2:H:89:GLU:HG3	4:H:233:HOH:O	2.15	0.45
2:H:159:THR:O	2:H:205:VAL:HA	2.16	0.45
1:A:48:ILE:HG21	1:A:52:SER:HA	1.96	0.45
1:A:66:GLY:HA3	1:A:71:TYR:CD2	2.52	0.45
1:L:36:TYR:CE2	2:H:111:TRP:HZ2	2.34	0.45
1:L:66:GLY:HA3	1:L:71:TYR:HA	1.98	0.45
1:A:6:GLN:HE21	1:A:99:GLY:CA	2.26	0.45
1:L:31:ASN:HD22	1:L:51:THR:CG2	2.26	0.45
1:L:94:LEU:HD23	1:L:96:ARG:NH1	2.32	0.45
1:A:48:ILE:HA	1:A:54:LEU:O	2.16	0.45
1:L:108:ARG:HD3	1:L:109:ALA:O	2.17	0.45
2:H:19:LYS:HG2	2:H:82:GLN:CG	2.45	0.45
2:H:29:PHE:CE2	2:H:72:VAL:HG11	2.52	0.45
3:P:3:LEU:C	3:P:4:ILE:HG13	2.42	0.45
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.99	0.45
1:L:186:TYR:O	1:L:192:TYR:OH	2.34	0.45
2:H:12:VAL:HG23	2:H:12:VAL:O	2.17	0.45
2:H:40:ARG:HH22	2:H:89:GLU:HA	1.78	0.45
2:H:46:GLU:OE1	2:H:63:LYS:HE3	2.17	0.45
2:H:168:SER:O	2:H:171:VAL:HG23	2.17	0.45
2:H:212:THR:HG23	2:H:213:LYS:N	2.32	0.45
1:A:150:ILE:HD12	1:A:155:ARG:HD3	1.98	0.45
1:L:108:ARG:O	1:L:140:TYR:CE1	2.70	0.44
2:H:174:PHE:CD2	2:H:174:PHE:N	2.85	0.44
2:H:192:PRO:HB2	2:H:195:PRO:HD3	1.99	0.44
2:B:124:THR:HA	2:B:154:PHE:O	2.17	0.44
1:L:50:TYR:CD2	1:L:51:THR:HG22	2.53	0.44
1:L:82:ASP:O	1:L:86:TYR:OH	2.27	0.44
2:H:3:GLN:HG3	2:H:5:GLN:HE21	1.83	0.44
2:H:208:PRO:O	2:H:211:SER:N	2.36	0.44
1:L:70:ASP:O	1:L:71:TYR:CD2	2.71	0.44
2:H:174:PHE:HD2	2:H:186:SER:O	2.00	0.44
1:A:123:GLU:CD	1:A:123:GLU:H	2.24	0.44
2:B:153:TYR:O	2:B:154:PHE:HB2	2.18	0.44
1:L:142:LYS:CB	1:L:173:TYR:CE2	2.99	0.44
1:A:67:SER:O	1:A:69:THR:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:4:ILE:HG21	3:P:7:PRO:CA	2.46	0.44
1:L:33:LEU:HD11	1:L:88:CYS:HB2	1.99	0.44
2:H:27:TYR:CE1	2:H:98:ARG:HD2	2.53	0.44
1:L:78:LEU:HD12	1:L:82:ASP:HB2	1.98	0.44
1:A:31:ASN:O	1:A:51:THR:CA	2.66	0.44
1:L:12:SER:CB	1:L:107:LYS:HD3	2.47	0.44
2:H:29:PHE:CE2	2:H:53:PRO:HB3	2.53	0.44
1:A:37:GLN:HG3	1:A:86:TYR:CE2	2.53	0.43
1:A:140:TYR:CD1	1:A:141:PRO:N	2.86	0.43
2:B:144:VAL:O	2:B:144:VAL:HG13	2.18	0.43
1:L:11:LEU:O	1:L:104:LEU:HA	2.18	0.43
1:L:18:ARG:HG3	1:L:76:SER:HA	1.99	0.43
2:H:196:ARG:HG3	2:H:201:VAL:HG21	2.00	0.43
1:A:108:ARG:HD3	1:A:109:ALA:O	2.17	0.43
2:H:26:GLY:O	2:H:27:TYR:HB3	2.17	0.43
2:H:107:TYR:CD1	2:H:107:TYR:C	2.95	0.43
2:B:167:LEU:O	2:B:171:VAL:HG21	2.18	0.43
3:P:1:ARG:O	3:P:2:LEU:HB2	2.18	0.43
2:B:101:TYR:O	2:B:105:SER:O	2.37	0.43
2:B:196:ARG:CD	2:B:197:PRO:HA	2.43	0.43
1:L:140:TYR:HA	1:L:141:PRO:C	2.42	0.43
1:A:108:ARG:NH2	4:A:228:HOH:O	2.51	0.43
1:L:151:ASP:OD2	1:L:189:HIS:CB	2.66	0.43
1:L:193:THR:HA	1:L:208:SER:HB3	2.00	0.43
2:H:86:LEU:CD2	2:H:90:ASP:OD2	2.67	0.43
1:A:57:GLY:CA	4:A:225:HOH:O	2.57	0.43
1:A:112:ALA:CB	1:A:200:THR:HG21	2.48	0.43
1:A:117:ILE:HG12	1:A:209:PHE:CD2	2.54	0.43
1:L:99:GLY:O	1:L:100:GLY:C	2.61	0.43
1:A:49:TYR:CZ	1:A:54:LEU:HD12	2.54	0.43
1:A:193:THR:HA	1:A:208:SER:HB3	2.01	0.43
1:L:140:TYR:CE2	1:L:141:PRO:HA	2.54	0.43
2:H:29:PHE:HE2	2:H:72:VAL:HG11	1.83	0.43
1:A:108:ARG:HG3	1:A:108:ARG:HH11	1.84	0.43
1:L:52:SER:HB3	1:L:64:GLY:HA3	2.02	0.42
1:A:2:ILE:HD11	1:A:93:THR:CB	2.49	0.42
1:A:92:ASN:HA	4:A:224:HOH:O	2.18	0.42
1:A:154:GLU:OE1	1:A:154:GLU:HA	2.18	0.42
3:P:4:ILE:HG23	3:P:6:ASP:H	1.84	0.42
2:H:42:GLY:O	2:H:43:GLN:O	2.37	0.42
1:A:77:ASN:O	1:A:77:ASN:CG	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:SER:O	1:A:53:ARG:CB	2.67	0.42
3:P:3:LEU:C	3:P:4:ILE:CG1	2.92	0.42
3:P:4:ILE:HG22	3:P:6:ASP:N	2.34	0.42
1:L:19:VAL:HG21	1:L:78:LEU:HD22	2.00	0.42
1:A:40:PRO:O	1:A:42:GLY:N	2.52	0.42
1:L:33:LEU:HD12	1:L:89:GLN:C	2.44	0.42
2:H:148:CYS:HB2	2:H:162:TRP:CH2	2.54	0.42
1:A:38:GLN:O	1:A:84:ALA:HB1	2.18	0.42
1:A:69:THR:HG22	1:A:70:ASP:OD2	2.18	0.42
2:B:69:THR:HG22	2:B:69:THR:O	2.20	0.42
1:L:38:GLN:O	1:L:84:ALA:HB1	2.19	0.42
1:L:137:ASN:HB3	1:L:138:ASN:ND2	2.34	0.42
1:L:155:ARG:HD2	1:L:155:ARG:HA	1.63	0.42
2:H:8:GLY:O	2:H:115:THR:HG23	2.20	0.42
2:H:196:ARG:HG3	2:H:201:VAL:CG2	2.50	0.42
1:A:48:ILE:HG22	1:A:49:TYR:N	2.35	0.42
1:L:94:LEU:CD1	2:H:59:LYS:HE2	2.48	0.42
2:H:98:ARG:O	2:H:108:PHE:HA	2.18	0.42
1:L:34:ASN:OD1	1:L:49:TYR:HB2	2.20	0.42
2:B:127:PRO:CB	2:B:153:TYR:HB3	2.47	0.42
1:L:29:ILE:HG22	1:L:32:TYR:N	2.30	0.41
2:H:35:ASN:O	2:H:96:CYS:HA	2.20	0.41
1:A:7:THR:O	1:A:8:THR:CB	2.68	0.41
3:P:4:ILE:HG23	3:P:6:ASP:N	2.35	0.41
1:A:210:ASN:HB3	1:A:212:ASN:OD1	2.19	0.41
2:H:61:ASN:C	2:H:61:ASN:ND2	2.76	0.41
2:B:6:GLN:CA	2:B:113:GLN:HE22	2.33	0.41
2:B:51:ILE:CD1	2:B:58:THR:HG22	2.48	0.41
2:B:171:VAL:O	2:B:172:HIS:HD2	2.03	0.41
3:P:2:LEU:HB3	3:P:10:PRO:CB	2.45	0.41
1:A:13:ALA:O	1:A:106:ILE:HA	2.20	0.41
1:A:136:LEU:HD23	1:A:144:ILE:HD11	2.02	0.41
2:H:196:ARG:HE	2:H:196:ARG:HB3	1.35	0.41
1:A:50:TYR:O	1:A:51:THR:C	2.63	0.41
1:A:186:TYR:CE2	1:A:211:ARG:HD2	2.56	0.41
2:B:141:ASN:O	2:B:193:SER:OG	2.37	0.41
2:H:6:GLN:OE1	2:H:95:PHE:HA	2.20	0.41
1:A:30:SER:O	1:A:31:ASN:HB2	2.19	0.41
2:B:29:PHE:CE2	2:B:77:SER:HA	2.55	0.41
1:A:52:SER:HB3	1:A:64:GLY:CA	2.50	0.41
2:H:55:ASN:C	2:H:57:TYR:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:SER:O	1:A:126:THR:HG23	2.19	0.41
1:A:136:LEU:HD23	1:A:144:ILE:CD1	2.50	0.41
1:A:25:ALA:O	1:A:69:THR:HG23	2.20	0.41
1:A:46:LEU:HG	1:A:47:LEU:N	2.35	0.41
1:A:193:THR:HG22	1:A:194:CYS:N	2.36	0.41
2:B:2:VAL:HB	2:B:110:TYR:CD1	2.55	0.41
1:L:94:LEU:HD22	2:H:47:TRP:CZ3	2.56	0.41
2:H:55:ASN:ND2	2:H:57:TYR:CB	2.66	0.41
2:H:174:PHE:HA	2:H:175:PRO:HD3	1.95	0.41
2:B:98:ARG:O	2:B:108:PHE:HA	2.21	0.41
2:B:153:TYR:CD2	2:B:153:TYR:C	2.99	0.41
1:L:183:LYS:O	1:L:187:GLU:HG3	2.21	0.40
2:B:51:ILE:O	2:B:51:ILE:HG23	2.21	0.40
1:L:116:SER:O	1:L:134:CYS:HA	2.22	0.40
1:L:140:TYR:HA	1:L:141:PRO:O	2.22	0.40
1:L:142:LYS:HB3	1:L:173:TYR:CE1	2.55	0.40
2:H:204:ASN:ND2	2:H:215:ASP:OD1	2.42	0.40
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.97	0.40
1:A:118:PHE:HA	1:A:119:PRO:HD3	1.83	0.40
2:B:40:ARG:O	2:B:42:GLY:N	2.55	0.40
2:B:141:ASN:O	2:B:143:MET:N	2.54	0.40
1:L:173:TYR:N	1:L:173:TYR:CD1	2.90	0.40
2:H:100:VAL:CG1	2:H:101:TYR:N	2.84	0.40
2:B:69:THR:HG22	2:B:71:THR:CG2	2.52	0.40
2:H:197:PRO:O	2:H:198:SER:C	2.62	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	212/214 (99%)	187 (88%)	16 (8%)	9 (4%)	2 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	212/214 (99%)	185 (87%)	19 (9%)	8 (4%)	2	10
2	B	215/222 (97%)	183 (85%)	25 (12%)	7 (3%)	3	13
2	H	214/222 (96%)	185 (86%)	22 (10%)	7 (3%)	3	13
3	P	10/12 (83%)	3 (30%)	3 (30%)	4 (40%)	0	0
All	All	863/884 (98%)	743 (86%)	85 (10%)	35 (4%)	2	9

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	8	THR
2	H	43	GLN
2	H	102	TYR
1	A	154	GLU
1	A	155	ARG
2	B	43	GLN
2	B	102	TYR
3	P	4	ILE
3	P	9	SER
3	P	10	PRO
1	L	53	ARG
1	L	100	GLY
2	H	62	GLU
2	H	103	GLY
2	H	221	ARG
1	A	8	THR
1	A	41	ASP
1	A	68	GLY
2	B	16	SER
2	B	103	GLY
3	P	2	LEU
1	L	50	TYR
1	L	56	SER
1	A	51	THR
1	A	52	SER
1	L	41	ASP
1	L	112	ALA
1	L	155	ARG
2	H	74	LYS
2	B	142	SER
2	B	179	GLN
2	H	179	GLN

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Mol	Chain	Res	Type
1	A	112	ALA
1	A	57	GLY
2	B	48	ILE

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	190/192 (99%)	169 (89%)	21 (11%)	6	20
1	L	189/192 (98%)	176 (93%)	13 (7%)	14	41
2	B	185/190 (97%)	158 (85%)	27 (15%)	3	10
2	H	185/190 (97%)	161 (87%)	24 (13%)	4	13
3	P	11/11 (100%)	8 (73%)	3 (27%)	0	1
All	All	760/775 (98%)	672 (88%)	88 (12%)	5	18

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	MET
1	L	9	SER
1	L	14	SER
1	L	53	ARG
1	L	58	VAL
1	L	103	LYS
1	L	108	ARG
1	L	117	ILE
1	L	138	ASN
1	L	155	ARG
1	L	162	SER
1	L	179	LEU
1	L	200	THR
2	H	13	ARG
2	H	25	SER
2	H	38	LYS

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Mol	Chain	Res	Type
2	H	50	TYR
2	H	51	ILE
2	H	55	ASN
2	H	61	ASN
2	H	63	LYS
2	H	72	VAL
2	H	99	SER
2	H	113	GLN
2	H	124	THR
2	H	125	THR
2	H	150	VAL
2	H	169	SER
2	H	177	VAL
2	H	178	LEU
2	H	185	LEU
2	H	190	THR
2	H	196	ARG
2	H	203	CYS
2	H	205	VAL
2	H	212	THR
2	H	216	LYS
1	A	3	GLN
1	A	10	SER
1	A	43	THR
1	A	46	LEU
1	A	53	ARG
1	A	54	LEU
1	A	58	VAL
1	A	60	SER
1	A	67	SER
1	A	77	ASN
1	A	79	GLU
1	A	105	GLU
1	A	108	ARG
1	A	153	SER
1	A	168	SER
1	A	169	LYS
1	A	176	SER
1	A	191	SER
1	A	200	THR
1	A	211	ARG
1	A	214	CYS

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Mol	Chain	Res	Type
2	B	5	GLN
2	B	6	GLN
2	B	11	LEU
2	B	13	ARG
2	B	21	SER
2	B	52	ASN
2	B	55	ASN
2	B	61	ASN
2	B	71	THR
2	B	72	VAL
2	B	73	ASP
2	B	113	GLN
2	B	123	LYS
2	B	136	SER
2	B	168	SER
2	B	169	SER
2	B	185	LEU
2	B	190	THR
2	B	191	VAL
2	B	194	SER
2	B	196	ARG
2	B	198	SER
2	B	200	THR
2	B	202	THR
2	B	203	CYS
2	B	213	LYS
2	B	222	ASP
3	P	6	ASP
3	P	7	PRO
3	P	12	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	31	ASN
1	L	92	ASN
1	L	137	ASN
1	L	138	ASN
1	L	161	ASN
1	L	189	HIS
2	H	3	GLN

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Mol	Chain	Res	Type
2	H	5	GLN
2	H	35	ASN
2	H	61	ASN
2	H	113	GLN
1	A	3	GLN
1	A	6	GLN
1	A	37	GLN
1	A	55	HIS
1	A	161	ASN
2	B	5	GLN
2	B	35	ASN
2	B	52	ASN
2	B	61	ASN
2	B	82	GLN
2	B	113	GLN
2	B	172	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 ⓘ

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%)	0.10	3 (1%) 73 65	3, 16, 31, 38	0
1	L	214/214 (100%)	0.49	14 (6%) 25 20	8, 22, 43, 49	0
2	B	219/222 (98%)	0.41	9 (4%) 41 33	3, 21, 38, 57	0
2	H	218/222 (98%)	0.73	21 (9%) 13 11	6, 31, 49, 60	0
3	P	12/12 (100%)	2.33	8 (66%) 0 0	61, 64, 69, 69	0
All	All	877/884 (99%)	0.46	55 (6%) 26 20	3, 22, 46, 69	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	33	GLY	4.2
3	P	2	LEU	3.6
2	H	49	GLY	3.6
2	B	222	ASP	3.5
2	H	103	GLY	3.4
1	L	52	SER	3.4
3	P	9	SER	3.3
1	L	53	ARG	3.2
1	L	2	ILE	3.1
2	H	89	GLU	3.1
1	A	212	ASN	3.0
3	P	5	ALA	3.0
2	H	222	ASP	2.9
1	L	71	TYR	2.9
2	H	101	TYR	2.9
2	H	50	TYR	2.8
1	L	29	ILE	2.8
1	A	214	CYS	2.8
2	H	47	TRP	2.7
1	L	76	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	29	PHE	2.6
2	B	57	TYR	2.6
3	P	7	PRO	2.6
1	L	51	THR	2.6
1	L	214	CYS	2.6
3	P	3	LEU	2.5
2	B	170	GLY	2.5
2	B	179	GLN	2.4
2	H	7	SER	2.4
1	L	30	SER	2.4
1	L	55	HIS	2.4
1	L	32	TYR	2.4
2	B	50	TYR	2.3
2	H	12	VAL	2.3
1	A	213	GLU	2.3
2	H	179	GLN	2.3
3	P	6	ASP	2.2
2	H	51	ILE	2.2
2	B	43	GLN	2.2
2	B	89	GLU	2.2
3	P	10	PRO	2.2
1	L	7	THR	2.2
2	B	124	THR	2.2
1	L	68	GLY	2.2
2	H	62	GLU	2.2
3	P	4	ILE	2.1
2	H	136	SER	2.1
2	H	43	GLN	2.1
2	H	1	GLU	2.1
2	H	180	SER	2.1
2	H	3	GLN	2.1
1	L	54	LEU	2.1
2	H	97	ALA	2.0
2	H	57	TYR	2.0
2	B	140	THR	2.0

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

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.