



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:52 AM UTC

PDB ID : 3MLT / pdb_00003mlt
Title : Crystal structure of anti-HIV-1 V3 Fab 2557 in complex with a UG1033 V3 peptide
Authors : Kong, X.-P.
Deposited on : 2010-04-18
Resolution : 2.49 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

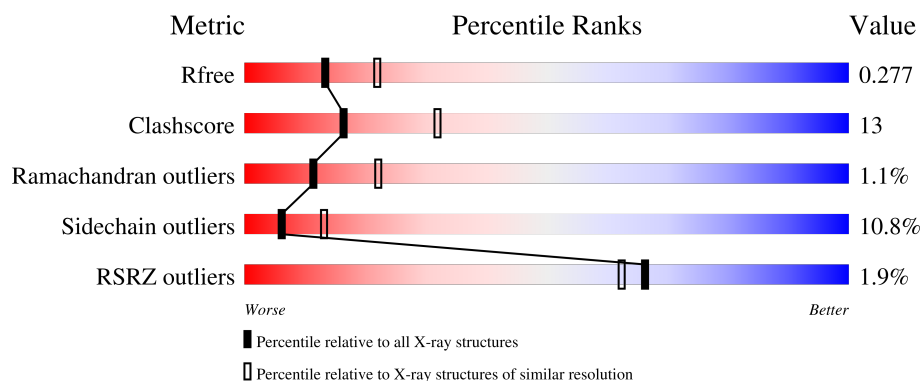
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	219	5% 61% 33% ..
1	D	219	% 65% 27% 5% .
1	G	219	70% 23% ..
1	L	219	2% 68% 27% ..
2	B	226	73% 19% 5% .

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Mol	Chain	Length	Quality of chain
2	E	226	3% 69% 21% 7%
2	H	226	2% 67% 26% 5%
2	I	226	77% 17%
3	C	23	13% 43% 17% 39%
3	P	23	30% 22% 9% 39%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13628 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 Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1623	1019	266	333	5			
1	A	215	Total	C	N	O	S	0	0	0
			1619	1017	265	332	5			
1	D	213	Total	C	N	O	S	0	0	0
			1608	1011	263	329	5			
1	G	213	Total	C	N	O	S	0	1	0
			1614	1015	263	331	5			

- Molecule 2 is a protein called Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1633	1044	263	320	6			
2	B	219	Total	C	N	O	S	0	0	0
			1659	1059	267	327	6			
2	E	219	Total	C	N	O	S	0	0	0
			1659	1059	267	327	6			
2	I	219	Total	C	N	O	S	0	0	0
			1659	1059	267	327	6			

- Molecule 3 is a protein called HIV-1 gp120 third variable region (V3) crown.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	14	Total	C	N	O	0	0	0
			113	73	23	17			
3	C	14	Total	C	N	O	0	0	0
			113	73	23	17			

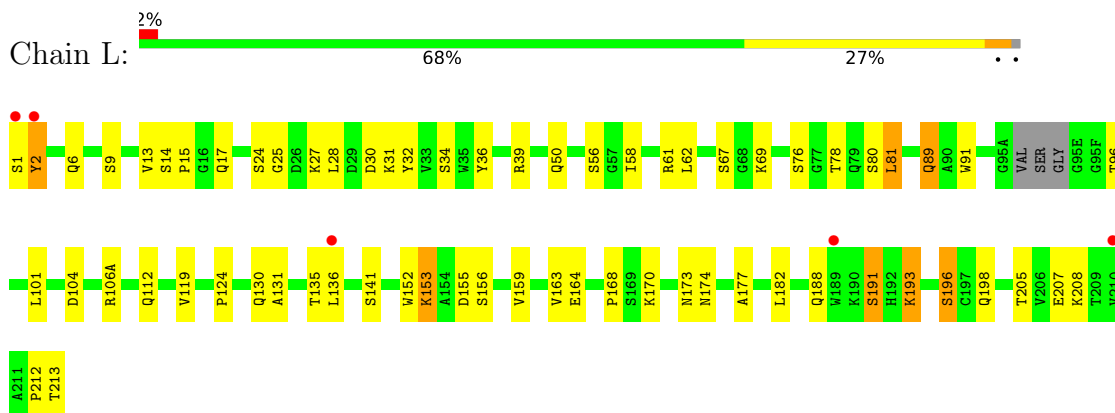
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	55	Total 55	O 55	0	0
4	H	44	Total 44	O 44	0	0
4	P	3	Total 3	O 3	0	0
4	A	12	Total 12	O 12	0	0
4	B	30	Total 30	O 30	0	0
4	C	1	Total 1	O 1	0	0
4	D	31	Total 31	O 31	0	0
4	E	49	Total 49	O 49	0	0
4	G	48	Total 48	O 48	0	0
4	I	55	Total 55	O 55	0	0

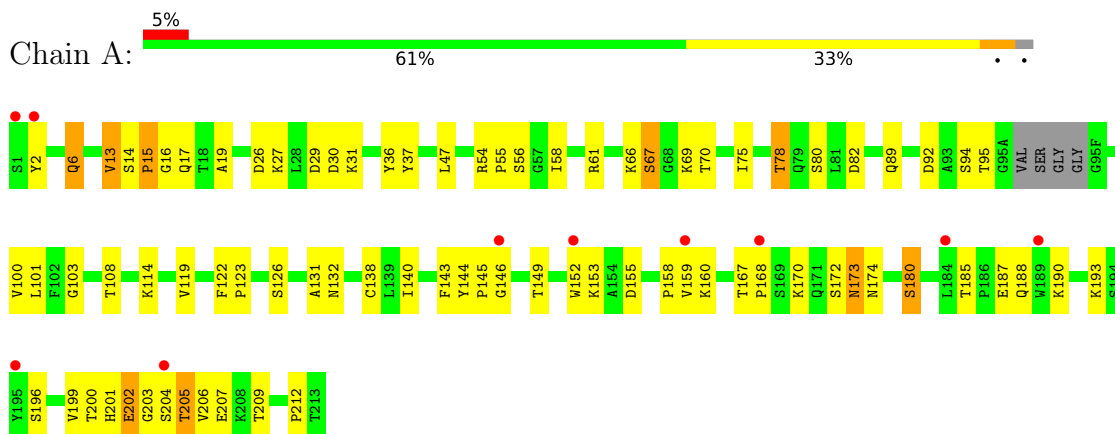
3 Residue-property plots

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.

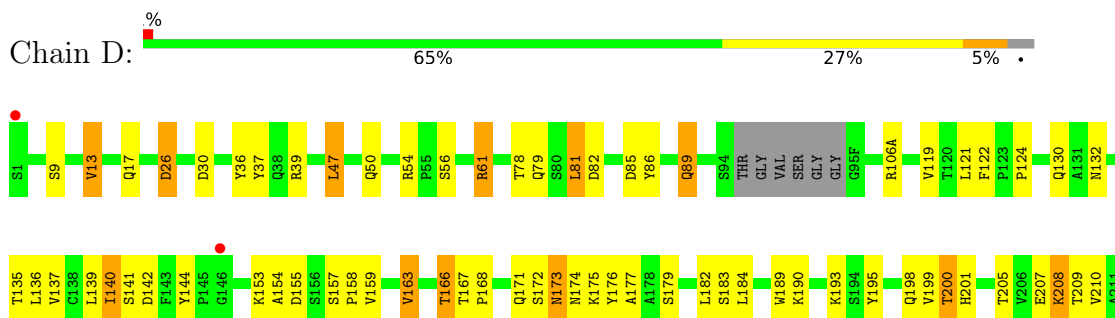
- Molecule 1: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab light chain



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P212
T213

- Molecule 1: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab light chain

Chain G:  70% 23%

S1 Y2 D3 Q6 S12 V13 Q17 S24 Q25 D26 K27 L28 D29 D30 K31 Y36 Y37 Q38 R39 L47 Q50 Q51 D52 F52 K53 E60 R61 L62 S63 T72 Q79 S80 L81 D82 Q89 S94 THR GLY VAL SER GLY G95F T96 K97 L98 T99 V100 L101

F102 G103 Q112 P113 P124 K133 L136 S141 D142 D155 S156 S157 P158 V159 E164 T167 P168 S169 K170 Q171 S172 N173 K53 S179 P186 W189 K190 Q198 V199 T200 T205 P212 T213

- Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab heavy chain

Chain H:  2% 67% 26% 5%

E1 V2 Q3 E6 Q13 P14 G15 K19 K23 N28 F29 L30 D31 I40 P41 P52A D53 D54 S55 D56 A57 H58 Q65 G66 V67 K73 S74 I75 S76 T82A T82B Q100B S100C S100D N100E A100F F100G D101 L102 Q105 M108 S113 P119 A125

P126 SER LYS SER THR SER GLY G134 T135 A136 A137 L138 G139 K143 D144 Y145 P149 V150 L159 G162 V163 H164 T165 F166 P167 A168 V169 S172 L178 S179 S180 V181 V182 P185 SER SER SER LEU G190 T191 Q192 T193 Y194 C196 K201 N204 T205 P213

K214 S215

- Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab heavy chain

Chain B:  73% 19% 5%

E1 L4 V5 E6 Q13 Q16 I20 K23 F29 L30 I34 Q39 I40 P41 V47 I48 G49 P52A D53 D54 S55 D56 Q66 Q67 I75 Q81 W82 Q83 Q84 S85 D86 K89 Y90 F91 L95 M100E L102 Q105 I109

G114 K117 G118 P119 A125 P126 SER LYS SER THR SER SER GLY G134 L138 G139 Y145 V150 V154 V163 L170 L175 L178 V181 V182 T191 C196 K210 V211 E212 S215

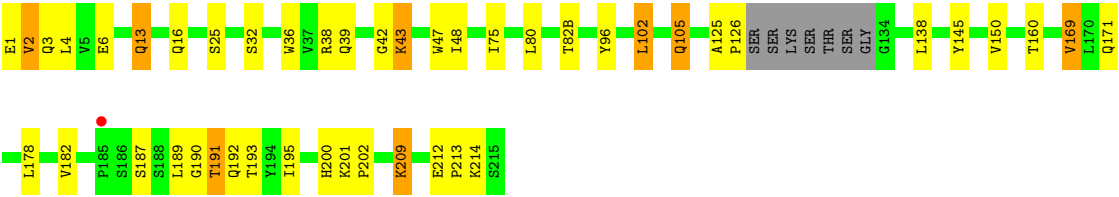
- Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab heavy chain

Chain E:  3% 69% 21% 7%

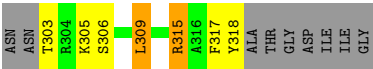
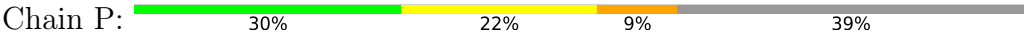
E1 V2 Q3 E6 Q13 S17 L18 K19 R38 Q39 I40 P41 G42 K43 I48 D54 E64 G65 L80 T82A Q83 T93 R94 L95 Y96 S97 F98 E99 S100C S100D N100E A100F F100G D101 L102 Q105 T115 P123 L124 A125 P126 SER SER LYS SER

THR SER GLY G134 A137 L138 K143 V150 V154 N155 S156 G157 A158 L159 T160 S161 G162 V163 F166 V169 Y176 S177 L178 V182 T183 P184 P185 S186 S187 S188 L189 Q192 T193 I194 I195 C196 K201 K209 V210 E212 P213 K214 S215

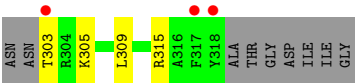
- Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab heavy chain



• Molecule 3: HIV-1 gp120 third variable region (V3) crown



• Molecule 3: HIV-1 gp120 third variable region (V3) crown



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.68Å 142.93Å 85.01Å 90.00° 95.00° 90.00°	Depositor
Resolution (Å)	35.74 – 2.49 35.74 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.3 (35.74-2.49) 99.3 (35.74-2.49)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.48Å)	Xtriage
Refinement program	CNS, REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.280 0.204 , 0.277	Depositor DCC
R_{free} test set	3177 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13628	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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	0.89	0/1658	1.05	4/2261 (0.2%)
1	D	0.91	1/1647 (0.1%)	1.04	3/2246 (0.1%)
1	G	0.95	0/1656	1.16	13/2258 (0.6%)
1	L	0.97	0/1662	1.10	9/2266 (0.4%)
2	B	0.89	0/1702	1.05	3/2319 (0.1%)
2	E	0.98	1/1702 (0.1%)	1.09	4/2319 (0.2%)
2	H	0.99	0/1675	1.10	10/2281 (0.4%)
2	I	0.97	0/1702	1.10	9/2319 (0.4%)
3	C	0.95	0/116	1.02	0/154
3	P	0.94	0/116	1.01	0/154
All	All	0.94	2/13636 (0.0%)	1.09	55/18577 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	200	THR	CA-CB	5.21	1.60	1.53
2	E	82(A)	THR	CA-CB	5.04	1.61	1.53

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	167	THR	CB-CA-C	7.06	119.70	109.11
2	H	195	ILE	N-CA-C	6.93	117.81	108.11
1	G	26	ASP	N-CA-C	6.83	119.59	111.33
2	H	139	GLY	N-CA-C	6.67	120.00	110.46
1	G	167	THR	CA-C-N	-6.63	113.96	120.52
1	G	167	THR	C-N-CA	-6.63	113.96	120.52
2	E	3	GLN	N-CA-C	6.29	117.70	108.14
2	E	100(D)	SER	N-CA-C	-6.22	100.45	109.59
2	I	169	VAL	CB-CA-C	-6.05	102.45	110.98
2	H	3	GLN	N-CA-C	5.99	117.89	108.96
2	H	163	VAL	N-CA-C	5.93	115.28	106.85
2	H	143	LYS	N-CA-C	5.90	118.51	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	157	SER	CA-C-N	5.90	127.21	119.84
1	G	157	SER	C-N-CA	5.90	127.21	119.84
1	G	24	SER	N-CA-C	5.85	118.50	109.07
2	E	186	SER	N-CA-C	5.83	118.41	111.71
1	G	39	ARG	N-CA-C	-5.82	102.73	110.07
2	B	139	GLY	N-CA-C	5.78	119.56	111.19
1	D	54	ARG	N-CA-C	5.75	116.90	109.72
1	G	112	GLN	CA-C-N	-5.59	114.83	120.31
1	G	112	GLN	C-N-CA	-5.59	114.83	120.31
1	D	141	SER	N-CA-C	5.59	117.46	109.14
1	L	96	THR	N-CA-C	5.58	117.82	108.96
2	H	201	LYS	CA-C-N	-5.58	113.00	119.47
2	H	201	LYS	C-N-CA	-5.58	113.00	119.47
2	I	201	LYS	CA-C-N	-5.55	113.03	119.47
2	I	201	LYS	C-N-CA	-5.55	113.03	119.47
1	G	2	TYR	N-CA-C	5.50	118.21	109.96
2	I	3	GLN	N-CA-C	5.48	117.41	109.07
2	I	212	GLU	CA-C-N	5.42	126.61	119.84
2	I	212	GLU	C-N-CA	5.42	126.61	119.84
2	I	82(B)	THR	CB-CA-C	-5.41	102.73	110.62
2	H	82(A)	THR	N-CA-C	-5.40	104.94	112.45
1	L	80	SER	N-CA-C	5.35	117.80	111.33
1	D	47	LEU	N-CA-C	-5.23	107.92	114.56
1	G	141	SER	N-CA-C	5.22	117.13	109.24
2	I	190	GLY	N-CA-C	-5.16	107.05	115.46
2	H	163	VAL	CB-CA-C	-5.15	104.83	111.53
1	L	112	GLN	CA-C-N	-5.14	114.94	120.03
1	L	112	GLN	C-N-CA	-5.14	114.94	120.03
1	L	25	GLY	N-CA-C	5.14	117.98	110.38
1	G	200	THR	CB-CA-C	-5.14	101.87	110.19
1	A	95	THR	N-CA-C	5.13	117.61	111.71
1	L	58	ILE	CA-C-N	-5.12	114.71	120.14
1	L	58	ILE	C-N-CA	-5.12	114.71	120.14
1	L	196	SER	N-CA-C	5.10	117.21	108.90
2	B	48	ILE	N-CA-C	-5.10	107.77	111.90
2	B	125	ALA	N-CA-C	5.06	116.90	109.71
1	L	141	SER	N-CA-C	5.05	117.36	109.52
1	A	167	THR	CA-C-N	5.05	126.16	119.84
1	A	167	THR	C-N-CA	5.05	126.16	119.84
2	H	55	SER	N-CA-C	5.05	119.02	112.86
2	E	184	VAL	N-CA-C	5.04	114.00	108.05
2	I	75	ILE	N-CA-C	5.04	117.02	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	ALA	N-CA-C	-5.02	104.96	112.54

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	1619	0	1578	60	0
1	D	1608	0	1568	49	0
1	G	1614	0	1574	39	0
1	L	1623	0	1581	38	0
2	B	1659	0	1618	35	0
2	E	1659	0	1618	55	0
2	H	1633	0	1591	39	0
2	I	1659	0	1618	31	0
3	C	113	0	115	7	0
3	P	113	0	115	8	0
4	A	12	0	0	0	0
4	B	30	0	0	0	0
4	C	1	0	0	0	0
4	D	31	0	0	1	0
4	E	49	0	0	1	0
4	G	48	0	0	2	0
4	H	44	0	0	0	0
4	I	55	0	0	1	0
4	L	55	0	0	4	0
4	P	3	0	0	0	0
All	All	13628	0	12976	341	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 13.

All (341) 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)
2:I:42:GLY:O	2:I:43:LYS:HE3	1.43	1.15
1:A:31:LYS:NZ	3:C:309:LEU:HD13	1.61	1.13
3:P:315:ARG:HG3	3:P:315:ARG:HH11	1.14	1.12
2:E:212:GLU:HB3	2:E:213:PRO:CD	1.79	1.11
2:E:212:GLU:HB3	2:E:213:PRO:HD3	1.12	1.05
2:H:192:GLN:NE2	2:H:193:THR:H	1.57	1.02
3:C:309:LEU:HD11	3:C:315:ARG:HD3	1.43	1.01
2:I:105:GLN:HE21	2:I:105:GLN:H	1.02	1.00
1:A:2:TYR:O	1:A:2:TYR:CD1	2.16	0.98
2:B:13:GLN:H	2:B:16:GLN:HE21	1.03	0.97
1:L:36:TYR:HE1	1:L:89:GLN:HG2	1.28	0.95
2:I:43:LYS:HA	2:I:43:LYS:CE	1.96	0.95
1:A:2:TYR:OH	1:A:31:LYS:HD2	1.67	0.95
2:H:192:GLN:HE21	2:H:193:THR:H	1.14	0.94
1:G:198:GLN:HG3	1:G:205:THR:CG2	1.98	0.93
2:I:13:GLN:HG2	2:I:16:GLN:NE2	1.84	0.92
1:D:166:THR:CG2	1:D:179:SER:H	1.82	0.92
2:H:149:PRO:HG3	2:E:201:LYS:HG3	1.51	0.91
2:H:105:GLN:H	2:H:105:GLN:HE21	0.99	0.91
1:A:205:THR:HG23	1:A:206:VAL:N	1.84	0.90
1:L:2:TYR:HE2	1:L:31:LYS:HZ2	1.17	0.90
2:E:105:GLN:H	2:E:105:GLN:HE21	0.94	0.90
1:L:17:GLN:O	1:L:78:THR:HG23	1.72	0.89
2:I:13:GLN:H	2:I:16:GLN:HE21	1.17	0.89
2:E:105:GLN:H	2:E:105:GLN:NE2	1.70	0.88
2:H:105:GLN:H	2:H:105:GLN:NE2	1.73	0.87
2:B:23:LYS:NZ	2:B:75:ILE:O	2.08	0.87
2:B:6:GLU:H	2:B:105:GLN:HE22	1.18	0.86
2:H:192:GLN:HE21	2:H:193:THR:N	1.75	0.85
2:B:105:GLN:HE21	2:B:105:GLN:H	1.24	0.85
1:A:31:LYS:HZ2	3:C:309:LEU:HD13	1.39	0.85
1:G:198:GLN:HG3	1:G:205:THR:HG21	1.56	0.84
2:H:105:GLN:HE21	2:H:105:GLN:N	1.76	0.83
1:D:171:GLN:HE21	1:D:177:ALA:HB2	1.43	0.83
1:G:171:GLN:HE21	1:G:173:ASN:HD21	1.26	0.83
1:G:37:TYR:HB2	1:G:47:LEU:HD11	1.61	0.83
1:G:36:TYR:HE1	1:G:89:GLN:HG2	1.43	0.82
1:L:36:TYR:CE1	1:L:89:GLN:HG2	2.13	0.82
2:E:105:GLN:HE21	2:E:105:GLN:N	1.76	0.82
2:H:40:ILE:HG23	2:H:41:PRO:HD2	1.61	0.82
1:D:36:TYR:HE1	1:D:89:GLN:HG2	1.45	0.82
2:E:1:GLU:OE2	2:E:1:GLU:N	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:43:LYS:HA	2:I:43:LYS:HE2	1.62	0.80
2:B:13:GLN:H	2:B:16:GLN:NE2	1.82	0.78
2:I:6:GLU:H	2:I:105:GLN:HE22	1.31	0.78
2:H:6:GLU:H	2:H:105:GLN:HE22	1.32	0.77
2:I:105:GLN:H	2:I:105:GLN:NE2	1.79	0.77
1:A:2:TYR:O	1:A:2:TYR:CG	2.38	0.76
3:P:315:ARG:HG3	3:P:315:ARG:NH1	1.95	0.76
2:I:105:GLN:HE21	2:I:105:GLN:N	1.83	0.75
2:B:105:GLN:H	2:B:105:GLN:NE2	1.83	0.75
1:A:153:LYS:HA	1:A:158:PRO:HA	1.68	0.74
2:H:149:PRO:HG3	2:E:201:LYS:CG	2.16	0.74
1:D:37:TYR:HB2	1:D:47:LEU:HD11	1.70	0.74
1:G:38:GLN:OE1	2:I:39:GLN:NE2	2.16	0.73
2:B:82:TRP:NE1	2:B:86:ASP:OD1	2.21	0.73
1:A:36:TYR:HE1	1:A:89:GLN:HG2	1.53	0.73
1:L:153:LYS:HD2	1:L:198:GLN:HE22	1.52	0.73
1:L:188:GLN:HA	1:L:191:SER:HB3	1.72	0.72
1:D:142:ASP:H	1:D:171:GLN:HE22	1.36	0.71
2:E:212:GLU:CB	2:E:213:PRO:CD	2.65	0.71
1:A:31:LYS:HZ3	3:C:309:LEU:HD13	1.55	0.70
1:A:173:ASN:C	1:A:173:ASN:HD22	1.99	0.70
1:A:170:LYS:HE3	1:A:174:ASN:ND2	2.07	0.70
1:G:173:ASN:HD22	1:G:173:ASN:N	1.88	0.70
1:L:163:VAL:HG22	1:L:182:LEU:CD1	2.21	0.69
2:E:163:VAL:HG22	2:E:182:VAL:HG22	1.73	0.69
1:G:164:GLU:HG2	2:I:171:GLN:HA	1.73	0.69
2:B:13:GLN:HG2	2:B:16:GLN:NE2	2.07	0.69
2:E:126:PRO:HD3	2:E:212:GLU:O	1.92	0.69
1:G:36:TYR:CE1	1:G:89:GLN:HG2	2.27	0.69
1:D:166:THR:HG22	1:D:179:SER:O	1.93	0.68
1:D:39:ARG:NH2	1:D:81:LEU:HD22	2.09	0.68
1:A:114:LYS:HE3	1:A:202:GLU:OE2	1.94	0.68
2:E:98:PHE:H	2:E:100(E):ASN:ND2	1.91	0.68
1:A:13:VAL:HG22	1:A:14:SER:N	2.09	0.68
1:G:173:ASN:HD22	1:G:173:ASN:H	1.42	0.68
1:D:171:GLN:NE2	1:D:177:ALA:HB2	2.09	0.67
2:E:150:VAL:HG22	2:E:178:LEU:HD21	1.77	0.67
1:D:163:VAL:HG23	1:D:182:LEU:HD13	1.77	0.67
1:A:201:HIS:C	1:A:202:GLU:HG3	2.20	0.66
1:D:119:VAL:O	1:D:208:LYS:HE3	1.95	0.66
3:C:309:LEU:HD11	3:C:315:ARG:CD	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:SER:O	1:A:15:PRO:O	2.14	0.66
2:I:13:GLN:H	2:I:16:GLN:NE2	1.93	0.66
2:I:43:LYS:HE3	2:I:43:LYS:HA	1.75	0.66
2:H:192:GLN:NE2	2:H:193:THR:N	2.35	0.65
2:H:192:GLN:NE2	2:H:193:THR:OG1	2.30	0.65
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.78	0.65
1:A:201:HIS:O	1:A:202:GLU:CB	2.45	0.65
1:L:104:ASP:HB2	4:L:238:HOH:O	1.98	0.64
2:E:186:SER:HA	2:E:189:LEU:HD13	1.79	0.63
2:B:54:ASP:OD2	2:B:56:ASP:HB2	1.98	0.63
2:B:1:GLU:CD	2:B:1:GLU:N	2.56	0.62
2:E:154:TRP:O	2:E:155:ASN:HB2	1.99	0.62
2:E:195:ILE:HA	2:E:209:LYS:O	2.00	0.62
2:E:1:GLU:H3	2:E:1:GLU:CD	2.04	0.62
1:A:36:TYR:CE1	1:A:89:GLN:HG2	2.33	0.62
1:A:67:SER:O	1:A:70:THR:HG22	1.99	0.61
1:L:173:ASN:O	1:L:174:ASN:HB2	2.00	0.61
2:B:6:GLU:H	2:B:105:GLN:NE2	1.95	0.61
1:G:50:GLN:HE21	1:G:53:LYS:HZ2	1.49	0.61
1:G:124:PRO:HD3	1:G:136:LEU:HD23	1.83	0.60
1:D:130:GLN:C	1:D:132:ASN:H	2.09	0.60
1:L:50:GLN:NE2	4:L:216:HOH:O	2.20	0.60
2:E:201:LYS:H	2:E:201:LYS:HZ2	1.49	0.60
1:D:200:THR:OG1	1:D:205:THR:HG22	2.01	0.60
1:A:55:PRO:HD2	1:A:58:ILE:HG13	1.83	0.59
2:B:6:GLU:N	2:B:105:GLN:HE22	1.96	0.59
2:E:100(C):SER:HB3	2:E:100(E):ASN:ND2	2.18	0.59
1:L:106(A):ARG:NH1	4:L:247:HOH:O	2.20	0.59
3:P:305:LYS:HE2	3:P:318:TYR:CD2	2.38	0.58
1:A:201:HIS:O	1:A:202:GLU:HG3	2.02	0.58
1:L:164:GLU:HB3	2:H:169:VAL:HG11	1.85	0.58
1:A:37:TYR:HB2	1:A:47:LEU:HD11	1.84	0.58
1:A:173:ASN:C	1:A:173:ASN:ND2	2.61	0.58
2:B:1:GLU:CD	2:B:1:GLU:H3	2.11	0.58
1:D:61:ARG:NH2	1:D:82:ASP:OD1	2.34	0.58
1:A:13:VAL:CG2	1:A:14:SER:N	2.66	0.58
1:L:153:LYS:HB3	1:L:196:SER:HB2	1.83	0.58
1:L:32:TYR:OH	2:H:100(B):GLN:HG3	2.04	0.58
2:E:160:THR:O	2:E:160:THR:OG1	2.22	0.57
1:A:201:HIS:O	1:A:202:GLU:HB2	2.02	0.57
1:G:173:ASN:H	1:G:173:ASN:ND2	2.00	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:96:THR:HG23	1:G:97:LYS:N	2.18	0.57
2:E:123:PRO:HD3	2:E:209:LYS:HE2	1.87	0.57
2:H:28:ASN:HD21	2:H:31:ASP:CG	2.12	0.56
1:G:50:GLN:HE21	1:G:53:LYS:NZ	2.02	0.56
2:B:210:LYS:HD2	2:B:212:GLU:HG3	1.86	0.56
2:E:2:VAL:HG13	2:E:102:LEU:HD11	1.87	0.56
1:D:173:ASN:HD21	1:D:175:LYS:HB2	1.70	0.56
2:I:150:VAL:CG2	2:I:178:LEU:HD21	2.36	0.56
1:L:2:TYR:OH	1:L:31:LYS:HD2	2.06	0.56
1:L:163:VAL:HG22	1:L:182:LEU:HD11	1.88	0.55
1:L:36:TYR:HE1	1:L:89:GLN:CG	2.10	0.55
1:D:13:VAL:HG22	1:D:17:GLN:HB2	1.88	0.55
2:B:105:GLN:HE21	2:B:105:GLN:N	1.98	0.55
2:H:19:LYS:HZ2	1:A:203:GLY:HA3	1.71	0.55
1:D:166:THR:HG23	1:D:179:SER:H	1.66	0.55
1:A:152:TRP:HE1	1:A:180:SER:HB3	1.70	0.55
2:E:134:GLY:O	2:E:185:PRO:HA	2.07	0.55
1:G:72:THR:OG1	4:G:276:HOH:O	2.17	0.55
1:G:36:TYR:HE1	1:G:89:GLN:CG	2.16	0.55
1:A:143:PHE:HE2	1:A:146:GLY:HA2	1.72	0.54
2:E:100(D):SER:O	2:E:100(D):SER:OG	2.23	0.54
1:A:201:HIS:C	1:A:202:GLU:CG	2.77	0.54
2:I:13:GLN:HG2	2:I:16:GLN:HE21	1.65	0.54
2:H:28:ASN:ND2	2:H:31:ASP:CG	2.65	0.54
1:G:171:GLN:NE2	1:G:173:ASN:HD21	2.01	0.54
2:H:19:LYS:NZ	1:A:203:GLY:HA3	2.22	0.54
1:A:153:LYS:HB2	1:A:196:SER:HB3	1.90	0.54
2:E:138:LEU:HD23	2:E:182:VAL:O	2.08	0.54
1:A:144:TYR:O	1:A:201:HIS:CE1	2.61	0.53
2:E:201:LYS:H	2:E:201:LYS:NZ	2.06	0.53
1:G:142:ASP:OD1	1:G:171:GLN:NE2	2.40	0.53
1:D:130:GLN:C	1:D:132:ASN:N	2.65	0.53
1:A:14:SER:O	1:A:15:PRO:C	2.52	0.53
2:E:138:LEU:HD23	2:E:138:LEU:H	1.73	0.53
1:D:140:ILE:HD12	1:D:199:VAL:HG21	1.90	0.52
1:L:39:ARG:NH2	1:L:81:LEU:HD22	2.24	0.52
2:H:193:THR:O	2:H:194:TYR:HB2	2.08	0.52
1:A:114:LYS:CE	1:A:202:GLU:OE2	2.56	0.52
1:D:173:ASN:ND2	1:D:175:LYS:H	2.08	0.52
2:H:149:PRO:CG	2:E:201:LYS:HG3	2.32	0.52
2:H:162:GLY:O	2:H:182:VAL:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:TYR:OH	1:A:31:LYS:CD	2.48	0.51
1:G:171:GLN:HE21	1:G:173:ASN:ND2	2.02	0.51
1:A:61:ARG:NH2	1:A:82:ASP:OD1	2.37	0.51
1:L:2:TYR:HE2	1:L:31:LYS:NZ	1.98	0.51
2:B:210:LYS:NZ	2:B:211:VAL:O	2.43	0.51
1:D:163:VAL:HG23	1:D:182:LEU:CD1	2.40	0.51
2:I:126:PRO:HG3	2:I:138:LEU:HD23	1.93	0.51
1:D:184:LEU:HD11	1:D:195:TYR:CZ	2.46	0.51
2:E:138:LEU:HD12	2:E:211:VAL:HB	1.92	0.51
1:G:171:GLN:HB2	1:G:173:ASN:HD21	1.76	0.51
1:A:17:GLN:O	1:A:78:THR:HG23	2.11	0.51
1:G:2:TYR:CZ	1:G:27:LYS:HB2	2.46	0.51
1:G:171:GLN:HB2	1:G:173:ASN:ND2	2.26	0.51
2:B:89:LYS:HD3	2:B:91:PHE:CZ	2.45	0.50
1:A:13:VAL:CG2	1:A:14:SER:H	2.23	0.50
1:D:140:ILE:HD12	1:D:199:VAL:CG2	2.42	0.50
1:L:119:VAL:O	1:L:208:LYS:NZ	2.45	0.50
1:D:153:LYS:HE2	1:D:198:GLN:NE2	2.27	0.50
2:I:4:LEU:HG	2:I:102:LEU:HD13	1.92	0.50
1:L:2:TYR:HB2	4:L:226:HOH:O	2.12	0.50
1:L:124:PRO:HD3	1:L:136:LEU:HD23	1.94	0.49
1:D:144:TYR:O	1:D:201:HIS:HE1	1.95	0.49
2:H:138:LEU:O	2:H:181:VAL:HG23	2.12	0.49
2:B:4:LEU:HG	2:B:102:LEU:HD13	1.94	0.49
1:D:36:TYR:CE1	1:D:89:GLN:HG2	2.36	0.49
1:D:198:GLN:HG2	1:D:207:GLU:HB2	1.94	0.49
1:D:85:ASP:OD1	1:D:106(A):ARG:HD3	2.13	0.49
1:L:168:PRO:HA	1:L:177:ALA:O	2.13	0.49
1:G:112:GLN:HB2	1:G:113:PRO:HD2	1.95	0.49
2:E:38:ARG:HB2	2:E:48:ILE:HD11	1.93	0.49
1:L:153:LYS:HG2	1:L:156:SER:HA	1.95	0.49
2:H:178:LEU:HD12	2:H:178:LEU:C	2.38	0.49
2:E:184:VAL:HG11	2:E:194:TYR:CE1	2.49	0.48
1:L:14:SER:O	1:L:15:PRO:C	2.55	0.48
2:H:119:PRO:HD2	2:H:205:THR:HG21	1.94	0.48
2:H:40:ILE:CG2	2:H:41:PRO:HD2	2.40	0.48
2:B:210:LYS:CD	2:B:212:GLU:HG3	2.42	0.48
2:H:54:ASP:OD2	2:H:56:ASP:HB2	2.13	0.48
2:B:178:LEU:C	2:B:178:LEU:HD12	2.38	0.48
1:L:152:TRP:CD2	1:L:182:LEU:HD13	2.49	0.48
2:B:154:TRP:CH2	2:B:196:CYS:HB3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:GLN:O	1:G:51:ASP:HB2	2.13	0.48
1:D:163:VAL:CG2	1:D:182:LEU:HD13	2.43	0.48
1:G:99:THR:HG22	1:G:101:LEU:HD23	1.95	0.48
2:H:28:ASN:ND2	2:H:31:ASP:HB2	2.28	0.48
3:C:305:LYS:O	3:C:305:LYS:HG2	2.12	0.47
2:I:145:TYR:CE1	2:I:150:VAL:HG13	2.48	0.47
2:I:1:GLU:HG2	2:I:2:VAL:N	2.28	0.47
2:E:17:SER:HB3	2:E:82(A):THR:O	2.14	0.47
1:D:166:THR:HG21	1:D:179:SER:H	1.74	0.47
2:B:30:LEU:HD13	2:B:53:ASP:OD1	2.14	0.47
1:A:26:ASP:OD2	1:A:69:LYS:NZ	2.46	0.47
1:D:124:PRO:HD3	1:D:136:LEU:HD23	1.96	0.47
3:P:315:ARG:HH11	3:P:315:ARG:CG	2.01	0.47
1:G:13:VAL:HG22	1:G:17:GLN:HB2	1.97	0.47
2:B:29:PHE:CE2	2:B:52(A):PRO:HB3	2.49	0.47
2:E:95:LEU:HD21	2:E:97:LEU:HG	1.97	0.47
2:B:83:GLN:HG2	2:B:84:ALA:N	2.30	0.47
2:E:2:VAL:O	2:E:3:GLN:HB3	2.15	0.47
1:D:122:PHE:HE1	2:E:125:ALA:O	1.97	0.46
1:G:186:PRO:O	1:G:190:LYS:HG3	2.15	0.46
1:A:201:HIS:O	1:A:202:GLU:CG	2.62	0.46
2:B:163:VAL:HG22	2:B:182:VAL:HG13	1.97	0.46
1:D:26:ASP:OD1	1:D:26:ASP:N	2.41	0.46
1:A:61:ARG:HH22	1:A:82:ASP:CG	2.20	0.46
1:A:54:ARG:NH1	1:A:58:ILE:O	2.44	0.46
2:I:191:THR:HG22	2:I:192:GLN:N	2.31	0.46
1:L:27:LYS:HB2	1:L:31:LYS:HE3	1.98	0.46
2:H:75:ILE:O	2:H:76:SER:HB2	2.15	0.46
2:B:150:VAL:CG2	2:B:178:LEU:HD21	2.46	0.46
2:E:2:VAL:CG1	2:E:102:LEU:HD11	2.46	0.46
2:B:82:TRP:CD1	2:B:86:ASP:OD1	2.69	0.46
1:A:2:TYR:CZ	1:A:31:LYS:HD2	2.48	0.46
1:A:205:THR:O	1:A:206:VAL:HG23	2.16	0.46
2:B:20:ILE:HG21	2:B:109:ILE:HD11	1.98	0.46
1:D:171:GLN:NE2	1:D:176:TYR:O	2.49	0.46
4:D:222:HOH:O	2:E:143:LYS:HG2	2.16	0.46
1:G:189:TRP:CZ2	1:G:212:PRO:HA	2.51	0.46
1:A:100:VAL:HB	2:B:47:TRP:CG	2.51	0.45
1:L:17:GLN:O	1:L:78:THR:CG2	2.54	0.45
1:A:140:ILE:HG12	1:A:199:VAL:HG21	1.97	0.45
1:D:167:THR:O	1:D:168:PRO:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:TRP:CZ2	1:D:212:PRO:HA	2.51	0.45
1:A:19:ALA:N	1:A:75:ILE:O	2.40	0.45
2:I:200:HIS:CD2	2:I:202:PRO:HD2	2.50	0.45
2:E:82(A):THR:N	4:E:227:HOH:O	2.49	0.45
1:G:89:GLN:HA	1:G:101:LEU:O	2.17	0.45
1:A:2:TYR:CD1	1:A:2:TYR:C	2.92	0.45
1:A:144:TYR:CG	1:A:145:PRO:HA	2.51	0.45
2:E:19:LYS:HA	2:E:80:LEU:O	2.17	0.45
2:E:154:TRP:O	2:E:156:SER:N	2.50	0.45
1:D:166:THR:CG2	1:D:179:SER:N	2.66	0.45
1:G:96:THR:CG2	1:G:97:LYS:N	2.79	0.45
1:G:133:LYS:HE3	1:G:133:LYS:HA	1.99	0.45
2:I:38:ARG:HB2	2:I:48:ILE:HD11	1.99	0.45
2:B:95:LEU:HD11	2:B:100(E):ASN:HB3	1.99	0.45
1:L:152:TRP:CG	1:L:182:LEU:HD13	2.52	0.44
2:H:15:GLY:HA2	2:H:82(B):THR:HG23	1.99	0.44
2:I:43:LYS:CE	2:I:43:LYS:CA	2.82	0.44
2:E:40:ILE:HG23	2:E:41:PRO:HD2	1.99	0.44
1:D:79:GLN:NE2	1:D:82:ASP:OD2	2.51	0.44
2:E:138:LEU:CD2	2:E:184:VAL:HG22	2.47	0.44
2:E:155:ASN:N	2:E:195:ILE:O	2.34	0.44
1:G:169:SER:HB3	4:G:245:HOH:O	2.18	0.44
2:H:54:ASP:OD1	3:P:305:LYS:NZ	2.50	0.43
1:A:144:TYR:CD1	1:A:145:PRO:HA	2.53	0.43
1:G:60:GLU:H	1:G:60:GLU:CD	2.23	0.43
1:L:198:GLN:HG3	1:L:207:GLU:HG3	2.00	0.43
1:D:13:VAL:HG11	1:D:78:THR:HG21	2.00	0.43
1:L:177:ALA:HB3	2:H:164:HIS:CE1	2.54	0.43
1:D:39:ARG:HH21	1:D:81:LEU:HD22	1.77	0.43
1:D:139:LEU:HD22	2:E:166:PHE:CE1	2.53	0.43
2:E:212:GLU:CB	2:E:213:PRO:HD3	2.07	0.43
2:I:36:TRP:CE3	2:I:80:LEU:HD22	2.54	0.43
1:A:190:LYS:HA	1:A:212:PRO:HG3	2.00	0.43
1:D:154:ALA:HB2	1:D:195:TYR:CE2	2.53	0.43
1:D:172:SER:C	1:D:174:ASN:H	2.26	0.43
2:E:93:THR:HG23	2:E:100(G):PHE:CD1	2.54	0.43
1:G:61:ARG:HH22	1:G:82:ASP:CG	2.26	0.43
1:A:14:SER:C	1:A:15:PRO:O	2.62	0.43
1:A:92:ASP:HB2	1:A:101:LEU:HD11	2.01	0.43
1:A:185:THR:C	1:A:187:GLU:N	2.76	0.43
2:H:125:ALA:HB1	2:H:213:PRO:HA	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:ASP:OD1	1:D:193:LYS:HB2	2.19	0.42
1:A:31:LYS:O	1:A:66:LYS:NZ	2.51	0.42
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.55	0.42
2:E:154:TRP:CZ3	2:E:196:CYS:HB3	2.54	0.42
2:I:178:LEU:C	2:I:178:LEU:HD12	2.44	0.42
2:I:209:LYS:HD2	2:I:209:LYS:HA	1.85	0.42
1:L:2:TYR:OH	1:L:31:LYS:CD	2.67	0.42
1:A:14:SER:O	1:A:17:GLN:HB3	2.19	0.42
3:C:309:LEU:C	3:C:309:LEU:HD12	2.44	0.42
2:E:100(C):SER:HB3	2:E:100(E):ASN:HD21	1.84	0.42
1:G:31:LYS:HD2	1:G:31:LYS:HA	1.84	0.42
2:H:30:LEU:HA	2:H:52(A):PRO:HB2	2.01	0.42
1:L:61:ARG:HD2	1:L:76:SER:O	2.19	0.42
2:H:145:TYR:CZ	2:H:150:VAL:HG13	2.55	0.42
3:P:309:LEU:N	3:P:309:LEU:HD23	2.34	0.42
2:E:162:GLY:O	2:E:183:THR:N	2.41	0.42
1:D:157:SER:HA	1:D:158:PRO:HD3	1.94	0.42
2:I:150:VAL:HG22	2:I:178:LEU:HD21	2.01	0.42
3:P:309:LEU:HG	3:P:317:PHE:HE1	1.84	0.42
1:D:36:TYR:O	1:D:86:TYR:HA	2.19	0.42
2:E:54:ASP:OD2	2:E:54:ASP:C	2.62	0.42
1:G:100:VAL:HB	2:I:47:TRP:CD2	2.54	0.42
1:L:31:LYS:HD3	1:L:91:TRP:O	2.20	0.41
1:L:193:LYS:O	1:L:212:PRO:HD2	2.20	0.41
2:I:214:LYS:NZ	4:I:230:HOH:O	2.44	0.41
2:H:29:PHE:CE2	2:H:52(A):PRO:HB3	2.54	0.41
2:H:58:HIS:NE2	3:P:318:TYR:OH	2.45	0.41
1:A:185:THR:C	1:A:187:GLU:H	2.28	0.41
1:A:122:PHE:HA	1:A:123:PRO:HD3	1.90	0.41
1:A:138:CYS:HB2	1:A:152:TRP:CZ2	2.56	0.41
2:I:125:ALA:HA	2:I:126:PRO:HD3	1.87	0.41
2:B:138:LEU:O	2:B:181:VAL:HA	2.20	0.41
1:L:89:GLN:HA	1:L:101:LEU:O	2.21	0.41
1:G:89:GLN:HB2	1:G:101:LEU:O	2.20	0.41
2:H:166:PHE:C	2:H:167:PRO:O	2.60	0.41
1:A:6:GLN:OE1	1:A:103:GLY:HA3	2.21	0.41
2:E:169:VAL:O	2:E:176:TYR:HA	2.21	0.41
1:D:144:TYR:O	1:D:201:HIS:CE1	2.72	0.41
1:L:212:PRO:HA	1:L:213:THR:HA	1.61	0.41
1:D:173:ASN:ND2	1:D:173:ASN:C	2.78	0.41
2:E:6:GLU:H	2:E:105:GLN:HE22	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:THR:OG1	2:E:143:LYS:HE2	2.20	0.40
1:G:6:GLN:OE1	1:G:103:GLY:HA3	2.21	0.40
2:I:32:SER:HB3	2:I:96:TYR:CE2	2.56	0.40
2:E:42:GLY:C	2:E:43:LYS:HD2	2.47	0.40
2:E:209:LYS:HA	2:E:209:LYS:HD3	1.85	0.40
1:D:121:LEU:HD12	1:D:137:VAL:O	2.20	0.40
1:L:34:SER:HB2	1:L:89:GLN:HG3	2.03	0.40
2:H:53:ASP:O	2:H:73:LYS:NZ	2.47	0.40
1:A:89:GLN:HA	1:A:101:LEU:O	2.20	0.40
2:B:83:GLN:HG2	2:B:84:ALA:H	1.86	0.40
2:H:40:ILE:HG23	2:H:41:PRO:CD	2.40	0.40
2:B:154:TRP:CZ3	2:B:196:CYS:HB3	2.56	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	211/219 (96%)	187 (89%)	19 (9%)	5 (2%)	4	8
1	D	209/219 (95%)	196 (94%)	13 (6%)	0	100	100
1	G	210/219 (96%)	199 (95%)	9 (4%)	2 (1%)	12	24
1	L	212/219 (97%)	198 (93%)	10 (5%)	4 (2%)	6	11
2	B	215/226 (95%)	202 (94%)	11 (5%)	2 (1%)	14	27
2	E	215/226 (95%)	196 (91%)	16 (7%)	3 (1%)	9	17
2	H	209/226 (92%)	194 (93%)	13 (6%)	2 (1%)	12	24
2	I	215/226 (95%)	203 (94%)	11 (5%)	1 (0%)	24	43
3	C	12/23 (52%)	12 (100%)	0	0	100	100
3	P	12/23 (52%)	12 (100%)	0	0	100	100
All	All	1720/1826 (94%)	1599 (93%)	102 (6%)	19 (1%)	11	22

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	2	TYR
2	E	156	SER
2	E	212	GLU
1	L	131	ALA
1	A	15	PRO
1	A	16	GLY
1	A	168	PRO
2	B	114	GLY
2	H	65	GLY
1	A	67	SER
2	B	41	PRO
1	G	155	ASP
2	I	213	PRO
1	L	155	ASP
1	A	202	GLU
1	L	191	SER
2	H	172	SER
2	E	65	GLY
1	G	158	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	184/186 (99%)	157 (85%)	27 (15%)	3	6
1	D	183/186 (98%)	163 (89%)	20 (11%)	6	13
1	G	184/186 (99%)	166 (90%)	18 (10%)	7	16
1	L	184/186 (99%)	164 (89%)	20 (11%)	6	13
2	B	188/194 (97%)	168 (89%)	20 (11%)	6	14
2	E	188/194 (97%)	170 (90%)	18 (10%)	8	17
2	H	184/194 (95%)	164 (89%)	20 (11%)	6	13
2	I	188/194 (97%)	173 (92%)	15 (8%)	11	24
3	C	11/17 (65%)	10 (91%)	1 (9%)	9	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	P	11/17 (65%)	7 (64%)	4 (36%)	0 0
All	All	1505/1554 (97%)	1342 (89%)	163 (11%)	6 13

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	SER
1	L	6	GLN
1	L	9	SER
1	L	13	VAL
1	L	24	SER
1	L	28	LEU
1	L	30	ASP
1	L	56	SER
1	L	62	LEU
1	L	67	SER
1	L	69	LYS
1	L	81	LEU
1	L	89	GLN
1	L	130	GLN
1	L	135	THR
1	L	153	LYS
1	L	159	VAL
1	L	170	LYS
1	L	193	LYS
1	L	205	THR
2	H	13	GLN
2	H	23	LYS
2	H	67	VAL
2	H	73	LYS
2	H	100(B)	GLN
2	H	100(C)	SER
2	H	100(D)	SER
2	H	100(E)	ASN
2	H	100(G)	PHE
2	H	102	LEU
2	H	105	GLN
2	H	108	MET
2	H	113	SER
2	H	150	VAL
2	H	159	LEU
2	H	178	LEU

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Mol	Chain	Res	Type
2	H	179	SER
2	H	191	THR
2	H	196	CYS
2	H	204	ASN
3	P	303	THR
3	P	306	SER
3	P	309	LEU
3	P	315	ARG
1	A	6	GLN
1	A	13	VAL
1	A	27	LYS
1	A	29	ASP
1	A	30	ASP
1	A	56	SER
1	A	78	THR
1	A	80	SER
1	A	94	SER
1	A	108	THR
1	A	119	VAL
1	A	126	SER
1	A	132	ASN
1	A	149	THR
1	A	155	ASP
1	A	159	VAL
1	A	160	LYS
1	A	172	SER
1	A	173	ASN
1	A	180	SER
1	A	188	GLN
1	A	193	LYS
1	A	200	THR
1	A	204	SER
1	A	205	THR
1	A	207	GLU
1	A	209	THR
2	B	1	GLU
2	B	13	GLN
2	B	23	LYS
2	B	34	ILE
2	B	39	GLN
2	B	66	GLN
2	B	67	VAL

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Mol	Chain	Res	Type
2	B	81	GLN
2	B	83	GLN
2	B	86	ASP
2	B	102	LEU
2	B	105	GLN
2	B	117	LYS
2	B	138	LEU
2	B	170	LEU
2	B	175	LEU
2	B	178	LEU
2	B	182	VAL
2	B	191	THR
2	B	210	LYS
3	C	303	THR
1	D	9	SER
1	D	13	VAL
1	D	26	ASP
1	D	30	ASP
1	D	50	GLN
1	D	56	SER
1	D	61	ARG
1	D	81	LEU
1	D	89	GLN
1	D	140	ILE
1	D	159	VAL
1	D	163	VAL
1	D	166	THR
1	D	173	ASN
1	D	183	SER
1	D	190	LYS
1	D	208	LYS
1	D	209	THR
1	D	210	VAL
1	D	213	THR
2	E	1	GLU
2	E	13	GLN
2	E	43	LYS
2	E	64	GLU
2	E	83	GLN
2	E	97	LEU
2	E	99	GLU
2	E	105	GLN

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Mol	Chain	Res	Type
2	E	115	THR
2	E	150	VAL
2	E	156	SER
2	E	160	THR
2	E	161	SER
2	E	169	VAL
2	E	183	THR
2	E	192	GLN
2	E	201	LYS
2	E	209	LYS
1	G	1	SER
1	G	3	ASP
1	G	12	SER
1	G	13	VAL
1	G	28	LEU
1	G	29	ASP
1	G	63	SER
1	G	79	GLN
1	G	80	SER
1	G	89	GLN
1	G	97	LYS
1	G	133	LYS
1	G	159	VAL
1	G	164	GLU
1	G	173	ASN
1	G	179	SER
1	G	200	THR
1	G	213	THR
2	I	2	VAL
2	I	13	GLN
2	I	25	SER
2	I	43	LYS
2	I	102	LEU
2	I	105	GLN
2	I	160	THR
2	I	169	VAL
2	I	182	VAL
2	I	187	SER
2	I	189	LEU
2	I	191	THR
2	I	193	THR
2	I	195	ILE

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Mol	Chain	Res	Type
2	I	209	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	50	GLN
1	L	112	GLN
1	L	198	GLN
1	L	201	HIS
2	H	3	GLN
2	H	28	ASN
2	H	81	GLN
2	H	105	GLN
2	H	164	HIS
2	H	192	GLN
2	H	199	ASN
1	A	79	GLN
1	A	130	GLN
1	A	132	ASN
1	A	173	ASN
1	A	174	ASN
1	A	198	GLN
1	A	201	HIS
2	B	3	GLN
2	B	16	GLN
2	B	66	GLN
2	B	81	GLN
2	B	83	GLN
2	B	105	GLN
2	B	192	GLN
2	B	204	ASN
1	D	42	GLN
1	D	171	GLN
1	D	173	ASN
1	D	174	ASN
1	D	192	HIS
1	D	201	HIS
2	E	3	GLN
2	E	13	GLN
2	E	16	GLN
2	E	81	GLN
2	E	100(E)	ASN

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Mol	Chain	Res	Type
2	E	105	GLN
2	E	192	GLN
1	G	50	GLN
1	G	79	GLN
1	G	173	ASN
1	G	192	HIS
1	G	198	GLN
2	I	16	GLN
2	I	28	ASN
2	I	100(E)	ASN
2	I	105	GLN

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](#)

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	215/219 (98%)	0.49	10 (4%) 36 32	26, 58, 87, 92	0
1	D	213/219 (97%)	0.09	3 (1%) 73 70	25, 46, 66, 74	0
1	G	213/219 (97%)	-0.19	1 (0%) 87 85	22, 41, 60, 67	1 (0%)
1	L	216/219 (98%)	-0.03	5 (2%) 61 57	21, 37, 73, 76	0
2	B	219/226 (96%)	-0.06	0 100 100	25, 43, 59, 69	0
2	E	219/226 (96%)	-0.12	6 (2%) 56 51	23, 37, 78, 88	0
2	H	215/226 (95%)	0.00	5 (2%) 61 57	22, 39, 71, 80	0
2	I	219/226 (96%)	-0.23	1 (0%) 87 85	18, 34, 66, 80	0
3	C	14/23 (60%)	1.28	3 (21%) 2 2	64, 74, 87, 88	0
3	P	14/23 (60%)	0.46	0 100 100	43, 51, 62, 65	0
All	All	1757/1826 (96%)	0.01	34 (1%) 66 62	18, 42, 74, 92	1 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TYR	5.2
1	A	189	TRP	3.8
2	H	134	GLY	3.8
3	C	317	PHE	3.7
1	L	2	TYR	3.6
1	A	159	VAL	3.1
1	A	184	LEU	2.9
1	D	1	SER	2.8
1	A	1	SER	2.8
1	L	1	SER	2.7
2	E	185	PRO	2.6
2	E	188	SER	2.5
3	C	318	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	2	TYR	2.3
1	L	189	TRP	2.3
2	H	190	GLY	2.3
3	C	303	THR	2.3
1	A	195	TYR	2.3
2	E	137	ALA	2.2
1	L	136	LEU	2.1
2	E	159	LEU	2.1
1	A	152	TRP	2.1
1	A	146	GLY	2.1
2	E	158	ALA	2.1
1	A	168	PRO	2.1
1	L	210	VAL	2.0
1	D	146	GLY	2.0
1	A	204	SER	2.0
2	H	136	ALA	2.0
2	H	137	ALA	2.0
1	D	213	THR	2.0
2	H	185	PRO	2.0
2	I	185	PRO	2.0
2	E	187	SER	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.