



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 02:36 AM UTC

PDB ID : 6D0U / pdb_00006d0u
Title : Crystal structure of C05 V110P/A117E mutant bound to H3 influenza hemagglutinin, HA1 subunit
Authors : Wu, N.C.; Wilson, I.A.
Deposited on : 2018-04-11
Resolution : 3.25 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:

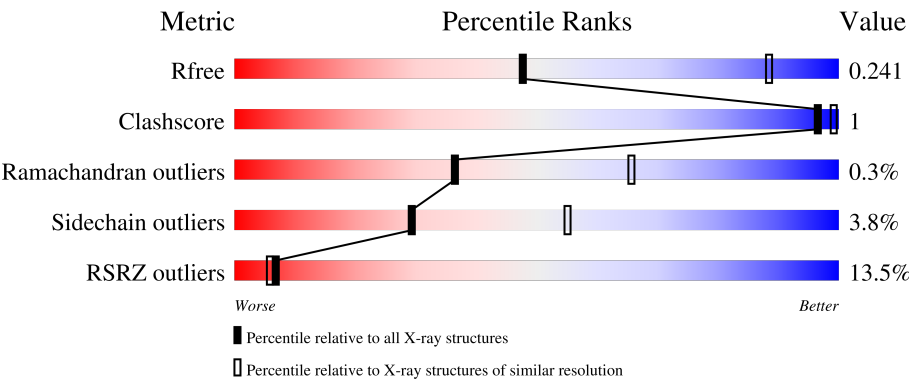
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	274	18% 95%
1	B	274	14% 94%
1	G	274	14% 92% 5%
1	J	274	14% 92%
2	C	247	13% 94%

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Mol	Chain	Length	Quality of chain
2	E	247	10% 86% 9%
2	H	247	10% 87% 9%
2	K	247	17% 91%
3	D	214	15% 93% 7%
3	F	214	10% 92% 7%
3	I	214	7% 94% 6%
3	L	214	15% 88% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21964 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2073	1303	363	396	11			
1	B	267	Total	C	N	O	S	0	0	0
			2073	1303	363	396	11			
1	J	267	Total	C	N	O	S	0	0	0
			2073	1303	363	396	11			
1	G	267	Total	C	N	O	S	0	0	0
			2073	1303	363	396	11			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLY	-	expression tag	UNP Q91MA7
A	311	HIS	-	expression tag	UNP Q91MA7
A	312	HIS	-	expression tag	UNP Q91MA7
A	313	HIS	-	expression tag	UNP Q91MA7
A	314	HIS	-	expression tag	UNP Q91MA7
A	315	HIS	-	expression tag	UNP Q91MA7
A	316	HIS	-	expression tag	UNP Q91MA7
B	310	GLY	-	expression tag	UNP Q91MA7
B	311	HIS	-	expression tag	UNP Q91MA7
B	312	HIS	-	expression tag	UNP Q91MA7
B	313	HIS	-	expression tag	UNP Q91MA7
B	314	HIS	-	expression tag	UNP Q91MA7
B	315	HIS	-	expression tag	UNP Q91MA7
B	316	HIS	-	expression tag	UNP Q91MA7
J	310	GLY	-	expression tag	UNP Q91MA7
J	311	HIS	-	expression tag	UNP Q91MA7
J	312	HIS	-	expression tag	UNP Q91MA7
J	313	HIS	-	expression tag	UNP Q91MA7
J	314	HIS	-	expression tag	UNP Q91MA7
J	315	HIS	-	expression tag	UNP Q91MA7
J	316	HIS	-	expression tag	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	310	GLY	-	expression tag	UNP Q91MA7
G	311	HIS	-	expression tag	UNP Q91MA7
G	312	HIS	-	expression tag	UNP Q91MA7
G	313	HIS	-	expression tag	UNP Q91MA7
G	314	HIS	-	expression tag	UNP Q91MA7
G	315	HIS	-	expression tag	UNP Q91MA7
G	316	HIS	-	expression tag	UNP Q91MA7

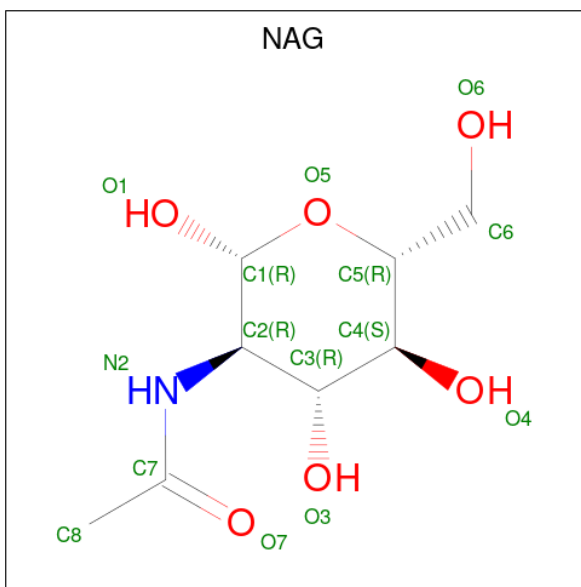
- Molecule 2 is a protein called Antibody C05 V110P/A117E mutant, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	238	Total	C	N	O	S	0	1	0
			1777	1111	298	360	8			
2	C	238	Total	C	N	O	S	0	0	0
			1771	1108	297	358	8			
2	K	238	Total	C	N	O	S	0	0	0
			1771	1108	297	358	8			
2	H	238	Total	C	N	O	S	0	1	0
			1777	1111	298	360	8			

- Molecule 3 is a protein called Antibody C05, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	213	Total	C	N	O	S	0	0	0
			1637	1027	277	329	4			
3	D	213	Total	C	N	O	S	0	0	0
			1637	1027	277	329	4			
3	L	213	Total	C	N	O	S	0	0	0
			1637	1027	277	329	4			
3	I	213	Total	C	N	O	S	0	0	0
			1637	1027	277	329	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

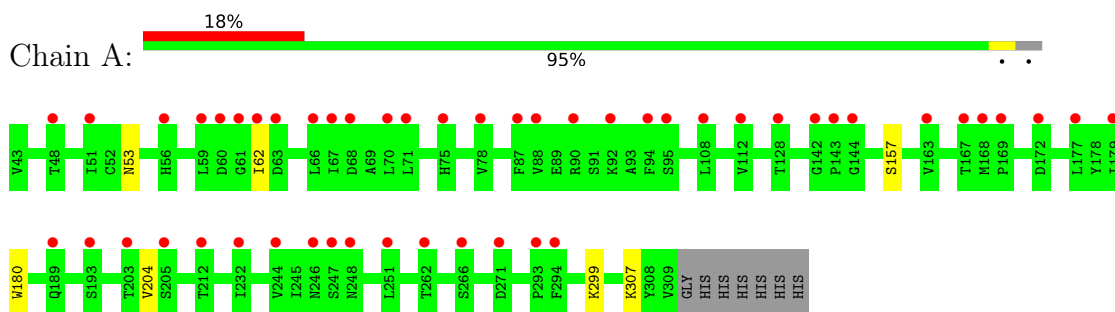


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	J	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		

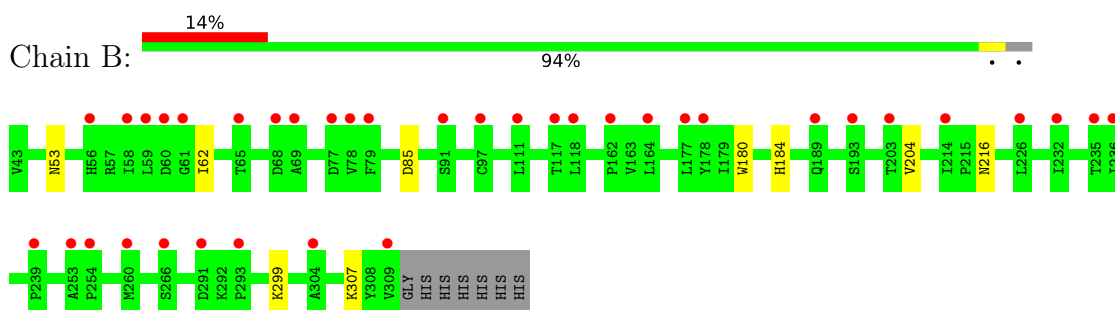
3 Residue-property plots [i](#)

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.

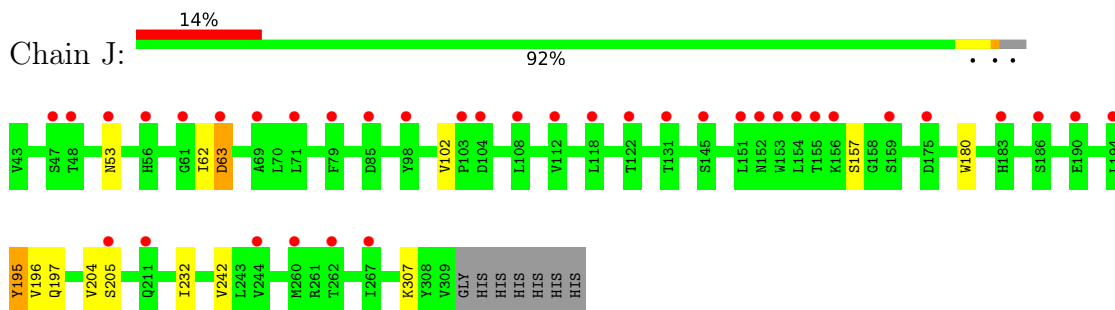
- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin

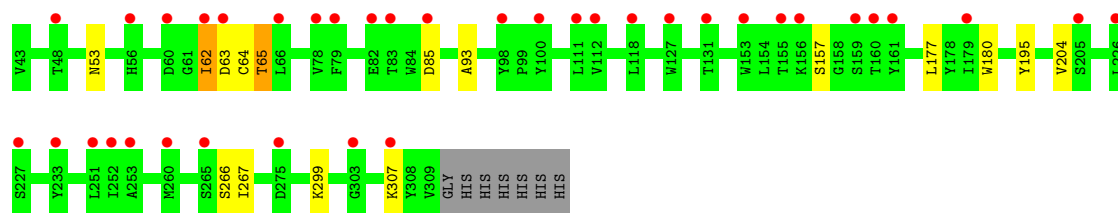


- Molecule 1: Hemagglutinin

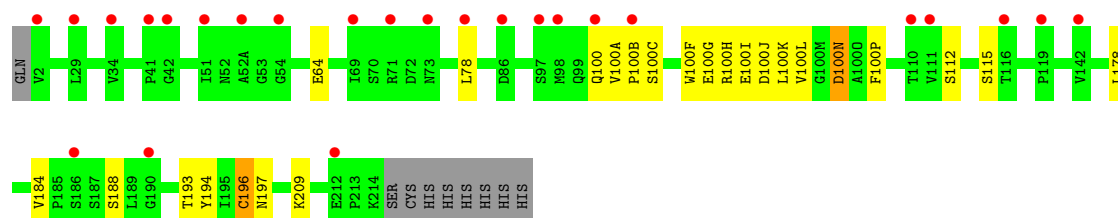
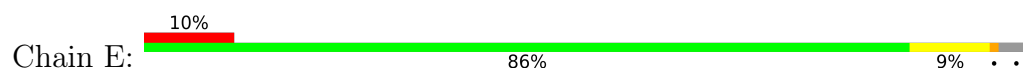


- Molecule 1: Hemagglutinin

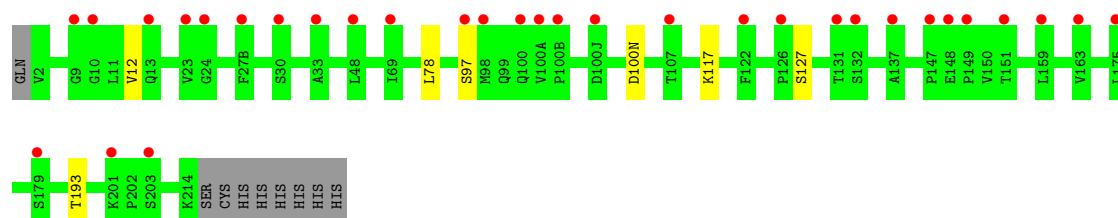




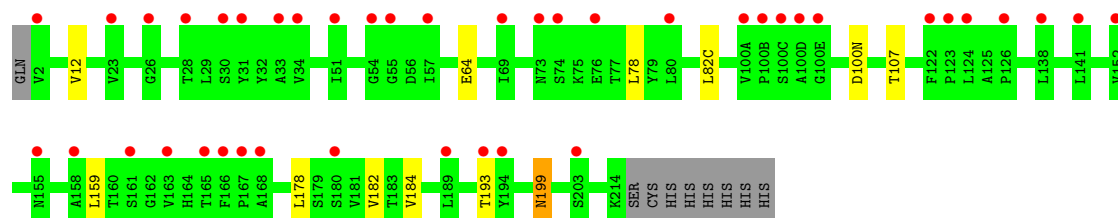
- Molecule 2: Antibody C05 V110P/A117E mutant, heavy chain



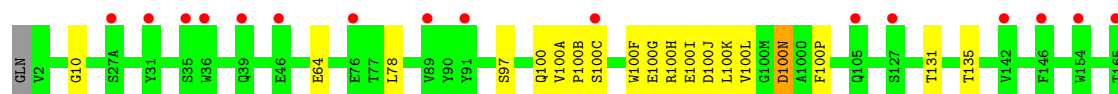
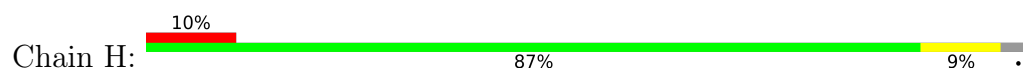
- Molecule 2: Antibody C05 V110P/A117E mutant, heavy chain

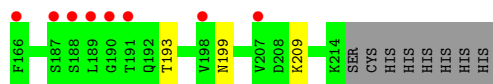


- Molecule 2: Antibody C05 V110P/A117E mutant, heavy chain

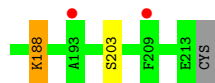
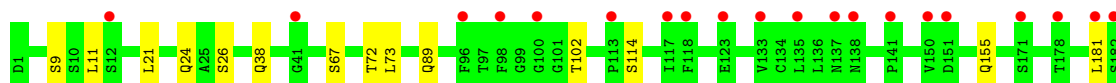
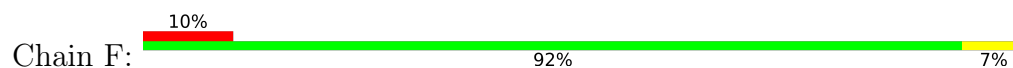


- Molecule 2: Antibody C05 V110P/A117E mutant, heavy chain

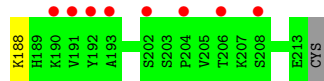
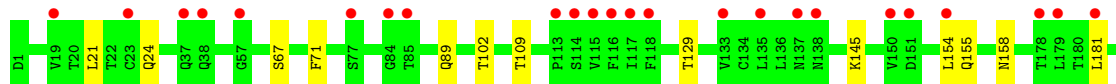
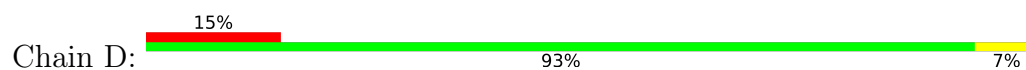




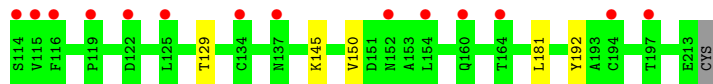
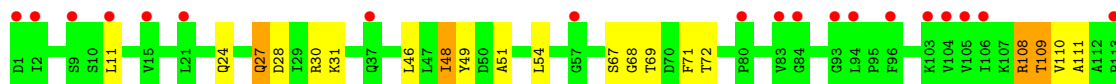
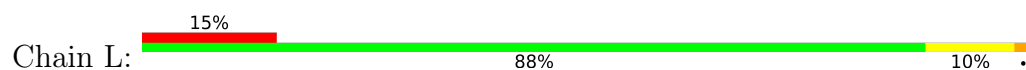
- Molecule 3: Antibody C05, light chain



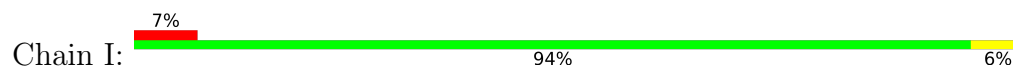
- Molecule 3: Antibody C05, light chain



- Molecule 3: Antibody C05, light chain



- Molecule 3: Antibody C05, light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.61Å 258.42Å 91.88Å 90.00° 90.54° 90.00°	Depositor
Resolution (Å)	50.00 – 3.25 50.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	94.0 (50.00-3.25) 99.3 (50.00-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.254 , 0.268 0.231 , 0.241	Depositor DCC
R_{free} test set	3191 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	96.0	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.035 for l,k,-h 0.043 for h,-k,-l 0.032 for l,-k,h	Xtriage
Reported twinning fraction	0.473 for H, K, L 0.527 for -L, K, H	Depositor
Outliers	0 of 66894 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	21964	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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](#)

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

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	0.88	1/2125 (0.0%)	0.92	0/2895
1	B	0.87	1/2125 (0.0%)	0.94	0/2895
1	G	0.90	3/2125 (0.1%)	0.95	0/2895
1	J	0.89	1/2125 (0.0%)	0.95	1/2895 (0.0%)
2	C	0.85	1/1810 (0.1%)	0.91	0/2463
2	E	0.90	1/1816 (0.1%)	0.89	1/2471 (0.0%)
2	H	0.89	1/1816 (0.1%)	0.91	0/2471
2	K	0.91	3/1810 (0.2%)	0.92	0/2463
3	D	0.96	1/1671 (0.1%)	0.96	1/2266 (0.0%)
3	F	0.95	3/1671 (0.2%)	0.96	2/2266 (0.1%)
3	I	0.95	2/1671 (0.1%)	0.95	0/2266
3	L	0.97	2/1671 (0.1%)	0.99	1/2266 (0.0%)
All	All	0.91	20/22436 (0.1%)	0.94	6/30512 (0.0%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	177	LEU	C-O	-7.41	1.15	1.24
3	L	48	ILE	C-O	-7.03	1.16	1.24
1	G	157	SER	C-O	-6.96	1.16	1.24
2	E	196	CYS	C-O	-6.64	1.16	1.24
1	B	85	ASP	C-O	-6.38	1.15	1.24
2	K	184	VAL	C-O	6.19	1.28	1.24
3	L	181	LEU	C-O	6.00	1.31	1.23
3	D	89	GLN	C-O	-5.97	1.16	1.23
1	J	157	SER	C-O	-5.82	1.17	1.24
1	A	157	SER	C-O	-5.82	1.17	1.24
3	F	89	GLN	C-O	-5.80	1.17	1.23
2	K	199	ASN	C-O	-5.72	1.17	1.24
2	H	10	GLY	C-O	-5.32	1.17	1.23
3	I	38	GLN	C-O	-5.24	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	12	VAL	C-O	-5.24	1.18	1.23
1	G	85	ASP	C-O	-5.15	1.17	1.24
3	F	9	SER	C-O	-5.02	1.17	1.24
3	I	154	LEU	C-O	5.01	1.29	1.24
2	K	107	THR	C-O	5.01	1.29	1.23
3	F	38	GLN	C-O	-5.00	1.17	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	242	VAL	N-CA-C	6.50	117.24	107.75
3	L	11	LEU	N-CA-C	6.26	118.58	109.07
3	D	188	LYS	N-CA-C	6.11	118.74	111.71
3	F	188	LYS	N-CA-C	5.66	118.22	111.71
3	F	11	LEU	N-CA-C	5.41	117.28	109.07
2	E	112	SER	CA-C-O	5.32	126.62	121.14

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	2073	0	2015	1	0
1	B	2073	0	2015	3	0
1	G	2073	0	2015	7	0
1	J	2073	0	2014	5	0
2	C	1771	0	1716	0	0
2	E	1777	0	1720	2	0
2	H	1777	0	1720	1	0
2	K	1771	0	1716	2	0
3	D	1637	0	1602	3	0
3	F	1637	0	1602	2	0
3	I	1637	0	1602	3	0
3	L	1637	0	1602	12	0
4	G	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	14	0	13	0	0
All	All	21964	0	21365	41	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 1.

All (41) 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:27:GLN:O	3:L:69:THR:HG22	1.93	0.68
1:G:63:ASP:HA	1:G:93:ALA:HA	1.78	0.65
3:D:155:GLN:HE21	3:D:158:ASN:HD21	1.44	0.64
3:D:67:SER:HA	3:D:71:PHE:CZ	2.33	0.64
3:L:108:ARG:NE	3:L:109:THR:O	2.31	0.63
3:L:30:ARG:O	3:L:71:PHE:HZ	1.85	0.58
1:G:64:CYS:O	1:G:65:THR:O	2.23	0.57
1:B:184:HIS:HD1	1:B:216:ASN:H	1.55	0.54
1:G:64:CYS:O	1:G:65:THR:C	2.50	0.54
3:L:108:ARG:NH2	3:L:111:ALA:HB2	2.24	0.53
3:I:50:ASP:OD1	3:I:91:TYR:OH	2.22	0.52
3:I:33:LEU:HA	3:I:89:GLN:O	2.11	0.51
1:J:180:TRP:CE2	1:J:204:VAL:HG21	2.46	0.50
1:B:180:TRP:CE2	1:B:204:VAL:HG21	2.47	0.49
1:G:64:CYS:C	1:G:65:THR:O	2.56	0.49
2:E:184:VAL:HG11	2:E:194:TYR:CE2	2.47	0.49
3:L:108:ARG:HH21	3:L:110:VAL:C	2.21	0.48
3:F:21:LEU:HD22	3:F:73:LEU:HD23	1.96	0.47
1:G:266:SER:OG	1:G:267:ILE:N	2.47	0.47
3:D:21:LEU:HG	3:D:102:THR:HG21	1.96	0.46
1:G:62:ILE:H	1:G:62:ILE:HD12	1.81	0.46
3:L:150:VAL:HG13	3:L:192:TYR:CE1	2.50	0.45
3:F:21:LEU:HG	3:F:102:THR:HG21	1.98	0.45
2:H:131:THR:HA	2:H:135:THR:O	2.17	0.45
3:I:21:LEU:HG	3:I:102:THR:HG21	1.98	0.45
2:E:196:CYS:O	2:E:196:CYS:SG	2.75	0.44
2:K:159:LEU:HD21	2:K:182:VAL:HG21	1.99	0.44
1:J:102:VAL:HG22	1:J:232:ILE:HB	2.01	0.43
3:L:108:ARG:HH21	3:L:111:ALA:HB2	1.83	0.43
3:L:108:ARG:NH2	3:L:110:VAL:O	2.53	0.42
1:A:180:TRP:CD2	1:A:204:VAL:HG21	2.54	0.42
1:B:180:TRP:CD2	1:B:204:VAL:HG21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:12:VAL:HG21	2:K:82(C):LEU:HD13	2.02	0.41
3:L:46:LEU:HD11	3:L:49:TYR:HB3	2.02	0.41
3:L:48:ILE:HD13	3:L:54:LEU:HA	2.01	0.41
1:J:63:ASP:OD1	1:J:63:ASP:N	2.54	0.41
1:J:195:TYR:O	1:J:197:GLN:N	2.53	0.41
3:L:46:LEU:HD21	3:L:49:TYR:HB3	2.02	0.41
1:G:180:TRP:CE2	1:G:204:VAL:HG21	2.56	0.41
3:L:28:ASP:OD1	3:L:68:GLY:HA2	2.21	0.41
1:J:180:TRP:CD2	1:J:204:VAL:HG21	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	265/274 (97%)	251 (95%)	13 (5%)	1 (0%)	30	59
1	B	265/274 (97%)	252 (95%)	12 (4%)	1 (0%)	30	59
1	G	265/274 (97%)	251 (95%)	13 (5%)	1 (0%)	30	59
1	J	265/274 (97%)	254 (96%)	10 (4%)	1 (0%)	30	59
2	C	236/247 (96%)	227 (96%)	8 (3%)	1 (0%)	30	59
2	E	237/247 (96%)	228 (96%)	8 (3%)	1 (0%)	30	59
2	H	237/247 (96%)	226 (95%)	10 (4%)	1 (0%)	30	59
2	K	236/247 (96%)	228 (97%)	7 (3%)	1 (0%)	30	59
3	D	211/214 (99%)	202 (96%)	9 (4%)	0	100	100
3	F	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
3	I	211/214 (99%)	206 (98%)	5 (2%)	0	100	100
3	L	211/214 (99%)	205 (97%)	5 (2%)	1 (0%)	24	55
All	All	2850/2940 (97%)	2735 (96%)	106 (4%)	9 (0%)	36	66

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	65	THR
3	L	51	ALA
2	C	100(N)	ASP
2	K	100(N)	ASP
2	H	100(N)	ASP
1	A	62	ILE
2	E	100(N)	ASP
1	B	62	ILE
1	J	196	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/242 (98%)	233 (99%)	3 (1%)	61	73
1	B	236/242 (98%)	233 (99%)	3 (1%)	61	73
1	G	236/242 (98%)	231 (98%)	5 (2%)	47	66
1	J	236/242 (98%)	230 (98%)	6 (2%)	42	63
2	C	199/208 (96%)	194 (98%)	5 (2%)	42	63
2	E	200/208 (96%)	179 (90%)	21 (10%)	6	24
2	H	200/208 (96%)	181 (90%)	19 (10%)	8	28
2	K	199/208 (96%)	194 (98%)	5 (2%)	42	63
3	D	186/187 (100%)	180 (97%)	6 (3%)	34	58
3	F	186/187 (100%)	177 (95%)	9 (5%)	23	50
3	I	186/187 (100%)	182 (98%)	4 (2%)	45	65
3	L	186/187 (100%)	177 (95%)	9 (5%)	23	50
All	All	2486/2548 (98%)	2391 (96%)	95 (4%)	29	55

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	299	LYS
1	A	307	LYS
2	E	64	GLU
2	E	78	LEU
2	E	100	GLN
2	E	100(A)	VAL
2	E	100(B)	PRO
2	E	100(C)	SER
2	E	100(F)	TRP
2	E	100(G)	GLU
2	E	100(H)	ARG
2	E	100(I)	GLU
2	E	100(J)	ASP
2	E	100(K)	LEU
2	E	100(L)	VAL
2	E	100(N)	ASP
2	E	100(P)	PHE
2	E	115	SER
2	E	178	LEU
2	E	188	SER
2	E	193	THR
2	E	197	ASN
2	E	209	LYS
3	F	24	GLN
3	F	26	SER
3	F	67	SER
3	F	72	THR
3	F	114	SER
3	F	155	GLN
3	F	181	LEU
3	F	188	LYS
3	F	203	SER
1	B	53	ASN
1	B	299	LYS
1	B	307	LYS
2	C	78	LEU
2	C	97	SER
2	C	117	LYS
2	C	127	SER
2	C	193	THR
3	D	24	GLN
3	D	109	THR

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Mol	Chain	Res	Type
3	D	129	THR
3	D	145	LYS
3	D	154	LEU
3	D	181	LEU
1	J	53	ASN
1	J	62	ILE
1	J	63	ASP
1	J	195	TYR
1	J	205	SER
1	J	307	LYS
2	K	64	GLU
2	K	78	LEU
2	K	178	LEU
2	K	193	THR
2	K	199	ASN
3	L	24	GLN
3	L	27	GLN
3	L	31	LYS
3	L	67	SER
3	L	72	THR
3	L	108	ARG
3	L	109	THR
3	L	129	THR
3	L	145	LYS
2	H	64	GLU
2	H	78	LEU
2	H	97	SER
2	H	100	GLN
2	H	100(A)	VAL
2	H	100(B)	PRO
2	H	100(C)	SER
2	H	100(F)	TRP
2	H	100(G)	GLU
2	H	100(H)	ARG
2	H	100(I)	GLU
2	H	100(J)	ASP
2	H	100(K)	LEU
2	H	100(L)	VAL
2	H	100(N)	ASP
2	H	100(P)	PHE
2	H	193	THR
2	H	199	ASN

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Mol	Chain	Res	Type
2	H	209	LYS
3	I	37	GLN
3	I	109	THR
3	I	155	GLN
3	I	181	LEU
1	G	53	ASN
1	G	62	ILE
1	G	195	TYR
1	G	299	LYS
1	G	307	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	56	HIS
1	A	75	HIS
1	A	81	ASN
1	A	171	ASN
1	A	197	GLN
2	E	164	HIS
2	E	171	GLN
3	F	3	GLN
3	F	37	GLN
3	F	53	ASN
3	F	137	ASN
3	F	138	ASN
3	F	199	GLN
1	B	53	ASN
1	B	75	HIS
1	B	197	GLN
2	C	39	GLN
2	C	81	GLN
2	C	100	GLN
2	C	164	HIS
2	C	199	ASN
3	D	24	GLN
3	D	38	GLN
3	D	55	GLN
3	D	137	ASN
3	D	138	ASN
3	D	155	GLN

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Mol	Chain	Res	Type
1	J	44	GLN
1	J	53	ASN
1	J	75	HIS
1	J	189	GLN
1	J	197	GLN
1	J	211	GLN
2	K	164	HIS
2	K	199	ASN
3	L	24	GLN
3	L	27	GLN
3	L	34	ASN
3	L	55	GLN
3	L	137	ASN
3	L	138	ASN
3	L	199	GLN
2	H	81	GLN
2	H	164	HIS
3	I	37	GLN
3	I	55	GLN
3	I	138	ASN
3	I	147	GLN
3	I	155	GLN
3	I	199	GLN
1	G	53	ASN
1	G	54	ASN
1	G	56	HIS
1	G	81	ASN
1	G	210	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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	NAG	J	401	1	14,14,15	0.37	0	17,19,21	0.76	0
4	NAG	G	401	-	14,14,15	0.33	0	17,19,21	0.95	1 (5%)

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	NAG	J	401	1	-	2/6/23/26	0/1/1/1
4	NAG	G	401	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	401	NAG	O5-C1-C2	-2.68	107.14	111.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	401	NAG	C4-C5-C6-O6
4	J	401	NAG	O5-C5-C6-O6

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	A	267/274 (97%)	1.02	50 (18%) 3 3	86, 107, 149, 166	0
1	B	267/274 (97%)	0.87	37 (13%) 6 5	82, 103, 165, 180	0
1	G	267/274 (97%)	0.88	37 (13%) 6 5	84, 112, 141, 160	0
1	J	267/274 (97%)	0.91	37 (13%) 6 5	90, 105, 147, 184	0
2	C	238/247 (96%)	0.98	32 (13%) 7 6	103, 124, 160, 173	0
2	E	238/247 (96%)	0.89	25 (10%) 11 9	57, 107, 132, 165	1 (0%)
2	H	238/247 (96%)	0.88	24 (10%) 12 10	58, 111, 140, 157	1 (0%)
2	K	238/247 (96%)	1.17	42 (17%) 4 3	105, 129, 166, 199	0
3	D	213/214 (99%)	1.05	32 (15%) 5 5	109, 126, 183, 249	0
3	F	213/214 (99%)	0.86	22 (10%) 12 10	86, 101, 116, 136	0
3	I	213/214 (99%)	0.70	16 (7%) 20 15	89, 99, 111, 123	0
3	L	213/214 (99%)	0.96	33 (15%) 5 4	120, 134, 184, 211	0
All	All	2872/2940 (97%)	0.93	387 (13%) 7 6	57, 111, 157, 249	2 (0%)

All (387) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	116	PHE	12.9
2	H	91	TYR	10.2
3	D	114	SER	10.1
2	K	74	SER	9.4
1	A	205	SER	9.3
1	A	60	ASP	7.9
2	K	100(C)	SER	7.8
2	C	132	SER	7.3
3	D	135	LEU	7.2
1	A	189	GLN	7.0
3	D	137	ASN	6.8

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Mol	Chain	Res	Type	RSRZ
3	F	150	VAL	6.7
1	J	155	THR	6.6
1	B	189	GLN	6.6
1	J	145	SER	6.4
1	J	190	GLU	6.1
3	F	151	ASP	6.1
2	E	100	GLN	6.0
1	J	98	TYR	6.0
1	A	246	ASN	5.9
1	B	193	SER	5.9
1	A	92	LYS	5.8
1	J	131	THR	5.7
3	I	42	LYS	5.7
3	L	94	LEU	5.5
2	K	166	PHE	5.4
1	A	59	LEU	5.4
3	L	134	CYS	5.3
3	I	152	ASN	5.3
2	E	41	PRO	5.3
3	D	115	VAL	5.2
2	C	148	GLU	5.1
2	K	203	SER	5.1
1	A	62	ILE	5.1
2	K	122	PHE	5.1
3	F	100	GLY	5.1
1	A	94	PHE	5.0
3	F	137	ASN	5.0
1	A	51	ILE	4.9
2	K	100(B)	PRO	4.9
1	G	56	HIS	4.9
1	G	78	VAL	4.8
2	K	100(D)	ALA	4.8
2	K	168	ALA	4.7
1	B	59	LEU	4.7
2	H	89	VAL	4.6
1	G	85	ASP	4.6
1	B	293	PRO	4.6
1	J	175	ASP	4.6
3	F	178	THR	4.6
2	E	42	GLY	4.6
1	J	56	HIS	4.6
1	A	169	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
2	K	123	PRO	4.4
3	L	194	CYS	4.4
1	B	65	THR	4.3
1	J	108	LEU	4.3
3	D	133	VAL	4.3
2	K	161	SER	4.3
2	H	187	SER	4.3
1	A	247	SER	4.3
3	I	72	THR	4.2
2	C	10	GLY	4.2
2	H	100(C)	SER	4.2
3	I	38	GLN	4.2
1	B	162	PRO	4.2
3	L	116	PHE	4.1
1	A	293	PRO	4.1
2	K	167	PRO	4.1
3	D	117	ILE	4.1
2	H	36	TRP	4.1
2	K	69	ILE	4.0
1	B	77	ASP	4.0
1	J	122	THR	4.0
3	D	154	LEU	4.0
1	J	260	MET	4.0
1	A	193	SER	4.0
2	C	137	ALA	3.9
1	A	61	GLY	3.9
3	D	118	PHE	3.9
2	C	98	MET	3.8
3	F	181	LEU	3.8
1	G	253	ALA	3.8
1	A	179	ILE	3.8
2	K	51	ILE	3.8
1	A	88	VAL	3.8
2	C	147	PRO	3.8
3	F	41	GLY	3.7
2	K	141	LEU	3.7
3	F	209	PHE	3.7
2	C	163	VAL	3.7
2	K	152	VAL	3.7
2	H	198	VAL	3.7
1	G	127	TRP	3.7
1	J	152	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
2	C	9	GLY	3.7
3	F	135	LEU	3.7
2	C	131	THR	3.6
2	H	166	PHE	3.6
3	L	15	VAL	3.6
2	H	191	THR	3.6
3	D	181	LEU	3.6
1	B	254	PRO	3.6
2	K	34	VAL	3.6
1	B	79	PHE	3.5
1	J	53	ASN	3.5
2	C	27(B)	PHE	3.5
1	G	227	SER	3.5
2	K	189	LEU	3.5
1	B	178	TYR	3.5
3	I	43	GLY	3.5
2	C	126	PRO	3.5
3	L	21	LEU	3.5
3	L	197	THR	3.4
1	G	260	MET	3.4
1	A	68	ASP	3.4
3	F	138	ASN	3.4
1	A	90	ARG	3.4
1	J	262	THR	3.4
3	D	85	THR	3.4
2	C	179	SER	3.3
2	E	86	ASP	3.3
2	C	24	GLY	3.3
3	L	105	VAL	3.3
2	K	80	LEU	3.3
1	B	304	ALA	3.2
1	B	68	ASP	3.2
1	J	61	GLY	3.2
3	L	154	LEU	3.2
2	E	100(B)	PRO	3.2
2	H	31	TYR	3.2
1	B	232	ILE	3.2
2	C	201	LYS	3.2
1	G	82	GLU	3.2
2	H	39	GLN	3.2
1	J	63	ASP	3.1
1	J	205	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	48	THR	3.1
3	I	19	VAL	3.1
1	A	248	ASN	3.1
3	L	119	PRO	3.1
1	A	112	VAL	3.1
2	K	165	THR	3.1
3	D	206	THR	3.1
2	K	2	VAL	3.1
3	L	1	ASP	3.1
1	B	236	ILE	3.1
3	D	193	ALA	3.0
3	L	160	GLN	3.0
2	K	100(E)	GLY	3.0
1	G	265	SER	3.0
3	I	148	TRP	3.0
1	B	253	ALA	3.0
2	E	78	LEU	3.0
1	J	211	GLN	3.0
2	H	127	SER	3.0
1	A	75	HIS	3.0
1	J	194	LEU	3.0
2	E	186	SER	3.0
1	B	78	VAL	3.0
3	L	37	GLN	3.0
2	K	138	LEU	3.0
2	E	54	GLY	3.0
1	A	168	MET	3.0
2	H	189	LEU	2.9
1	G	156	LYS	2.9
1	B	309	VAL	2.9
2	C	30	SER	2.9
1	A	203	THR	2.9
3	L	152	ASN	2.9
1	J	103	PRO	2.9
1	A	66	LEU	2.9
2	H	76	GLU	2.9
3	F	193	ALA	2.9
1	A	63	ASP	2.9
3	L	122	ASP	2.9
1	B	117	THR	2.9
1	G	83	THR	2.9
3	D	178	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	144	GLY	2.9
2	C	149	PRO	2.8
2	H	35	SER	2.8
1	B	235	THR	2.8
2	C	151	THR	2.8
1	J	151	LEU	2.8
2	E	69	ILE	2.8
1	B	69	ALA	2.8
1	J	156	LYS	2.8
2	C	100(J)	ASP	2.8
3	D	38	GLN	2.8
2	H	142	VAL	2.8
1	B	177	LEU	2.8
1	G	66	LEU	2.8
3	D	77	SER	2.8
1	G	131	THR	2.8
1	A	244	VAL	2.7
3	D	150	VAL	2.7
1	B	239	PRO	2.7
2	K	55	GLY	2.7
1	A	172	ASP	2.7
1	G	118	LEU	2.7
1	G	179	ILE	2.7
1	A	251	LEU	2.7
3	D	179	LEU	2.7
1	A	142	GLY	2.7
3	D	23	CYS	2.7
1	G	159	SER	2.7
3	L	114	SER	2.7
1	B	118	LEU	2.7
2	E	190	GLY	2.6
1	A	71	LEU	2.6
2	C	23	VAL	2.6
2	H	207	VAL	2.6
2	E	98	MET	2.6
3	I	142	ARG	2.6
1	A	212	THR	2.6
2	C	100	GLN	2.6
3	F	123	GLU	2.6
1	G	251	LEU	2.6
2	E	52(A)	ALA	2.6
2	K	28	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	97	CYS	2.6
1	B	291	ASP	2.6
1	G	275	ASP	2.6
1	A	108	LEU	2.6
2	K	124	LEU	2.6
2	E	34	VAL	2.6
2	C	100(A)	VAL	2.6
3	D	19	VAL	2.6
1	J	47	SER	2.5
2	K	73	ASN	2.5
2	K	31	TYR	2.5
1	B	111	LEU	2.5
1	B	60	ASP	2.5
2	K	126	PRO	2.5
2	K	54	GLY	2.5
2	H	190	GLY	2.5
1	A	266	SER	2.5
3	F	182	SER	2.5
1	J	104	ASP	2.5
1	A	87	PHE	2.5
1	J	48	THR	2.5
3	I	102	THR	2.5
2	E	29	LEU	2.5
1	J	159	SER	2.5
1	G	60	ASP	2.5
1	G	160	THR	2.5
1	B	56	HIS	2.5
2	C	13	GLN	2.5
3	D	208	SER	2.4
2	H	46	GLU	2.4
2	E	71	ARG	2.4
1	B	226	LEU	2.4
3	L	125	LEU	2.4
2	K	158	ALA	2.4
2	C	203	SER	2.4
1	G	233	TYR	2.4
3	I	104	VAL	2.4
1	A	177	LEU	2.4
2	C	100(B)	PRO	2.4
2	K	26	GLY	2.4
1	J	267	ILE	2.4
1	G	153	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	78	VAL	2.4
2	C	107	THR	2.4
2	K	163	VAL	2.4
1	A	56	HIS	2.4
3	L	93	GLY	2.4
2	E	2	VAL	2.4
2	K	33	ALA	2.3
3	D	138	ASN	2.3
3	L	106	ILE	2.3
1	G	63	ASP	2.3
3	F	96	PHE	2.3
2	E	142	VAL	2.3
3	L	83	VAL	2.3
2	E	116	THR	2.3
3	L	57	GLY	2.3
2	K	194	TYR	2.3
3	I	154	LEU	2.3
2	H	105	GLN	2.3
2	K	100(A)	VAL	2.3
3	F	133	VAL	2.3
1	G	62	ILE	2.3
2	K	30	SER	2.3
2	K	180	SER	2.3
2	H	188	SER	2.3
3	F	117	ILE	2.3
1	J	118	LEU	2.3
1	G	112	VAL	2.3
2	C	69	ILE	2.3
2	K	57	ILE	2.3
3	F	113	PRO	2.3
1	A	95	SER	2.3
1	A	167	THR	2.3
2	K	193	THR	2.3
1	J	71	LEU	2.3
1	J	183	HIS	2.3
1	G	226	LEU	2.3
2	H	146	PHE	2.3
3	F	98	PHE	2.3
3	I	151	ASP	2.3
2	E	212	GLU	2.3
3	L	2	ILE	2.3
3	D	84	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	175	LEU	2.3
1	G	205	SER	2.3
2	C	97	SER	2.3
2	C	122	PHE	2.3
3	D	202	SER	2.3
2	K	76	GLU	2.2
2	C	48	LEU	2.2
3	L	96	PHE	2.2
1	J	186	SER	2.2
3	F	12	SER	2.2
2	E	111	VAL	2.2
3	L	137	ASN	2.2
3	I	55	GLN	2.2
1	A	232	ILE	2.2
2	E	51	ILE	2.2
3	L	84	GLY	2.2
1	J	79	PHE	2.2
1	G	307	LYS	2.2
2	H	27(A)	SER	2.2
3	F	171	SER	2.2
1	B	58	ILE	2.2
1	B	164	LEU	2.2
2	H	154	TRP	2.2
1	J	244	VAL	2.2
3	L	115	VAL	2.2
1	B	266	SER	2.2
3	D	113	PRO	2.2
3	L	80	PRO	2.2
1	J	153	TRP	2.2
1	A	262	THR	2.2
2	H	165	THR	2.2
1	G	98	TYR	2.2
1	G	100	TYR	2.2
1	G	252	ILE	2.2
1	A	271	ASP	2.2
2	E	110	THR	2.1
1	A	67	ILE	2.1
1	G	111	LEU	2.1
3	L	11	LEU	2.1
1	B	260	MET	2.1
2	E	97	SER	2.1
3	D	190	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	L	9	SER	2.1
1	B	61	GLY	2.1
2	E	73	ASN	2.1
2	E	119	PRO	2.1
3	L	113	PRO	2.1
3	D	151	ASP	2.1
1	A	143	PRO	2.1
3	D	204	PRO	2.1
2	K	23	VAL	2.1
1	B	203	THR	2.1
3	D	192	TYR	2.1
1	A	294	PHE	2.1
3	F	118	PHE	2.1
1	J	69	ALA	2.1
3	D	191	VAL	2.1
2	K	155	ASN	2.1
3	L	103	LYS	2.1
1	J	85	ASP	2.1
1	G	155	THR	2.1
1	G	161	TYR	2.1
1	G	303	GLY	2.1
3	D	37	GLN	2.1
3	I	44	PRO	2.1
1	J	112	VAL	2.0
1	A	70	LEU	2.0
1	B	214	ILE	2.0
3	L	164	THR	2.0
3	F	141	PRO	2.0
1	B	91	SER	2.0
3	I	131	SER	2.0
1	A	48	THR	2.0
1	A	128	THR	2.0
2	C	33	ALA	2.0
3	I	86	TYR	2.0
1	G	79	PHE	2.0
3	D	57	GLY	2.0
1	A	163	VAL	2.0
3	L	104	VAL	2.0
1	J	154	LEU	2.0
2	C	159	LEU	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	NAG	G	401	14/15	0.77	0.09	110,110,110,110	0
4	NAG	J	401	14/15	0.81	0.11	77,78,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.