



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:03 AM UTC

PDB ID : 5WLG / pdb_00005wlg
Title : Crystal Structure of H-2Db with the GAP501 peptide (SQL)
Authors : Gras, S.; Farenc, C.; Josephs, T.; Rossjohn, J.
Deposited on : 2017-07-26
Resolution : 2.10 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:

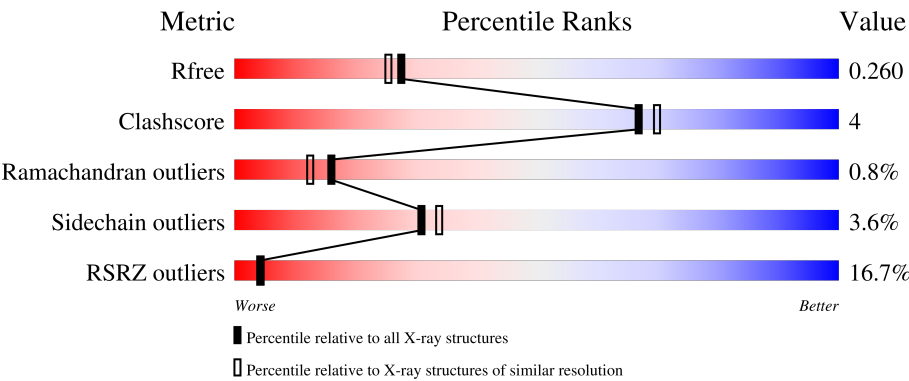
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	278	5% 87% 12% .
1	F	278	20% 82% 14% .
2	B	99	2% 95% . .
2	G	99	14% 88% 7% . . .
3	C	9	100%

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Mol	Chain	Length	Quality of chain
3	H	9	78% 11% 11%
4	D	182	8% 85% 13% ..
4	I	182	23% 82% 13% ...
5	E	243	22% 90% 9%
5	J	243	31% 91% 8% .

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 13901 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	1	0
			2290	1446	406	429	9			
1	F	277	Total	C	N	O	S	0	0	0
			2271	1435	401	426	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			810	517	137	149	7			
2	G	98	Total	C	N	O	S	0	0	0
			810	517	137	149	7			

- Molecule 3 is a protein called GAP50 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			74	48	12	14			
3	H	9	Total	C	N	O	0	0	0
			74	48	12	14			

- Molecule 4 is a protein called T cell receptor alpha variable 8D-2,Human nkt tcr alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	182	Total	C	N	O	S	0	2	0
			1431	879	249	293	10			
4	I	177	Total	C	N	O	S	0	2	0
			1386	851	242	283	10			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	91	VAL	-	linker	UNP A0A075B616
D	92	TYR	-	linker	UNP A0A075B616
D	93	ALA	-	linker	UNP A0A075B616
D	94	GLN	-	linker	UNP A0A075B616
D	95	GLY	-	linker	UNP A0A075B616
D	96	LEU	-	linker	UNP A0A075B616
D	97	THR	-	linker	UNP A0A075B616
D	98	PHE	-	linker	UNP A0A075B616
D	99	GLY	-	linker	UNP A0A075B616
D	100	LEU	-	linker	UNP A0A075B616
D	101	GLY	-	linker	UNP A0A075B616
D	102	THR	-	linker	UNP A0A075B616
D	103	ARG	-	linker	UNP A0A075B616
D	104	VAL	-	linker	UNP A0A075B616
D	105	SER	-	linker	UNP A0A075B616
D	106	VAL	-	linker	UNP A0A075B616
D	107	PHE	-	linker	UNP A0A075B616
D	108	PRO	-	linker	UNP A0A075B616
D	109	ASN	-	linker	UNP A0A075B616
I	92	VAL	-	linker	UNP A0A075B616
I	93	TYR	-	linker	UNP A0A075B616
I	94	ALA	-	linker	UNP A0A075B616
I	95	GLN	-	linker	UNP A0A075B616
I	96	GLY	-	linker	UNP A0A075B616
I	97	LEU	-	linker	UNP A0A075B616
I	98	THR	-	linker	UNP A0A075B616
I	99	PHE	-	linker	UNP A0A075B616
I	100	GLY	-	linker	UNP A0A075B616
I	101	LEU	-	linker	UNP A0A075B616
I	102	GLY	-	linker	UNP A0A075B616
I	103	THR	-	linker	UNP A0A075B616
I	104	ARG	-	linker	UNP A0A075B616
I	105	VAL	-	linker	UNP A0A075B616
I	106	SER	-	linker	UNP A0A075B616
I	107	VAL	-	linker	UNP A0A075B616
I	108	PHE	-	linker	UNP A0A075B616
I	109	PRO	-	linker	UNP A0A075B616
I	110	ASN	-	linker	UNP A0A075B616

- Molecule 5 is a protein called T-cell receptor beta chain V region C5,Human nkt tcr beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	243	Total 1933	C 1215	N 333	O 378	S 7	0	1	0
5	J	241	Total 1928	C 1212	N 333	O 376	S 7	0	2	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	95	ASP	GLY	conflict	UNP P04213
E	96	TRP	THR	conflict	UNP P04213
E	?	-	GLY	deletion	UNP P04213
E	?	-	ALA	deletion	UNP P04213
E	?	-	LEU	deletion	UNP P04213
E	100	GLY	-	insertion	UNP P04213
E	102	LEU	-	insertion	UNP P04213
E	106	GLU	PRO	conflict	UNP P04213
E	108	SER	THR	conflict	UNP P04213
E	109	LYS	ARG	conflict	UNP P04213
E	111	THR	LEU	conflict	UNP P04213
J	95	ASP	GLY	conflict	UNP P04213
J	96	TRP	THR	conflict	UNP P04213
J	?	-	GLY	deletion	UNP P04213
J	?	-	ALA	deletion	UNP P04213
J	?	-	LEU	deletion	UNP P04213
J	100	GLY	-	insertion	UNP P04213
J	102	LEU	-	insertion	UNP P04213
J	106	GLU	PRO	conflict	UNP P04213
J	108	SER	THR	conflict	UNP P04213
J	109	LYS	ARG	conflict	UNP P04213
J	111	THR	LEU	conflict	UNP P04213

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Na 1	0	0
6	G	1	Total 1	Na 1	0	0
6	I	1	Total 1	Na 1	0	0

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0

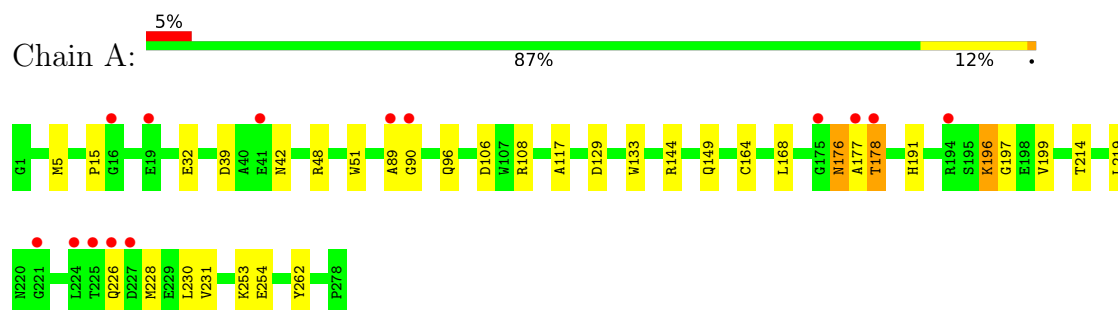
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	215	Total O 215 215	0	0
8	B	97	Total O 97 97	0	0
8	C	1	Total O 1 1	0	0
8	D	97	Total O 97 97	0	0
8	E	120	Total O 120 120	0	0
8	F	139	Total O 139 139	0	0
8	G	47	Total O 47 47	0	0
8	H	1	Total O 1 1	0	0
8	I	66	Total O 66 66	0	0
8	J	107	Total O 107 107	0	0

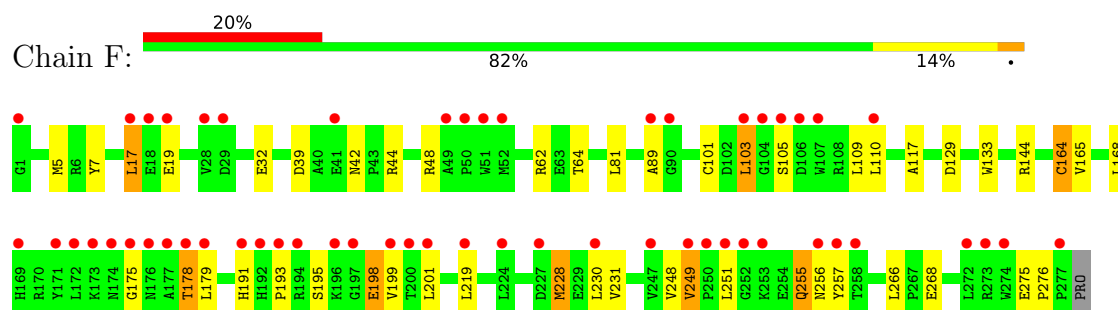
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

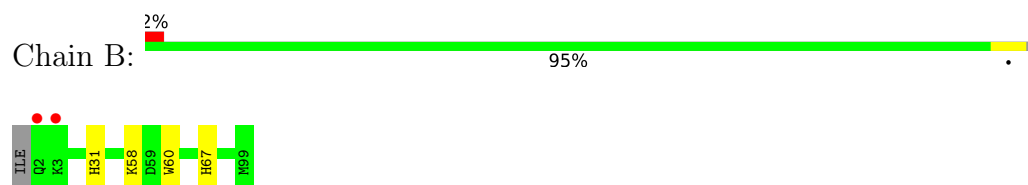
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



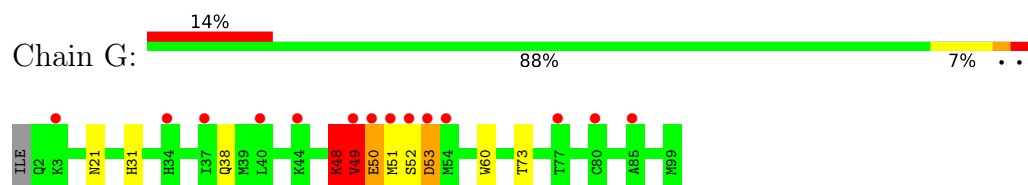
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: GAP50 peptide

Chain C:  100%

There are no outlier residues recorded for this chain.

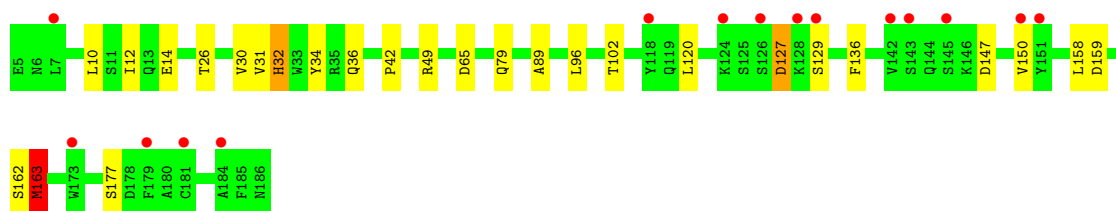
- Molecule 3: GAP50 peptide

Chain H:  78% 11% 11%



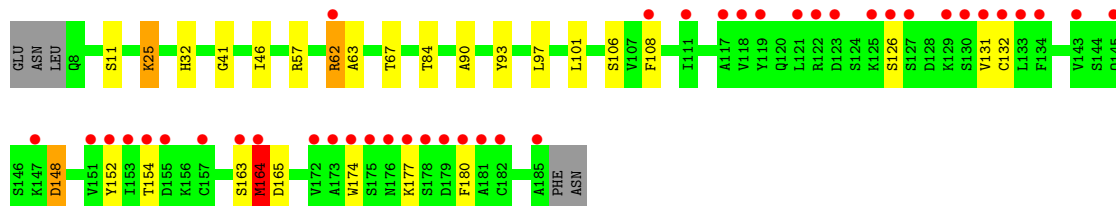
- Molecule 4: T cell receptor alpha variable 8D-2,Human nkt tcr alpha chain

Chain D:  8% 85% 13% ..



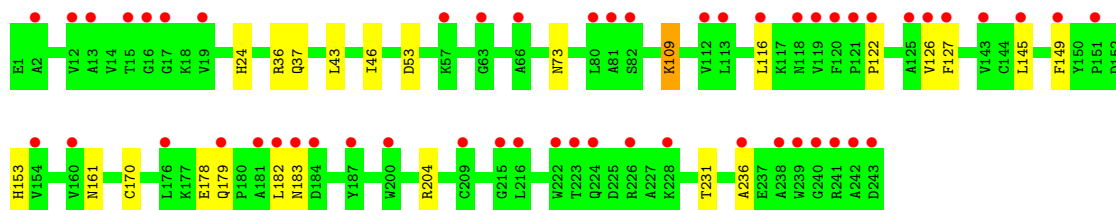
- Molecule 4: T cell receptor alpha variable 8D-2,Human nkt tcr alpha chain

Chain I:  23% 82% 13% ...



- Molecule 5: T-cell receptor beta chain V region C5,Human nkt tcr beta chain

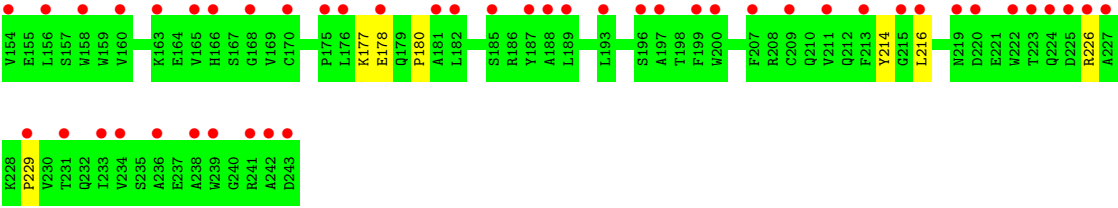
Chain E:  22% 90% 9%



- Molecule 5: T-cell receptor beta chain V region C5,Human nkt tcr beta chain

Chain J:  31% 91% 8%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	115.73Å 70.21Å 116.49Å 90.00° 108.28° 90.00°	Depositor
Resolution (Å)	47.05 – 2.10 47.05 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.05-2.10) 99.9 (47.05-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.218 , 0.249 0.227 , 0.260	Depositor DCC
R_{free} test set	5105 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.769	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13901	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: NA, CL

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	0.69	1/2359 (0.0%)	1.20	8/3204 (0.2%)
1	F	0.70	0/2339	1.24	12/3178 (0.4%)
2	B	0.70	0/836	1.05	0/1133
2	G	0.70	0/836	1.14	3/1133 (0.3%)
3	C	0.70	0/74	1.11	0/97
3	H	0.75	0/74	1.41	3/97 (3.1%)
4	D	0.70	0/1454	1.16	5/1967 (0.3%)
4	I	0.69	0/1408	1.18	6/1906 (0.3%)
5	E	0.65	0/1986	1.12	2/2705 (0.1%)
5	J	0.67	0/1981	1.12	1/2698 (0.0%)
All	All	0.68	1/13347 (0.0%)	1.17	40/18118 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	LYS	CA-C	6.76	1.59	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ALA	N-CA-C	-9.08	98.54	110.53
1	A	89	ALA	N-CA-C	-8.39	99.45	110.53
1	F	89	ALA	N-CA-C	-8.02	99.94	110.53
1	A	176	ASN	CA-CB-CG	7.70	120.30	112.60
1	F	276	PRO	N-CA-C	7.69	120.08	110.70
1	A	254	GLU	N-CA-C	-7.02	101.78	110.41
4	I	25	LYS	CA-C-N	6.48	133.37	121.70
4	I	25	LYS	C-N-CA	6.48	133.37	121.70
5	E	231	THR	CB-CA-C	6.41	120.14	109.89
4	I	148	ASP	CA-C-N	6.15	128.84	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	148	ASP	C-N-CA	6.15	128.84	120.54
1	A	219	LEU	N-CA-C	-6.08	105.77	113.43
1	F	248	VAL	N-CA-CB	6.06	118.31	111.21
1	F	129	ASP	CA-CB-CG	5.66	118.26	112.60
4	I	164	MET	CA-C-N	5.65	132.32	121.54
4	I	164	MET	C-N-CA	5.65	132.32	121.54
1	F	256	ASN	CA-CB-CG	5.62	118.22	112.60
5	J	42	GLY	N-CA-C	-5.60	103.84	112.85
3	H	2	GLN	N-CA-C	5.56	117.72	110.43
4	D	159	ASP	CA-CB-CG	5.55	118.15	112.60
1	F	164	CYS	CA-C-N	5.37	127.82	120.46
1	F	164	CYS	C-N-CA	5.37	127.82	120.46
1	F	249	VAL	N-CA-CB	-5.32	103.77	111.21
1	F	266	LEU	N-CA-C	5.29	116.31	109.65
1	A	129	ASP	CA-CB-CG	5.28	117.88	112.60
4	D	136	PHE	CA-C-N	5.22	128.63	120.75
4	D	136	PHE	C-N-CA	5.22	128.63	120.75
2	G	48	LYS	CA-C-N	5.18	131.03	121.70
2	G	48	LYS	C-N-CA	5.18	131.03	121.70
1	F	228	MET	N-CA-C	5.17	117.80	110.10
4	D	32	HIS	CA-CB-CG	5.16	118.96	113.80
4	D	31	VAL	N-CA-CB	5.15	118.82	111.82
2	G	21	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	164	CYS	CA-C-N	5.09	127.43	120.46
1	A	164	CYS	C-N-CA	5.09	127.43	120.46
5	E	178	GLU	N-CA-C	-5.08	101.47	109.25
1	F	81	LEU	CA-C-N	5.08	127.33	120.38
1	F	81	LEU	C-N-CA	5.08	127.33	120.38
3	H	1	SER	CA-C-N	5.02	129.35	120.87
3	H	1	SER	C-N-CA	5.02	129.35	120.87

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	2290	0	2162	17	0
1	F	2271	0	2145	21	0
2	B	810	0	783	4	0
2	G	810	0	783	8	0
3	C	74	0	81	0	0
3	H	74	0	81	2	0
4	D	1431	0	1368	13	0
4	I	1386	0	1330	15	0
5	E	1933	0	1817	12	0
5	J	1928	0	1812	13	0
6	A	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
7	A	1	0	0	0	0
8	A	215	0	0	1	0
8	B	97	0	0	2	0
8	C	1	0	0	0	0
8	D	97	0	0	0	0
8	E	120	0	0	0	0
8	F	139	0	0	1	0
8	G	47	0	0	1	0
8	H	1	0	0	0	0
8	I	66	0	0	0	0
8	J	107	0	0	0	0
All	All	13901	0	12362	92	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 4.

All (92) 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:G:48:LYS:HA	2:G:49:VAL:HG12	1.18	1.10
2:G:48:LYS:HA	2:G:49:VAL:CG1	2.00	0.91
1:A:196:LYS:HB3	1:A:197:GLY:HA3	1.54	0.90
1:F:103:LEU:HD11	1:F:165:VAL:HG22	1.52	0.90
1:A:196:LYS:CB	1:A:197:GLY:HA3	2.07	0.83
1:F:193:PRO:HA	1:F:199:VAL:HG23	1.66	0.76
1:F:103:LEU:HD13	1:F:168:LEU:HD23	1.69	0.75
4:D:36:GLN:HE22	5:E:37:GLN:HE22	1.35	0.74
1:F:32:GLU:OE2	1:F:48:ARG:HD2	1.91	0.70
5:E:24:HIS:HD2	5:E:73:ASN:HD21	1.39	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:MET:HE3	1:F:230:LEU:HD13	1.77	0.67
1:A:32:GLU:OE2	1:A:48:ARG:HD2	1.96	0.66
1:F:175:GLY:O	1:F:179:LEU:HD12	1.96	0.64
1:A:144:ARG:HD2	8:A:492:HOH:O	1.99	0.63
4:D:158:LEU:HB3	5:E:170[B]:CYS:HB2	1.81	0.63
5:E:36:ARG:HB2	5:E:46:ILE:HD11	1.81	0.62
4:I:90:ALA:HB1	4:I:97:LEU:HD22	1.82	0.62
4:D:30:VAL:HG12	4:D:49[B]:ARG:HG2	1.82	0.62
2:B:31:HIS:HD2	8:B:170:HOH:O	1.81	0.62
2:B:67:HIS:HD2	8:B:181:HOH:O	1.84	0.59
4:I:97:LEU:HG	5:J:98:ASP:HB3	1.85	0.58
5:J:24:HIS:HD2	5:J:73:ASN:HD21	1.49	0.58
1:F:103:LEU:HD21	1:F:165:VAL:HG13	1.86	0.58
1:A:228:MET:HE3	1:A:230:LEU:HD13	1.87	0.56
5:E:24:HIS:HD2	5:E:73:ASN:ND2	2.04	0.56
4:D:162:SER:O	4:D:163:MET:HB2	2.06	0.56
1:A:196:LYS:CB	1:A:197:GLY:CA	2.82	0.55
5:E:179:GLN:HB3	5:E:182:LEU:HD13	1.88	0.54
2:G:49:VAL:O	2:G:49:VAL:HG13	2.07	0.54
1:F:103:LEU:CD1	1:F:165:VAL:HG22	2.34	0.54
4:D:42:PRO:HG2	5:E:43:LEU:HD11	1.90	0.54
1:A:15:PRO:HB3	1:A:90:GLY:HA2	1.90	0.53
1:F:201:LEU:HD22	1:F:249:VAL:HG21	1.89	0.53
1:A:191:HIS:NE2	1:A:199:VAL:HG21	2.24	0.53
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.44	0.52
2:G:50:GLU:O	2:G:50:GLU:HG3	2.08	0.52
5:J:153:HIS:HB3	5:J:214:TYR:HB2	1.92	0.52
1:A:191:HIS:CE1	1:A:199:VAL:HG21	2.45	0.51
4:I:46:ILE:HG21	4:I:63:ALA:CB	2.40	0.51
1:A:96:GLN:OE1	2:B:31:HIS:HE1	1.92	0.51
5:E:122:PRO:HB3	5:E:149:PHE:HB3	1.91	0.51
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.92	0.51
1:F:44:ARG:HG3	1:F:64:THR:OG1	2.11	0.50
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.47	0.50
5:J:24:HIS:HD2	5:J:73:ASN:ND2	2.09	0.50
1:F:7:TYR:CD2	3:H:2:GLN:HG3	2.48	0.49
5:J:177:LYS:HD3	5:J:180:PRO:HA	1.96	0.48
2:G:48:LYS:HA	2:G:49:VAL:CB	2.44	0.48
1:A:106:ASP:OD2	1:A:108[A]:ARG:HD3	2.14	0.48
1:F:5:MET:HB2	1:F:168:LEU:HD13	1.95	0.47
5:J:119:VAL:HG12	5:J:229:PRO:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:198:GLU:HB2	1:F:249:VAL:O	2.15	0.47
8:F:333:HOH:O	3:H:2:GLN:HG2	2.14	0.46
4:I:177:LYS:HB2	4:I:180:PHE:HB2	1.97	0.46
4:I:46:ILE:HG21	4:I:63:ALA:HB3	1.98	0.46
4:I:57:ARG:HG2	4:I:62:ARG:HG3	1.97	0.46
1:F:255:GLN:H	1:F:255:GLN:HG3	1.53	0.46
4:D:120:LEU:HB3	5:E:127:PHE:HB3	1.97	0.46
4:I:131:VAL:HG12	4:I:174:TRP:HB3	1.97	0.46
4:D:32:HIS:HD2	4:D:34:TYR:OH	1.97	0.45
2:G:31:HIS:HD2	8:G:244:HOH:O	1.98	0.45
5:J:121:PRO:HD3	5:J:229:PRO:HB3	1.98	0.45
4:D:14:GLU:HG3	4:D:79:GLN:HA	1.99	0.45
4:D:32:HIS:HB2	4:D:89:ALA:HB3	1.98	0.45
5:J:116:LEU:HG	5:J:216:LEU:HD21	1.99	0.45
1:F:191:HIS:CE1	1:F:199:VAL:HG21	2.52	0.44
1:A:196:LYS:HB2	1:A:197:GLY:HA3	1.94	0.44
4:I:11:SER:HB3	4:I:108:PHE:HE2	1.82	0.44
4:D:10:LEU:HD12	4:D:102:THR:HG21	1.99	0.43
4:I:152:TYR:HE1	5:J:178:GLU:HA	1.82	0.43
5:J:10:SER:OG	5:J:153:HIS:HD2	2.02	0.43
1:F:62:ARG:HD2	4:I:93:TYR:O	2.19	0.43
1:F:101:CYS:CB	1:F:164:CYS:HG	2.26	0.43
1:F:219:LEU:HD13	1:F:257:TYR:CZ	2.54	0.43
5:J:111:THR:OG1	5:J:153:HIS:HE1	2.02	0.43
4:I:32:HIS:HB2	4:I:90:ALA:HB3	2.02	0.42
1:A:133:TRP:HB2	1:A:144:ARG:HG3	2.01	0.42
5:E:24:HIS:CD2	5:E:73:ASN:HD21	2.28	0.42
4:D:147:ASP:HA	4:I:164:MET:HE2	2.02	0.41
1:F:133:TRP:HB2	1:F:144:ARG:HG3	2.02	0.41
4:D:96:LEU:C	4:D:96:LEU:HD12	2.45	0.41
4:I:41:GLY:HA2	5:J:90:PHE:CE1	2.55	0.41
5:E:109:LYS:HD3	5:E:153:HIS:CD2	2.54	0.41
4:D:147:ASP:HB3	4:D:150:VAL:HB	2.02	0.41
2:G:52:SER:O	2:G:53:ASP:HB2	2.21	0.41
1:F:101:CYS:HB2	1:F:109:LEU:CD1	2.50	0.41
5:J:68:ARG:HD2	5:J:73:ASN:O	2.21	0.41
4:I:163:SER:HA	4:I:164:MET:HA	1.77	0.41
1:A:51:TRP:HD1	1:A:178:THR:HG21	1.85	0.40
4:I:84:THR:HG23	4:I:106:SER:HA	2.03	0.40
1:A:214:THR:HB	1:A:262:TYR:HB2	2.03	0.40
5:E:126:VAL:HG23	5:E:236:ALA:HB3	2.02	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	277/278 (100%)	262 (95%)	13 (5%)	2 (1%)	18	15
1	F	275/278 (99%)	261 (95%)	11 (4%)	3 (1%)	11	8
2	B	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
2	G	96/99 (97%)	91 (95%)	3 (3%)	2 (2%)	5	2
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	H	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	182/182 (100%)	174 (96%)	5 (3%)	3 (2%)	7	4
4	I	177/182 (97%)	169 (96%)	6 (3%)	2 (1%)	11	8
5	E	242/243 (100%)	236 (98%)	5 (2%)	1 (0%)	30	28
5	J	241/243 (99%)	233 (97%)	8 (3%)	0	100	100
All	All	1600/1622 (99%)	1532 (96%)	55 (3%)	13 (1%)	16	12

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	163	MET
1	F	178	THR
2	G	53	ASP
1	A	176	ASN
2	G	49	VAL
4	I	165	ASP
1	F	195	SER
1	A	226	GLN
4	D	26	THR
4	D	127	ASP
5	E	161	ASN
1	F	17	LEU

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Mol	Chain	Res	Type
4	I	126	SER

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	237/236 (100%)	231 (98%)	6 (2%)	42	48
1	F	235/236 (100%)	221 (94%)	14 (6%)	17	15
2	B	92/93 (99%)	91 (99%)	1 (1%)	65	74
2	G	92/93 (99%)	86 (94%)	6 (6%)	15	13
3	C	8/8 (100%)	8 (100%)	0	100	100
3	H	8/8 (100%)	8 (100%)	0	100	100
4	D	163/161 (101%)	157 (96%)	6 (4%)	30	33
4	I	158/161 (98%)	150 (95%)	8 (5%)	21	21
5	E	210/209 (100%)	204 (97%)	6 (3%)	37	42
5	J	210/209 (100%)	207 (99%)	3 (1%)	59	67
All	All	1413/1414 (100%)	1363 (96%)	50 (4%)	31	35

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	42	ASN
1	A	149	GLN
1	A	178	THR
1	A	231	VAL
1	A	253	LYS
2	B	58	LYS
4	D	12	ILE
4	D	65	ASP
4	D	127	ASP
4	D	129	SER
4	D	163	MET

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Mol	Chain	Res	Type
4	D	177	SER
5	E	53	ASP
5	E	109	LYS
5	E	116	LEU
5	E	145	LEU
5	E	183	ASN
5	E	204	ARG
1	F	17	LEU
1	F	19	GLU
1	F	39	ASP
1	F	42	ASN
1	F	103	LEU
1	F	105	SER
1	F	110	LEU
1	F	178	THR
1	F	198	GLU
1	F	231	VAL
1	F	251	LEU
1	F	255	GLN
1	F	268	GLU
1	F	275	GLU
2	G	38	GLN
2	G	48	LYS
2	G	49	VAL
2	G	50	GLU
2	G	51	MET
2	G	73	THR
4	I	25	LYS
4	I	62	ARG
4	I	67	THR
4	I	101	LEU
4	I	132	CYS
4	I	148	ASP
4	I	154	THR
4	I	164	MET
5	J	109	LYS
5	J	116	LEU
5	J	226	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	174	ASN
1	A	220	ASN
1	A	255	GLN
2	B	2	GLN
2	B	31	HIS
2	B	38	GLN
4	D	32	HIS
4	D	112	ASN
4	D	186	ASN
5	E	24	HIS
5	E	37	GLN
5	E	73	ASN
5	E	174	GLN
5	E	183	ASN
1	F	96	GLN
1	F	149	GLN
1	F	220	ASN
1	F	255	GLN
1	F	256	ASN
2	G	2	GLN
2	G	17	ASN
2	G	31	HIS
2	G	67	HIS
4	I	21	ASN
4	I	80	GLN
4	I	113	ASN
5	J	24	HIS
5	J	73	ASN
5	J	153	HIS
5	J	166	HIS
5	J	174	GLN
5	J	202	ASN
5	J	212	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 4 ligands modelled in this entry, 4 are 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	A	278/278 (100%)	0.26	14 (5%) 34 36	18, 32, 69, 102	5 (1%)
1	F	277/278 (99%)	1.19	55 (19%) 3 3	28, 48, 92, 132	5 (1%)
2	B	98/99 (98%)	0.07	2 (2%) 65 67	20, 35, 63, 87	1 (1%)
2	G	98/99 (98%)	1.24	14 (14%) 6 6	36, 57, 89, 102	1 (1%)
3	C	9/9 (100%)	-0.54	0 100 100	19, 21, 29, 30	0
3	H	9/9 (100%)	0.02	0 100 100	27, 30, 40, 41	0
4	D	182/182 (100%)	0.78	15 (8%) 17 18	17, 47, 99, 119	2 (1%)
4	I	177/182 (97%)	1.28	41 (23%) 2 2	20, 58, 120, 134	8 (4%)
5	E	243/243 (100%)	1.16	53 (21%) 2 2	19, 52, 81, 120	1 (0%)
5	J	241/243 (99%)	1.44	76 (31%) 1 1	20, 58, 110, 138	4 (1%)
All	All	1612/1622 (99%)	0.95	270 (16%) 4 4	17, 48, 96, 138	27 (1%)

All (270) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	17	LEU	9.2
4	I	125	LYS	5.6
1	F	274	TRP	5.3
5	J	226	ARG	5.2
4	I	178	SER	5.1
4	I	185	ALA	5.0
5	J	119	VAL	4.8
4	I	129	LYS	4.8
4	I	133	LEU	4.8
1	F	199	VAL	4.8
4	I	174	TRP	4.6
5	J	116	LEU	4.5
1	F	1	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	251	LEU	4.5
4	I	131	VAL	4.4
1	F	51	TRP	4.3
2	G	51	MET	4.3
1	F	107	TRP	4.3
5	E	181	ALA	4.3
1	A	178	THR	4.3
2	G	49	VAL	4.2
1	A	224	LEU	4.2
5	J	165	VAL	4.2
4	I	180	PHE	4.2
5	E	120	PHE	4.1
4	I	118	VAL	3.9
5	J	241	ARG	3.9
5	J	236	ALA	3.9
1	F	177	ALA	3.8
4	I	121	LEU	3.8
4	I	172	VAL	3.8
4	I	173	ALA	3.8
5	J	127	PHE	3.8
1	F	256	ASN	3.7
5	J	126	VAL	3.7
1	F	249	VAL	3.7
5	E	113	LEU	3.6
5	J	182	LEU	3.6
4	I	132	CYS	3.6
5	J	12	VAL	3.6
5	E	182	LEU	3.6
5	J	224	GLN	3.6
1	F	172	LEU	3.6
1	F	178	THR	3.6
5	J	176	LEU	3.6
4	D	126	SER	3.5
1	F	257	TYR	3.5
4	I	119	TYR	3.5
5	J	118	ASN	3.5
4	D	179	PHE	3.5
1	F	201	LEU	3.4
5	J	234	VAL	3.4
5	J	122	PRO	3.4
5	J	222	TRP	3.3
1	F	171	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
5	E	223	THR	3.3
1	F	197	GLY	3.3
4	D	150	VAL	3.3
1	F	176	ASN	3.3
4	I	179	ASP	3.2
1	F	104	GLY	3.2
1	F	250	PRO	3.2
5	J	151	PRO	3.2
1	F	179	LEU	3.2
5	J	193	LEU	3.2
1	F	192	HIS	3.2
5	E	240	GLY	3.2
4	I	164	MET	3.2
1	F	174	ASN	3.2
1	F	103	LEU	3.2
1	A	225	THR	3.2
4	D	142	VAL	3.1
4	I	177	LYS	3.1
1	A	227	ASP	3.1
1	F	89	ALA	3.1
4	I	153	ILE	3.1
1	F	196	LYS	3.1
5	E	222	TRP	3.1
2	G	52	SER	3.1
5	J	239	TRP	3.0
5	J	229	PRO	3.0
5	E	242	ALA	3.0
5	J	125	ALA	3.0
5	J	146	ALA	3.0
5	J	188	ALA	3.0
5	J	207	PHE	3.0
4	I	127	SER	3.0
1	F	110	LEU	3.0
1	F	277	PRO	3.0
4	I	126	SER	2.9
4	I	157[A]	CYS	2.9
5	J	156	LEU	2.9
1	F	175	GLY	2.9
1	F	193	PRO	2.9
4	I	163	SER	2.9
1	F	28	VAL	2.9
1	F	247	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
4	D	118	TYR	2.9
2	B	3	LYS	2.9
5	J	199	PHE	2.9
4	D	173	TRP	2.9
5	E	116	LEU	2.8
5	J	189	LEU	2.8
5	J	149	PHE	2.8
2	G	53	ASP	2.8
5	E	13	ALA	2.8
5	J	215	GLY	2.8
5	J	243	ASP	2.8
1	F	18	GLU	2.8
5	E	149	PHE	2.8
5	J	124	VAL	2.8
5	J	160	VAL	2.8
1	A	90	GLY	2.8
5	J	238	ALA	2.8
5	J	147	THR	2.8
5	J	233	ILE	2.8
5	E	179	GLN	2.7
5	J	150	TYR	2.7
1	F	200	THR	2.7
1	F	105	SER	2.7
1	A	16	GLY	2.7
5	E	228	LYS	2.7
2	G	50	GLU	2.7
5	J	14	VAL	2.7
5	E	17	GLY	2.7
1	A	89	ALA	2.7
5	J	175	PRO	2.7
4	I	176	ASN	2.7
4	I	151	VAL	2.7
4	I	182	CYS	2.7
5	J	200	TRP	2.7
2	B	2	GLN	2.6
5	E	80	LEU	2.6
5	E	176	LEU	2.6
5	J	121	PRO	2.6
5	J	209	CYS	2.6
5	J	13	ALA	2.6
5	E	112	VAL	2.6
5	E	143	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	50	PRO	2.6
5	J	117	LYS	2.6
5	J	163	LYS	2.6
4	I	134	PHE	2.6
5	J	71[A]	GLN	2.6
5	J	211	VAL	2.6
1	F	19	GLU	2.6
1	F	173	LYS	2.6
1	A	177	ALA	2.6
1	F	194	ARG	2.6
4	I	181	ALA	2.6
5	J	227	ALA	2.6
5	J	120	PHE	2.5
5	E	224	GLN	2.5
1	F	41	GLU	2.5
5	E	119	VAL	2.5
5	E	126	VAL	2.5
4	I	62	ARG	2.5
4	I	154	THR	2.5
5	E	2	ALA	2.5
1	A	226	GLN	2.5
5	J	145	LEU	2.5
5	J	216	LEU	2.5
1	A	175	GLY	2.5
5	J	143	VAL	2.5
1	F	169	HIS	2.5
5	E	184	ASP	2.5
5	E	243	ASP	2.5
2	G	85	ALA	2.5
1	F	52	MET	2.5
4	I	143	VAL	2.5
5	J	187	TYR	2.5
1	F	258	THR	2.5
4	I	175	SER	2.5
5	E	15	THR	2.5
1	F	49	ALA	2.5
1	F	191	HIS	2.5
2	G	77	THR	2.4
4	D	143	SER	2.4
4	I	117	ALA	2.4
5	E	200	TRP	2.4
5	J	7	SER	2.4

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Mol	Chain	Res	Type	RSRZ
5	E	238	ALA	2.4
1	F	224	LEU	2.4
5	E	216	LEU	2.4
5	E	127	PHE	2.4
5	J	223	THR	2.4
5	J	178	GLU	2.4
1	F	90	GLY	2.4
5	E	215	GLY	2.4
4	I	155	ASP	2.4
5	E	226	ARG	2.4
1	F	253	LYS	2.3
5	E	121	PRO	2.3
1	F	106	ASP	2.3
5	J	115	ASP	2.3
5	E	19	VAL	2.3
5	E	122	PRO	2.3
5	J	219	ASN	2.3
5	J	3	ALA	2.3
5	J	242	ALA	2.3
1	F	230	LEU	2.3
4	D	7	LEU	2.3
4	I	122	ARG	2.3
4	I	123	ASP	2.3
2	G	80	CYS	2.3
4	I	147	LYS	2.3
5	J	113	LEU	2.3
5	J	135	SER	2.2
4	I	108	PHE	2.2
5	J	220	ASP	2.2
5	J	170[A]	CYS	2.2
1	F	272	LEU	2.2
5	J	166	HIS	2.2
5	J	213	PHE	2.2
2	G	44	LYS	2.2
4	I	111	ILE	2.2
1	F	29	ASP	2.2
5	E	66	ALA	2.2
5	E	236	ALA	2.2
5	J	181	ALA	2.2
5	E	160	VAL	2.2
5	E	125	ALA	2.2
4	D	151	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	G	3	LYS	2.2
5	E	183	ASN	2.2
5	E	151	PRO	2.1
1	A	41	GLU	2.1
5	E	16	GLY	2.1
1	F	273	ARG	2.1
4	D	181	CYS	2.1
1	A	19	GLU	2.1
1	F	227	ASP	2.1
5	E	63	GLY	2.1
5	J	154	VAL	2.1
4	D	184	ALA	2.1
5	J	197	ALA	2.1
4	D	129	SER	2.1
5	J	225	ASP	2.1
5	E	187	TYR	2.1
1	F	252	GLY	2.1
2	G	37	ILE	2.1
5	E	241	ARG	2.1
5	J	158	TRP	2.1
5	E	12	VAL	2.1
5	E	57	LYS	2.1
5	E	81	ALA	2.1
2	G	40	LEU	2.1
4	I	130	SER	2.1
5	J	108	SER	2.1
5	J	196	SER	2.1
2	G	54	MET	2.1
5	J	168	GLY	2.1
4	D	124	LYS	2.1
5	E	154	VAL	2.1
5	E	239	TRP	2.1
4	D	145	SER	2.1
5	J	185	SER	2.1
1	F	219	LEU	2.0
5	E	145	LEU	2.0
5	E	118	ASN	2.0
1	A	194	ARG	2.0
2	G	34	HIS	2.0
5	J	231	THR	2.0
5	J	109	LYS	2.0
1	A	221	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
5	E	82	SER	2.0
4	I	145	GLN	2.0
5	E	209	CYS	2.0
4	D	128	LYS	2.0
4	I	152	TYR	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
6	NA	G	101	1/1	0.83	0.19	66,66,66,66	0
6	NA	I	201	1/1	0.83	0.21	61,61,61,61	0
7	CL	A	302	1/1	0.91	0.12	67,67,67,67	0
6	NA	A	301	1/1	0.92	0.10	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.