



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:41 am BST

PDB ID : 5WJN
Title : Crystal Structure of HLA-A*11:01-GTS3
Authors : Gras, S.; Rossjohn, J.
Deposited on : 2017-07-23
Resolution : 2.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

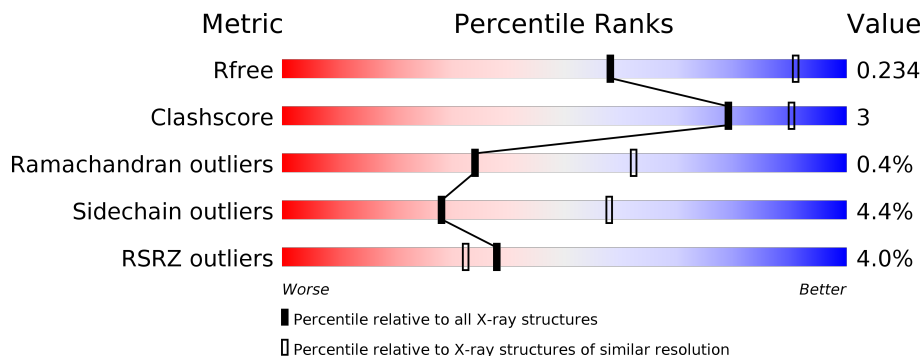
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 on 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	
2	H	100	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	10	 80% 10% 10%
3	F	10	 90% 10%
3	I	10	 10% 80% 10% 10%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9779 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
			Total	C	N	O	S			
1	A	274	Total 2246	C 1395	N 410	O 432	S 9	0	1	0
1	D	274	Total 2236	C 1389	N 407	O 431	S 9	0	0	0
1	G	274	Total 2236	C 1389	N 407	O 431	S 9	0	0	0

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

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

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 GTS3 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	10	Total 70	C 41	N 14	O 15	0	0	0
3	F	10	Total 70	C 41	N 14	O 15	0	0	0

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
			70	41	14	15			

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	74	Total	O	0	0
			74	74		
5	B	47	Total	O	0	0
			47	47		
5	C	6	Total	O	0	0
			6	6		
5	D	87	Total	O	0	0
			87	87		
5	E	36	Total	O	0	0
			36	36		
5	F	4	Total	O	0	0
			4	4		
5	G	57	Total	O	0	0
			57	57		
5	H	22	Total	O	0	0
			22	22		
5	I	6	Total	O	0	0
			6	6		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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.

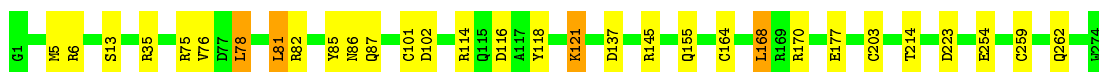
- Molecule 1: HLA class I histocompatibility antigen, A-11 alpha chain

Chain A: 




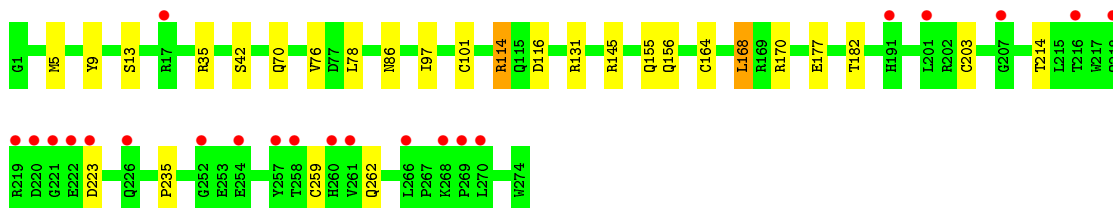
- Molecule 1: HLA class I histocompatibility antigen, A-11 alpha chain

Chain D: 




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

Chain G: 




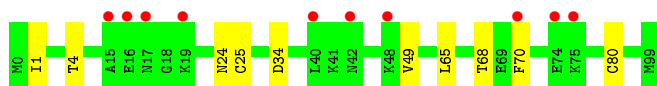
- Molecule 2: Beta-2-microglobulin

Chain B: 

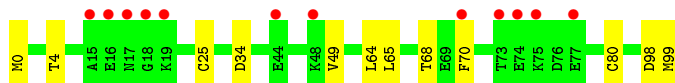
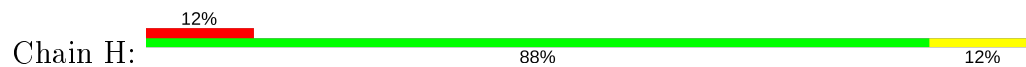


- Molecule 2: Beta-2-microglobulin

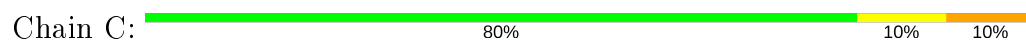
Chain E: 



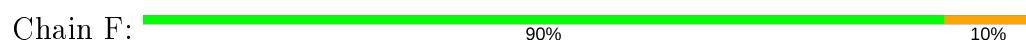
- Molecule 2: Beta-2-microglobulin



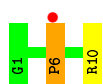
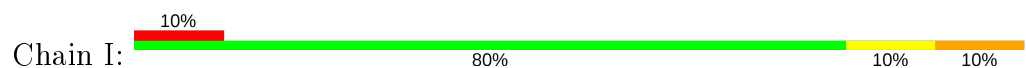
- Molecule 3: GTS3 peptide



- Molecule 3: GTS3 peptide



- Molecule 3: GTS3 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.32Å 145.52Å 106.30Å 90.00° 121.14° 90.00°	Depositor
Resolution (Å)	45.67 – 2.85 45.67 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.1 (45.67-2.85) 98.1 (45.67-2.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.86Å)	Xtrriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.201 , 0.230 0.208 , 0.234	Depositor DCC
R_{free} test set	2388 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtrriage
Anisotropy	0.043	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9779	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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:
K

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	0.35	0/2308	0.61	0/3132
1	D	0.41	0/2297	0.61	0/3117
1	G	0.36	0/2297	0.62	0/3117
2	B	0.34	0/860	0.59	0/1162
2	E	0.34	0/860	0.59	0/1162
2	H	0.46	0/860	0.61	0/1162
3	C	0.53	0/70	0.88	0/92
3	F	0.53	0/70	0.86	0/92
3	I	0.62	0/70	0.92	0/92
All	All	0.38	0/9692	0.62	0/13128

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2246	0	2095	11	0
1	D	2236	0	2089	13	0
1	G	2236	0	2089	12	0
2	B	837	0	805	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	837	0	805	4	0
2	H	837	0	805	4	0
3	C	70	0	73	2	0
3	F	70	0	73	1	0
3	I	70	0	73	2	0
4	B	1	0	0	0	0
5	A	74	0	0	0	0
5	B	47	0	0	0	0
5	C	6	0	0	0	0
5	D	87	0	0	0	0
5	E	36	0	0	0	0
5	F	4	0	0	0	0
5	G	57	0	0	0	0
5	H	22	0	0	0	0
5	I	6	0	0	0	0
All	All	9779	0	8907	45	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 3.

All (45) 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:101:CYS:HG	1:G:164:CYS:HG	1.00	0.92
1:D:101:CYS:HG	1:D:164:CYS:HG	0.87	0.84
2:E:25:CYS:HG	2:E:80:CYS:HG	0.81	0.79
1:D:155:GLN:HB3	3:F:6:PRO:HD3	1.69	0.73
1:G:235:PRO:HG2	2:H:65:LEU:HD22	1.75	0.68
1:A:155:GLN:HB3	3:C:6:PRO:HD3	1.82	0.61
1:A:101:CYS:HG	1:A:164:CYS:HG	1.08	0.61
1:G:203:CYS:HG	1:G:259:CYS:HG	1.50	0.59
1:D:85:TYR:OH	1:D:137:ASP:OD2	2.19	0.58
2:H:25:CYS:HG	2:H:80:CYS:HG	0.70	0.58
1:G:155:GLN:HB3	3:I:6:PRO:HD3	1.85	0.57
2:B:92:ILE:HD12	2:H:0:MET:O	2.04	0.57
1:D:203:CYS:HG	1:D:259:CYS:HG	1.47	0.56
1:D:203:CYS:SG	1:D:259:CYS:SG	3.00	0.56
1:G:203:CYS:SG	1:G:259:CYS:SG	3.04	0.54
1:G:214:THR:HB	1:G:262:GLN:HB2	1.93	0.51
1:A:214:THR:HB	1:A:262:GLN:HB2	1.93	0.50
1:D:214:THR:HB	1:D:262:GLN:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LYS:HB2	2:B:1:ILE:HD13	1.94	0.49
1:A:197[B]:HIS:HD2	1:A:198:GLU:HG3	1.77	0.48
1:G:5:MET:HB2	1:G:168:LEU:HG	1.96	0.48
1:G:13:SER:HB3	1:G:78:LEU:HD13	1.96	0.47
1:D:82:ARG:HG2	1:D:87:GLN:HB2	1.97	0.46
1:G:114:ARG:HG3	1:G:156:GLN:NE2	2.31	0.45
1:A:13:SER:HB3	1:A:78:LEU:HD13	1.98	0.45
1:D:6:ARG:NH2	1:D:102:ASP:OD1	2.47	0.45
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.47	0.45
1:A:97:ILE:HD11	3:C:10:ARG:HH22	1.80	0.45
1:G:97:ILE:HD11	3:I:10:ARG:HH22	1.82	0.45
1:D:5:MET:HB2	1:D:168:LEU:HG	2.00	0.44
1:A:82:ARG:HB2	1:A:87:GLN:HB2	2.01	0.43
1:G:101:CYS:HG	1:G:164:CYS:CB	2.30	0.42
2:B:49:VAL:HG22	2:B:68:THR:HB	2.02	0.42
1:D:81:LEU:HD23	1:D:118:TYR:CD1	2.55	0.42
2:E:49:VAL:HG22	2:E:68:THR:HB	2.02	0.42
2:H:49:VAL:HG22	2:H:68:THR:HB	2.02	0.41
1:D:13:SER:HB3	1:D:78:LEU:HG	2.03	0.41
2:E:24:ASN:HB3	2:E:65:LEU:HD11	2.01	0.41
2:B:29:GLY:HA2	2:B:61:SER:HB3	2.02	0.41
1:D:121:LYS:HB2	2:E:1:ILE:HD13	2.03	0.41
1:D:85:TYR:O	1:D:86:ASN:HB2	2.20	0.41
2:B:24:ASN:HB3	2:B:65:LEU:HD11	2.02	0.41
1:A:101:CYS:HG	1:A:164:CYS:CB	2.33	0.41
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.56	0.40
1:G:9:TYR:CD2	1:G:70:GLN:HG2	2.57	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	273/274 (100%)	267 (98%)	6 (2%)	0	100	100
1	D	272/274 (99%)	260 (96%)	12 (4%)	0	100	100
1	G	272/274 (99%)	266 (98%)	6 (2%)	0	100	100
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	E	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	H	98/100 (98%)	96 (98%)	1 (1%)	1 (1%)	15	40
3	C	8/10 (80%)	5 (62%)	2 (25%)	1 (12%)	0	0
3	F	8/10 (80%)	5 (62%)	2 (25%)	1 (12%)	0	0
3	I	8/10 (80%)	5 (62%)	2 (25%)	1 (12%)	0	0
All	All	1135/1152 (98%)	1094 (96%)	37 (3%)	4 (0%)	34	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	98	ASP
3	C	6	PRO
3	F	6	PRO
3	I	6	PRO

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	232/231 (100%)	225 (97%)	7 (3%)	41	72
1	D	231/231 (100%)	217 (94%)	14 (6%)	18	43
1	G	231/231 (100%)	218 (94%)	13 (6%)	21	47
2	B	95/95 (100%)	93 (98%)	2 (2%)	53	79
2	E	95/95 (100%)	92 (97%)	3 (3%)	39	69
2	H	95/95 (100%)	90 (95%)	5 (5%)	22	50
3	C	8/8 (100%)	8 (100%)	0	100	100
3	F	8/8 (100%)	8 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	8/8 (100%)	8 (100%)	0	100	100
All	All	1003/1002 (100%)	959 (96%)	44 (4%)	28	58

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	VAL
1	A	75	ARG
1	A	86	ASN
1	A	116	ASP
1	A	145	ARG
1	A	181	ARG
1	A	254	GLU
2	B	70	PHE
2	B	99	MET
1	D	35	ARG
1	D	75	ARG
1	D	76	VAL
1	D	78	LEU
1	D	81	LEU
1	D	114	ARG
1	D	116	ASP
1	D	121	LYS
1	D	145	ARG
1	D	168	LEU
1	D	170	ARG
1	D	177	GLU
1	D	223	ASP
1	D	254	GLU
2	E	4	THR
2	E	34	ASP
2	E	70	PHE
1	G	35	ARG
1	G	42	SER
1	G	76	VAL
1	G	86	ASN
1	G	114	ARG
1	G	116	ASP
1	G	131	ARG
1	G	145	ARG
1	G	168	LEU
1	G	170	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	177	GLU
1	G	182	THR
1	G	223	ASP
2	H	4	THR
2	H	34	ASP
2	H	64	LEU
2	H	70	PHE
2	H	99	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	D	72	GLN
1	D	255	GLN
1	G	156	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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

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	274/274 (100%)	-0.13	0 100 100	25, 47, 73, 94	0
1	D	274/274 (100%)	-0.07	0 100 100	28, 51, 73, 93	0
1	G	274/274 (100%)	0.35	22 (8%) 12 9	33, 59, 110, 129	0
2	B	100/100 (100%)	-0.03	1 (1%) 82 81	33, 48, 80, 95	0
2	E	100/100 (100%)	0.49	10 (10%) 7 5	35, 61, 92, 101	0
2	H	100/100 (100%)	0.75	12 (12%) 4 3	40, 70, 105, 119	0
3	C	10/10 (100%)	0.32	0 100 100	25, 49, 64, 66	0
3	F	10/10 (100%)	0.32	0 100 100	36, 51, 67, 68	0
3	I	10/10 (100%)	0.44	1 (10%) 7 5	37, 51, 73, 73	0
All	All	1152/1152 (100%)	0.15	46 (3%) 38 32	25, 54, 96, 129	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	74	GLU	6.5
2	H	75	LYS	5.7
1	G	260	HIS	4.8
1	G	266	LEU	4.1
1	G	218	GLN	4.0
1	G	268	LYS	3.9
1	G	258	THR	3.8
1	G	220	ASP	3.7
2	H	19	LYS	3.6
2	E	16	GLU	3.4
2	E	75	LYS	3.4
1	G	257	TYR	3.4
1	G	221	GLY	3.4
1	G	222	GLU	3.3
2	H	16	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	I	6	PRO	3.1
1	G	216	THR	3.0
2	H	44	GLU	3.0
2	H	18	GLY	2.9
1	G	226	GLN	2.9
1	G	223	ASP	2.9
2	H	15	ALA	2.8
1	G	207	GLY	2.7
1	G	261	VAL	2.6
2	B	16	GLU	2.6
1	G	191	HIS	2.6
1	G	201	LEU	2.6
2	H	77	GLU	2.6
1	G	270	LEU	2.5
2	E	17	ASN	2.5
2	E	40	LEU	2.4
2	E	42	ASN	2.4
1	G	17	ARG	2.4
2	H	17	ASN	2.4
1	G	254	GLU	2.3
2	H	73	THR	2.3
1	G	252	GLY	2.3
2	E	70	PHE	2.2
2	H	48	LYS	2.2
2	E	48	LYS	2.2
2	E	74	GLU	2.2
2	E	15	ALA	2.1
2	E	19	LYS	2.1
2	H	70	PHE	2.1
1	G	219	ARG	2.1
1	G	269	PRO	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 carbohydrates 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	K	B	101	1/1	0.93	0.14	89,89,89,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.