



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 07:50 AM EDT

PDB ID : 1OAU
Title : Fv Structure of the IgE SPE-7 in complex with DNP-Ser (immunising hapten)
Authors : James, L.C.; Roversi, P.; Tawfik, D.
Deposited on : 2003-01-21
Resolution : 1.80 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:

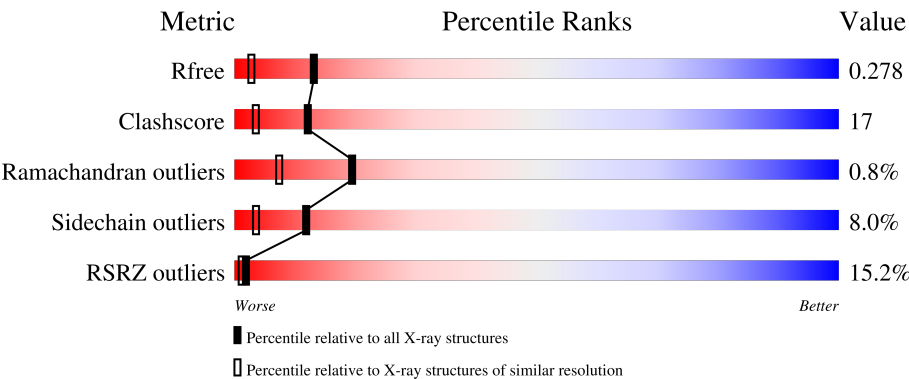
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	H	122	<div><div>2%</div><div>84%</div><div>14%</div><div></div></div>
1	I	122	<div><div>13%</div><div>11%</div><div>7%</div><div>82%</div></div>
1	J	122	<div><div>2%</div><div>84%</div><div>13%</div><div></div></div>
1	K	122	<div><div>16%</div><div>7%</div><div>11%</div><div>82%</div></div>
2	L	110	<div><div>%</div><div>82%</div><div>13%</div><div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	M	110	<div><div></div><div>25%</div><div>50%</div><div>25%</div><div>5%</div><div>•</div><div>18%</div></div>
2	N	110	<div><div>%</div><div></div><div>80%</div><div>15%</div><div>•••</div></div>
2	O	110	<div><div>30%</div><div>46%</div><div>30%</div><div>5%</div><div>•</div><div>16%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5631 atoms, of which 10 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.

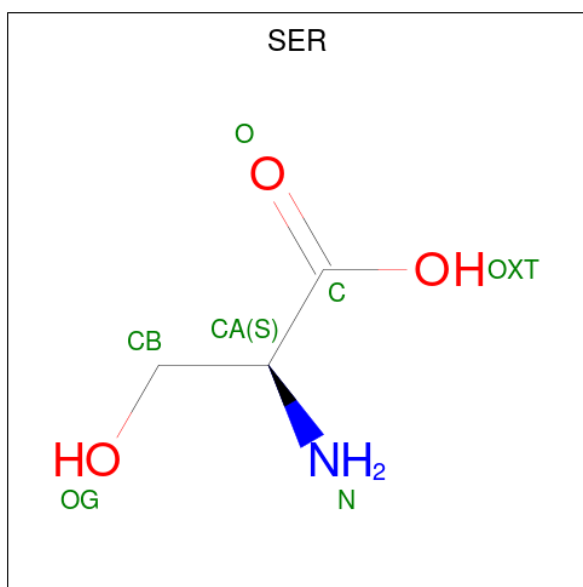
- Molecule 1 is a protein called IMMUNOGLOBULIN E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	122	Total	C	N	O	S	0	0	0
			964	617	158	184	5			
1	I	22	Total	C	N	O	S	0	0	1
			164	105	31	25	3			
1	J	122	Total	C	N	O	S	0	0	0
			964	617	158	184	5			
1	K	22	Total	C	N	O	S	0	0	1
			163	103	30	28	2			

- Molecule 2 is a protein called IMMUNOGLOBULIN E.

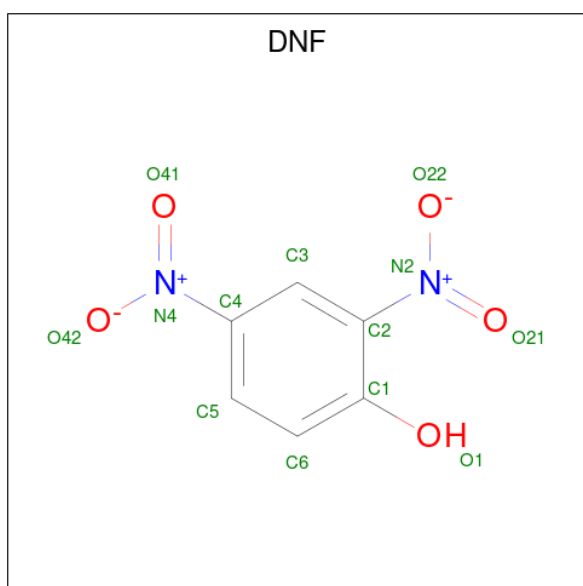
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	108	Total	C	N	O	S	0	0	0
			795	500	135	158	2			
2	M	90	Total	C	N	O	S	0	0	0
			661	411	113	135	2			
2	N	108	Total	C	N	O	S	0	0	0
			795	500	135	158	2			
2	O	92	Total	C	N	O	S	0	0	0
			672	417	115	138	2			

- Molecule 3 is SERINE (three-letter code: SER) (formula: C₃H₇NO₃).



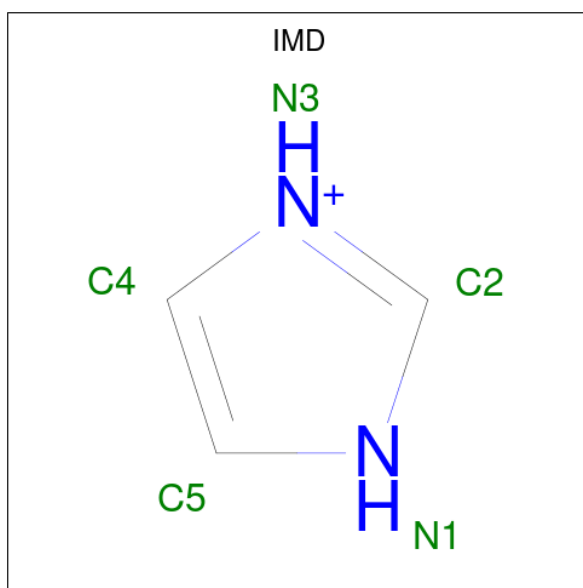
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			7	3	1	3		
3	J	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 4 is 2,4-DINITROPHENOL (three-letter code: DNF) (formula: $C_6H_4N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			12	6	2	4		
4	J	1	Total	C	N	O	0	0
			12	6	2	4		

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	H	N	0	0
			10	3	5	2		
5	N	1	Total	C	H	N	0	0
			10	3	5	2		

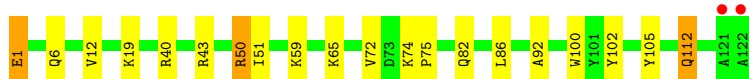
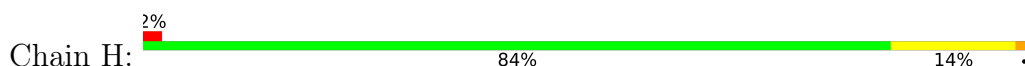
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	112	Total	O	0	0
			112	112		
6	I	3	Total	O	0	0
			3	3		
6	J	70	Total	O	0	0
			70	70		
6	K	10	Total	O	0	0
			10	10		
6	L	105	Total	O	0	0
			105	105		
6	M	25	Total	O	0	0
			25	25		
6	N	53	Total	O	0	0
			53	53		
6	O	17	Total	O	0	0
			17	17		

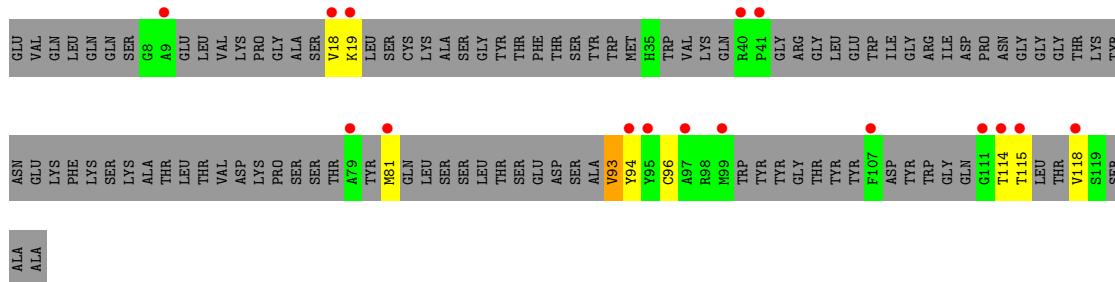
3 Residue-property plots [i](#)

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.

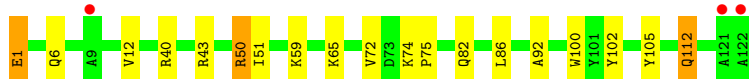
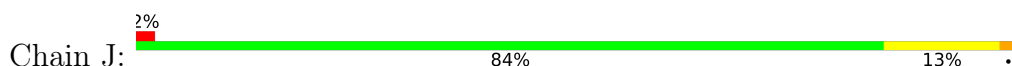
- Molecule 1: IMMUNOGLOBULIN E



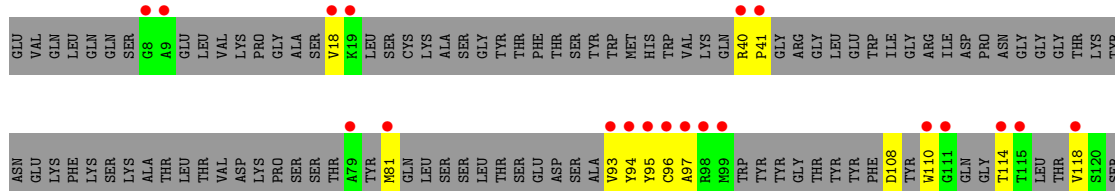
- Molecule 1: IMMUNOGLOBULIN E



- Molecule 1: IMMUNOGLOBULIN E




- Molecule 1: IMMUNOGLOBULIN E



ALA
ALA

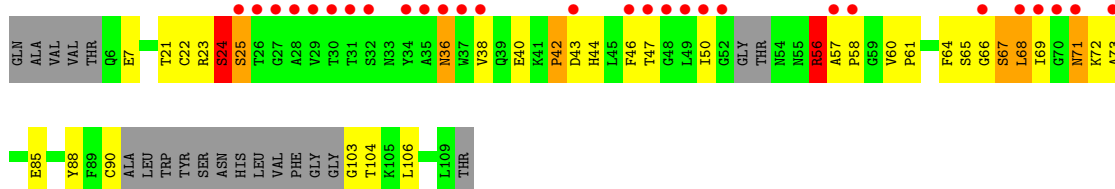
● Molecule 2: IMMUNOGLOBULIN E

Chain L:  82% 13% ...




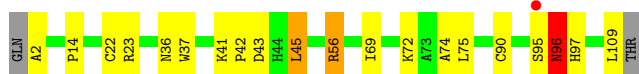
● Molecule 2: IMMUNOGLOBULIN E

Chain M:  25% 50% 25% 5% 18%



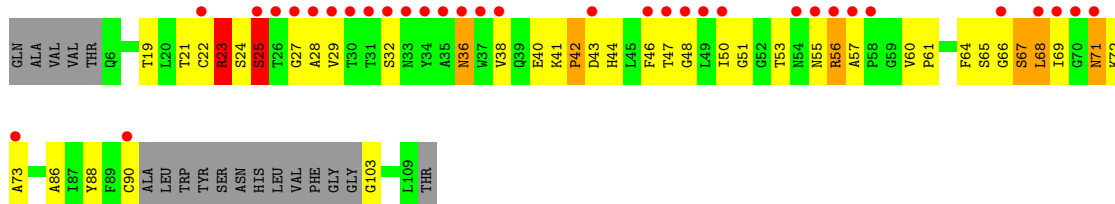
● Molecule 2: IMMUNOGLOBULIN E

Chain N:  80% 15% ...



● Molecule 2: IMMUNOGLOBULIN E

Chain O:  30% 46% 30% 5% 16%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.46Å 79.48Å 168.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.02 – 1.80 30.05 – 1.81	Depositor EDS
% Data completeness (in resolution range)	91.4 (30.02-1.80) 91.6 (30.05-1.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.226 , 0.264 0.271 , 0.278	Depositor DCC
R_{free} test set	4529 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.479 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5631	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.45% 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

5.1 Standard geometry

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

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	H	0.45	0/992	0.58	0/1345
1	I	0.24	0/158	0.41	0/196
1	J	0.45	0/992	0.58	0/1345
1	K	0.23	0/155	0.40	0/194
2	L	0.50	0/811	0.60	0/1109
2	M	0.75	1/669 (0.1%)	0.90	6/908 (0.7%)
2	N	0.50	0/811	0.60	0/1109
2	O	0.76	2/681 (0.3%)	0.73	2/926 (0.2%)
All	All	0.55	3/5269 (0.1%)	0.65	8/7132 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
2	M	0	3
2	N	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	56	ARG	C-N	-10.83	1.09	1.34
2	O	25	SER	N-CA	10.73	1.67	1.46
2	O	25	SER	CA-C	-7.61	1.33	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	24	SER	O-C-N	-9.81	107.00	122.70
2	M	56	ARG	C-N-CA	-8.44	100.61	121.70
2	M	56	ARG	CA-C-N	-7.20	101.36	117.20
2	O	25	SER	CB-CA-C	7.06	123.51	110.10
2	M	24	SER	CB-CA-C	-6.86	97.06	110.10
2	M	24	SER	C-N-CA	5.72	135.99	121.70
2	M	25	SER	CA-C-N	-5.50	105.10	117.20
2	O	25	SER	CA-C-O	-5.26	109.06	120.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	96	ASN	Mainchain
2	M	24	SER	Mainchain
2	M	25	SER	Mainchain
2	M	56	ARG	Mainchain
2	N	96	ASN	Mainchain

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	H	964	0	924	20	0
1	I	164	0	154	6	0
1	J	964	0	924	19	0
1	K	163	0	144	9	0
2	L	795	0	779	18	0
2	M	661	0	644	22	0
2	N	795	0	779	18	0
2	O	672	0	657	61	0
3	H	7	0	4	0	0
3	J	7	0	4	0	0
4	H	12	0	3	1	0
4	J	12	0	3	1	0
5	L	5	5	5	0	0
5	N	5	5	5	0	0
6	H	112	0	0	7	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	3	0	0	2	0
6	J	70	0	0	5	0
6	K	10	0	0	3	0
6	L	105	0	0	4	1
6	M	25	0	0	1	0
6	N	53	0	0	3	0
6	O	17	0	0	0	0
All	All	5621	10	5029	172	1

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 17.

All (172) 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:O:25:SER:N	2:O:25:SER:CA	1.67	1.55
2:O:24:SER:HB3	2:O:29:VAL:N	1.56	1.18
2:O:23:ARG:HA	2:O:72:LYS:HA	1.37	1.03
2:O:24:SER:N	2:O:29:VAL:HG23	1.75	1.01
2:O:24:SER:HB2	2:O:29:VAL:HG22	1.40	1.00
2:N:23:ARG:HD2	2:N:72:LYS:HD3	1.47	0.94
2:L:23:ARG:HD2	2:L:72:LYS:HD3	1.49	0.94
1:J:112:GLN:HE21	1:J:112:GLN:H	1.15	0.93
1:K:96:CYS:HB2	6:K:2010:HOH:O	1.68	0.91
2:O:24:SER:HB2	2:O:29:VAL:CG2	2.01	0.91
2:N:96:ASN:OD1	2:N:97:HIS:ND1	2.05	0.90
2:O:24:SER:CB	2:O:29:VAL:CG2	2.50	0.89
1:H:112:GLN:H	1:H:112:GLN:HE21	1.15	0.88
2:L:96:ASN:OD1	2:L:97:HIS:ND1	2.05	0.88
2:O:56:ARG:HD3	2:O:64:PHE:O	1.77	0.84
1:J:12:VAL:HG21	1:J:86:LEU:HD13	1.61	0.82
2:O:53:THR:HG21	2:O:68:LEU:HD21	1.61	0.82
1:H:12:VAL:HG21	1:H:86:LEU:HD13	1.61	0.82
2:O:23:ARG:NE	2:O:71:ASN:O	2.16	0.79
2:O:23:ARG:HA	2:O:72:LYS:CA	2.09	0.79
2:O:24:SER:HB3	2:O:29:VAL:CA	2.15	0.77
2:O:24:SER:CB	2:O:29:VAL:HG23	2.14	0.77
1:H:12:VAL:HG21	1:H:86:LEU:CD1	2.15	0.77
1:J:12:VAL:HG21	1:J:86:LEU:CD1	2.15	0.76
2:N:36:ASN:HB2	6:N:2027:HOH:O	1.88	0.74
1:J:6:GLN:H	1:J:112:GLN:HE22	1.35	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:24:SER:HB3	2:O:28:ALA:C	2.06	0.74
2:O:23:ARG:HD2	2:O:72:LYS:HD2	1.68	0.74
1:H:6:GLN:H	1:H:112:GLN:HE22	1.35	0.72
1:I:19:LYS:HB3	6:I:2001:HOH:O	1.89	0.71
1:J:51:ILE:HD13	1:J:72:VAL:HG13	1.72	0.71
1:H:51:ILE:HD13	1:H:72:VAL:HG13	1.72	0.71
1:J:65:LYS:HG2	6:J:2044:HOH:O	1.90	0.71
2:N:56:ARG:NH2	6:N:2034:HOH:O	2.23	0.71
2:L:36:ASN:HB2	6:L:2050:HOH:O	1.91	0.71
2:O:24:SER:CB	2:O:29:VAL:N	2.47	0.68
1:K:94:TYR:O	1:K:114:THR:N	2.28	0.67
1:I:94:TYR:O	1:I:114:THR:N	2.28	0.66
2:L:95:SER:OG	6:L:2095:HOH:O	2.15	0.65
2:O:71:ASN:N	2:O:71:ASN:OD1	2.30	0.65
2:O:24:SER:CB	2:O:29:VAL:CA	2.75	0.65
2:M:71:ASN:N	2:M:71:ASN:OD1	2.30	0.65
2:O:25:SER:N	2:O:25:SER:C	2.44	0.64
2:O:68:LEU:HD23	2:O:68:LEU:N	2.13	0.64
2:O:21:THR:HB	2:O:72:LYS:HE2	1.81	0.63
2:O:56:ARG:HB2	2:O:56:ARG:CZ	2.27	0.63
1:J:74:LYS:HE3	6:J:2048:HOH:O	1.97	0.63
2:M:22:CYS:HB3	2:M:73:ALA:HB3	1.80	0.63
1:J:50:ARG:HD3	4:J:501:DNF:O22	1.99	0.63
2:M:21:THR:HB	2:M:72:LYS:HE2	1.81	0.63
2:M:68:LEU:N	2:M:68:LEU:HD23	2.13	0.62
2:N:22:CYS:CB	2:N:90:CYS:HG	2.11	0.62
1:H:50:ARG:HD3	4:H:501:DNF:O22	1.99	0.62
1:H:112:GLN:HE21	1:H:112:GLN:N	1.93	0.62
1:H:19:LYS:HE3	6:H:2020:HOH:O	1.98	0.61
1:K:97:ALA:HB2	1:K:110:TRP:HA	1.82	0.61
6:H:2098:HOH:O	2:O:69:ILE:HG13	2.01	0.61
2:O:24:SER:CA	2:O:29:VAL:HG23	2.30	0.61
1:J:112:GLN:HE21	1:J:112:GLN:N	1.93	0.60
2:M:36:ASN:O	2:M:90:CYS:HA	2.00	0.60
2:O:23:ARG:HE	2:O:72:LYS:HG3	1.66	0.60
2:O:24:SER:CB	2:O:29:VAL:HG22	2.17	0.59
2:N:22:CYS:CB	2:N:90:CYS:SG	2.91	0.59
2:O:23:ARG:CD	2:O:72:LYS:HD2	2.31	0.59
2:O:88:TYR:O	2:O:103:GLY:HA2	2.01	0.59
1:K:108:ASP:HA	2:O:48:GLY:HA3	1.85	0.59
1:H:112:GLN:H	1:H:112:GLN:NE2	1.95	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:22:CYS:HG	2:L:90:CYS:HG	0.62	0.58
2:L:56:ARG:NH2	6:L:2070:HOH:O	2.36	0.58
2:N:22:CYS:HG	2:N:90:CYS:HG	0.58	0.58
2:L:47:THR:HG22	6:L:2060:HOH:O	2.02	0.58
2:L:23:ARG:HD2	2:L:72:LYS:CD	2.27	0.58
2:O:61:PRO:HG2	2:O:64:PHE:CD1	2.39	0.58
2:M:38:VAL:HG13	2:M:47:THR:O	2.04	0.58
2:O:24:SER:N	2:O:29:VAL:CG2	2.60	0.57
1:H:74:LYS:HB2	1:H:75:PRO:HD3	1.87	0.57
6:H:2098:HOH:O	2:O:69:ILE:HG21	2.04	0.57
2:M:61:PRO:HG2	2:M:64:PHE:CD1	2.39	0.57
6:J:2061:HOH:O	2:M:69:ILE:HG21	2.05	0.57
2:O:38:VAL:HG13	2:O:47:THR:O	2.04	0.57
2:O:53:THR:HG21	2:O:68:LEU:CD2	2.32	0.57
2:O:56:ARG:HD2	2:O:61:PRO:O	2.04	0.57
1:J:43:ARG:NH1	6:J:2029:HOH:O	2.27	0.56
1:J:74:LYS:HB2	1:J:75:PRO:HD3	1.87	0.56
2:L:22:CYS:CB	2:L:90:CYS:SG	2.93	0.56
2:N:42:PRO:O	2:N:43:ASP:HB2	2.05	0.56
1:J:12:VAL:CG2	1:J:86:LEU:HD13	2.34	0.56
2:L:22:CYS:CB	2:L:90:CYS:HG	2.16	0.56
2:L:42:PRO:O	2:L:43:ASP:HB2	2.05	0.55
2:M:43:ASP:OD1	2:M:43:ASP:O	2.25	0.55
2:L:23:ARG:CD	2:L:72:LYS:HD3	2.28	0.55
2:N:22:CYS:HB2	2:N:90:CYS:SG	2.47	0.54
2:O:43:ASP:O	2:O:43:ASP:OD1	2.25	0.54
1:H:12:VAL:CG2	1:H:86:LEU:HD13	2.34	0.53
1:H:43:ARG:NH1	6:H:2048:HOH:O	2.28	0.53
2:M:40:GLU:HB2	2:M:46:PHE:CE2	2.44	0.53
2:O:40:GLU:HB2	2:O:46:PHE:CE2	2.44	0.52
1:H:74:LYS:HE3	6:H:2059:HOH:O	2.10	0.52
2:L:22:CYS:HB2	2:L:90:CYS:SG	2.50	0.52
2:M:61:PRO:HG2	2:M:64:PHE:HD1	1.74	0.52
2:O:23:ARG:NE	2:O:72:LYS:HG3	2.18	0.52
2:O:61:PRO:HG2	2:O:64:PHE:HD1	1.74	0.52
2:O:23:ARG:HE	2:O:71:ASN:C	2.10	0.51
2:O:24:SER:CB	2:O:29:VAL:HA	2.40	0.51
2:O:24:SER:CB	2:O:28:ALA:C	2.76	0.51
2:L:69:ILE:HD12	2:L:74:ALA:CB	2.40	0.51
2:N:69:ILE:HD12	2:N:74:ALA:CB	2.40	0.51
1:J:1:GLU:HB2	6:J:2001:HOH:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:24:SER:HB3	2:O:29:VAL:HG23	1.90	0.50
2:O:50:ILE:HD13	2:O:66:GLY:N	2.26	0.50
1:K:94:TYR:HA	6:K:2007:HOH:O	2.12	0.50
2:O:23:ARG:C	2:O:29:VAL:HG23	2.31	0.50
2:O:24:SER:OG	2:O:27:GLY:O	2.29	0.49
2:O:23:ARG:HG3	2:O:24:SER:N	2.26	0.49
2:M:50:ILE:HD13	2:M:66:GLY:N	2.28	0.49
1:J:112:GLN:H	1:J:112:GLN:NE2	1.95	0.49
1:J:50:ARG:NH2	1:J:59:LYS:HD2	2.28	0.48
1:J:100:TRP:O	1:J:105:TYR:HA	2.14	0.48
1:H:100:TRP:O	1:H:105:TYR:HA	2.14	0.48
2:M:57:ALA:O	2:M:60:VAL:HB	2.13	0.48
1:H:1:GLU:O	1:H:1:GLU:HG2	2.13	0.48
1:H:50:ARG:NH2	1:H:59:LYS:HD2	2.28	0.48
1:J:1:GLU:HG2	1:J:1:GLU:O	2.13	0.48
2:O:36:ASN:O	2:O:90:CYS:HA	2.14	0.48
2:O:24:SER:HB3	2:O:29:VAL:CG2	2.39	0.47
2:O:57:ALA:O	2:O:60:VAL:HB	2.13	0.47
2:N:2:ALA:N	6:N:2005:HOH:O	2.49	0.46
1:J:40:ARG:CG	1:J:92:ALA:HB2	2.46	0.46
1:J:40:ARG:HG2	1:J:92:ALA:HB2	1.98	0.46
2:N:23:ARG:HD2	2:N:72:LYS:CD	2.32	0.46
1:H:40:ARG:CG	1:H:92:ALA:HB2	2.46	0.46
1:I:93:VAL:N	6:I:2003:HOH:O	2.48	0.46
2:M:50:ILE:CD1	2:M:66:GLY:N	2.79	0.46
2:M:58:PRO:HD2	6:M:2014:HOH:O	2.16	0.45
2:L:42:PRO:O	2:L:45:LEU:HD22	2.17	0.45
2:N:36:ASN:O	2:N:90:CYS:HA	2.17	0.44
2:N:42:PRO:O	2:N:45:LEU:HD22	2.17	0.44
2:O:24:SER:CA	2:O:29:VAL:CG2	2.93	0.44
2:O:53:THR:CG2	2:O:68:LEU:CD2	2.95	0.44
2:O:23:ARG:C	2:O:29:VAL:CG2	2.86	0.44
1:H:40:ARG:HG2	1:H:92:ALA:HB2	1.98	0.44
2:L:36:ASN:O	2:L:90:CYS:HA	2.17	0.44
2:M:67:SER:C	2:M:68:LEU:HD23	2.38	0.43
2:M:42:PRO:O	2:M:43:ASP:HB3	2.18	0.43
2:O:67:SER:C	2:O:68:LEU:HD23	2.38	0.43
2:M:36:ASN:O	2:M:90:CYS:CA	2.64	0.43
2:O:42:PRO:O	2:O:43:ASP:HB3	2.18	0.43
2:O:51:GLY:O	2:O:55:ASN:HB2	2.19	0.42
1:K:95:TYR:CD2	1:K:95:TYR:N	2.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:7:GLU:O	2:M:104:THR:OG1	2.29	0.42
2:M:88:TYR:O	2:M:103:GLY:HA2	2.19	0.42
2:O:29:VAL:HG11	2:O:73:ALA:HB2	2.02	0.42
1:K:118:VAL:O	1:K:118:VAL:HG12	2.19	0.41
2:L:37:TRP:CD2	2:L:75:LEU:HB2	2.55	0.41
2:O:22:CYS:HB3	2:O:73:ALA:HB3	2.01	0.41
2:N:37:TRP:CD2	2:N:75:LEU:HB2	2.55	0.41
2:M:85:GLU:HG3	2:M:106:LEU:O	2.20	0.41
1:K:40:ARG:HA	1:K:41:PRO:HD3	1.83	0.41
2:N:14:PRO:HD3	2:N:109:LEU:O	2.20	0.41
2:N:43:ASP:HB2	2:N:45:LEU:HD22	2.02	0.41
2:O:25:SER:N	2:O:25:SER:CB	2.71	0.41
1:I:96:CYS:O	1:I:96:CYS:SG	2.79	0.41
2:M:23:ARG:CG	2:M:24:SER:N	2.84	0.41
1:I:118:VAL:O	1:I:118:VAL:HG12	2.19	0.41
2:L:43:ASP:HB2	2:L:45:LEU:HD22	2.02	0.41
2:N:42:PRO:O	2:N:43:ASP:CB	2.69	0.41
6:H:2098:HOH:O	2:O:19:THR:HG21	2.21	0.40
2:O:41:LYS:CD	2:O:86:ALA:HB2	2.51	0.40
1:H:6:GLN:H	1:H:112:GLN:NE2	2.12	0.40
1:I:114:THR:HG22	1:I:115:THR:N	2.37	0.40
1:K:40:ARG:O	6:K:2003:HOH:O	2.22	0.40
1:H:65:LYS:HG2	6:H:2071:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:2025:HOH:O	6:L:2073:HOH:O[4_466]	2.19	0.01

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	H	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
1	I	5/122 (4%)	5 (100%)	0	0	100	100
1	J	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
1	K	5/122 (4%)	5 (100%)	0	0	100	100
2	L	106/110 (96%)	97 (92%)	8 (8%)	1 (1%)	17	6
2	M	83/110 (76%)	75 (90%)	7 (8%)	1 (1%)	13	3
2	N	106/110 (96%)	97 (92%)	8 (8%)	1 (1%)	17	6
2	O	86/110 (78%)	75 (87%)	9 (10%)	2 (2%)	6	1
All	All	631/928 (68%)	588 (93%)	38 (6%)	5 (1%)	19	7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	O	23	ARG
2	L	96	ASN
2	N	96	ASN
2	M	42	PRO
2	O	42	PRO

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	H	101/101 (100%)	96 (95%)	5 (5%)	24	10
1	I	16/101 (16%)	13 (81%)	3 (19%)	1	0
1	J	101/101 (100%)	96 (95%)	5 (5%)	24	10
1	K	15/101 (15%)	12 (80%)	3 (20%)	1	0
2	L	85/87 (98%)	81 (95%)	4 (5%)	26	12
2	M	72/87 (83%)	64 (89%)	8 (11%)	6	1
2	N	85/87 (98%)	81 (95%)	4 (5%)	26	12
2	O	73/87 (84%)	63 (86%)	10 (14%)	3	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	548/752 (73%)	506 (92%)	42 (8%)	12 4

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	GLU
1	H	50	ARG
1	H	82	GLN
1	H	102	TYR
1	H	112	GLN
1	I	18	VAL
1	I	81	MET
1	I	93	VAL
1	J	1	GLU
1	J	50	ARG
1	J	82	GLN
1	J	102	TYR
1	J	112	GLN
1	K	18	VAL
1	K	81	MET
1	K	93	VAL
2	L	41	LYS
2	L	45	LEU
2	L	56	ARG
2	L	95	SER
2	M	24	SER
2	M	36	ASN
2	M	44	HIS
2	M	56	ARG
2	M	65	SER
2	M	67	SER
2	M	68	LEU
2	M	71	ASN
2	N	41	LYS
2	N	45	LEU
2	N	56	ARG
2	N	95	SER
2	O	23	ARG
2	O	25	SER
2	O	32	SER
2	O	36	ASN
2	O	44	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	56	ARG
2	O	65	SER
2	O	67	SER
2	O	68	LEU
2	O	71	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	5	GLN
1	H	112	GLN
1	J	5	GLN
1	J	112	GLN
2	L	36	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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
5	IMD	N	200	-	3,5,5	0.41	0	4,5,5	0.60	0
3	SER	J	500	4	5,6,6	0.42	0	5,7,7	7.07	3 (60%)
3	SER	H	500	4	5,6,6	0.42	0	5,7,7	7.08	3 (60%)
5	IMD	L	200	-	3,5,5	0.42	0	4,5,5	0.60	0
4	DNF	H	501	3	10,12,13	1.29	0	12,16,18	3.22	10 (83%)
4	DNF	J	501	3	10,12,13	1.28	0	12,16,18	3.24	10 (83%)

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
5	IMD	N	200	-	-	-	0/1/1/1
3	SER	J	500	4	-	3/6/6/6	-
3	SER	H	500	4	-	3/6/6/6	-
5	IMD	L	200	-	-	-	0/1/1/1
4	DNF	H	501	3	-	0/4/8/8	0/1/1/1
4	DNF	J	501	3	-	0/4/8/8	0/1/1/1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	500	SER	OXT-C-O	-13.53	93.38	124.09
3	J	500	SER	OXT-C-O	-13.51	93.41	124.09
3	H	500	SER	OXT-C-CA	7.52	139.01	113.38
3	J	500	SER	OXT-C-CA	7.51	138.98	113.38
4	J	501	DNF	C5-C4-N4	-5.44	115.28	119.38
4	H	501	DNF	C5-C4-N4	-5.40	115.31	119.38
4	J	501	DNF	C5-C4-C3	5.07	126.51	120.09
4	H	501	DNF	C5-C4-C3	5.06	126.51	120.09
4	J	501	DNF	O21-N2-C2	4.19	124.73	118.80
4	H	501	DNF	O21-N2-C2	4.18	124.72	118.80
4	J	501	DNF	C6-C5-C4	-3.71	114.25	119.41
4	H	501	DNF	C6-C5-C4	-3.68	114.29	119.41
3	H	500	SER	OG-CB-CA	3.16	119.20	110.85
3	J	500	SER	OG-CB-CA	3.15	119.17	110.85
4	J	501	DNF	C3-C2-N2	-3.12	115.99	118.75
4	H	501	DNF	C3-C2-N2	-3.07	116.04	118.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	501	DNF	C1-C2-N2	2.55	121.30	119.38
4	H	501	DNF	C1-C2-N2	2.54	121.28	119.38
4	J	501	DNF	C5-C6-C1	2.31	123.52	120.25
4	H	501	DNF	C5-C6-C1	2.30	123.52	120.25
4	J	501	DNF	O41-N4-C4	-2.24	115.63	118.80
4	H	501	DNF	O41-N4-C4	-2.23	115.64	118.80
4	J	501	DNF	C4-C3-C2	-2.09	116.23	119.57
4	J	501	DNF	C1-C2-C3	2.07	122.72	120.09
4	H	501	DNF	C4-C3-C2	-2.07	116.27	119.57
4	H	501	DNF	C1-C2-C3	2.04	122.67	120.09

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	500	SER	N-CA-CB-OG
3	H	500	SER	C-CA-CB-OG
3	J	500	SER	N-CA-CB-OG
3	J	500	SER	C-CA-CB-OG
3	H	500	SER	OXT-C-CA-N
3	J	500	SER	OXT-C-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	501	DNF	1	0
4	J	501	DNF	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	M	2

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
1	I	1
1	K	1
2	O	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	111:GLY	C	114:THR	N	8.17
1	M	50:ILE	C	52:GLY	N	5.31
1	K	118:VAL	C	120:SER	N	4.83
1	O	24:SER	C	25:SER	N	3.98
1	M	56:ARG	C	57:ALA	N	1.09

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	H	122/122 (100%)	0.04	2 (1%) 72 68	21, 30, 47, 54	0
1	I	22/122 (18%)	3.63	16 (72%) 0 0	75, 83, 90, 105	0
1	J	122/122 (100%)	0.03	3 (2%) 57 52	21, 30, 47, 54	0
1	K	22/122 (18%)	5.89	20 (90%) 0 0	90, 98, 108, 112	0
2	L	108/110 (98%)	-0.05	1 (0%) 84 82	22, 28, 38, 42	0
2	M	90/110 (81%)	1.89	28 (31%) 0 0	30, 51, 85, 94	0
2	N	108/110 (98%)	-0.03	1 (0%) 84 82	21, 28, 37, 42	0
2	O	92/110 (83%)	2.04	33 (35%) 0 0	34, 57, 87, 97	0
All	All	686/928 (73%)	0.83	104 (15%) 2 1	21, 34, 87, 112	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	18	VAL	11.8
1	K	118	VAL	11.6
1	K	40	ARG	10.5
2	M	58	PRO	10.4
2	M	27	GLY	8.9
2	O	56	ARG	7.9
2	O	34	TYR	7.9
2	O	70	GLY	7.9
2	O	55	ASN	7.9
1	K	95	TYR	7.8
2	O	58	PRO	7.8
1	K	81	MET	7.8
2	O	35	ALA	7.8
2	M	34	TYR	7.7
2	M	71	ASN	7.4
1	I	79	ALA	7.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	9	ALA	7.1
1	K	114	THR	7.1
1	I	18	VAL	7.0
1	K	98	ARG	6.9
1	K	111	GLY	6.7
2	O	43	ASP	6.6
1	K	96	CYS	6.6
2	M	52	GLY	6.3
1	K	94	TYR	6.3
1	K	115	THR	6.2
1	I	40	ARG	6.0
2	O	38	VAL	5.9
2	O	26	THR	5.9
2	M	28	ALA	5.7
2	O	57	ALA	5.6
2	M	32	SER	5.6
2	O	25	SER	5.6
1	K	19	LYS	5.6
2	O	32	SER	5.5
2	M	29	VAL	5.4
1	I	111	GLY	5.3
2	O	30	THR	5.3
2	M	43	ASP	5.3
2	O	71	ASN	5.2
1	I	81	MET	5.2
2	O	69	ILE	5.1
2	M	68	LEU	5.1
1	I	19	LYS	5.1
2	M	26	THR	5.1
2	M	57	ALA	5.1
2	M	25	SER	5.1
2	O	54	ASN	5.1
2	M	35	ALA	4.9
2	O	31	THR	4.9
1	K	110	TRP	4.9
2	M	70	GLY	4.8
2	O	68	LEU	4.7
1	I	118	VAL	4.7
2	M	38	VAL	4.7
2	M	36	ASN	4.6
1	I	114	THR	4.6
2	M	31	THR	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	122	ALA	4.5
1	K	97	ALA	4.3
1	I	107	PHE	4.3
2	O	37	TRP	4.1
1	I	94	TYR	4.1
2	O	36	ASN	4.0
1	I	95	TYR	3.9
2	M	30	THR	3.9
2	M	46	PHE	3.9
1	I	97	ALA	3.8
2	O	28	ALA	3.6
2	M	48	GLY	3.6
1	J	122	ALA	3.6
2	O	46	PHE	3.6
2	N	95	SER	3.4
2	M	47	THR	3.4
1	K	93	VAL	3.4
1	K	79	ALA	3.3
2	O	47	THR	3.3
1	K	41	PRO	3.2
2	O	66	GLY	3.2
2	O	48	GLY	3.2
2	L	95	SER	3.1
2	M	69	ILE	3.1
1	K	99	MET	3.1
2	O	29	VAL	3.0
2	M	66	GLY	2.9
2	O	22	CYS	2.9
2	M	50	ILE	2.8
2	O	50	ILE	2.8
1	I	99	MET	2.8
1	I	9	ALA	2.8
1	I	115	THR	2.7
2	O	49	LEU	2.6
1	J	9	ALA	2.6
1	K	8	GLY	2.6
2	M	37	TRP	2.6
2	O	27	GLY	2.6
2	O	73	ALA	2.5
2	M	73	ALA	2.4
1	H	121	ALA	2.4
1	J	121	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	41	PRO	2.4
2	O	33	ASN	2.3
2	M	49	LEU	2.3
2	O	90	CYS	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 monosaccharides 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(\AA^2)	Q<0.9
5	IMD	L	200	5/5	0.70	0.20	20,20,20,20	0
5	IMD	N	200	5/5	0.78	0.25	20,20,20,20	0
3	SER	H	500	7/7	0.79	0.13	39,44,50,56	0
3	SER	J	500	7/7	0.84	0.13	39,44,50,56	0
4	DNF	J	501	12/13	0.94	0.11	29,33,44,45	0
4	DNF	H	501	12/13	0.96	0.11	29,33,44,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.