



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:06 PM UTC

PDB ID : 5WJL / pdb_00005wjl
Title : Crystal Structure of HLA-A*11:01 with GTS1 peptide
Authors : Gras, S.; Rossjohn, J.
Deposited on : 2017-07-23
Resolution : 3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

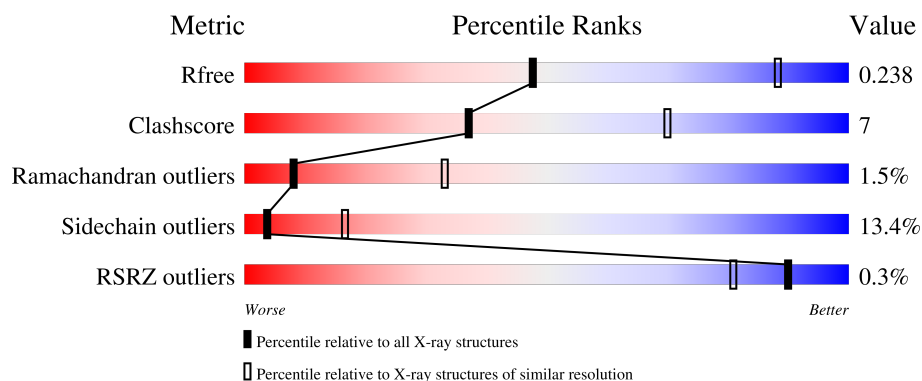
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	
1	D	274	
1	G	274	
2	B	100	
2	E	100	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	100	66% 30%
3	C	10	60% 30% 10%
3	F	10	60% 30% 10%
3	I	10	10% 40% 40% 20%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9520 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 HLA class I histocompatibility antigen, A-11 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2236	1389	407	431	9			
1	D	274	Total	C	N	O	S	0	0	0
			2236	1389	407	431	9			
1	G	274	Total	C	N	O	S	0	0	0
			2236	1389	407	431	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	E	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	H	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
E	0	MET	-	initiating methionine	UNP P61769
H	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called GTS1 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			69	40	14	15			
3	F	10	Total	C	N	O	0	0	0
			69	40	14	15			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	10	Total	C	N	O	0	0	0
			69	40	14	15			

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		

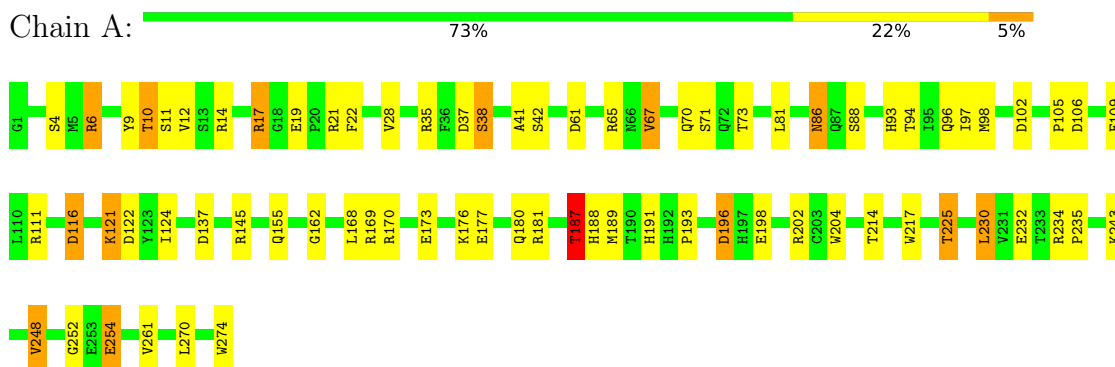
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		
5	B	7	Total	O	0	0
			7	7		
5	C	2	Total	O	0	0
			2	2		
5	D	28	Total	O	0	0
			28	28		
5	E	6	Total	O	0	0
			6	6		
5	F	3	Total	O	0	0
			3	3		
5	G	20	Total	O	0	0
			20	20		
5	H	4	Total	O	0	0
			4	4		
5	I	1	Total	O	0	0
			1	1		

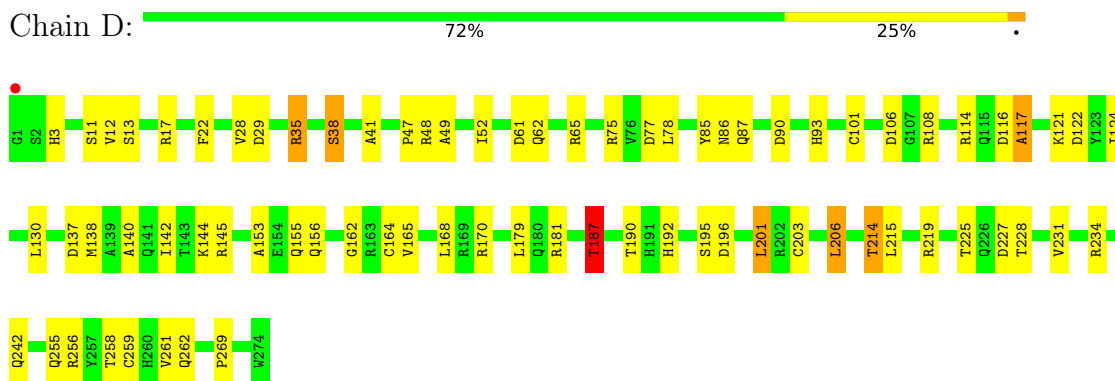
3 Residue-property plots [i](#)

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.

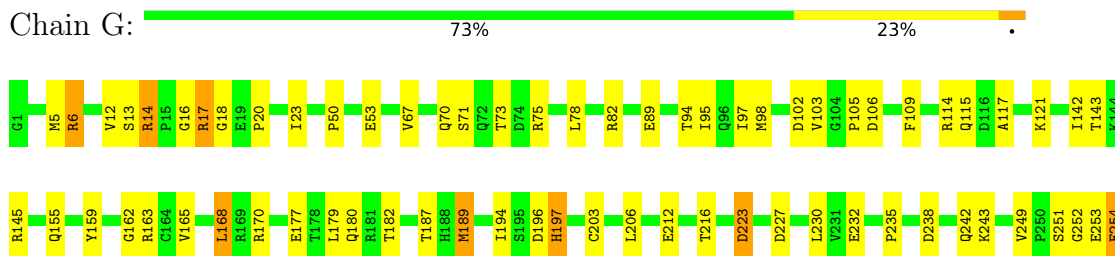
- Molecule 1: HLA class I histocompatibility antigen, A-11 alpha chain

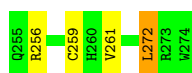


- Molecule 1: HLA class I histocompatibility antigen, A-11 alpha chain



- Molecule 1: HLA class I histocompatibility antigen, A-11 alpha chain





- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



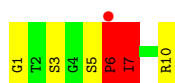
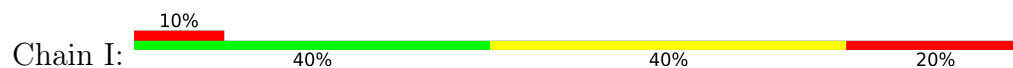
- Molecule 3: GTS1 peptide



- Molecule 3: GTS1 peptide



- Molecule 3: GTS1 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.50Å 150.20Å 105.83Å 90.00° 120.53° 90.00°	Depositor
Resolution (Å)	46.90 – 3.15 46.90 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.90-3.15) 99.9 (46.90-3.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.177 , 0.231 0.188 , 0.238	Depositor DCC
R_{free} test set	1815 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	83.4	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 88.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9520	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: 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	0.90	1/2297 (0.0%)	1.43	22/3117 (0.7%)
1	D	0.84	0/2297	1.41	20/3117 (0.6%)
1	G	0.86	0/2297	1.39	15/3117 (0.5%)
2	B	0.94	0/860	1.45	10/1162 (0.9%)
2	E	0.82	0/860	1.39	6/1162 (0.5%)
2	H	0.82	0/860	1.37	9/1162 (0.8%)
3	C	1.43	1/69 (1.4%)	1.67	0/91
3	F	1.05	0/69	1.80	1/91 (1.1%)
3	I	1.17	0/69	1.82	3/91 (3.3%)
All	All	0.87	2/9678 (0.0%)	1.42	86/13110 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	GLY	C-N	5.16	1.40	1.33
1	A	98	MET	SD-CE	5.08	1.92	1.79

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	58	LYS	CA-C-N	9.08	133.36	120.28
2	B	58	LYS	C-N-CA	9.08	133.36	120.28
1	A	162	GLY	N-CA-C	8.93	118.33	110.21
1	D	162	GLY	N-CA-C	8.62	118.05	110.21
2	E	58	LYS	CA-C-N	8.00	132.06	120.38
2	E	58	LYS	C-N-CA	8.00	132.06	120.38
2	B	87	LEU	CA-C-N	7.92	131.23	120.38
2	B	87	LEU	C-N-CA	7.92	131.23	120.38
1	D	179	LEU	N-CA-C	7.72	119.78	111.36
1	A	196	ASP	N-CA-C	-7.36	104.33	113.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	SER	N-CA-C	7.18	119.78	111.02
1	D	41	ALA	CA-C-N	7.08	131.44	120.82
1	D	41	ALA	C-N-CA	7.08	131.44	120.82
2	E	70	PHE	CA-CB-CG	7.06	120.86	113.80
2	H	30	PHE	N-CA-C	6.76	120.34	109.79
2	H	4	THR	N-CA-C	6.69	118.53	109.24
1	G	67	VAL	N-CA-CB	6.64	117.86	110.62
1	A	65	ARG	CA-C-N	6.55	129.38	120.54
1	A	65	ARG	C-N-CA	6.55	129.38	120.54
2	E	59	ASP	CA-CB-CG	6.54	119.14	112.60
1	A	187	THR	N-CA-C	6.52	119.34	108.20
1	A	61	ASP	CA-CB-CG	6.49	119.08	112.60
1	D	187	THR	N-CA-C	6.31	119.94	109.46
1	D	106	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	105	PRO	CA-C-N	6.09	128.76	120.54
1	A	105	PRO	C-N-CA	6.09	128.76	120.54
3	I	6	PRO	CA-C-N	6.07	132.89	121.97
3	I	6	PRO	C-N-CA	6.07	132.89	121.97
1	G	223	ASP	N-CA-C	6.05	117.87	109.15
1	A	116	ASP	CA-CB-CG	6.03	118.63	112.60
1	G	256	ARG	CA-C-N	6.01	130.09	121.50
1	G	256	ARG	C-N-CA	6.01	130.09	121.50
2	H	87	LEU	CA-C-N	6.00	128.91	120.28
2	H	87	LEU	C-N-CA	6.00	128.91	120.28
1	G	253	GLU	CA-C-N	5.97	128.60	120.54
1	G	253	GLU	C-N-CA	5.97	128.60	120.54
3	F	5	SER	N-CA-C	-5.96	102.27	109.83
1	D	61	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	137	ASP	CA-CB-CG	5.76	118.36	112.60
2	E	28	SER	N-CA-C	5.73	115.84	108.34
2	H	71	THR	CB-CA-C	5.70	120.01	110.55
1	A	137	ASP	N-CA-C	5.68	116.06	108.38
1	D	231	VAL	N-CA-CB	5.67	118.39	110.56
1	A	122	ASP	CA-CB-CG	5.65	118.25	112.60
1	D	12	VAL	N-CA-C	5.62	115.69	107.37
1	D	28	VAL	N-CA-CB	5.58	118.94	111.90
1	G	179	LEU	N-CA-C	5.55	117.41	111.36
1	D	3	HIS	N-CA-C	5.55	118.30	110.14
2	H	24	ASN	CA-CB-CG	5.55	118.15	112.60
2	B	76	ASP	N-CA-C	5.54	117.76	108.96
1	A	169	ARG	CA-C-N	5.53	127.62	120.44
1	A	169	ARG	C-N-CA	5.53	127.62	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	59	ASP	CA-CB-CG	5.51	118.11	112.60
3	I	5	SER	CB-CA-C	5.51	117.44	109.45
1	D	153	ALA	CA-C-N	5.49	127.94	120.54
1	D	153	ALA	C-N-CA	5.49	127.94	120.54
1	G	182	THR	CB-CA-C	5.45	119.86	111.95
2	H	15	ALA	N-CA-C	5.43	118.23	110.24
1	A	225	THR	N-CA-C	-5.40	107.70	114.56
1	A	248	VAL	N-CA-CB	5.34	117.09	111.00
1	A	93	HIS	N-CA-C	5.33	117.52	109.41
1	G	95	ILE	N-CA-CB	5.33	118.50	111.25
1	A	28	VAL	N-CA-C	-5.26	100.06	107.75
1	D	269	PRO	CA-C-N	5.19	129.05	121.31
1	D	269	PRO	C-N-CA	5.19	129.05	121.31
2	E	9	VAL	N-CA-CB	5.17	117.20	110.99
1	D	29	ASP	CB-CA-C	-5.17	110.20	117.23
1	G	142	ILE	CA-C-N	5.16	127.15	120.44
1	G	142	ILE	C-N-CA	5.16	127.15	120.44
1	A	67	VAL	N-CA-CB	-5.14	104.54	110.55
1	A	41	ALA	CA-C-N	5.13	127.93	120.79
1	A	41	ALA	C-N-CA	5.13	127.93	120.79
1	G	94	THR	N-CA-C	5.12	116.75	108.41
1	D	117	ALA	N-CA-C	5.10	116.91	108.13
1	D	108	ARG	CA-C-N	5.09	128.43	120.75
1	D	108	ARG	C-N-CA	5.09	128.43	120.75
2	B	44	GLU	CA-C-N	5.08	131.25	121.54
2	B	44	GLU	C-N-CA	5.08	131.25	121.54
2	H	32	PRO	CA-C-N	5.08	127.40	120.54
2	H	32	PRO	C-N-CA	5.08	127.40	120.54
1	G	105	PRO	CA-C-N	5.07	127.03	120.44
1	G	105	PRO	C-N-CA	5.07	127.03	120.44
2	B	70	PHE	CA-CB-CG	5.07	118.87	113.80
2	B	70	PHE	N-CA-C	5.05	116.49	108.96
1	D	93	HIS	N-CA-C	5.04	117.53	109.81
1	G	82	ARG	N-CA-C	-5.01	106.43	112.54

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	2236	0	2089	23	0
1	D	2236	0	2089	31	0
1	G	2236	0	2089	29	0
2	B	837	0	805	15	0
2	E	837	0	805	13	0
2	H	837	0	804	22	0
3	C	69	0	71	3	0
3	F	69	0	71	3	0
3	I	69	0	71	6	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	1	0
5	A	20	0	0	0	0
5	B	7	0	0	0	0
5	C	2	0	0	0	0
5	D	28	0	0	0	0
5	E	6	0	0	0	0
5	F	3	0	0	0	0
5	G	20	0	0	0	0
5	H	4	0	0	1	0
5	I	1	0	0	0	0
All	All	9520	0	8894	121	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 7.

All (121) 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)
1:G:203:CYS:HG	1:G:259:CYS:HG	1.09	0.94
1:D:203:CYS:HG	1:D:259:CYS:HG	0.98	0.86
2:H:33:SER:N	2:H:62:PHE:HE2	1.75	0.84
1:A:155:GLN:HB3	3:C:6:PRO:HD3	1.63	0.79
1:G:155:GLN:HB2	3:I:6:PRO:HD3	1.65	0.77
2:H:33:SER:HA	2:H:62:PHE:CE2	2.21	0.76
1:A:97:ILE:HD11	3:C:10:ARG:HH22	1.49	0.76
2:H:25:CYS:HG	2:H:80:CYS:HG	0.78	0.75
2:E:25:CYS:HG	2:E:80:CYS:HG	0.78	0.75
2:H:33:SER:CA	2:H:62:PHE:CE2	2.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:21:ASN:HB3	2:H:70:PHE:CE1	2.22	0.74
2:H:33:SER:N	2:H:62:PHE:CE2	2.55	0.74
2:H:21:ASN:HB3	2:H:70:PHE:HE1	1.56	0.70
1:D:155:GLN:HB3	3:F:6:PRO:HD3	1.74	0.69
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.74	0.68
1:D:214:THR:HB	1:D:262:GLN:HB3	1.76	0.67
1:G:98:MET:HG3	5:H:103:HOH:O	1.95	0.67
1:D:35:ARG:HG2	1:D:48:ARG:HD2	1.80	0.63
1:D:62:GLN:HE21	1:D:65:ARG:HH11	1.46	0.63
1:D:101:CYS:HG	1:D:164:CYS:HG	0.63	0.62
1:G:159:TYR:OH	3:I:1:GLY:O	2.16	0.62
2:H:33:SER:HA	2:H:62:PHE:CD2	2.35	0.62
1:G:235:PRO:HG2	2:H:65:LEU:HD22	1.81	0.61
1:G:189:MET:HE1	1:G:272:LEU:HB2	1.81	0.61
1:D:85:TYR:HB2	1:D:87:GLN:HE21	1.67	0.59
1:D:48:ARG:NH1	2:E:53:ASP:OD2	2.29	0.59
2:H:7:ILE:HG12	2:H:82:VAL:HG21	1.86	0.58
1:D:62:GLN:NE2	1:D:65:ARG:HD2	2.19	0.57
1:G:16:GLY:C	1:G:18:GLY:H	2.13	0.57
1:A:97:ILE:HD11	3:C:10:ARG:NH2	2.19	0.56
1:D:203:CYS:HG	1:D:259:CYS:CB	2.17	0.56
1:G:238:ASP:HB3	2:H:12:ARG:HD3	1.88	0.56
2:B:38:ASP:OD1	2:B:45:ARG:HD3	2.06	0.56
1:D:62:GLN:HE21	1:D:65:ARG:NH1	2.04	0.56
1:G:155:GLN:CB	3:I:6:PRO:HD3	2.35	0.55
1:D:101:CYS:CB	1:D:164:CYS:SG	2.95	0.54
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.41	0.54
1:A:121:LYS:HB2	2:B:1:ILE:HD13	1.90	0.54
1:A:14:ARG:HB2	1:A:17:ARG:HD3	1.89	0.54
1:A:22:PHE:H	1:A:38:SER:HB3	1.73	0.54
1:D:187:THR:HG21	1:D:261:VAL:HG21	1.89	0.54
1:G:206:LEU:HG	1:G:242:GLN:HG2	1.89	0.54
1:D:85:TYR:CB	1:D:87:GLN:HE21	2.21	0.53
1:G:50:PRO:HA	1:G:53:GLU:HG3	1.90	0.53
2:H:63:TYR:C	2:H:63:TYR:CD1	2.85	0.53
1:D:22:PHE:H	1:D:38:SER:HB3	1.72	0.53
1:A:21:ARG:HH21	1:A:37:ASP:CG	2.16	0.53
1:D:62:GLN:NE2	1:D:65:ARG:HH11	2.06	0.53
1:D:101:CYS:HB3	1:D:164:CYS:SG	2.50	0.52
1:G:14:ARG:HB2	1:G:17:ARG:HB2	1.91	0.52
1:G:97:ILE:HD11	3:I:10:ARG:HH22	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:ILE:HD12	2:E:1:ILE:H	1.73	0.52
2:E:40:LEU:HD11	2:E:81:ARG:HB2	1.92	0.52
2:E:89:GLN:HG3	2:E:90:PRO:HD2	1.92	0.52
1:G:162:GLY:O	1:G:165:VAL:HG22	2.10	0.51
1:G:203:CYS:CB	1:G:259:CYS:HG	2.22	0.51
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.93	0.50
1:G:70:GLN:HA	3:I:7:ILE:HD11	1.92	0.50
2:E:16:GLU:HB3	2:E:19:LYS:HD2	1.92	0.50
2:E:96:ASP:HB3	2:E:99:MET:HB2	1.92	0.50
1:D:234:ARG:HG2	1:D:242:GLN:HB2	1.94	0.49
1:G:235:PRO:CG	2:H:65:LEU:HD22	2.42	0.49
2:H:62:PHE:O	2:H:63:TYR:HB3	2.11	0.49
2:H:27:VAL:HG21	2:H:37:VAL:HG21	1.93	0.49
1:G:20:PRO:HD2	1:G:75:ARG:HD2	1.93	0.49
1:G:97:ILE:HD11	3:I:10:ARG:NH2	2.27	0.49
2:B:11:SER:HB2	2:B:13:HIS:O	2.12	0.48
1:D:206:LEU:HG	1:D:242:GLN:HG2	1.96	0.48
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.49	0.48
1:G:230:LEU:HD22	1:G:243:LYS:HE3	1.96	0.47
1:A:176:LYS:HA	1:A:180:GLN:HG3	1.96	0.47
1:G:13:SER:HB3	1:G:78:LEU:HD13	1.97	0.46
1:D:137:ASP:H	1:D:140:ALA:HB3	1.80	0.46
1:G:6:ARG:NH2	1:G:102:ASP:OD1	2.49	0.46
2:E:49:VAL:HG22	2:E:68:THR:HB	1.97	0.46
2:B:96:ASP:HB3	2:B:99:MET:HB2	1.98	0.46
1:A:9:TYR:CD2	1:A:70:GLN:HG2	2.51	0.46
1:A:234:ARG:HD3	2:B:8:GLN:OE1	2.15	0.46
1:G:5:MET:HB2	1:G:168:LEU:HG	1.97	0.46
2:B:8:GLN:O	2:B:10:TYR:CD1	2.69	0.45
1:G:103:VAL:HG22	1:G:168:LEU:HD13	1.98	0.45
2:B:31:HIS:CD2	2:B:62:PHE:CE2	3.05	0.45
1:A:10:THR:HG23	1:A:96:GLN:HG2	1.98	0.45
1:D:47:PRO:HB3	1:D:52:ILE:HG23	1.99	0.45
1:A:188:HIS:CE1	1:A:204:TRP:HB2	2.52	0.45
1:G:187:THR:HG21	1:G:261:VAL:HG21	1.98	0.45
2:H:63:TYR:CD1	2:H:63:TYR:O	2.70	0.45
2:B:57:SER:HB2	2:B:59:ASP:HB3	1.99	0.44
2:E:31:HIS:CD2	2:E:62:PHE:CE2	3.05	0.44
1:A:252:GLY:C	1:A:254:GLU:H	2.25	0.44
2:B:39:LEU:HD23	2:B:39:LEU:HA	1.85	0.44
1:A:191:HIS:CE1	1:A:193:PRO:HD3	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HD22	1:A:243:LYS:HE2	1.99	0.43
1:D:77:ASP:OD2	3:F:10:ARG:NH1	2.51	0.43
1:A:116:ASP:HB2	1:A:124:ILE:HG22	1.99	0.43
2:E:87:LEU:O	4:E:101:CL:CL	2.73	0.43
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.53	0.43
2:H:70:PHE:C	2:H:70:PHE:CD1	2.93	0.43
1:D:138:MET:O	1:D:142:ILE:HD12	2.18	0.42
1:A:191:HIS:HB3	1:A:274:TRP:CZ2	2.54	0.42
1:A:189:MET:HE2	1:A:217:TRP:CH2	2.55	0.42
1:D:114:ARG:NH1	1:D:116:ASP:OD1	2.52	0.42
1:A:121:LYS:HB2	2:B:1:ILE:CD1	2.49	0.42
2:B:4:THR:HG23	2:B:86:THR:HB	2.01	0.42
1:D:116:ASP:HB2	1:D:124:ILE:HG22	2.01	0.42
2:H:32:PRO:C	2:H:62:PHE:HE2	2.28	0.42
1:D:201:LEU:HD12	1:D:201:LEU:HA	1.91	0.41
1:D:49:ALA:O	1:D:52:ILE:HG22	2.21	0.41
1:G:12:VAL:HG11	2:H:33:SER:HB3	2.01	0.41
1:A:235:PRO:HD2	2:B:10:TYR:OH	2.20	0.41
2:H:37:VAL:HG22	2:H:82:VAL:HG22	2.00	0.41
1:G:252:GLY:C	1:G:254:GLU:H	2.29	0.41
2:E:25:CYS:CB	2:E:80:CYS:HG	2.27	0.41
2:H:42:ASN:OD1	2:H:77:GLU:N	2.48	0.41
1:A:10:THR:HG21	2:B:62:PHE:CE1	2.56	0.41
2:B:39:LEU:HB3	2:B:46:ILE:HD12	2.02	0.41
1:D:155:GLN:HB3	3:F:6:PRO:CD	2.46	0.41
1:D:255:GLN:HE21	1:D:256:ARG:HG3	1.85	0.41
2:E:59:ASP:HB3	2:E:61:SER:OG	2.21	0.41
1:G:197:HIS:HA	1:G:251:SER:HB2	2.02	0.40
1:D:190:THR:HB	1:D:192:HIS:CE1	2.57	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	272/274 (99%)	252 (93%)	18 (7%)	2 (1%)	18	49
1	D	272/274 (99%)	253 (93%)	18 (7%)	1 (0%)	30	59
1	G	272/274 (99%)	245 (90%)	24 (9%)	3 (1%)	11	39
2	B	98/100 (98%)	85 (87%)	11 (11%)	2 (2%)	6	27
2	E	98/100 (98%)	88 (90%)	10 (10%)	0	100	100
2	H	98/100 (98%)	85 (87%)	9 (9%)	4 (4%)	2	14
3	C	8/10 (80%)	6 (75%)	1 (12%)	1 (12%)	0	1
3	F	8/10 (80%)	6 (75%)	0	2 (25%)	0	0
3	I	8/10 (80%)	5 (62%)	1 (12%)	2 (25%)	0	0
All	All	1134/1152 (98%)	1025 (90%)	92 (8%)	17 (2%)	8	33

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	6	PRO
3	F	6	PRO
2	H	98	ASP
3	I	6	PRO
1	A	109	PHE
2	B	15	ALA
1	D	17	ARG
1	G	17	ARG
1	G	109	PHE
2	H	29	GLY
1	A	86	ASN
2	H	31	HIS
2	H	62	PHE
2	B	18	GLY
1	G	227	ASP
3	I	7	ILE
3	F	7	ILE

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	231/231 (100%)	195 (84%)	36 (16%)	2	12
1	D	231/231 (100%)	201 (87%)	30 (13%)	4	17
1	G	231/231 (100%)	203 (88%)	28 (12%)	5	20
2	B	95/95 (100%)	79 (83%)	16 (17%)	2	10
2	E	95/95 (100%)	84 (88%)	11 (12%)	5	21
2	H	95/95 (100%)	85 (90%)	10 (10%)	6	24
3	C	8/8 (100%)	7 (88%)	1 (12%)	4	19
3	F	8/8 (100%)	8 (100%)	0	100	100
3	I	8/8 (100%)	6 (75%)	2 (25%)	0	3
All	All	1002/1002 (100%)	868 (87%)	134 (13%)	4	16

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	6	ARG
1	A	10	THR
1	A	11	SER
1	A	12	VAL
1	A	17	ARG
1	A	19	GLU
1	A	35	ARG
1	A	38	SER
1	A	67	VAL
1	A	71	SER
1	A	73	THR
1	A	81	LEU
1	A	86	ASN
1	A	88	SER
1	A	94	THR
1	A	106	ASP
1	A	111	ARG
1	A	121	LYS
1	A	145	ARG
1	A	168	LEU
1	A	170	ARG
1	A	173	GLU
1	A	177	GLU
1	A	181	ARG
1	A	187	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	196	ASP
1	A	198	GLU
1	A	202	ARG
1	A	214	THR
1	A	225	THR
1	A	230	LEU
1	A	232	GLU
1	A	248	VAL
1	A	254	GLU
1	A	270	LEU
2	B	2	GLN
2	B	4	THR
2	B	7	ILE
2	B	9	VAL
2	B	11	SER
2	B	17	ASN
2	B	27	VAL
2	B	33	SER
2	B	35	ILE
2	B	45	ARG
2	B	68	THR
2	B	70	PHE
2	B	71	THR
2	B	88	SER
2	B	89	GLN
2	B	99	MET
3	C	7	ILE
1	D	11	SER
1	D	13	SER
1	D	35	ARG
1	D	38	SER
1	D	75	ARG
1	D	78	LEU
1	D	86	ASN
1	D	90	ASP
1	D	121	LYS
1	D	122	ASP
1	D	130	LEU
1	D	144	LYS
1	D	145	ARG
1	D	156	GLN
1	D	165	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	168	LEU
1	D	170	ARG
1	D	181	ARG
1	D	187	THR
1	D	195	SER
1	D	196	ASP
1	D	201	LEU
1	D	206	LEU
1	D	214	THR
1	D	215	LEU
1	D	219	ARG
1	D	225	THR
1	D	227	ASP
1	D	228	THR
1	D	258	THR
2	E	4	THR
2	E	16	GLU
2	E	33	SER
2	E	34	ASP
2	E	36	GLU
2	E	40	LEU
2	E	61	SER
2	E	64	LEU
2	E	68	THR
2	E	69	GLU
2	E	70	PHE
1	G	6	ARG
1	G	14	ARG
1	G	23	ILE
1	G	71	SER
1	G	73	THR
1	G	89	GLU
1	G	106	ASP
1	G	114	ARG
1	G	115	GLN
1	G	121	LYS
1	G	143	THR
1	G	145	ARG
1	G	163	ARG
1	G	168	LEU
1	G	170	ARG
1	G	177	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	180	GLN
1	G	189	MET
1	G	194	ILE
1	G	196	ASP
1	G	197	HIS
1	G	212	GLU
1	G	216	THR
1	G	223	ASP
1	G	232	GLU
1	G	249	VAL
1	G	254	GLU
1	G	272	LEU
2	H	0	MET
2	H	2	GLN
2	H	4	THR
2	H	16	GLU
2	H	35	ILE
2	H	61	SER
2	H	70	PHE
2	H	73	THR
2	H	75	LYS
2	H	89	GLN
3	I	3	SER
3	I	7	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	191	HIS
1	A	224	GLN
1	A	262	GLN
2	B	31	HIS
3	C	9	ASN
1	D	62	GLN
1	D	72	GLN
1	D	86	ASN
1	D	87	GLN
1	D	93	HIS
1	D	115	GLN
1	D	141	GLN
1	D	156	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	180	GLN
1	D	191	HIS
1	D	255	GLN
2	E	24	ASN
2	E	31	HIS
1	G	32	GLN
1	G	72	GLN
1	G	86	ASN
1	G	96	GLN
1	G	180	GLN
1	G	224	GLN
1	G	242	GLN
2	H	2	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 [i](#)

Of 3 ligands modelled in this entry, 3 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 [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, 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	274/274 (100%)	-0.41	0 100 100	46, 80, 132, 152	0
1	D	274/274 (100%)	-0.36	1 (0%) 88 78	55, 86, 121, 148	0
1	G	274/274 (100%)	-0.32	0 100 100	55, 92, 142, 173	0
2	B	100/100 (100%)	-0.00	0 100 100	57, 98, 137, 147	0
2	E	100/100 (100%)	-0.16	1 (1%) 79 62	73, 105, 132, 145	0
2	H	100/100 (100%)	-0.03	0 100 100	72, 108, 143, 161	0
3	C	10/10 (100%)	-0.20	0 100 100	50, 62, 80, 85	0
3	F	10/10 (100%)	-0.01	0 100 100	58, 84, 99, 103	0
3	I	10/10 (100%)	0.11	1 (10%) 12 7	56, 78, 103, 109	0
All	All	1152/1152 (100%)	-0.28	3 (0%) 90 81	46, 91, 135, 173	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	6	PRO	2.9
2	E	1	ILE	2.8
1	D	1	GLY	2.1

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(Å ²)	Q<0.9
4	CL	E	101	1/1	0.91	0.09	117,117,117,117	0
4	CL	D	301	1/1	0.94	0.19	90,90,90,90	0
4	CL	C	101	1/1	0.98	0.08	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.