



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:51 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 wwPDB X-ray Structure Validation Summary 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
Xtrriage (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

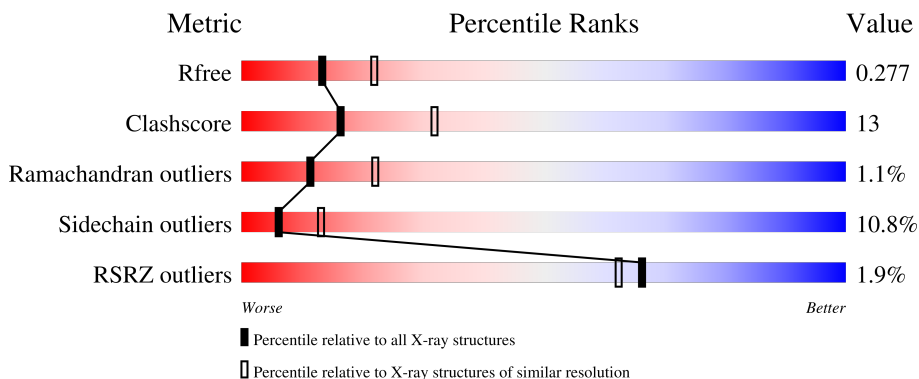
1 Overall quality at a glance

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	<p>3% 69% 21% 7% .</p>
2	H	226	<p>2% 67% 26% . 5%</p>
2	I	226	<p>77% 17% . .</p>
3	C	23	<p>13% 43% 17% 39%</p>
3	P	23	<p>30% 22% 9% 39%</p>

2 Entry composition [i](#)

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

- 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
			Total	C	N	O	S			
2	H	215	Total 1633	C 1044	N 263	O 320	S 6	0	0	0
2	B	219	Total 1659	C 1059	N 267	O 327	S 6	0	0	0
2	E	219	Total 1659	C 1059	N 267	O 327	S 6	0	0	0
2	I	219	Total 1659	C 1059	N 267	O 327	S 6	0	0	0

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

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

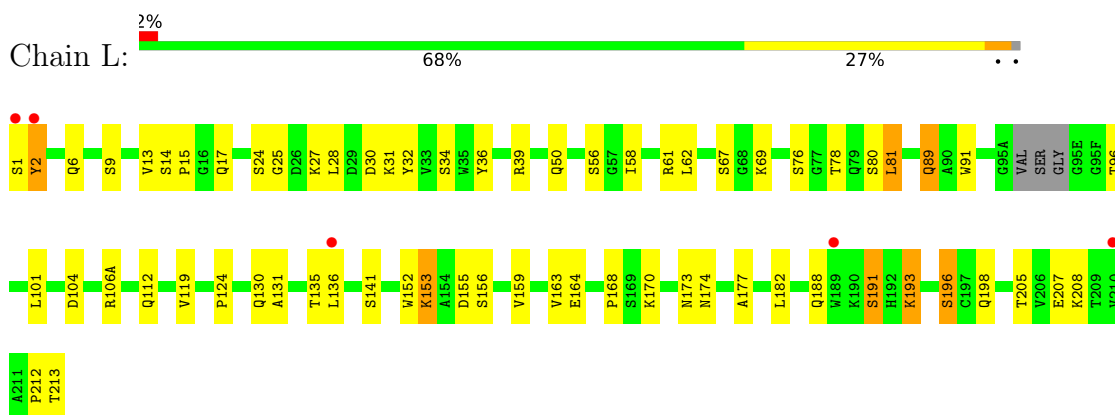
- Molecule 4 is water.

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

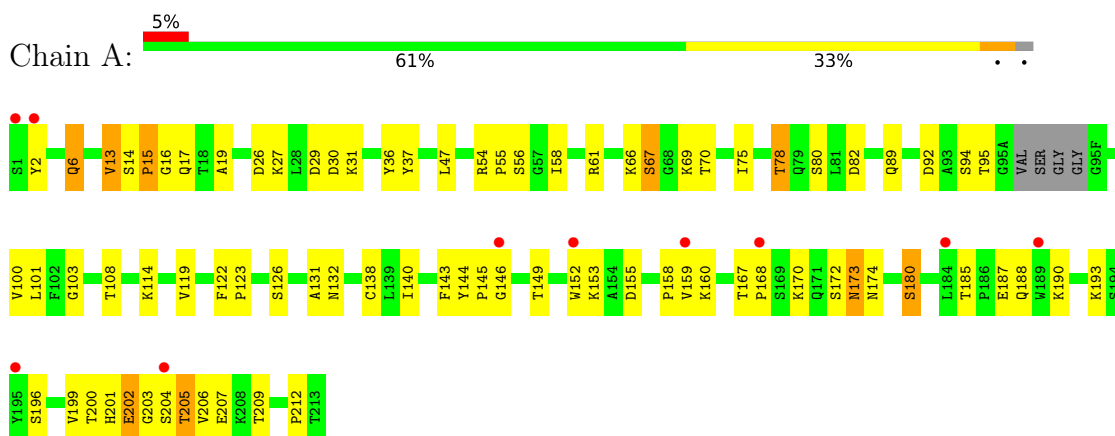
3 Residue-property plots [i](#)

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.

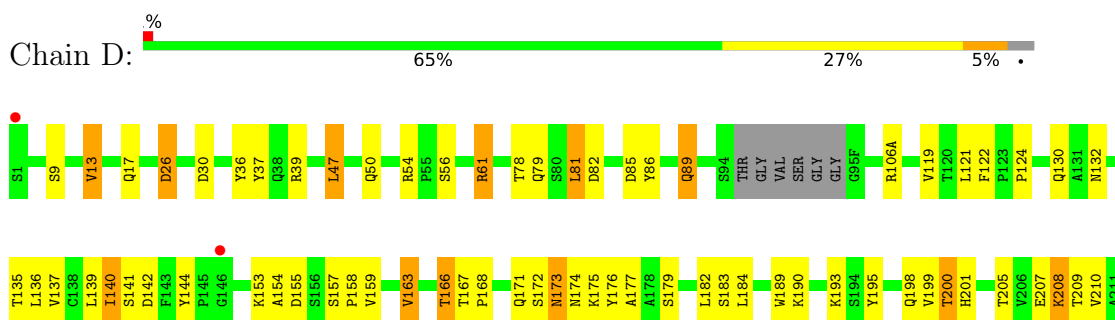
- Molecule 1: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab light chain



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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 D51 F52 K53 E60 R61 L62 S63 T72 Q79 S80 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 F172 S173 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 M28 F29 L30 D31 I40 P41 P52A D53 D54 S55 D56 H58 H59 G65 G66 V67 K73 S74 I75 S76 T82A T82B Q100B S100C S100D N100E A100F F100G D101 L102 Q105 M108 S113 P119 A125

P126 SER LYS THR SER GLY G134 T135 A136 A137 L138 G139 K143 D144 Y145 P149 V150 L159 G162 V163 H164 D165 F166 P167 A168 V169 S172 L178 S179 S180 V181 V182 P185 SER SER SER LEU G190 T191 Q192 T193 I194 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 V6 E6 Q13 Q16 I20 K23 F29 L30 I34 Q39 I40 P41 N47 I48 G49 P52A D54 D55 S55 D56 H58 H59 G65 D66 Q66 V67 Q68 V69 I75 I76 Q81 W82 Q83 A84 S85 D86 K89 Y90 F91 L95 M100E L102 Q105 I109

G114 K117 G118 P119 A125 F126 SER LYS THR SER SER SER GLY G134 L138 G139 Y145 V150 W154 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

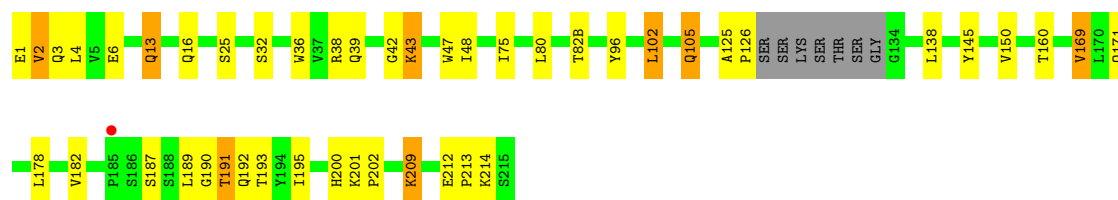
Chain E:  3% 69% 21% 7%

E1 V2 Q3 E6 Q13 S17 L18 K19 R38 Q39 I40 P41 K43 I48 D54 E64 G65 L80 T82A Q83 T93 R94 L95 S96 Y96 F98 E99 S100C S100D A84 M100E F100G D101 L102 Q105 T115 P123 L124 A125 P126 SER SER LYS SER


THR SER GLY G134 A137 L138 K143 V150 W154 N155 S156 G157 A158 L159 T160 S161 G162 V163 F166 V169 Y176 S177 L178 V182 T183 R184 P185 S186 Y186 S187 S188 L189 Q192 T193 Y194 I195 C196 K201 K209 K210 E212 P213 K214 S215

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

Chain I:  77% 17%



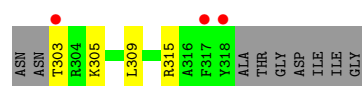
- Molecule 3: HIV-1 gp120 third variable region (V3) crown

Chain P:  30% 22% 9% 39%



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

Chain C:  13% 43% 17% 39%



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)	Xtrriage
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	Xtrriage
Anisotropy	0.050	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [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	0.89	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

The worst 5 of 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

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.

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

5 of 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

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	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
3	P	11/17 (65%)	7 (64%)	4 (36%)	0	0
All	All	1505/1554 (97%)	1342 (89%)	163 (11%)	6	13

5 of 163 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	64	GLU
1	G	164	GLU
2	E	105	GLN
1	G	1	SER
2	I	25	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	173	ASN
2	E	81	GLN
1	D	174	ASN
2	E	3	GLN
2	E	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)

The worst 5 of 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

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.