



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:19 PM UTC

PDB ID : 4I3S / pdb_00004i3s
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

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

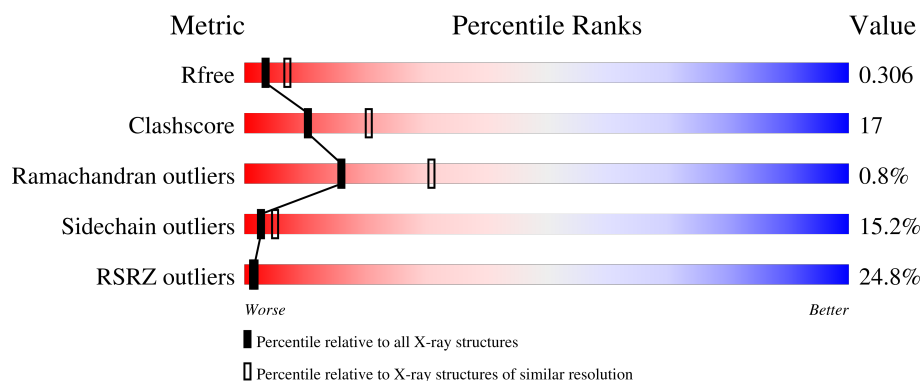
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	G	190	
2	H	228	
3	L	208	

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			

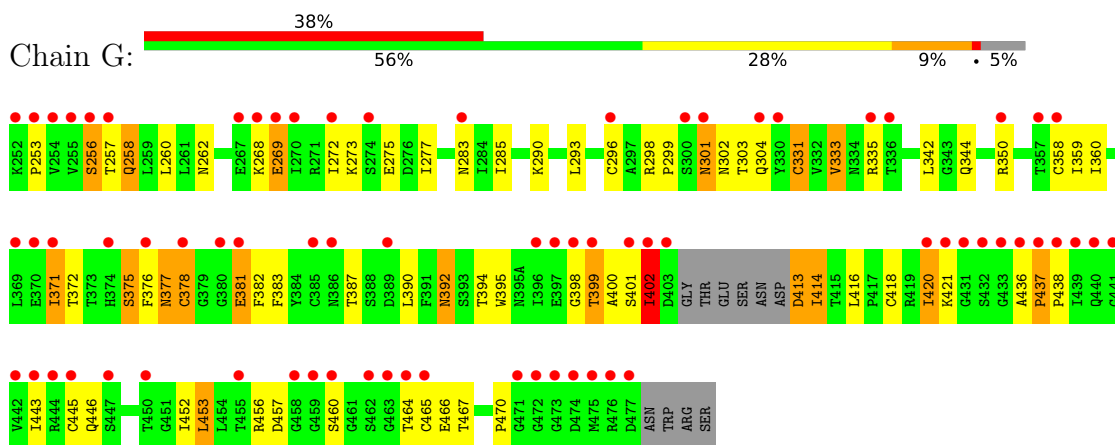
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

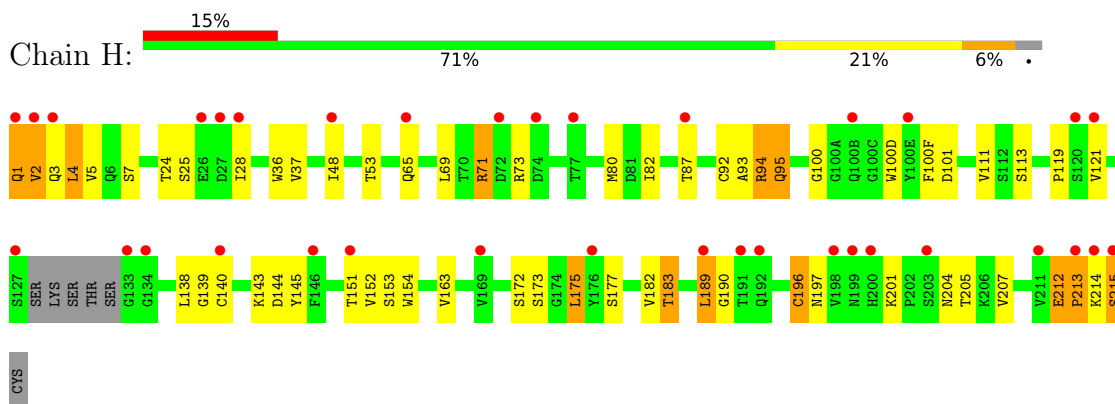
3 Residue-property plots

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.

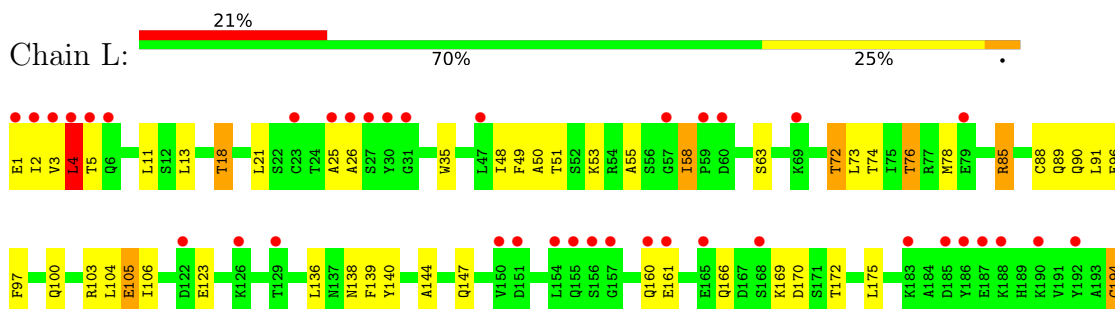
- Molecule 1: Outer domain of HIV-1 gp120 (KER2018 OD4.2.2)



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.248 , 0.320 0.272 , 0.306	Depositor DCC
R_{free} test set	1075 reflections (6.14%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

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

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	0.78	0/1394	1.31	7/1890 (0.4%)
2	H	0.78	2/1740 (0.1%)	1.23	7/2369 (0.3%)
3	L	0.80	0/1669	1.20	3/2260 (0.1%)
All	All	0.79	2/4803 (0.0%)	1.25	17/6519 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	212	GLU	C-N	5.65	1.41	1.33
2	H	213	PRO	N-CD	5.17	1.54	1.47

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	138	ASN	N-CA-C	7.89	122.28	111.39
2	H	144	ASP	N-CA-C	6.77	120.51	111.30
1	G	359	ILE	N-CA-C	6.73	118.17	108.48
2	H	212	GLU	CA-C-N	-6.54	113.02	119.76
2	H	212	GLU	C-N-CA	-6.54	113.02	119.76
1	G	437	PRO	N-CA-C	6.39	118.49	110.70
1	G	402	ILE	N-CA-C	6.28	116.45	110.42
3	L	72	THR	N-CA-C	6.25	119.66	109.59
2	H	183	THR	CB-CA-C	6.18	120.20	110.19
1	G	258	GLN	N-CA-C	6.04	117.94	111.36
2	H	5	VAL	N-CA-C	5.37	115.98	108.89
2	H	1	GLN	CA-C-N	5.31	131.26	121.70
2	H	1	GLN	C-N-CA	5.31	131.26	121.70
1	G	269	GLU	CA-C-N	5.07	127.30	120.50
1	G	269	GLU	C-N-CA	5.07	127.30	120.50
1	G	262	ASN	N-CA-C	5.07	118.75	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	58	ILE	CB-CA-C	5.04	115.76	110.37

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	G	1372	0	1346	71	0
2	H	1696	0	1671	30	0
3	L	1629	0	1600	58	0
4	L	1	0	0	0	0
All	All	4698	0	4617	152	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 17.

All (152) 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:SG	2.28	1.22
1:G:378:CYS:CB	1:G:445:CYS:HG	1.53	1.21
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:2:ILE:HG13	3:L:3:VAL:H	1.32	0.92
3:L:3:VAL:HG12	3:L:26:ALA:HB2	1.51	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
3:L:2:ILE:HG13	3:L:3:VAL:N	1.88	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:375:SER:HG	1:G:382:PHE:HZ	1.28	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
1:G:378:CYS:HB3	1:G:445:CYS:HG	1.11	0.79
1:G:457:ASP:CG	1:G:467:THR:HG23	2.08	0.79
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
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
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:378:CYS:SG	1:G:445:CYS:HB3	2.31	0.70
2:H:4:LEU:H	2:H:4:LEU:HD23	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
2:H:215:SER:OG	3:L:214:CYS:C	2.39	0.66
1:G:457:ASP:CG	1:G:467:THR:CG2	2.71	0.63
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
3:L:78:MET:HE1	3:L:104:LEU:HD23	1.81	0.61
1:G:381:GLU:HB2	1:G:420:ILE:CD1	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:257:THR:HG22	1:G:258:GLN:N	2.17	0.60
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
3:L:160:GLN:C	3:L:161:GLU:HG3	2.27	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
1:G:402:ILE:C	1:G:402:ILE:HD13	2.29	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
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
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
2:H:80:MET:HE3	2:H:82:ILE:HD11	1.92	0.51
1:G:375:SER:OG	1:G:382:PHE:CZ	2.53	0.50
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:4:LEU:CD2	3:L:97:PHE:C	2.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:283:ASN:HD21	1:G:453:LEU:HG	1.79	0.47
1:G:377:ASN:ND2	1:G:377:ASN:C	2.73	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:376:PHE:C	1:G:382:PHE:CE1	2.94	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:89:GLN:NE2	3:L:91:LEU:O	2.49	0.45
3:L:195:GLU:HA	3:L:205:VAL:O	2.16	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
3:L:140:TYR:C	3:L:140:TYR:CD1	2.95	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
3:L:170:ASP:OD1	3:L:172:THR:OG1	2.32	0.44
1:G:335:ARG:HD3	1:G:414:ILE:HG12	1.99	0.44
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:HD21	3:L:97:PHE:C	2.44	0.43
1:G:376:PHE:C	1:G:382:PHE:CD1	2.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:213:PRO:C	2:H:214:LYS:HG2	2.45	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: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:ND2	1:G:377:ASN:O	2.52	0.40
3:L:4:LEU:CD2	3:L:97:PHE:CB	2.99	0.40
3:L:90:GLN:O	3:L:91:LEU:HB2	2.20	0.40
3:L:194:CYS:O	3:L:194:CYS:SG	2.79	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 [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	G	176/190 (93%)	158 (90%)	15 (8%)	3 (2%)	7	16
2	H	218/228 (96%)	207 (95%)	10 (5%)	1 (0%)	24	42
3	L	207/208 (100%)	197 (95%)	9 (4%)	1 (0%)	24	42
All	All	601/626 (96%)	562 (94%)	34 (6%)	5 (1%)	16	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	392	ASN
2	H	2	VAL
3	L	4	LEU

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Mol	Chain	Res	Type
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%)	124 (80%)	32 (20%)	1	1
2	H	187/193 (97%)	159 (85%)	28 (15%)	3	5
3	L	183/182 (100%)	163 (89%)	20 (11%)	6	12
All	All	526/540 (97%)	446 (85%)	80 (15%)	3	5

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	256	SER
1	G	268	LYS
1	G	269	GLU
1	G	272	ILE
1	G	277	ILE
1	G	290	LYS
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	342	LEU
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

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Mol	Chain	Res	Type
1	G	392	ASN
1	G	399	THR
1	G	401	SER
1	G	402	ILE
1	G	413	ASP
1	G	414	ILE
1	G	420	ILE
1	G	421	LYS
1	G	446	GLN
1	G	452	ILE
1	G	453	LEU
1	G	464	THR
2	H	1	GLN
2	H	4	LEU
2	H	7	SER
2	H	37	VAL
2	H	48	ILE
2	H	65	GLN
2	H	71	ARG
2	H	92	CYS
2	H	94	ARG
2	H	95	GLN
2	H	113	SER
2	H	121	VAL
2	H	138	LEU
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	201	LYS
2	H	204	ASN
2	H	205	THR
2	H	207	VAL
2	H	212	GLU
2	H	215	SER
3	L	4	LEU
3	L	11	LEU

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Mol	Chain	Res	Type
3	L	13	LEU
3	L	18	THR
3	L	51	THR
3	L	53	LYS
3	L	72	THR
3	L	76	THR
3	L	85	ARG
3	L	96	GLU
3	L	105	GLU
3	L	106	ILE
3	L	123	GLU
3	L	147	GLN
3	L	169	LYS
3	L	194	CYS
3	L	197	THR
3	L	201	LEU
3	L	203	SER
3	L	207	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	258	GLN
1	G	283	ASN
1	G	352	HIS
2	H	200	HIS
3	L	32	HIS
3	L	90	GLN
3	L	137	ASN
3	L	138	ASN
3	L	166	GLN
3	L	199	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

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, 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	G	180/190 (94%)	2.07	73 (40%)	0 0	24, 46, 88, 123	0
2	H	222/228 (97%)	1.09	35 (15%)	5 4	13, 33, 56, 87	0
3	L	208/208 (100%)	1.26	43 (20%)	2 2	17, 36, 66, 98	1 (0%)
All	All	610/626 (97%)	1.44	151 (24%)	2 1	13, 38, 74, 123	1 (0%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	442	VAL	7.5
1	G	443	ILE	7.3
1	G	253	PRO	7.0
1	G	438	PRO	6.7
1	G	403	ASP	6.5
1	G	252	LYS	6.3
3	L	3	VAL	6.0
1	G	256	SER	5.9
1	G	402	ILE	5.8
1	G	473	GLY	5.7
1	G	477	ASP	5.5
3	L	4	LEU	5.1
1	G	464	THR	5.1
1	G	437	PRO	5.0
2	H	127	SER	5.0
1	G	445	CYS	4.7
3	L	25	ALA	4.7
1	G	397	GLU	4.6
3	L	30	TYR	4.6
1	G	439	ILE	4.5
3	L	154	LEU	4.4
1	G	460	SER	4.4
3	L	2	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	G	436	ALA	4.3
1	G	401	SER	4.3
3	L	31	GLY	4.2
3	L	27	SER	4.1
1	G	444	ARG	4.0
2	H	189	LEU	4.0
1	G	472	GLY	4.0
2	H	215	SER	4.0
1	G	301	ASN	3.9
1	G	440	GLN	3.9
1	G	255	VAL	3.8
1	G	358	CYS	3.7
3	L	157	GLY	3.7
1	G	254	VAL	3.7
1	G	421	LYS	3.5
3	L	192	TYR	3.5
1	G	257	THR	3.5
2	H	3	GLN	3.4
1	G	398	GLY	3.4
1	G	462	SER	3.4
3	L	212	GLY	3.4
1	G	432	SER	3.4
1	G	381	GLU	3.4
3	L	214	CYS	3.4
1	G	433	GLY	3.3
3	L	122	ASP	3.3
3	L	155	GLN	3.3
2	H	27	ASP	3.2
1	G	474	ASP	3.2
1	G	357	THR	3.2
1	G	374	HIS	3.1
1	G	458	GLY	3.1
1	G	399	THR	3.1
2	H	192	GLN	3.0
1	G	378	CYS	3.0
3	L	187	GLU	3.0
1	G	475	MET	3.0
2	H	199	ASN	3.0
1	G	385	CYS	3.0
3	L	165	GLU	2.9
3	L	26	ALA	2.9
3	L	156	SER	2.9

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Mol	Chain	Res	Type	RSRZ
3	L	23	CYS	2.9
3	L	1	GLU	2.9
2	H	191	THR	2.9
3	L	57	GLY	2.8
2	H	213	PRO	2.8
3	L	168	SER	2.8
1	G	431	GLY	2.8
1	G	336	THR	2.8
1	G	476	ARG	2.8
2	H	121	VAL	2.7
1	G	267	GLU	2.7
2	H	211	VAL	2.7
1	G	270	ILE	2.6
1	G	272	ILE	2.6
3	L	188	LYS	2.6
1	G	380	GLY	2.6
1	G	369	LEU	2.6
1	G	274	SER	2.6
3	L	47	LEU	2.6
2	H	26	GLU	2.6
1	G	350	ARG	2.5
1	G	269	GLU	2.5
1	G	304	GLN	2.5
3	L	150	VAL	2.5
3	L	160	GLN	2.5
1	G	420	ILE	2.5
1	G	335	ARG	2.5
1	G	371	ILE	2.5
2	H	65	GLN	2.5
1	G	459	GLY	2.4
3	L	211	ARG	2.4
1	G	283	ASN	2.4
1	G	465	CYS	2.4
2	H	120	SER	2.4
1	G	296	CYS	2.4
1	G	463	GLY	2.4
2	H	133	GLY	2.4
2	H	74	ASP	2.4
2	H	214	LYS	2.4
1	G	370	GLU	2.4
2	H	151	THR	2.4
3	L	186	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
3	L	69	LYS	2.3
2	H	203	SER	2.3
3	L	151	ASP	2.3
1	G	300	SER	2.3
1	G	447	SER	2.3
2	H	100(B)	GLN	2.3
1	G	396	ILE	2.3
2	H	28	ILE	2.3
1	G	471	GLY	2.3
3	L	210	ASN	2.3
3	L	6	GLN	2.3
3	L	5	THR	2.3
1	G	441	GLY	2.3
2	H	140	CYS	2.2
1	G	330	TYR	2.2
2	H	100(E)	TYR	2.2
2	H	176	TYR	2.2
2	H	48	ILE	2.2
3	L	60	ASP	2.2
1	G	455	THR	2.2
1	G	386	ASN	2.2
2	H	200	HIS	2.2
1	G	389	ASP	2.2
2	H	198	VAL	2.2
3	L	190	LYS	2.1
2	H	72	ASP	2.1
3	L	185	ASP	2.1
2	H	77	THR	2.1
3	L	208	SER	2.1
2	H	1	GLN	2.1
2	H	169	VAL	2.1
2	H	134	GLY	2.1
1	G	376	PHE	2.1
3	L	79	GLU	2.1
3	L	161	GLU	2.1
1	G	268	LYS	2.1
3	L	59	PRO	2.1
1	G	450	THR	2.1
3	L	126	LYS	2.0
3	L	183	LYS	2.0
2	H	146	PHE	2.0
2	H	87	THR	2.0

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Mol	Chain	Res	Type	RSRZ
3	L	129	THR	2.0
2	H	2	VAL	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](#)

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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	L	301	1/1	0.66	0.15	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.