



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:39 pm GMT

PDB ID : 4I3S  
Title : Crystal structure of the outer domain of HIV-1 gp120 in complex with VRC-PG04 space group P21  
Authors : Joyce, M.G.; Biertumpfel, C.; Nabel, G.J.; Kwong, P.D.  
Deposited on : 2012-11-26  
Resolution : 2.85 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

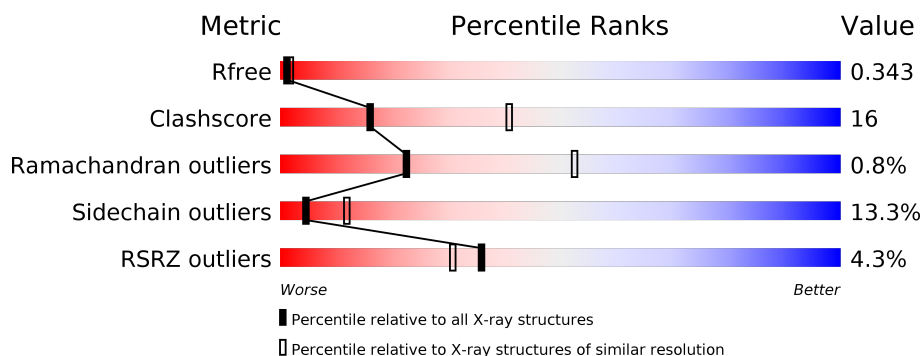
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
$R_{free}$	100719	2469 (2.90-2.82)
Clashscore	112137	2749 (2.90-2.82)
Ramachandran outliers	110173	2687 (2.90-2.82)
Sidechain outliers	110143	2690 (2.90-2.82)
RSRZ outliers	101464	2487 (2.90-2.82)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	G	190	<div> <div>11%</div> <div>60%</div> <div>28%</div> <div>6%</div> <div>5%</div> </div>
2	H	228	<div> <div>%</div> <div>73%</div> <div>20%</div> <div>.</div> <div>.</div> </div>
3	L	208	<div> <div>2%</div> <div>72%</div> <div>25%</div> <div>.</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4698 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 Outer domain of HIV-1 gp120 (KER2018 OD4.2.2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	180	Total	C	N	O	S	0	0	0
			1372	848	244	271	9			

- Molecule 2 is a protein called Heavy chain of VRC-PG04 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1696	1078	294	319	5			

- Molecule 3 is a protein called Light chain of VRC-PG04 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	208	Total	C	N	O	S	0	1	0
			1629	1024	278	320	7			

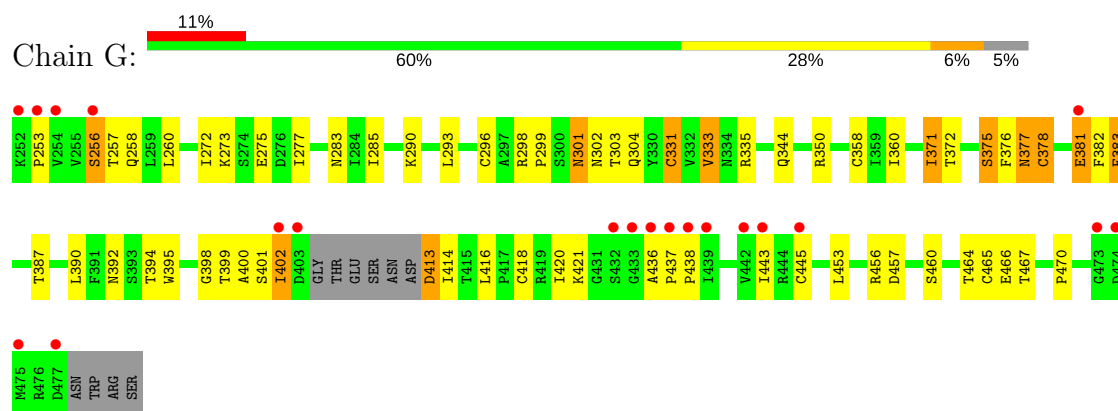
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	Ca	0	0
			1	1		

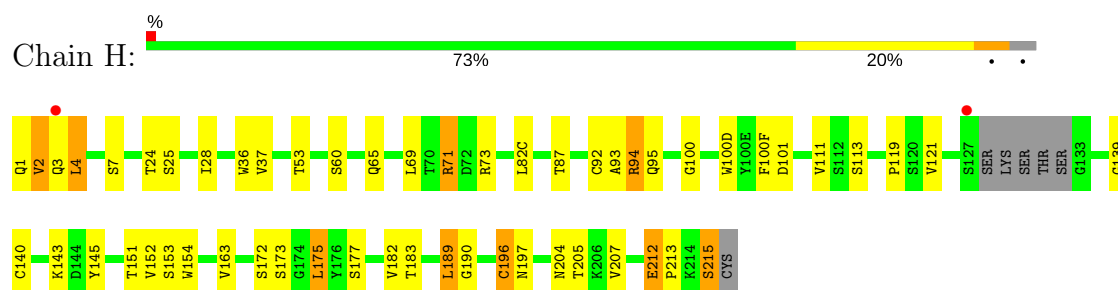
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

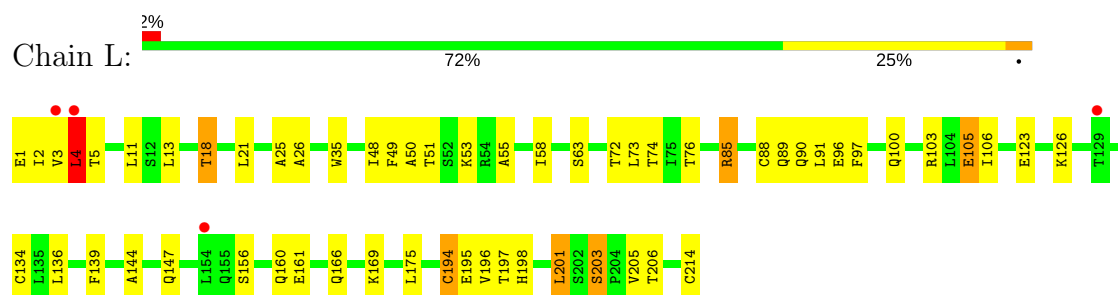
- Molecule 1: Outer domain of HIV-1 gp120 (KER2018 OD4.2.2)



- Molecule 2: Heavy chain of VRC-PG04 Fab



- Molecule 3: Light chain of VRC-PG04 Fab



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.65Å 73.47Å 109.29Å 90.00° 100.94° 90.00°	Depositor
Resolution (Å)	46.78 – 2.85 46.78 – 2.85	Depositor EDS
% Data completeness (in resolution range)	85.4 (46.78-2.85) 85.3 (46.78-2.85)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	0.23	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.248 , 0.320 0.276 , 0.343	Depositor DCC
$R_{free}$ test set	1075 reflections (7.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 29.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	4698	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	G	0.45	0/1394	0.70	0/1890
2	H	0.47	1/1740 (0.1%)	0.73	1/2369 (0.0%)
3	L	0.45	0/1669	0.68	0/2260
All	All	0.46	1/4803 (0.0%)	0.70	1/6519 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	213	PRO	N-CD	5.10	1.54	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	212	GLU	C-N-CD	5.66	140.28	128.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1372	0	1346	71	0
2	H	1696	0	1671	28	0
3	L	1629	0	1600	54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	1	0	0	0	0
All	All	4698	0	4617	146	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 16.

All (146) 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:L:3:VAL:HG12	3:L:26:ALA:CB	1.43	1.47
3:L:3:VAL:CG1	3:L:26:ALA:HB3	1.41	1.47
1:G:378:CYS:HB3	1:G:445:CYS:SG	1.67	1.34
1:G:383:PHE:HD2	1:G:418:CYS:SG	1.60	1.25
1:G:378:CYS:CB	1:G:445:CYS:HG	1.52	1.23
1:G:378:CYS:CB	1:G:445:CYS:SG	2.28	1.22
1:G:383:PHE:CD2	1:G:418:CYS:SG	2.39	1.14
1:G:457:ASP:HB2	1:G:467:THR:HG23	1.50	0.92
3:L:3:VAL:HG12	3:L:26:ALA:HB2	1.51	0.92
3:L:2:ILE:HG13	3:L:3:VAL:H	1.32	0.92
1:G:383:PHE:CE1	1:G:420:ILE:HD11	2.05	0.92
3:L:3:VAL:HG11	3:L:26:ALA:HB3	1.48	0.92
1:G:381:GLU:OE2	1:G:420:ILE:HD11	1.70	0.91
3:L:3:VAL:HG12	3:L:26:ALA:HB3	0.93	0.90
1:G:375:SER:HG	1:G:382:PHE:HZ	1.17	0.89
3:L:2:ILE:HG13	3:L:3:VAL:N	1.88	0.89
1:G:457:ASP:HB2	1:G:467:THR:CG2	2.03	0.88
2:H:87:THR:HG22	2:H:111:VAL:H	1.42	0.84
1:G:381:GLU:OE2	1:G:383:PHE:HE1	1.61	0.84
1:G:436:ALA:HB1	1:G:437:PRO:HD2	1.60	0.83
1:G:381:GLU:OE2	1:G:420:ILE:CD1	2.27	0.82
1:G:457:ASP:CB	1:G:467:THR:HG23	2.09	0.82
3:L:2:ILE:HG13	3:L:3:VAL:HG13	1.60	0.81
2:H:215:SER:OG	3:L:214:CYS:SG	2.22	0.80
3:L:3:VAL:O	3:L:4:LEU:HB2	1.80	0.80
3:L:201:LEU:HD22	3:L:203:SER:O	1.84	0.78
1:G:381:GLU:HB2	1:G:420:ILE:HD13	1.65	0.78
1:G:378:CYS:HB3	1:G:445:CYS:HG	1.10	0.77
3:L:2:ILE:CG1	3:L:3:VAL:H	1.97	0.77
3:L:4:LEU:CD1	3:L:97:PHE:HB2	2.15	0.76
2:H:140:CYS:HG	2:H:196:CYS:HG	1.33	0.74
2:H:189:LEU:HD12	2:H:190:GLY:H	1.51	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:4:LEU:HD11	3:L:97:PHE:HB2	1.68	0.74
3:L:4:LEU:HD13	3:L:97:PHE:CB	2.18	0.74
1:G:381:GLU:OE2	1:G:383:PHE:CE1	2.41	0.73
1:G:457:ASP:CG	1:G:467:THR:HG23	2.08	0.73
1:G:378:CYS:SG	1:G:445:CYS:HB3	2.31	0.70
2:H:4:LEU:HD23	2:H:4:LEU:H	1.56	0.70
2:H:189:LEU:HD12	2:H:190:GLY:N	2.07	0.69
1:G:358:CYS:HG	1:G:465:CYS:HG	0.78	0.69
1:G:383:PHE:CE2	1:G:418:CYS:SG	2.86	0.69
1:G:375:SER:OG	1:G:382:PHE:HZ	1.75	0.69
3:L:4:LEU:CD1	3:L:97:PHE:CB	2.71	0.68
1:G:378:CYS:SG	1:G:445:CYS:CB	2.84	0.66
3:L:89:GLN:HA	3:L:97:PHE:O	1.99	0.62
1:G:350:ARG:HH22	1:G:399:THR:HG23	1.63	0.62
1:G:350:ARG:NH2	1:G:399:THR:CG2	2.63	0.62
1:G:296:CYS:HB2	1:G:445:CYS:HB2	1.81	0.62
1:G:358:CYS:SG	1:G:465:CYS:CB	2.88	0.62
1:G:381:GLU:HB2	1:G:420:ILE:CD1	2.31	0.61
2:H:215:SER:OG	3:L:214:CYS:C	2.39	0.61
1:G:457:ASP:CB	1:G:467:THR:CG2	2.71	0.61
3:L:35:TRP:HB2	3:L:48:ILE:HB	1.83	0.61
2:H:93:ALA:HB1	2:H:100(F):PHE:HB3	1.81	0.61
1:G:257:THR:HG22	1:G:258:GLN:N	2.17	0.60
1:G:457:ASP:CG	1:G:467:THR:CG2	2.71	0.59
1:G:358:CYS:HG	1:G:465:CYS:CB	2.15	0.59
1:G:350:ARG:HH22	1:G:399:THR:CG2	2.16	0.59
1:G:333:VAL:HG21	1:G:390:LEU:HD21	1.85	0.59
2:H:215:SER:HG	3:L:214:CYS:CB	2.16	0.58
3:L:3:VAL:HG23	3:L:4:LEU:HD12	1.86	0.58
1:G:376:PHE:N	1:G:382:PHE:HE1	2.02	0.57
2:H:173:SER:CB	2:H:175:LEU:HD12	2.34	0.57
3:L:4:LEU:HD13	3:L:97:PHE:HB3	1.85	0.57
3:L:49:PHE:O	3:L:50:ALA:HB3	2.05	0.56
1:G:331:CYS:HB3	1:G:416:LEU:HB2	1.86	0.56
1:G:456:ARG:HD2	1:G:466:GLU:OE1	2.06	0.56
1:G:258:GLN:HG2	1:G:470:PRO:HB2	1.87	0.56
1:G:383:PHE:CD1	1:G:420:ILE:HD11	2.42	0.55
2:H:163:VAL:HG22	2:H:182:VAL:HG12	1.89	0.55
1:G:335:ARG:HD3	1:G:414:ILE:CD1	2.37	0.54
1:G:378:CYS:HG	1:G:445:CYS:CB	2.19	0.54
3:L:160:GLN:C	3:L:161:GLU:HG3	2.27	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:21:LEU:HD13	3:L:73:LEU:HD23	1.89	0.54
2:H:2:VAL:HG22	2:H:3:GLN:H	1.73	0.54
3:L:4:LEU:HD22	3:L:97:PHE:HB3	1.89	0.54
1:G:335:ARG:HD3	1:G:414:ILE:HD11	1.89	0.53
3:L:89:GLN:O	3:L:89:GLN:HG3	2.09	0.53
2:H:25:SER:HB2	2:H:28:ILE:HD12	1.91	0.53
3:L:3:VAL:CB	3:L:26:ALA:HB3	2.30	0.53
1:G:402:ILE:HD13	1:G:402:ILE:C	2.29	0.52
3:L:55:ALA:HB3	3:L:58:ILE:HD13	1.91	0.52
3:L:63:SER:HB2	3:L:74:THR:HG23	1.92	0.51
3:L:25:ALA:HB1	3:L:90:GLN:NE2	2.26	0.51
3:L:5:THR:HG23	3:L:100:GLN:OE1	2.11	0.50
2:H:153:SER:HB3	2:H:197:ASN:HB2	1.95	0.49
1:G:273:LYS:HB2	1:G:285:ILE:HB	1.94	0.49
1:G:457:ASP:OD2	1:G:467:THR:HG21	2.12	0.48
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.95	0.48
2:H:4:LEU:HD23	2:H:4:LEU:N	2.26	0.48
3:L:105:GLU:HB2	3:L:166:GLN:HE22	1.78	0.48
1:G:358:CYS:O	1:G:465:CYS:HB3	2.13	0.48
3:L:3:VAL:HB	3:L:26:ALA:H	1.79	0.48
1:G:395:TRP:HA	1:G:400:ALA:O	2.14	0.48
2:H:94:ARG:HD2	2:H:101:ASP:OD1	2.14	0.48
2:H:36:TRP:CD1	2:H:69:LEU:HD22	2.48	0.47
1:G:258:GLN:NE2	1:G:387:THR:OG1	2.47	0.47
1:G:381:GLU:OE1	1:G:443:ILE:HD13	2.14	0.47
1:G:378:CYS:HG	1:G:445:CYS:HB3	1.77	0.47
1:G:283:ASN:HD21	1:G:453:LEU:HG	1.79	0.47
3:L:35:TRP:CZ3	3:L:88:CYS:SG	3.08	0.47
3:L:3:VAL:CG1	3:L:26:ALA:CB	2.25	0.46
1:G:301:ASN:HA	1:G:302:ASN:HA	1.70	0.46
1:G:256:SER:O	1:G:257:THR:OG1	2.26	0.46
1:G:360:ILE:HD12	1:G:465:CYS:HB2	1.98	0.46
1:G:376:PHE:O	1:G:382:PHE:HD1	1.99	0.45
3:L:195:GLU:HA	3:L:205:VAL:O	2.16	0.45
3:L:89:GLN:NE2	3:L:91:LEU:O	2.49	0.45
3:L:195:GLU:HG3	3:L:206:THR:OG1	2.17	0.45
3:L:201:LEU:CD2	3:L:203:SER:O	2.61	0.45
1:G:275:GLU:HB3	2:H:100:GLY:HA3	1.99	0.45
1:G:460:SER:HB3	3:L:1:GLU:OE2	2.17	0.44
3:L:136:LEU:HD11	3:L:196:VAL:HG21	1.98	0.44
1:G:335:ARG:HD3	1:G:414:ILE:HG12	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:85:ARG:HE	3:L:103:ARG:HB2	1.83	0.44
3:L:18:THR:HB	3:L:76:THR:HA	2.00	0.44
2:H:173:SER:HB3	2:H:175:LEU:HD12	1.99	0.44
2:H:71:ARG:NH1	2:H:73:ARG:HD2	2.33	0.44
1:G:371:ILE:HG21	2:H:53:THR:OG1	2.17	0.43
3:L:4:LEU:CD2	3:L:97:PHE:C	2.87	0.43
3:L:136:LEU:HB2	3:L:175:LEU:HB3	1.99	0.43
1:G:360:ILE:HG12	1:G:394:THR:HG22	2.00	0.43
2:H:215:SER:OG	3:L:214:CYS:O	2.38	0.42
1:G:376:PHE:N	1:G:382:PHE:CE1	2.86	0.42
1:G:257:THR:CG2	1:G:258:GLN:N	2.83	0.42
2:H:139:GLY:HA2	2:H:154:TRP:CZ2	2.54	0.42
1:G:376:PHE:CA	1:G:382:PHE:HE1	2.32	0.42
1:G:377:ASN:ND2	1:G:377:ASN:C	2.73	0.42
1:G:299:PRO:HD2	1:G:303:THR:HG23	2.02	0.42
1:G:413:ASP:HB3	1:G:414:ILE:H	1.64	0.41
3:L:4:LEU:HD21	3:L:97:PHE:O	2.20	0.41
3:L:144:ALA:HB2	3:L:198:HIS:HD2	1.84	0.41
1:G:358:CYS:SG	1:G:465:CYS:CA	3.09	0.41
2:H:95:GLN:NE2	2:H:100(D):TRP:HA	2.35	0.41
2:H:4:LEU:HB3	2:H:24:THR:HB	2.01	0.41
2:H:71:ARG:HH11	2:H:73:ARG:HD2	1.85	0.41
1:G:437:PRO:HA	1:G:438:PRO:HD3	1.99	0.41
3:L:139:PHE:CD1	3:L:139:PHE:N	2.89	0.41
1:G:376:PHE:C	1:G:382:PHE:CE1	2.94	0.41
1:G:260:LEU:HD21	1:G:453:LEU:HD13	2.02	0.41
2:H:94:ARG:O	2:H:100(F):PHE:HA	2.21	0.41
1:G:377:ASN:O	1:G:377:ASN:ND2	2.52	0.40
3:L:194:CYS:O	3:L:194:CYS:SG	2.79	0.40
3:L:90:GLN:O	3:L:91:LEU:HB2	2.20	0.40
3:L:4:LEU:CD2	3:L:97:PHE:CB	2.99	0.40
3:L:35:TRP:CH2	3:L:88:CYS:SG	3.15	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	G	176/190 (93%)	158 (90%)	15 (8%)	3 (2%)	11	32
2	H	218/228 (96%)	207 (95%)	10 (5%)	1 (0%)	32	64
3	L	207/208 (100%)	197 (95%)	9 (4%)	1 (0%)	32	64
All	All	601/626 (96%)	562 (94%)	34 (6%)	5 (1%)	22	52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	392	ASN
2	H	2	VAL
3	L	4	LEU
1	G	398	GLY
1	G	253	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	G	156/165 (94%)	133 (85%)	23 (15%)	3	9
2	H	187/193 (97%)	161 (86%)	26 (14%)	4	10
3	L	183/182 (100%)	162 (88%)	21 (12%)	6	17
All	All	526/540 (97%)	456 (87%)	70 (13%)	4	12

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	256	SER
1	G	272	ILE
1	G	277	ILE
1	G	290	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	293	LEU
1	G	298	ARG
1	G	301	ASN
1	G	304	GLN
1	G	331	CYS
1	G	333	VAL
1	G	344	GLN
1	G	371	ILE
1	G	372	THR
1	G	375	SER
1	G	377	ASN
1	G	378	CYS
1	G	381	GLU
1	G	383	PHE
1	G	401	SER
1	G	402	ILE
1	G	413	ASP
1	G	421	LYS
1	G	464	THR
2	H	1	GLN
2	H	4	LEU
2	H	7	SER
2	H	37	VAL
2	H	60	SER
2	H	65	GLN
2	H	71	ARG
2	H	82(C)	LEU
2	H	92	CYS
2	H	94	ARG
2	H	113	SER
2	H	121	VAL
2	H	143	LYS
2	H	151	THR
2	H	152	VAL
2	H	172	SER
2	H	175	LEU
2	H	177	SER
2	H	183	THR
2	H	189	LEU
2	H	196	CYS
2	H	204	ASN
2	H	205	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	H	207	VAL
2	H	212	GLU
2	H	215	SER
3	L	4	LEU
3	L	11	LEU
3	L	13	LEU
3	L	18	THR
3	L	51	THR
3	L	53	LYS
3	L	72	THR
3	L	85	ARG
3	L	96	GLU
3	L	105	GLU
3	L	106	ILE
3	L	123	GLU
3	L	126	LYS
3	L	134	CYS
3	L	147	GLN
3	L	156	SER
3	L	169	LYS
3	L	194	CYS
3	L	197	THR
3	L	201	LEU
3	L	203	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	258	GLN
1	G	283	ASN
1	G	352	HIS
2	H	95	GLN
2	H	164	HIS
2	H	200	HIS
3	L	32	HIS
3	L	90	GLN
3	L	138	ASN
3	L	166	GLN
3	L	199	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	G	180/190 (94%)	0.62	20 (11%) <b>6</b> <b>4</b>	24, 46, 88, 123	0
2	H	222/228 (97%)	-0.05	2 (0%) <b>84</b> <b>83</b>	13, 33, 56, 87	0
3	L	208/208 (100%)	0.08	4 (1%) <b>67</b> <b>64</b>	17, 36, 66, 98	0
All	All	610/626 (97%)	0.19	26 (4%) <b>36</b> <b>31</b>	13, 38, 74, 123	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	438	PRO	6.2
1	G	253	PRO	5.2
1	G	402	ILE	5.1
1	G	443	ILE	4.6
1	G	477	ASP	4.4
3	L	4	LEU	3.7
1	G	256	SER	3.6
1	G	403	ASP	3.5
1	G	254	VAL	3.4
1	G	252	LYS	3.3
3	L	3	VAL	3.2
1	G	475	MET	3.0
3	L	154	LEU	2.9
2	H	127	SER	2.9
1	G	439	ILE	2.9
1	G	437	PRO	2.8
1	G	432	SER	2.6
1	G	474	ASP	2.4
1	G	445	CYS	2.4
1	G	442	VAL	2.3
1	G	436	ALA	2.3
3	L	129	THR	2.2
1	G	433	GLY	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	3	GLN	2.2
1	G	473	GLY	2.2
1	G	381	GLU	2.2

## 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	L	301	1/1	0.85	0.11	-3.40	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.