



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 09:25 PM UTC

PDB ID : 3QA3 / pdb\_00003qa3  
Title : Crystal Structure of A-domain in complex with antibody  
Authors : Mahalingam, B.; Xiong, J.P.; Arnaout, M.A.  
Deposited on : 2011-01-10  
Resolution : 3.00 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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
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

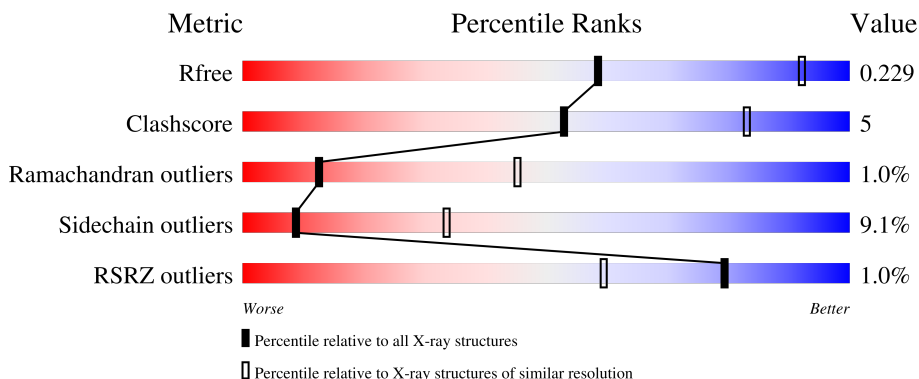
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


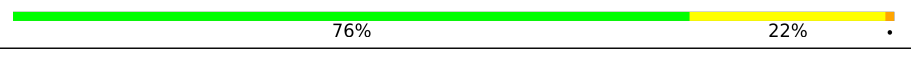
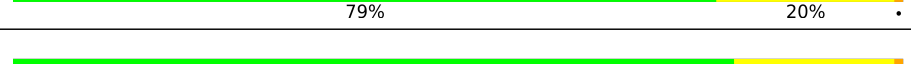

The reported resolution of this entry is 3.00 Å.

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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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  $\geq 3$ , 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	220	
1	C	220	
1	F	220	
1	J	220	
2	B	224	

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Mol	Chain	Length	Quality of chain	
2	D	224		80% 18% .
2	H	224		81% 16% .
2	K	224		84% 13% .
3	E	190		74% 21% ...
3	G	190		74% 22% ..
3	I	190		75% 21% ..
3	L	190		77% 19% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	D	2	-	-	X	-
5	GOL	G	5	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19772 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 Antibody Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	220	1718	1074	283	353	8	0	0	0
1	A	220	1718	1074	283	353	8	0	0	0
1	F	220	1718	1074	283	353	8	0	0	0
1	J	220	1718	1074	283	353	8	0	0	0

- Molecule 2 is a protein called Antibody Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	224	1689	1062	277	342	8	0	0	0
2	B	224	1689	1062	277	342	8	0	0	0
2	H	224	1689	1062	277	342	8	0	0	0
2	K	224	1689	1062	277	342	8	0	0	0

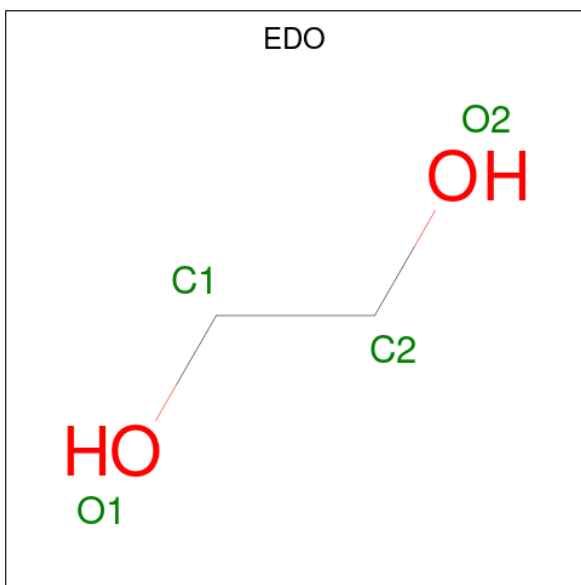
- Molecule 3 is a protein called Integrin alpha-M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	187	1510	960	269	278	3	0	0	0
3	E	186	1505	957	268	277	3	0	0	0
3	I	185	1494	948	267	276	3	0	0	0
3	L	185	1494	948	267	276	3	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	316	GLY	ILE	engineered mutation	UNP P11215
E	316	GLY	ILE	engineered mutation	UNP P11215
I	316	GLY	ILE	engineered mutation	UNP P11215
L	316	GLY	ILE	engineered mutation	UNP P11215

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0
4	K	1	Total C O 4 2 2	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 6 3 3	0	0
5	G	1	Total C O 6 3 3	0	0
5	G	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total Ca 1 1	0	0
6	E	1	Total Ca 1 1	0	0
6	I	1	Total Ca 1 1	0	0
6	L	1	Total Ca 1 1	0	0

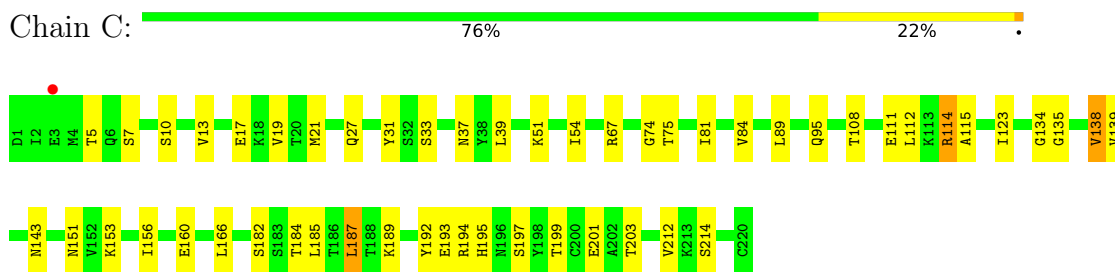
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	9	Total O 9 9	0	0
7	D	5	Total O 5 5	0	0
7	G	4	Total O 4 4	0	0
7	A	2	Total O 2 2	0	0
7	B	8	Total O 8 8	0	0
7	E	6	Total O 6 6	0	0
7	F	8	Total O 8 8	0	0
7	H	6	Total O 6 6	0	0
7	I	3	Total O 3 3	0	0
7	J	9	Total O 9 9	0	0
7	K	10	Total O 10 10	0	0
7	L	5	Total O 5 5	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.

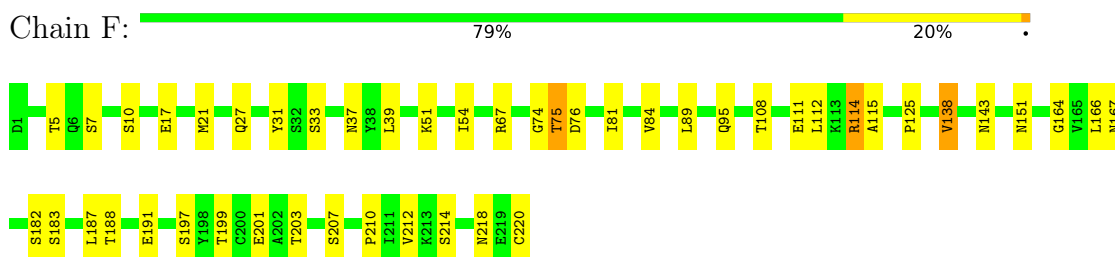
- Molecule 1: Antibody Light chain



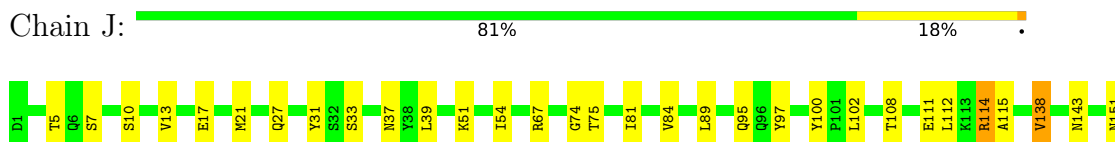
- Molecule 1: Antibody Light chain



- Molecule 1: Antibody Light chain

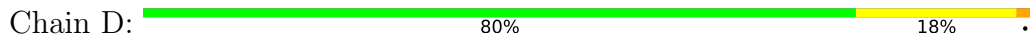


- Molecule 1: Antibody Light chain

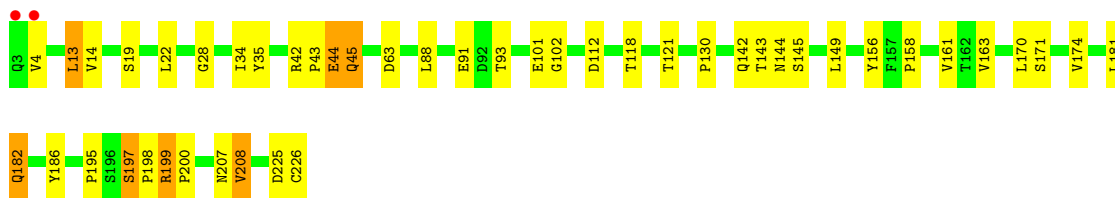
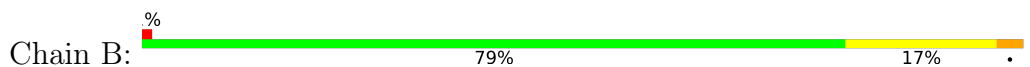




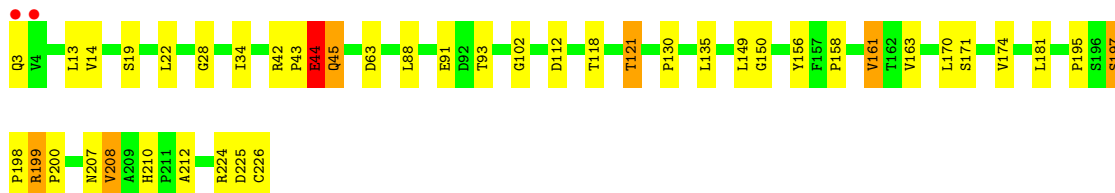
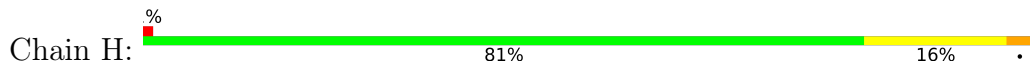
• Molecule 2: Antibody Heavy chain



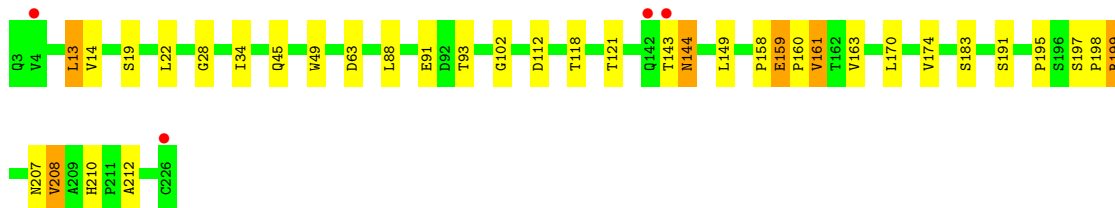
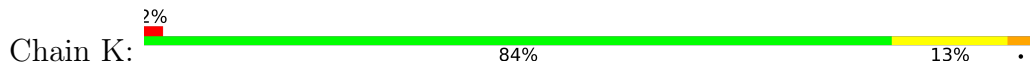
• Molecule 2: Antibody Heavy chain



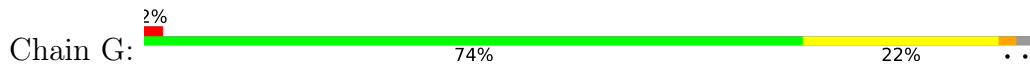
• Molecule 2: Antibody Heavy chain

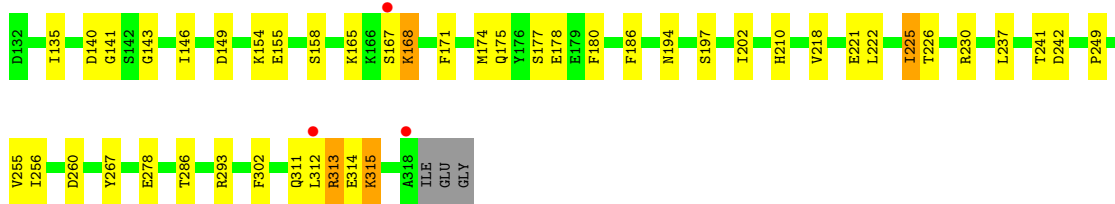


• Molecule 2: Antibody Heavy chain

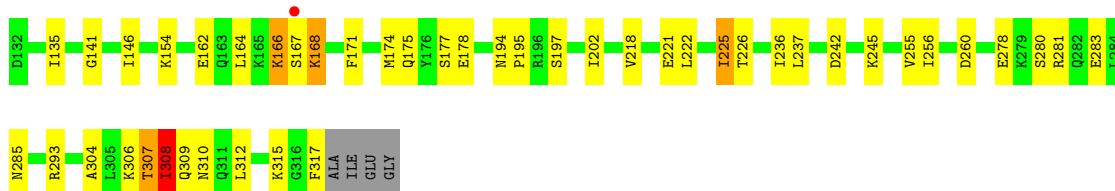
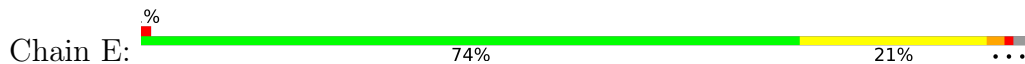


• Molecule 3: Integrin alpha-M

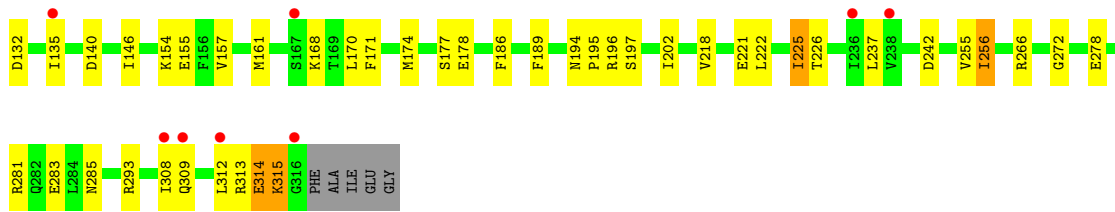




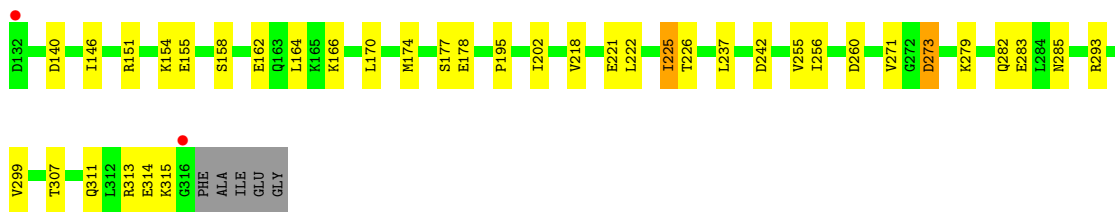
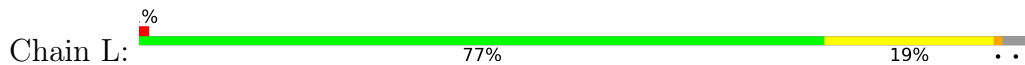
• Molecule 3: Integrin alpha-M



• Molecule 3: Integrin alpha-M



• Molecule 3: Integrin alpha-M



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.60Å 158.35Å 233.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.65 – 3.00 47.65 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.65-3.00) 98.2 (47.65-3.00)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 3.01Å)	Xtrriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.194 , 0.224 0.201 , 0.229	Depositor DCC
$R_{free}$ test set	3095 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.1	Xtrriage
Anisotropy	0.092	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	19772	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: GOL, EDO, 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	A	0.71	0/1757	1.16	6/2384 (0.3%)
1	C	0.74	0/1757	1.13	1/2384 (0.0%)
1	F	0.72	0/1757	1.15	6/2384 (0.3%)
1	J	0.73	0/1757	1.20	8/2384 (0.3%)
2	B	0.78	2/1732 (0.1%)	1.21	5/2368 (0.2%)
2	D	0.75	0/1732	1.25	5/2368 (0.2%)
2	H	0.73	1/1732 (0.1%)	1.23	4/2368 (0.2%)
2	K	0.75	0/1732	1.22	5/2368 (0.2%)
3	E	0.78	1/1534 (0.1%)	1.38	10/2063 (0.5%)
3	G	0.80	1/1539 (0.1%)	1.39	12/2070 (0.6%)
3	I	0.80	1/1522 (0.1%)	1.39	11/2047 (0.5%)
3	L	0.80	1/1522 (0.1%)	1.41	13/2047 (0.6%)
All	All	0.76	7/20073 (0.0%)	1.26	86/27235 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	197	SER	C-N	6.20	1.39	1.33
3	L	256	ILE	CA-CB	5.92	1.57	1.54
2	B	45	GLN	CA-C	5.78	1.57	1.52
3	I	256	ILE	CA-CB	5.59	1.56	1.54
2	H	197	SER	C-N	5.49	1.39	1.33
3	G	256	ILE	CA-CB	5.02	1.56	1.54
3	E	256	ILE	CA-CB	5.02	1.56	1.54

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	44	GLU	CA-C-N	8.07	136.22	121.70
2	H	44	GLU	C-N-CA	8.07	136.22	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	285	ASN	CA-CB-CG	7.85	120.45	112.60
2	D	91	GLU	CB-CG-CD	7.76	125.80	112.60
3	L	140	ASP	CA-CB-CG	7.28	119.88	112.60
3	G	140	ASP	CA-CB-CG	7.24	119.84	112.60
1	J	163	ASN	CA-C-N	7.20	132.80	123.08
1	J	163	ASN	C-N-CA	7.20	132.80	123.08
3	E	285	ASN	CA-CB-CG	7.13	119.73	112.60
2	D	112	ASP	CA-CB-CG	6.93	119.53	112.60
3	I	140	ASP	CA-CB-CG	6.84	119.44	112.60
3	E	178	GLU	N-CA-C	-6.84	104.83	113.72
3	G	178	GLU	N-CA-C	-6.78	104.91	113.72
3	L	285	ASN	CA-CB-CG	6.75	119.35	112.60
2	K	112	ASP	CA-CB-CG	6.75	119.35	112.60
2	K	144	ASN	CA-CB-CG	6.73	119.33	112.60
2	K	63	ASP	N-CA-C	-6.71	101.19	109.65
3	L	255	VAL	N-CA-C	6.71	117.33	111.56
2	H	63	ASP	N-CA-C	-6.69	101.22	109.65
2	D	112	ASP	N-CA-C	6.67	118.63	111.36
2	H	112	ASP	N-CA-C	6.66	118.62	111.36
2	B	63	ASP	N-CA-C	-6.65	101.27	109.65
3	I	178	GLU	N-CA-C	-6.63	105.10	113.72
2	D	63	ASP	N-CA-C	-6.59	101.35	109.65
1	A	3	GLU	CB-CG-CD	6.58	123.78	112.60
1	J	164	GLY	N-CA-C	-6.54	106.13	114.37
3	L	178	GLU	N-CA-C	-6.53	105.23	113.72
3	E	255	VAL	N-CA-C	6.43	117.09	111.56
3	G	255	VAL	N-CA-C	6.42	117.08	111.56
3	I	255	VAL	N-CA-C	6.42	117.08	111.56
1	A	194	ARG	N-CA-C	-6.10	101.75	110.59
3	L	164	LEU	CA-C-N	6.08	128.35	120.44
3	L	164	LEU	C-N-CA	6.08	128.35	120.44
2	B	112	ASP	CA-CB-CG	6.06	118.66	112.60
1	F	143	ASN	N-CA-C	5.96	119.53	109.76
3	G	260	ASP	CA-C-N	5.82	128.35	120.38
3	G	260	ASP	C-N-CA	5.82	128.35	120.38
2	D	181	LEU	N-CA-C	5.79	118.17	107.99
1	J	138	VAL	CB-CA-C	5.78	118.98	110.77
1	J	143	ASN	N-CA-C	5.73	119.16	109.76
2	B	44	GLU	CA-C-N	5.72	128.97	119.35
2	B	44	GLU	C-N-CA	5.72	128.97	119.35
3	I	186	PHE	CA-C-N	5.71	127.87	120.44
3	I	186	PHE	C-N-CA	5.71	127.87	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	308	ILE	CB-CA-C	5.71	120.65	111.29
1	F	164	GLY	CA-C-N	5.68	128.81	120.91
1	F	164	GLY	C-N-CA	5.68	128.81	120.91
3	I	255	VAL	CA-C-N	5.63	125.84	120.43
3	I	255	VAL	C-N-CA	5.63	125.84	120.43
1	A	143	ASN	N-CA-C	5.60	118.94	109.76
1	F	138	VAL	CB-CA-C	5.60	118.97	111.19
3	L	255	VAL	CA-C-N	5.59	125.80	120.43
3	L	255	VAL	C-N-CA	5.59	125.80	120.43
2	K	112	ASP	N-CA-C	5.58	117.45	111.36
3	G	255	VAL	CA-C-N	5.57	125.78	120.43
3	G	255	VAL	C-N-CA	5.57	125.78	120.43
1	J	164	GLY	CA-C-N	5.56	128.54	120.98
1	J	164	GLY	C-N-CA	5.56	128.54	120.98
1	J	190	ASP	N-CA-C	5.55	117.01	111.07
3	E	255	VAL	CA-C-N	5.54	125.75	120.43
3	E	255	VAL	C-N-CA	5.54	125.75	120.43
1	A	207	SER	CA-C-N	5.50	127.65	120.28
1	A	207	SER	C-N-CA	5.50	127.65	120.28
3	G	186	PHE	CA-C-N	5.50	127.58	120.44
3	G	186	PHE	C-N-CA	5.50	127.58	120.44
3	E	260	ASP	CA-C-N	5.44	127.83	120.38
3	E	260	ASP	C-N-CA	5.44	127.83	120.38
3	L	314	GLU	CA-C-N	5.40	131.42	121.70
3	L	314	GLU	C-N-CA	5.40	131.42	121.70
1	A	141	PHE	CA-CB-CG	5.36	119.16	113.80
1	C	143	ASN	N-CA-C	5.34	118.76	110.17
3	I	272	GLY	CA-C-N	5.33	129.13	120.60
3	I	272	GLY	C-N-CA	5.33	129.13	120.60
3	L	273	ASP	CA-CB-CG	5.30	117.90	112.60
2	B	144	ASN	CA-CB-CG	5.23	117.83	112.60
3	G	314	GLU	CB-CG-CD	5.20	121.43	112.60
2	K	159	GLU	N-CA-C	-5.19	102.67	110.24
3	E	306	LYS	CA-C-N	5.18	131.44	121.54
3	E	306	LYS	C-N-CA	5.18	131.44	121.54
3	I	315	LYS	N-CA-C	5.17	117.99	108.58
3	L	260	ASP	CA-C-N	5.13	127.16	120.28
3	L	260	ASP	C-N-CA	5.13	127.16	120.28
1	F	207	SER	CA-C-N	5.08	127.09	120.28
1	F	207	SER	C-N-CA	5.08	127.09	120.28
3	G	241	THR	N-CA-C	5.03	117.44	109.50
3	G	313	ARG	N-CA-C	-5.01	105.82	111.28

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	1718	0	1647	16	0
1	C	1718	0	1647	19	0
1	F	1718	0	1647	15	0
1	J	1718	0	1647	13	0
2	B	1689	0	1638	20	0
2	D	1689	0	1638	22	0
2	H	1689	0	1638	20	0
2	K	1689	0	1638	18	0
3	E	1505	0	1515	14	0
3	G	1510	0	1520	18	0
3	I	1494	0	1506	16	0
3	L	1494	0	1506	7	0
4	C	8	0	12	0	0
4	D	8	0	12	6	0
4	H	4	0	6	0	0
4	J	8	0	12	0	0
4	K	4	0	6	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	D	6	0	8	0	0
5	G	12	0	16	5	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
6	L	1	0	0	0	0
7	A	2	0	0	0	0
7	B	8	0	0	0	0
7	C	9	0	0	1	0
7	D	5	0	0	0	0
7	E	6	0	0	1	0
7	F	8	0	0	0	0
7	G	4	0	0	0	0
7	H	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I	3	0	0	0	0
7	J	9	0	0	0	0
7	K	10	0	0	0	0
7	L	5	0	0	0	0
All	All	19772	0	19275	194	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 5.

All (194) 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:K:199:ARG:HH11	2:K:199:ARG:HG3	1.09	1.17
2:B:199:ARG:HG3	2:B:199:ARG:HH11	1.19	1.03
2:H:199:ARG:HH11	2:H:199:ARG:HG3	1.18	1.03
2:D:199:ARG:HH11	2:D:199:ARG:HG3	1.30	0.95
2:K:199:ARG:HH11	2:K:199:ARG:CG	1.87	0.86
2:K:199:ARG:HG3	2:K:199:ARG:NH1	1.87	0.84
2:H:199:ARG:HG3	2:H:199:ARG:NH1	1.88	0.83
2:H:199:ARG:HD2	2:H:200:PRO:HA	1.65	0.79
2:D:199:ARG:HH11	2:D:199:ARG:CG	1.96	0.78
2:H:149:LEU:HD11	2:H:199:ARG:HG2	1.65	0.77
1:C:134:GLY:O	1:C:189:LYS:HB2	1.88	0.73
2:B:199:ARG:HH11	2:B:199:ARG:CG	1.99	0.73
3:L:218:VAL:HG11	3:L:237:LEU:HD13	1.73	0.70
3:E:218:VAL:HG11	3:E:237:LEU:HD13	1.73	0.70
1:F:201:GLU:HG3	1:F:212:VAL:HG22	1.74	0.70
3:I:218:VAL:HG11	3:I:237:LEU:HD13	1.74	0.69
1:C:37:ASN:HD21	1:C:74:GLY:H	1.40	0.69
1:F:37:ASN:HD21	1:F:74:GLY:H	1.41	0.68
3:L:162:GLU:HG2	3:L:195:PRO:HG2	1.75	0.68
2:B:199:ARG:HG3	2:B:199:ARG:NH1	1.99	0.68
3:G:218:VAL:HG11	3:G:237:LEU:HD13	1.76	0.68
1:A:37:ASN:HD21	1:A:74:GLY:H	1.41	0.68
1:J:37:ASN:HD21	1:J:74:GLY:H	1.41	0.66
3:G:180:PHE:O	5:G:6:GOL:H12	1.96	0.65
2:D:106:TYR:O	4:D:2:EDO:H22	1.96	0.64
3:E:308:ILE:O	3:E:310:ASN:N	2.30	0.64
3:G:249:PRO:HG3	5:G:5:GOL:H2	1.80	0.64
2:H:44:GLU:HA	2:H:45:GLN:O	1.97	0.63
2:D:199:ARG:HG3	2:D:199:ARG:NH1	2.08	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:34:ILE:HG22	2:K:102:GLY:HA2	1.82	0.61
3:E:304:ALA:O	3:E:307:THR:HB	2.01	0.61
2:D:103:HIS:HA	4:D:2:EDO:H21	1.83	0.60
2:D:34:ILE:HG22	2:D:102:GLY:HA2	1.85	0.59
1:C:37:ASN:ND2	1:C:74:GLY:H	2.00	0.59
1:J:37:ASN:ND2	1:J:74:GLY:H	2.01	0.59
1:C:187:LEU:HD13	1:C:192:TYR:HB2	1.84	0.58
1:A:37:ASN:ND2	1:A:74:GLY:H	2.01	0.58
3:L:279:LYS:O	3:L:282:GLN:HG2	2.03	0.58
1:F:37:ASN:ND2	1:F:74:GLY:H	2.01	0.58
1:F:188:THR:H	1:F:191:GLU:HB2	1.69	0.58
2:D:93:THR:HG23	2:D:121:THR:HA	1.87	0.57
2:B:149:LEU:HD11	2:B:199:ARG:HG2	1.85	0.57
2:H:42:ARG:O	2:H:44:GLU:N	2.39	0.56
3:I:194:ASN:HD22	3:I:197:SER:HB3	1.71	0.56
2:B:195:PRO:HB2	2:B:198:PRO:HD2	1.87	0.56
2:B:130:PRO:HB3	2:B:156:TYR:HB3	1.88	0.56
2:D:3:GLN:HE21	3:I:194:ASN:ND2	2.03	0.55
3:E:162:GLU:HG3	3:E:195:PRO:HG2	1.89	0.55
3:G:194:ASN:HD22	3:G:197:SER:HB3	1.72	0.54
1:F:201:GLU:HG2	1:F:210:PRO:HB2	1.89	0.54
3:E:194:ASN:HD22	3:E:197:SER:HB3	1.73	0.54
2:D:158:PRO:HD2	2:D:212:ALA:CB	2.37	0.54
3:E:174:MET:HB2	3:E:222:LEU:HD11	1.90	0.54
2:K:199:ARG:CG	2:K:199:ARG:NH1	2.58	0.54
3:I:174:MET:HB2	3:I:222:LEU:HD11	1.90	0.54
3:G:174:MET:HB2	3:G:222:LEU:HD11	1.90	0.53
2:D:103:HIS:HB3	4:D:2:EDO:H12	1.91	0.53
2:B:14:VAL:HG21	2:B:88:LEU:HD13	1.91	0.53
1:A:196:ASN:HD21	1:A:218:ASN:HB2	1.73	0.52
3:L:174:MET:HB2	3:L:222:LEU:HD11	1.90	0.52
1:J:156:ILE:HD11	1:J:185:LEU:HD21	1.91	0.52
1:F:31:TYR:CZ	1:F:33:SER:HB2	2.45	0.52
2:D:14:VAL:HG21	2:D:88:LEU:HD13	1.92	0.51
2:H:14:VAL:HG21	2:H:88:LEU:HD13	1.91	0.51
2:D:195:PRO:O	2:D:198:PRO:HD2	2.09	0.51
2:H:195:PRO:HB2	2:H:198:PRO:HD2	1.91	0.51
1:J:31:TYR:CZ	1:J:33:SER:HB2	2.46	0.51
2:D:195:PRO:HB2	2:D:198:PRO:HD2	1.92	0.51
2:K:22:LEU:HD22	2:K:118:THR:HG21	1.92	0.51
1:C:31:TYR:CZ	1:C:33:SER:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:TYR:CZ	1:A:33:SER:HB2	2.46	0.50
4:D:2:EDO:H11	3:G:143:GLY:CA	2.41	0.50
2:K:149:LEU:HD11	2:K:199:ARG:HG2	1.92	0.50
2:D:22:LEU:HD22	2:D:118:THR:HG21	1.94	0.50
2:B:199:ARG:HD2	2:B:200:PRO:HA	1.93	0.50
2:H:34:ILE:HG22	2:H:102:GLY:HA2	1.93	0.50
2:K:14:VAL:HG21	2:K:88:LEU:HD13	1.94	0.50
2:H:22:LEU:HD22	2:H:118:THR:HG21	1.94	0.49
2:K:93:THR:HG23	2:K:121:THR:HA	1.93	0.49
2:D:195:PRO:C	2:D:198:PRO:HD2	2.38	0.49
2:D:199:ARG:CG	2:D:199:ARG:NH1	2.65	0.49
1:C:21:MET:HG2	1:C:108:THR:HG21	1.95	0.49
3:G:210:HIS:CE1	5:G:5:GOL:H31	2.48	0.49
1:A:21:MET:HG2	1:A:108:THR:HG21	1.95	0.49
3:G:210:HIS:HE1	5:G:5:GOL:H31	1.78	0.48
1:C:21:MET:HB3	7:C:223:HOH:O	2.12	0.48
3:G:249:PRO:CG	5:G:5:GOL:H2	2.43	0.48
1:F:21:MET:HG2	1:F:108:THR:HG21	1.96	0.48
2:B:22:LEU:HD22	2:B:118:THR:HG21	1.95	0.48
3:G:267:TYR:CE2	3:G:315:LYS:HG2	2.49	0.47
3:I:170:LEU:HD23	3:I:189:PHE:HD2	1.79	0.47
2:B:13:LEU:HD21	2:B:158:PRO:HB3	1.95	0.47
1:J:67:ARG:HG3	1:J:81:ILE:HG23	1.96	0.47
1:A:67:ARG:HG3	1:A:81:ILE:HG23	1.96	0.47
2:H:130:PRO:HB3	2:H:156:TYR:HB3	1.97	0.47
2:B:181:LEU:HB2	2:B:186:TYR:CE1	2.50	0.47
1:J:100:TYR:HD1	2:K:49:TRP:CH2	2.32	0.47
1:A:166:LEU:HD21	2:B:182:GLN:HG3	1.96	0.47
2:B:34:ILE:HG22	2:B:102:GLY:HA2	1.96	0.47
2:B:195:PRO:O	2:B:198:PRO:HD2	2.15	0.46
1:F:67:ARG:HG3	1:F:81:ILE:HG23	1.97	0.46
2:H:158:PRO:HD2	2:H:212:ALA:CB	2.45	0.46
3:E:236:ILE:HG21	3:E:317:PHE:HB3	1.97	0.46
2:H:44:GLU:HA	2:H:45:GLN:C	2.41	0.46
1:J:21:MET:HG2	1:J:108:THR:HG21	1.97	0.46
2:K:195:PRO:HB2	2:K:198:PRO:HD2	1.97	0.46
2:B:195:PRO:C	2:B:198:PRO:HD2	2.41	0.46
2:B:35:TYR:HB2	2:B:101:GLU:HB3	1.97	0.45
3:E:166:LYS:O	3:E:168:LYS:N	2.49	0.45
3:I:256:ILE:HG23	3:I:266:ARG:HH21	1.80	0.45
1:C:67:ARG:HG3	1:C:81:ILE:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:195:PRO:O	2:K:198:PRO:HD2	2.16	0.45
2:D:163:VAL:HG22	2:D:208:VAL:HB	1.99	0.45
2:K:161:VAL:HG23	2:K:210:HIS:HD2	1.82	0.45
1:C:89:LEU:HD11	1:C:112:LEU:HD13	1.98	0.45
3:G:135:ILE:O	3:G:171:PHE:HA	2.17	0.44
2:H:225:ASP:HB3	2:H:226:CYS:HB3	2.00	0.44
3:I:312:LEU:C	3:I:314:GLU:H	2.25	0.44
1:A:89:LEU:HD11	1:A:112:LEU:HD13	2.00	0.44
4:D:2:EDO:H11	3:G:143:GLY:HA2	1.99	0.44
1:F:89:LEU:HD11	1:F:112:LEU:HD13	1.99	0.44
2:H:93:THR:HG23	2:H:121:THR:HA	2.00	0.44
2:H:163:VAL:HG22	2:H:208:VAL:HB	2.00	0.44
1:A:138:VAL:HG13	1:A:185:LEU:HB3	1.99	0.43
2:K:13:LEU:HD12	2:K:121:THR:HB	2.00	0.43
2:D:149:LEU:HD11	2:D:199:ARG:HG2	2.00	0.43
3:I:132:ASP:N	3:I:168:LYS:HB3	2.33	0.43
2:B:93:THR:HG23	2:B:121:THR:HA	1.99	0.43
1:C:138:VAL:HG13	1:C:185:LEU:HB3	2.00	0.43
1:F:114:ARG:HD3	1:F:115:ALA:O	2.17	0.43
3:I:157:VAL:HG12	3:I:161:MET:HE2	1.99	0.43
3:I:170:LEU:CD2	3:I:189:PHE:HD2	2.31	0.43
1:J:89:LEU:HD11	1:J:112:LEU:HD13	2.00	0.43
4:D:2:EDO:H11	3:G:143:GLY:HA3	2.00	0.43
1:A:17:GLU:O	1:A:84:VAL:HG23	2.19	0.43
3:E:225:ILE:H	3:E:225:ILE:HG13	1.64	0.43
2:B:195:PRO:HB2	2:B:198:PRO:CD	2.48	0.43
1:F:125:PRO:HB2	2:H:224:ARG:NH2	2.34	0.43
1:C:156:ILE:HD11	1:C:185:LEU:HD21	2.00	0.43
2:H:161:VAL:HG23	2:H:210:HIS:HD2	1.83	0.43
2:B:163:VAL:HG22	2:B:208:VAL:HB	2.01	0.43
1:J:17:GLU:O	1:J:84:VAL:HG23	2.19	0.43
1:A:199:THR:HG23	1:A:214:SER:HB2	2.00	0.43
1:C:199:THR:HG23	1:C:214:SER:HB2	2.00	0.42
1:C:201:GLU:HG2	1:C:212:VAL:HG22	2.01	0.42
2:D:195:PRO:HD2	2:D:198:PRO:HG3	2.01	0.42
1:A:114:ARG:HD3	1:A:115:ALA:O	2.19	0.42
3:L:154:LYS:HD3	3:L:202:ILE:HB	2.01	0.42
2:K:158:PRO:HD2	2:K:212:ALA:CB	2.49	0.42
1:J:114:ARG:HD3	1:J:115:ALA:O	2.19	0.42
2:D:195:PRO:HB2	2:D:198:PRO:CD	2.50	0.42
1:C:139:VAL:HG22	1:C:184:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:GLU:O	1:F:84:VAL:HG23	2.19	0.42
2:K:163:VAL:HG22	2:K:208:VAL:HB	2.02	0.42
1:C:114:ARG:HD3	1:C:115:ALA:O	2.20	0.42
2:B:42:ARG:O	2:B:43:PRO:C	2.62	0.42
1:J:199:THR:HG23	1:J:214:SER:HB2	2.01	0.42
1:F:199:THR:HG23	1:F:214:SER:HB2	2.01	0.42
3:I:312:LEU:HG	3:I:313:ARG:H	1.85	0.42
1:F:167:ASN:ND2	1:F:183:SER:OG	2.52	0.41
1:C:17:GLU:O	1:C:84:VAL:HG23	2.20	0.41
3:E:135:ILE:O	3:E:171:PHE:HA	2.21	0.41
3:E:280:SER:O	3:E:283:GLU:HB3	2.21	0.41
3:L:271:VAL:HG13	3:L:299:VAL:HG23	2.03	0.41
3:I:170:LEU:HD23	3:I:189:PHE:CD2	2.56	0.41
3:G:154:LYS:HD3	3:G:202:ILE:HB	2.02	0.41
2:K:159:GLU:HG3	2:K:160:PRO:HA	2.03	0.41
3:L:225:ILE:H	3:L:225:ILE:HG13	1.64	0.41
2:K:210:HIS:CE1	2:K:212:ALA:HB3	2.56	0.41
1:C:153:LYS:HB2	1:C:201:GLU:HB2	2.03	0.41
2:D:49:TRP:CZ2	2:D:51:GLY:HA2	2.56	0.41
1:A:13:VAL:HG22	1:A:19:VAL:HG11	2.03	0.41
1:A:201:GLU:HG2	1:A:212:VAL:HG22	2.02	0.41
2:H:195:PRO:O	2:H:198:PRO:HD2	2.20	0.41
3:G:149:ASP:HB3	3:G:302:PHE:CD2	2.56	0.41
3:G:168:LYS:HG3	3:G:230:ARG:NH2	2.36	0.41
3:E:245:LYS:NZ	7:E:39:HOH:O	2.49	0.41
2:H:135:LEU:HB2	2:H:150:GLY:CA	2.51	0.41
1:C:189:LYS:O	1:C:193:GLU:HG3	2.21	0.40
3:E:154:LYS:HD3	3:E:202:ILE:HB	2.03	0.40
3:I:161:MET:HE3	3:I:195:PRO:HB3	2.03	0.40
3:I:225:ILE:H	3:I:225:ILE:HG13	1.63	0.40
1:J:97:TYR:HA	1:J:102:LEU:HD22	2.03	0.40
1:C:13:VAL:HG22	1:C:19:VAL:HG11	2.03	0.40
2:D:130:PRO:HB3	2:D:156:TYR:HB3	2.04	0.40
3:G:141:GLY:HA3	3:G:175:GLN:OE1	2.21	0.40
3:G:225:ILE:H	3:G:225:ILE:HG13	1.65	0.40
1:F:75:THR:HG22	1:F:76:ASP:OD1	2.22	0.40
3:I:154:LYS:HD3	3:I:202:ILE:HB	2.02	0.40
1:A:75:THR:HG22	1:A:76:ASP:OD1	2.22	0.40
1:A:97:TYR:HA	1:A:102:LEU:HD22	2.04	0.40
3:E:141:GLY:HA3	3:E:175:GLN:OE1	2.21	0.40
3:I:135:ILE:O	3:I:171:PHE:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:13:VAL:HG11	1:J:84:VAL:HG11	2.04	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	A	218/220 (99%)	209 (96%)	9 (4%)	0	100	100
1	C	218/220 (99%)	209 (96%)	8 (4%)	1 (0%)	24	60
1	F	218/220 (99%)	208 (95%)	10 (5%)	0	100	100
1	J	218/220 (99%)	208 (95%)	9 (4%)	1 (0%)	24	60
2	B	222/224 (99%)	208 (94%)	10 (4%)	4 (2%)	6	31
2	D	222/224 (99%)	213 (96%)	5 (2%)	4 (2%)	6	31
2	H	222/224 (99%)	213 (96%)	5 (2%)	4 (2%)	6	31
2	K	222/224 (99%)	210 (95%)	9 (4%)	3 (1%)	9	36
3	E	184/190 (97%)	170 (92%)	10 (5%)	4 (2%)	5	26
3	G	185/190 (97%)	172 (93%)	11 (6%)	2 (1%)	11	43
3	I	183/190 (96%)	173 (94%)	9 (5%)	1 (0%)	24	60
3	L	183/190 (96%)	173 (94%)	8 (4%)	2 (1%)	11	43
All	All	2495/2536 (98%)	2366 (95%)	103 (4%)	26 (1%)	12	45

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	43	PRO
2	B	225	ASP
3	E	167	SER

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Mol	Chain	Res	Type
3	E	309	GLN
2	H	45	GLN
2	B	143	THR
3	E	308	ILE
2	H	43	PRO
2	D	183	SER
2	D	225	ASP
2	H	44	GLU
2	K	143	THR
3	L	315	LYS
3	G	167	SER
3	G	177	SER
1	J	163	ASN
3	E	177	SER
3	I	177	SER
2	K	183	SER
3	L	177	SER
1	C	135	GLY
2	D	28	GLY
2	B	28	GLY
2	H	28	GLY
2	K	28	GLY
2	B	4	VAL

### 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	197/197 (100%)	177 (90%)	20 (10%)	7 29
1	C	197/197 (100%)	175 (89%)	22 (11%)	6 24
1	F	197/197 (100%)	177 (90%)	20 (10%)	7 29
1	J	197/197 (100%)	180 (91%)	17 (9%)	10 36
2	B	192/192 (100%)	175 (91%)	17 (9%)	9 34
2	D	192/192 (100%)	174 (91%)	18 (9%)	8 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	192/192 (100%)	178 (93%)	14 (7%)	13	42
2	K	192/192 (100%)	179 (93%)	13 (7%)	14	45
3	E	166/168 (99%)	152 (92%)	14 (8%)	10	37
3	G	166/168 (99%)	150 (90%)	16 (10%)	8	31
3	I	165/168 (98%)	150 (91%)	15 (9%)	9	33
3	L	165/168 (98%)	149 (90%)	16 (10%)	8	30
All	All	2218/2228 (100%)	2016 (91%)	202 (9%)	9	33

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	5	THR
1	C	7	SER
1	C	10	SER
1	C	27	GLN
1	C	39	LEU
1	C	51	LYS
1	C	54	ILE
1	C	75	THR
1	C	95	GLN
1	C	111	GLU
1	C	114	ARG
1	C	123	ILE
1	C	138	VAL
1	C	151	ASN
1	C	160	GLU
1	C	166	LEU
1	C	182	SER
1	C	187	LEU
1	C	194	ARG
1	C	195	HIS
1	C	197	SER
1	C	203	THR
2	D	13	LEU
2	D	19	SER
2	D	45	GLN
2	D	91	GLU
2	D	119	THR
2	D	143	THR
2	D	161	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	D	170	LEU
2	D	171	SER
2	D	174	VAL
2	D	181	LEU
2	D	184	ASP
2	D	185	LEU
2	D	189	SER
2	D	197	SER
2	D	199	ARG
2	D	207	ASN
2	D	208	VAL
3	G	146	ILE
3	G	155	GLU
3	G	158	SER
3	G	165	LYS
3	G	168	LYS
3	G	221	GLU
3	G	225	ILE
3	G	226	THR
3	G	242	ASP
3	G	278	GLU
3	G	286	THR
3	G	293	ARG
3	G	311	GLN
3	G	312	LEU
3	G	313	ARG
3	G	315	LYS
1	A	3	GLU
1	A	5	THR
1	A	7	SER
1	A	10	SER
1	A	18	LYS
1	A	27	GLN
1	A	39	LEU
1	A	51	LYS
1	A	54	ILE
1	A	75	THR
1	A	95	GLN
1	A	111	GLU
1	A	114	ARG
1	A	123	ILE
1	A	138	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	151	ASN
1	A	166	LEU
1	A	182	SER
1	A	197	SER
1	A	203	THR
2	B	13	LEU
2	B	19	SER
2	B	44	GLU
2	B	45	GLN
2	B	91	GLU
2	B	142	GLN
2	B	145	SER
2	B	161	VAL
2	B	170	LEU
2	B	171	SER
2	B	174	VAL
2	B	182	GLN
2	B	197	SER
2	B	199	ARG
2	B	207	ASN
2	B	208	VAL
2	B	226	CYS
3	E	146	ILE
3	E	164	LEU
3	E	166	LYS
3	E	168	LYS
3	E	221	GLU
3	E	225	ILE
3	E	226	THR
3	E	242	ASP
3	E	278	GLU
3	E	281	ARG
3	E	293	ARG
3	E	307	THR
3	E	312	LEU
3	E	315	LYS
1	F	5	THR
1	F	7	SER
1	F	10	SER
1	F	27	GLN
1	F	39	LEU
1	F	51	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	54	ILE
1	F	75	THR
1	F	95	GLN
1	F	111	GLU
1	F	114	ARG
1	F	138	VAL
1	F	151	ASN
1	F	166	LEU
1	F	182	SER
1	F	187	LEU
1	F	197	SER
1	F	203	THR
1	F	218	ASN
1	F	220	CYS
2	H	3	GLN
2	H	13	LEU
2	H	19	SER
2	H	91	GLU
2	H	121	THR
2	H	161	VAL
2	H	170	LEU
2	H	171	SER
2	H	174	VAL
2	H	181	LEU
2	H	197	SER
2	H	199	ARG
2	H	207	ASN
2	H	208	VAL
3	I	146	ILE
3	I	155	GLU
3	I	196	ARG
3	I	221	GLU
3	I	225	ILE
3	I	226	THR
3	I	242	ASP
3	I	278	GLU
3	I	281	ARG
3	I	283	GLU
3	I	293	ARG
3	I	308	ILE
3	I	309	GLN
3	I	314	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	I	315	LYS
1	J	5	THR
1	J	7	SER
1	J	10	SER
1	J	27	GLN
1	J	39	LEU
1	J	51	LYS
1	J	54	ILE
1	J	75	THR
1	J	95	GLN
1	J	111	GLU
1	J	114	ARG
1	J	138	VAL
1	J	151	ASN
1	J	166	LEU
1	J	182	SER
1	J	187	LEU
1	J	203	THR
2	K	13	LEU
2	K	19	SER
2	K	45	GLN
2	K	91	GLU
2	K	144	ASN
2	K	161	VAL
2	K	170	LEU
2	K	174	VAL
2	K	191	SER
2	K	197	SER
2	K	199	ARG
2	K	207	ASN
2	K	208	VAL
3	L	146	ILE
3	L	151	ARG
3	L	155	GLU
3	L	158	SER
3	L	166	LYS
3	L	170	LEU
3	L	221	GLU
3	L	225	ILE
3	L	226	THR
3	L	242	ASP
3	L	273	ASP

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Mol	Chain	Res	Type
3	L	283	GLU
3	L	293	ARG
3	L	307	THR
3	L	311	GLN
3	L	313	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	37	ASN
1	C	44	GLN
1	C	95	GLN
1	C	143	ASN
1	C	195	HIS
1	C	216	ASN
2	D	7	GLN
2	D	30	ASN
2	D	41	GLN
2	D	45	GLN
2	D	84	GLN
3	G	194	ASN
3	G	298	GLN
3	G	311	GLN
1	A	37	ASN
1	A	44	GLN
1	A	95	GLN
1	A	143	ASN
1	A	167	ASN
1	A	196	ASN
1	A	218	ASN
2	B	3	GLN
2	B	7	GLN
2	B	30	ASN
2	B	41	GLN
2	B	45	GLN
2	B	142	GLN
3	E	163	GLN
3	E	191	ASN
3	E	194	ASN
3	E	224	ASN
3	E	285	ASN
1	F	37	ASN

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Mol	Chain	Res	Type
1	F	44	GLN
1	F	95	GLN
1	F	167	ASN
1	F	196	ASN
2	H	7	GLN
2	H	30	ASN
2	H	41	GLN
2	H	45	GLN
2	H	144	ASN
2	H	182	GLN
3	I	194	ASN
3	I	309	GLN
1	J	35	GLN
1	J	37	ASN
1	J	44	GLN
1	J	95	GLN
1	J	163	ASN
1	J	167	ASN
2	K	3	GLN
2	K	7	GLN
2	K	30	ASN
2	K	41	GLN
2	K	142	GLN
3	L	282	GLN
3	L	285	ASN
3	L	300	ASN
3	L	311	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

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	H	227	-	3,3,3	0.52	0	2,2,2	0.25	0
4	EDO	D	2	-	3,3,3	0.57	0	2,2,2	0.07	0
5	GOL	D	227	-	5,5,5	1.15	0	5,5,5	0.76	0
4	EDO	C	221	-	3,3,3	0.49	0	2,2,2	0.06	0
4	EDO	K	227	-	3,3,3	0.47	0	2,2,2	0.23	0
5	GOL	B	1	-	5,5,5	0.91	0	5,5,5	0.90	0
4	EDO	D	228	-	3,3,3	0.53	0	2,2,2	0.23	0
5	GOL	A	221	-	5,5,5	0.88	0	5,5,5	0.97	0
4	EDO	C	222	-	3,3,3	0.46	0	2,2,2	0.45	0
4	EDO	J	221	-	3,3,3	0.58	0	2,2,2	0.11	0
4	EDO	J	222	-	3,3,3	0.59	0	2,2,2	0.09	0
5	GOL	G	6	-	5,5,5	1.01	0	5,5,5	0.93	0
5	GOL	G	5	-	5,5,5	0.83	0	5,5,5	1.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	H	227	-	-	1/1/1/1	-
4	EDO	D	2	-	-	0/1/1/1	-
5	GOL	D	227	-	-	4/4/4/4	-
4	EDO	C	221	-	-	0/1/1/1	-
4	EDO	K	227	-	-	0/1/1/1	-
5	GOL	B	1	-	-	4/4/4/4	-
4	EDO	D	228	-	-	0/1/1/1	-
5	GOL	A	221	-	-	0/4/4/4	-
4	EDO	C	222	-	-	0/1/1/1	-
4	EDO	J	221	-	-	0/1/1/1	-
4	EDO	J	222	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	G	6	-	-	2/4/4/4	-
5	GOL	G	5	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	227	GOL	O1-C1-C2-C3
5	G	5	GOL	O1-C1-C2-O2
5	G	5	GOL	C1-C2-C3-O3
5	G	6	GOL	O1-C1-C2-C3
5	G	5	GOL	O2-C2-C3-O3
5	D	227	GOL	C1-C2-C3-O3
5	G	5	GOL	O1-C1-C2-C3
5	B	1	GOL	O1-C1-C2-C3
5	D	227	GOL	O1-C1-C2-O2
5	D	227	GOL	O2-C2-C3-O3
5	G	6	GOL	O1-C1-C2-O2
4	J	222	EDO	O1-C1-C2-O2
5	B	1	GOL	O2-C2-C3-O3
4	H	227	EDO	O1-C1-C2-O2
5	B	1	GOL	C1-C2-C3-O3
5	B	1	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	EDO	6	0
5	G	6	GOL	1	0
5	G	5	GOL	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 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	A	220/220 (100%)	0.11	2 (0%) 81 61	32, 55, 88, 111	0
1	C	220/220 (100%)	-0.12	1 (0%) 87 72	22, 39, 78, 110	0
1	F	220/220 (100%)	-0.24	0 100 100	23, 43, 66, 111	0
1	J	220/220 (100%)	-0.19	1 (0%) 87 72	24, 43, 63, 109	0
2	B	224/224 (100%)	-0.29	2 (0%) 81 61	21, 39, 77, 104	0
2	D	224/224 (100%)	-0.28	0 100 100	19, 36, 68, 106	0
2	H	224/224 (100%)	-0.05	2 (0%) 81 61	21, 44, 77, 105	0
2	K	224/224 (100%)	-0.19	4 (1%) 67 44	23, 41, 75, 104	0
3	E	186/190 (97%)	-0.09	1 (0%) 87 72	27, 53, 86, 99	0
3	G	187/190 (98%)	-0.18	3 (1%) 70 47	24, 42, 77, 100	0
3	I	185/190 (97%)	0.66	8 (4%) 40 21	39, 79, 113, 126	0
3	L	185/190 (97%)	-0.09	2 (1%) 78 57	28, 51, 85, 102	0
All	All	2519/2536 (99%)	-0.09	26 (1%) 79 59	19, 44, 87, 126	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	312	LEU	4.6
3	L	316	GLY	4.2
3	I	167	SER	3.4
2	K	226	CYS	3.1
3	G	312	LEU	3.0
2	B	3	GLN	3.0
2	H	4	VAL	2.9
2	K	143	THR	2.9
2	K	4	VAL	2.9
3	I	316	GLY	2.8
3	G	167	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	3	GLU	2.5
2	K	142	GLN	2.4
3	E	167	SER	2.3
1	A	156	ILE	2.3
3	I	238	VAL	2.3
3	I	236	ILE	2.3
2	H	3	GLN	2.3
3	G	318	ALA	2.3
2	B	4	VAL	2.3
3	I	135	ILE	2.2
3	L	132	ASP	2.2
1	A	158	GLY	2.1
3	I	308	ILE	2.0
1	J	220	CYS	2.0
3	I	309	GLN	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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	D	228	4/4	0.64	0.24	64,65,65,70	0
4	EDO	J	222	4/4	0.73	0.19	48,49,49,53	0
4	EDO	H	227	4/4	0.75	0.14	53,55,56,56	0
4	EDO	D	2	4/4	0.82	0.21	49,50,51,54	0
4	EDO	K	227	4/4	0.82	0.14	53,55,56,57	0
5	GOL	D	227	6/6	0.82	0.14	58,59,59,59	0
5	GOL	G	6	6/6	0.83	0.13	55,56,56,56	0
4	EDO	C	222	4/4	0.84	0.17	51,53,56,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	C	221	4/4	0.86	0.18	51,51,51,57	0
5	GOL	A	221	6/6	0.87	0.10	60,61,61,61	0
5	GOL	G	5	6/6	0.89	0.14	60,61,61,62	0
5	GOL	B	1	6/6	0.89	0.11	52,54,54,55	0
4	EDO	J	221	4/4	0.91	0.17	42,43,45,46	0
6	CA	G	500	1/1	0.99	0.02	28,28,28,28	0
6	CA	I	500	1/1	0.99	0.03	49,49,49,49	0
6	CA	L	500	1/1	0.99	0.02	49,49,49,49	0
6	CA	E	500	1/1	1.00	0.02	49,49,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.