



# Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2021 – 02:07 pm BST

PDB ID : 6RLM  
Title : Crystal structure of AT1412dm Fab fragment  
Authors : Neviani, V.; Pearce, N.M.; Pos, W.; Schotte, R.; Spits, H.; Gros, P.  
Deposited on : 2019-05-02  
Resolution : 2.50 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](mailto: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.

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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 : 2.18  
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) : 2.18

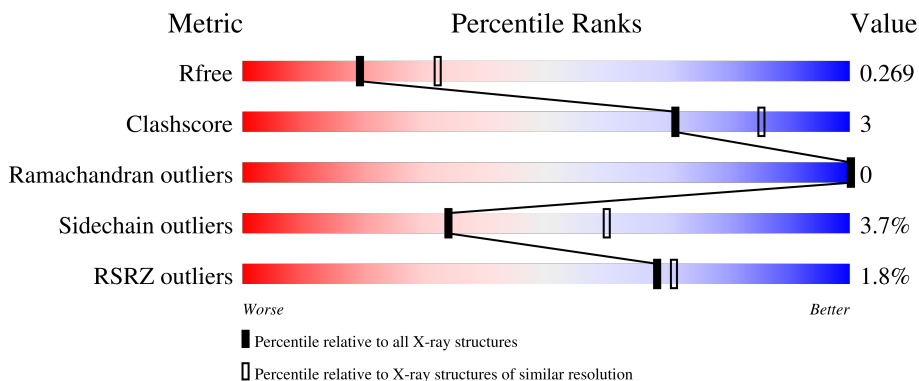
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	227	86% 9% 5%
1	C	227	87% 7% 6%
1	E	227	89% 7% . .
1	G	227	88% 6% 6%
1	I	227	90% 7% .

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Mol	Chain	Length	Quality of chain
1	K	227	<p>% 86% 7% 7%</p>
1	M	227	<p>% 89% 6% 5%</p>
1	O	227	<p>5% 82% 8% 9%</p>
2	B	220	<p>88% 11% .</p>
2	D	220	<p>% 88% 10% ..</p>
2	F	220	<p>90% 9% .</p>
2	H	220	<p>% 89% 10% ..</p>
2	J	220	<p>% 89% 10% .</p>
2	L	220	<p>2% 89% 10% .</p>
2	N	220	<p>% 86% 13%</p>
2	P	220	<p>7% 85% 14% .</p>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 26544 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 AT1412dm Fab (Heavy Chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	Total 1630	C 1041	N 271	O 313	S 5	0	0	0
1	C	214	Total 1622	C 1037	N 269	O 311	S 5	0	0	0
1	E	221	Total 1664	C 1060	N 277	O 322	S 5	0	0	0
1	G	213	Total 1613	C 1031	N 267	O 310	S 5	0	0	0
1	I	220	Total 1658	C 1057	N 276	O 320	S 5	0	0	0
1	K	211	Total 1601	C 1025	N 265	O 306	S 5	0	0	0
1	M	215	Total 1626	C 1039	N 270	O 312	S 5	0	0	0
1	O	206	Total 1566	C 1004	N 259	O 298	S 5	0	0	0

- Molecule 2 is a protein called AT1412dm Fab (Light Chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	219	Total 1697	C 1060	N 284	O 348	S 5	0	0	0
2	D	218	Total 1689	C 1056	N 283	O 345	S 5	0	0	0
2	F	219	Total 1697	C 1060	N 284	O 348	S 5	0	0	0
2	H	218	Total 1689	C 1056	N 283	O 345	S 5	0	0	0
2	J	219	Total 1697	C 1060	N 284	O 348	S 5	0	0	0
2	L	219	Total 1697	C 1060	N 284	O 348	S 5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	219	Total	C	N	O	S	0	0	0
			1697	1060	284	348	5			
2	P	219	Total	C	N	O	S	0	0	0
			1697	1060	284	348	5			


- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

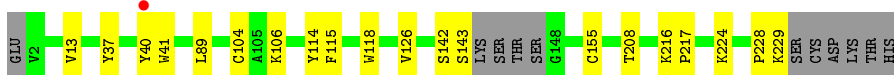
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Cl	0	0
			1	1		
3	G	1	Total	Cl	0	0
			1	1		
3	J	1	Total	Cl	0	0
			1	1		
3	K	1	Total	Cl	0	0
			1	1		

### 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.

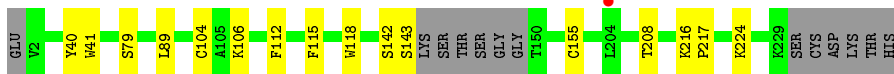
- Molecule 1: AT1412dm Fab (Heavy Chain)

Chain A: 




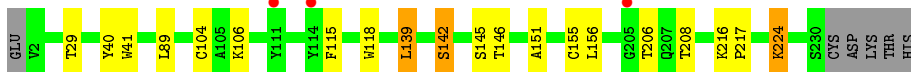
- Molecule 1: AT1412dm Fab (Heavy Chain)

Chain C: 




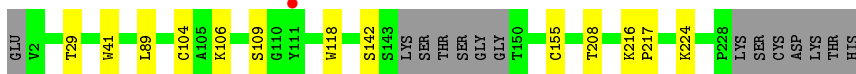
- Molecule 1: AT1412dm Fab (Heavy Chain)

Chain E: 




- Molecule 1: AT1412dm Fab (Heavy Chain)

Chain G: 

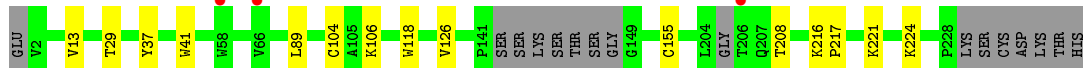
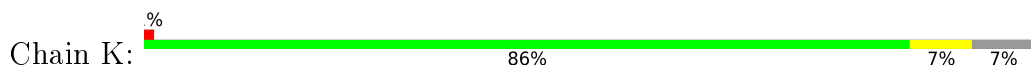


- Molecule 1: AT1412dm Fab (Heavy Chain)

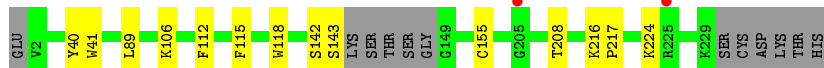
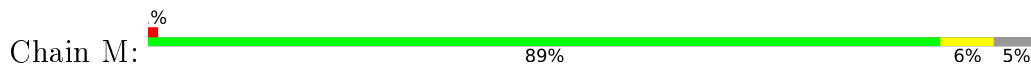
Chain I: 



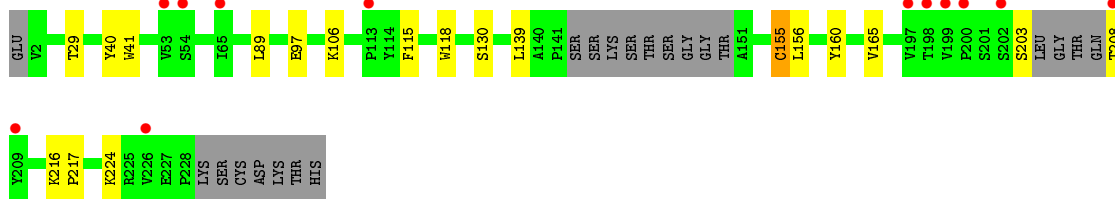
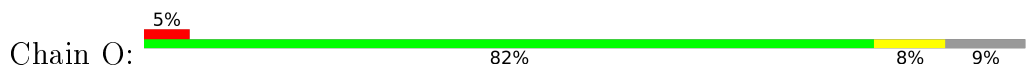
- Molecule 1: AT1412dm Fab (Heavy Chain)



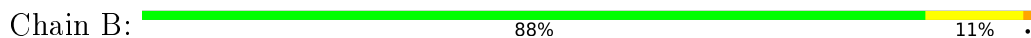
- Molecule 1: AT1412dm Fab (Heavy Chain)



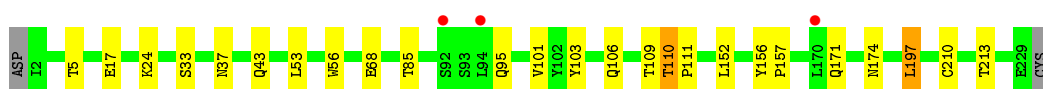
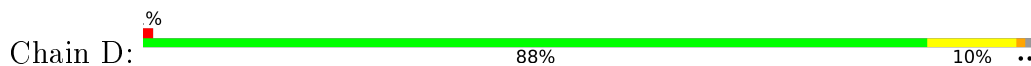
- Molecule 1: AT1412dm Fab (Heavy Chain)



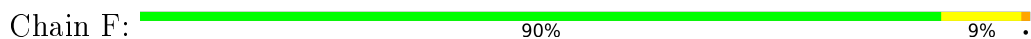
- Molecule 2: AT1412dm Fab (Light Chain)



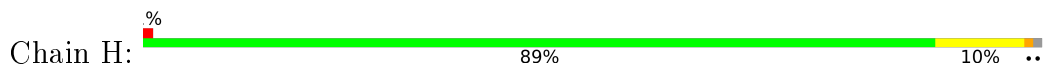
- Molecule 2: AT1412dm Fab (Light Chain)



- Molecule 2: AT1412dm Fab (Light Chain)

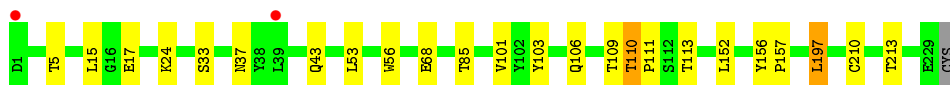
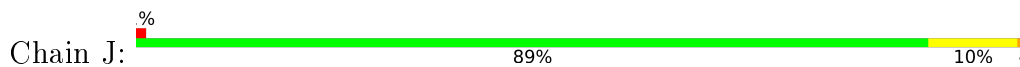


- Molecule 2: AT1412dm Fab (Light Chain)

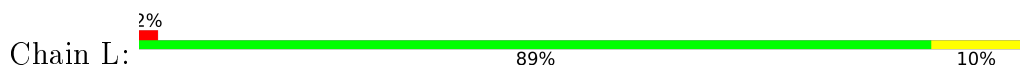




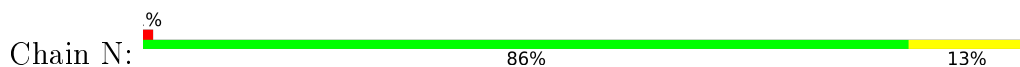
- Molecule 2: AT1412dm Fab (Light Chain)



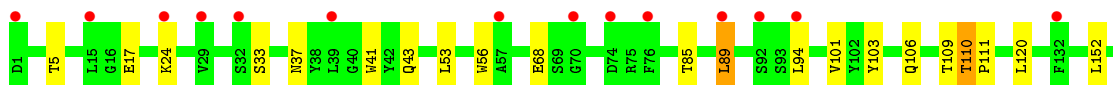
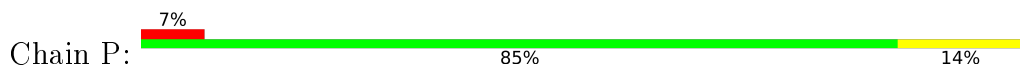
- Molecule 2: AT1412dm Fab (Light Chain)



- Molecule 2: AT1412dm Fab (Light Chain)



- Molecule 2: AT1412dm Fab (Light Chain)





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	224.91Å 238.59Å 209.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	163.66 – 2.50 163.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (163.66-2.50) 99.4 (163.66-2.50)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.52Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.242 , 0.267 0.246 , 0.269	Depositor DCC
$R_{free}$ test set	9440 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.6	Xtrriage
Anisotropy	0.607	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 39.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	26544	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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:  
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	0.68	0/1673	0.84	0/2280
1	C	0.70	0/1665	0.84	0/2270
1	E	0.70	0/1708	0.86	0/2328
1	G	0.67	0/1656	0.84	0/2259
1	I	0.69	0/1702	0.83	0/2320
1	K	0.66	0/1643	0.82	0/2240
1	M	0.67	0/1669	0.83	0/2275
1	O	0.69	0/1608	0.85	0/2192
2	B	0.68	0/1734	0.84	0/2356
2	D	0.70	0/1726	0.84	0/2345
2	F	0.72	0/1734	0.84	0/2356
2	H	0.70	1/1726 (0.1%)	0.85	0/2345
2	J	0.70	0/1734	0.84	0/2356
2	L	0.70	0/1734	0.83	0/2356
2	N	0.71	0/1734	0.84	0/2356
2	P	0.69	0/1734	0.83	0/2356
All	All	0.69	1/27180 (0.0%)	0.84	0/36990

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	97	GLU	CD-OE1	5.07	1.31	1.25

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	1630	0	1585	12	0
1	C	1622	0	1579	9	0
1	E	1664	0	1621	11	0
1	G	1613	0	1566	6	0
1	I	1658	0	1616	8	0
1	K	1601	0	1555	7	0
1	M	1626	0	1582	6	0
1	O	1566	0	1519	10	0
2	B	1697	0	1637	15	0
2	D	1689	0	1630	14	0
2	F	1697	0	1637	12	0
2	H	1689	0	1630	13	0
2	J	1697	0	1637	13	0
2	L	1697	0	1637	13	0
2	N	1697	0	1637	17	0
2	P	1697	0	1637	24	0
3	C	1	0	0	0	0
3	G	1	0	0	0	0
3	J	1	0	0	1	0
3	K	1	0	0	0	0
All	All	26544	0	25705	182	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 (182) 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:P:41:TRP:CG	2:P:89:LEU:HD23	1.61	1.36
2:P:41:TRP:CD2	2:P:89:LEU:HD23	2.02	0.95
2:P:41:TRP:CG	2:P:89:LEU:CD2	2.50	0.94
2:P:41:TRP:CD1	2:P:89:LEU:HD23	2.09	0.88
2:P:162:VAL:HG22	2:P:177:GLU:OE2	1.80	0.81
1:E:139:LEU:HD11	1:E:156:LEU:HB2	1.68	0.75
2:P:162:VAL:CG2	2:P:177:GLU:OE2	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:106:GLN:HE22	2:D:109:THR:CG2	2.09	0.66
2:H:106:GLN:HE22	2:H:109:THR:CG2	2.08	0.66
2:B:106:GLN:HE22	2:B:109:THR:CG2	2.08	0.66
1:I:142:SER:H	1:I:145:SER:HB3	1.60	0.66
2:P:106:GLN:HE22	2:P:109:THR:CG2	2.10	0.65
2:N:106:GLN:HE22	2:N:109:THR:CG2	2.09	0.65
2:L:106:GLN:HE22	2:L:109:THR:CG2	2.10	0.65
2:F:106:GLN:HE22	2:F:109:THR:CG2	2.09	0.64
2:J:106:GLN:HE22	2:J:109:THR:CG2	2.09	0.64
1:E:206:THR:HG22	1:G:109:SER:HB3	1.80	0.64
2:P:41:TRP:CD1	2:P:89:LEU:CD2	2.79	0.63
2:P:163:GLN:OE1	2:P:170:LEU:HD12	1.98	0.63
1:E:146:THR:HG22	1:E:151:ALA:HB2	1.83	0.60
2:P:41:TRP:CB	2:P:89:LEU:HD23	2.29	0.60
2:D:197:LEU:N	2:D:197:LEU:HD23	2.18	0.59
1:C:79:SER:HB3	1:I:205:GLY:HA3	1.85	0.58
2:B:106:GLN:HE22	2:B:109:THR:HG22	1.69	0.57
2:F:197:LEU:HD23	2:F:197:LEU:N	2.19	0.57
2:J:197:LEU:HD23	2:J:197:LEU:N	2.19	0.57
2:B:197:LEU:HD23	2:B:197:LEU:N	2.19	0.57
2:P:197:LEU:N	2:P:197:LEU:HD23	2.20	0.57
2:F:106:GLN:HE22	2:F:109:THR:HG22	1.71	0.56
2:F:110:THR:HA	2:F:111:PRO:C	2.26	0.56
2:L:197:LEU:N	2:L:197:LEU:HD23	2.21	0.56
2:P:110:THR:HA	2:P:111:PRO:C	2.26	0.56
2:J:110:THR:HA	2:J:111:PRO:C	2.26	0.56
2:D:106:GLN:HE22	2:D:109:THR:HG22	1.71	0.56
2:H:197:LEU:N	2:H:197:LEU:HD23	2.20	0.56
2:L:110:THR:HA	2:L:111:PRO:C	2.25	0.56
2:H:110:THR:HA	2:H:111:PRO:C	2.27	0.55
2:N:106:GLN:HE22	2:N:109:THR:HG22	1.71	0.55
2:B:110:THR:HA	2:B:111:PRO:C	2.26	0.55
1:E:206:THR:HG22	1:G:109:SER:CB	2.37	0.55
2:P:41:TRP:CB	2:P:89:LEU:CD2	2.84	0.55
2:N:110:THR:HA	2:N:111:PRO:C	2.26	0.55
2:H:106:GLN:HE22	2:H:109:THR:HG22	1.71	0.54
2:J:106:GLN:HE22	2:J:109:THR:HG22	1.72	0.54
2:D:110:THR:HA	2:D:111:PRO:C	2.27	0.54
2:L:106:GLN:HE22	2:L:109:THR:HG22	1.72	0.54
1:O:139:LEU:CD2	1:O:156:LEU:N	2.71	0.53
2:P:106:GLN:HE22	2:P:109:THR:HG22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:139:LEU:HD21	1:O:156:LEU:HB2	1.90	0.52
1:E:224:LYS:HE2	2:F:139:GLU:OE1	2.10	0.52
2:N:158:ARG:HH12	2:N:179:VAL:HG21	1.76	0.51
2:H:152:LEU:HD12	2:H:152:LEU:N	2.26	0.51
2:N:152:LEU:N	2:N:152:LEU:HD12	2.26	0.51
2:P:152:LEU:HD12	2:P:152:LEU:N	2.26	0.51
2:J:152:LEU:N	2:J:152:LEU:HD12	2.26	0.50
1:O:139:LEU:HD23	1:O:155:CYS:C	2.31	0.50
2:B:152:LEU:N	2:B:152:LEU:HD12	2.27	0.50
1:C:40:TYR:CD2	1:C:115:PHE:CE1	3.00	0.49
1:E:40:TYR:CD2	1:E:115:PHE:CE1	3.01	0.49
2:L:152:LEU:HD12	2:L:152:LEU:N	2.27	0.49
2:F:152:LEU:N	2:F:152:LEU:HD12	2.28	0.49
2:D:152:LEU:HD12	2:D:152:LEU:N	2.28	0.49
1:O:40:TYR:CD2	1:O:115:PHE:CE1	3.00	0.49
1:M:40:TYR:CD2	1:M:115:PHE:CE1	3.01	0.49
1:A:37:TYR:CE2	1:A:106:LYS:HD3	2.47	0.49
1:K:37:TYR:CD2	1:K:106:LYS:HG2	2.48	0.48
2:P:37:ASN:O	2:P:56:TRP:HA	2.14	0.48
1:I:40:TYR:CD2	1:I:115:PHE:CE1	3.02	0.47
2:N:37:ASN:O	2:N:56:TRP:HA	2.14	0.47
1:A:40:TYR:CD2	1:A:115:PHE:CE1	3.02	0.47
2:L:37:ASN:O	2:L:56:TRP:HA	2.15	0.47
2:B:37:ASN:O	2:B:56:TRP:HA	2.15	0.47
2:D:37:ASN:O	2:D:56:TRP:HA	2.15	0.47
2:D:156:TYR:CD1	2:D:157:PRO:HA	2.50	0.47
1:E:142:SER:O	1:E:146:THR:HG23	2.15	0.47
2:F:37:ASN:O	2:F:56:TRP:HA	2.15	0.47
2:J:37:ASN:O	2:J:56:TRP:HA	2.14	0.47
2:B:156:TYR:CG	2:B:157:PRO:HA	2.50	0.47
2:N:156:TYR:CD1	2:N:157:PRO:HA	2.50	0.46
2:P:24:LYS:HA	2:P:85:THR:O	2.15	0.46
2:B:156:TYR:CD1	2:B:157:PRO:HA	2.50	0.46
2:D:24:LYS:HA	2:D:85:THR:O	2.16	0.46
2:J:24:LYS:HA	2:J:85:THR:O	2.15	0.46
2:N:24:LYS:HA	2:N:85:THR:O	2.16	0.46
2:B:101:VAL:HG12	2:B:103:TYR:CE1	2.51	0.46
2:P:156:TYR:CD1	2:P:157:PRO:HA	2.50	0.46
2:H:156:TYR:CG	2:H:157:PRO:HA	2.50	0.46
2:L:156:TYR:CG	2:L:157:PRO:HA	2.50	0.46
1:A:228:PRO:O	1:A:229:LYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:37:ASN:O	2:H:56:TRP:HA	2.15	0.46
2:F:156:TYR:CG	2:F:157:PRO:HA	2.51	0.46
2:F:156:TYR:CD1	2:F:157:PRO:HA	2.51	0.46
2:J:156:TYR:CD1	2:J:157:PRO:HA	2.51	0.46
2:P:156:TYR:CG	2:P:157:PRO:HA	2.50	0.46
2:D:171:GLN:HE21	2:D:174:ASN:HD21	1.64	0.46
2:H:156:TYR:CD1	2:H:157:PRO:HA	2.50	0.46
2:H:24:LYS:HA	2:H:85:THR:O	2.16	0.45
1:E:106:LYS:HB2	1:E:118:TRP:CD1	2.52	0.45
2:N:158:ARG:NH1	2:N:179:VAL:HG21	2.31	0.45
2:L:156:TYR:CD1	2:L:157:PRO:HA	2.50	0.45
2:N:156:TYR:CG	2:N:157:PRO:HA	2.51	0.45
2:N:171:GLN:HE21	2:N:174:ASN:HD21	1.64	0.45
1:A:216:LYS:N	1:A:217:PRO:CD	2.79	0.45
1:M:41:TRP:NE1	1:M:89:LEU:HB2	2.32	0.45
2:F:101:VAL:HG12	2:F:103:TYR:CE1	2.52	0.45
2:H:106:GLN:HE22	2:H:109:THR:HG23	1.81	0.45
2:B:24:LYS:HA	2:B:85:THR:O	2.15	0.45
2:D:106:GLN:HE22	2:D:109:THR:HG23	1.82	0.45
1:O:139:LEU:HD21	1:O:156:LEU:N	2.32	0.45
2:J:106:GLN:HE22	2:J:109:THR:HG23	1.81	0.45
2:D:156:TYR:CG	2:D:157:PRO:HA	2.52	0.45
2:J:156:TYR:CG	2:J:157:PRO:HA	2.52	0.45
1:O:160:TYR:CE2	1:O:165:VAL:HG13	2.52	0.45
1:E:41:TRP:NE1	1:E:89:LEU:HB2	2.33	0.44
1:I:142:SER:N	1:I:145:SER:HB3	2.30	0.44
1:A:41:TRP:NE1	1:A:89:LEU:HB2	2.32	0.44
1:I:41:TRP:NE1	1:I:89:LEU:HB2	2.32	0.44
1:C:41:TRP:NE1	1:C:89:LEU:HB2	2.32	0.44
1:C:79:SER:CB	1:I:205:GLY:HA3	2.48	0.44
2:L:24:LYS:HA	2:L:85:THR:O	2.16	0.44
2:P:171:GLN:HE21	2:P:174:ASN:HD21	1.65	0.44
1:A:37:TYR:CD2	1:A:106:LYS:HG2	2.53	0.44
2:B:106:GLN:NE2	2:B:109:THR:HG22	2.31	0.44
2:F:24:LYS:HA	2:F:85:THR:O	2.16	0.44
1:K:106:LYS:HB2	1:K:118:TRP:CD1	2.53	0.44
1:O:41:TRP:NE1	1:O:89:LEU:HB2	2.32	0.44
2:J:43:GLN:HB2	2:J:53:LEU:HD11	2.00	0.44
1:G:41:TRP:NE1	1:G:89:LEU:HB2	2.33	0.44
1:M:216:LYS:N	1:M:217:PRO:CD	2.81	0.44
2:B:142:LYS:HE3	1:C:112:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:101:VAL:HG12	2:J:103:TYR:CE1	2.53	0.44
2:N:101:VAL:HG12	2:N:103:TYR:CE1	2.53	0.44
1:O:216:LYS:N	1:O:217:PRO:CD	2.81	0.44
1:K:41:TRP:NE1	1:K:89:LEU:HB2	2.33	0.43
2:D:43:GLN:HB2	2:D:53:LEU:HD11	2.00	0.43
2:P:101:VAL:HG12	2:P:103:TYR:CE1	2.53	0.43
1:C:104:CYS:HB2	1:C:118:TRP:O	2.17	0.43
1:G:216:LYS:N	1:G:217:PRO:CD	2.81	0.43
2:P:106:GLN:HE22	2:P:109:THR:HG23	1.81	0.43
2:H:171:GLN:HE21	2:H:174:ASN:HD21	1.65	0.43
1:I:216:LYS:N	1:I:217:PRO:CD	2.81	0.43
1:A:106:LYS:HB2	1:A:118:TRP:CD1	2.54	0.43
2:L:101:VAL:HG12	2:L:103:TYR:CE1	2.54	0.43
1:G:106:LYS:HB2	1:G:118:TRP:CD1	2.54	0.43
2:L:162:VAL:HG12	2:L:177:GLU:OE2	2.18	0.43
2:N:43:GLN:HB2	2:N:53:LEU:HD11	2.01	0.43
2:N:106:GLN:HE22	2:N:109:THR:HG23	1.82	0.43
1:E:216:LYS:N	1:E:217:PRO:CD	2.82	0.43
1:K:216:LYS:N	1:K:217:PRO:CD	2.81	0.43
1:C:216:LYS:N	1:C:217:PRO:CD	2.82	0.42
1:K:104:CYS:HB2	1:K:118:TRP:O	2.19	0.42
2:N:106:GLN:NE2	2:N:109:THR:HG22	2.33	0.42
1:C:106:LYS:HB2	1:C:118:TRP:CD1	2.54	0.42
2:H:43:GLN:HB2	2:H:53:LEU:HD11	2.01	0.42
2:B:94:LEU:HD11	2:B:120:LEU:HD21	2.01	0.42
2:D:106:GLN:NE2	2:D:109:THR:HG22	2.33	0.42
1:A:142:SER:O	1:A:143:SER:C	2.58	0.42
2:P:43:GLN:HB2	2:P:53:LEU:HD11	2.01	0.42
1:E:104:CYS:HB2	1:E:118:TRP:O	2.19	0.42
1:M:142:SER:O	1:M:143:SER:C	2.58	0.42
2:D:101:VAL:HG12	2:D:103:TYR:CE1	2.55	0.42
1:K:37:TYR:CD2	1:K:106:LYS:CD	3.03	0.42
2:H:106:GLN:NE2	2:H:109:THR:HG22	2.33	0.41
1:O:139:LEU:CD2	1:O:155:CYS:C	2.88	0.41
2:J:113:THR:HA	3:J:301:CL:CL	2.57	0.41
2:L:106:GLN:HE22	2:L:109:THR:HG23	1.83	0.41
1:O:106:LYS:HB2	1:O:118:TRP:CD1	2.55	0.41
1:A:114:TYR:CE2	2:B:55:TYR:HB2	2.56	0.41
1:G:104:CYS:HB2	1:G:118:TRP:O	2.19	0.41
2:L:43:GLN:HB2	2:L:53:LEU:HD11	2.03	0.41
2:B:43:GLN:HB2	2:B:53:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:13:VAL:O	1:K:126:VAL:HA	2.21	0.41
1:A:37:TYR:CD2	1:A:106:LYS:HD3	2.56	0.41
2:F:106:GLN:NE2	2:F:109:THR:HG22	2.33	0.41
1:M:106:LYS:HB2	1:M:118:TRP:CD1	2.55	0.41
1:A:104:CYS:HB2	1:A:118:TRP:O	2.20	0.41
1:A:13:VAL:O	1:A:126:VAL:HA	2.21	0.41
1:C:142:SER:O	1:C:143:SER:C	2.59	0.40
2:N:94:LEU:HD11	2:N:120:LEU:HD21	2.04	0.40
2:P:94:LEU:HD11	2:P:120:LEU:HD21	2.04	0.40
1:I:39:MET:HB3	1:I:87:LEU:HD22	2.04	0.40
1:M:112:PHE:HE2	2:N:55:TYR:CE2	2.39	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	212/227 (93%)	210 (99%)	2 (1%)	0	100	100
1	C	210/227 (92%)	207 (99%)	3 (1%)	0	100	100
1	E	219/227 (96%)	215 (98%)	4 (2%)	0	100	100
1	G	209/227 (92%)	207 (99%)	2 (1%)	0	100	100
1	I	218/227 (96%)	215 (99%)	3 (1%)	0	100	100
1	K	205/227 (90%)	201 (98%)	4 (2%)	0	100	100
1	M	211/227 (93%)	209 (99%)	2 (1%)	0	100	100
1	O	200/227 (88%)	197 (98%)	3 (2%)	0	100	100
2	B	217/220 (99%)	208 (96%)	9 (4%)	0	100	100
2	D	216/220 (98%)	206 (95%)	10 (5%)	0	100	100
2	F	217/220 (99%)	208 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	216/220 (98%)	208 (96%)	8 (4%)	0	100	100
2	J	217/220 (99%)	208 (96%)	9 (4%)	0	100	100
2	L	217/220 (99%)	209 (96%)	8 (4%)	0	100	100
2	N	217/220 (99%)	207 (95%)	10 (5%)	0	100	100
2	P	217/220 (99%)	207 (95%)	10 (5%)	0	100	100
All	All	3418/3576 (96%)	3322 (97%)	96 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	179/190 (94%)	176 (98%)	3 (2%)	60	82
1	C	179/190 (94%)	176 (98%)	3 (2%)	60	82
1	E	184/190 (97%)	177 (96%)	7 (4%)	33	58
1	G	178/190 (94%)	173 (97%)	5 (3%)	43	70
1	I	183/190 (96%)	177 (97%)	6 (3%)	38	64
1	K	176/190 (93%)	171 (97%)	5 (3%)	43	70
1	M	179/190 (94%)	176 (98%)	3 (2%)	60	82
1	O	172/190 (90%)	165 (96%)	7 (4%)	30	55
2	B	194/195 (100%)	186 (96%)	8 (4%)	30	55
2	D	193/195 (99%)	184 (95%)	9 (5%)	26	49
2	F	194/195 (100%)	185 (95%)	9 (5%)	27	50
2	H	193/195 (99%)	185 (96%)	8 (4%)	30	55
2	J	194/195 (100%)	185 (95%)	9 (5%)	27	50
2	L	194/195 (100%)	185 (95%)	9 (5%)	27	50
2	N	194/195 (100%)	186 (96%)	8 (4%)	30	55
2	P	194/195 (100%)	184 (95%)	10 (5%)	23	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2980/3080 (97%)	2871 (96%)	109 (4%)	34 60

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	CYS
1	A	208	THR
1	A	224	LYS
2	B	5	THR
2	B	17	GLU
2	B	33	SER
2	B	68	GLU
2	B	110	THR
2	B	197	LEU
2	B	213	THR
2	B	229	GLU
1	C	155	CYS
1	C	208	THR
1	C	224	LYS
2	D	5	THR
2	D	17	GLU
2	D	33	SER
2	D	68	GLU
2	D	95	GLN
2	D	110	THR
2	D	197	LEU
2	D	210	CYS
2	D	213	THR
1	E	29	THR
1	E	139	LEU
1	E	142	SER
1	E	145	SER
1	E	155	CYS
1	E	208	THR
1	E	224	LYS
2	F	5	THR
2	F	17	GLU
2	F	33	SER
2	F	68	GLU
2	F	110	THR
2	F	197	LEU
2	F	210	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	F	213	THR
2	F	229	GLU
1	G	29	THR
1	G	142	SER
1	G	155	CYS
1	G	208	THR
1	G	224	LYS
2	H	5	THR
2	H	17	GLU
2	H	33	SER
2	H	68	GLU
2	H	110	THR
2	H	197	LEU
2	H	213	THR
2	H	229	GLU
1	I	106	LYS
1	I	142	SER
1	I	155	CYS
1	I	208	THR
1	I	224	LYS
1	I	229	LYS
2	J	5	THR
2	J	15	LEU
2	J	17	GLU
2	J	33	SER
2	J	68	GLU
2	J	110	THR
2	J	197	LEU
2	J	210	CYS
2	J	213	THR
1	K	29	THR
1	K	155	CYS
1	K	208	THR
1	K	221	LYS
1	K	224	LYS
2	L	5	THR
2	L	17	GLU
2	L	33	SER
2	L	68	GLU
2	L	110	THR
2	L	162	VAL
2	L	197	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	L	213	THR
2	L	229	GLU
1	M	155	CYS
1	M	208	THR
1	M	224	LYS
2	N	5	THR
2	N	17	GLU
2	N	33	SER
2	N	68	GLU
2	N	110	THR
2	N	210	CYS
2	N	213	THR
2	N	229	GLU
1	O	29	THR
1	O	97	GLU
1	O	130	SER
1	O	155	CYS
1	O	203	SER
1	O	208	THR
1	O	224	LYS
2	P	5	THR
2	P	17	GLU
2	P	33	SER
2	P	68	GLU
2	P	89	LEU
2	P	110	THR
2	P	197	LEU
2	P	210	CYS
2	P	213	THR
2	P	229	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	207	GLN
2	B	226	ASN
1	C	207	GLN
2	D	171	GLN
2	D	226	ASN
1	E	207	GLN
2	F	163	GLN
2	F	226	ASN

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Mol	Chain	Res	Type
1	G	3	GLN
2	H	27	GLN
2	H	171	GLN
2	H	226	ASN
1	I	3	GLN
1	I	207	GLN
2	J	226	ASN
1	K	207	GLN
2	L	226	ASN
1	M	207	GLN
2	N	163	GLN
2	N	171	GLN
2	N	226	ASN
2	P	171	GLN
2	P	226	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](#)

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	216/227 (95%)	0.27	1 (0%) 91 91	42, 68, 96, 114	0
1	C	214/227 (94%)	0.42	1 (0%) 91 91	40, 62, 119, 136	0
1	E	221/227 (97%)	0.36	3 (1%) 75 77	48, 75, 105, 132	0
1	G	213/227 (93%)	0.29	1 (0%) 91 91	46, 66, 110, 128	0
1	I	220/227 (96%)	0.48	9 (4%) 37 40	51, 82, 116, 132	0
1	K	211/227 (92%)	0.42	3 (1%) 75 77	61, 86, 118, 137	0
1	M	215/227 (94%)	0.30	2 (0%) 84 86	51, 73, 108, 123	0
1	O	206/227 (90%)	0.61	12 (5%) 23 24	57, 82, 123, 157	0
2	B	219/220 (99%)	0.16	0 100 100	42, 66, 94, 124	0
2	D	218/220 (99%)	0.28	3 (1%) 75 77	49, 84, 116, 128	0
2	F	219/220 (99%)	0.18	0 100 100	48, 75, 104, 121	0
2	H	218/220 (99%)	0.17	2 (0%) 84 86	45, 72, 113, 132	0
2	J	219/220 (99%)	0.32	2 (0%) 84 86	56, 78, 106, 137	0
2	L	219/220 (99%)	0.33	5 (2%) 60 63	60, 89, 132, 147	0
2	N	219/220 (99%)	0.18	2 (0%) 84 86	53, 77, 104, 130	0
2	P	219/220 (99%)	0.43	15 (6%) 17 17	70, 105, 138, 148	0
All	All	3466/3576 (96%)	0.32	61 (1%) 68 71	40, 78, 118, 157	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	209	TYR	6.3
2	P	1	ASP	4.6
2	L	1	ASP	4.2
2	D	92	SER	4.0
2	L	197	LEU	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	O	202	SER	3.5
1	C	204	LEU	3.4
1	I	146	THR	3.4
1	O	65	ILE	3.3
2	P	94	LEU	3.0
2	P	39	LEU	3.0
1	I	55	GLY	3.0
2	P	74	ASP	3.0
2	H	163	GLN	2.9
1	E	205	GLY	2.9
1	E	111	TYR	2.9
1	K	66	VAL	2.8
2	H	170	LEU	2.8
2	P	170	LEU	2.8
1	M	225	ARG	2.8
2	P	57	ALA	2.8
1	O	200	PRO	2.8
1	O	199	VAL	2.7
1	A	40	TYR	2.7
2	L	212	VAL	2.6
2	J	39	LEU	2.6
2	P	32	SER	2.5
1	I	202	SER	2.5
2	P	15	LEU	2.4
1	I	145	SER	2.4
1	I	144	LYS	2.4
1	K	58	TRP	2.4
1	K	206	THR	2.4
2	J	1	ASP	2.4
1	O	226	VAL	2.4
1	O	198	THR	2.4
2	N	170	LEU	2.4
1	G	111	TYR	2.3
1	I	66	VAL	2.3
2	P	89	LEU	2.3
1	O	53	VAL	2.3
2	P	92	SER	2.3
2	D	94	LEU	2.3
1	O	113	PRO	2.2
2	P	132	PHE	2.2
2	L	108	TYR	2.2
2	P	24	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	N	1	ASP	2.1
2	P	70	GLY	2.1
1	O	54	SER	2.1
1	O	197	VAL	2.1
1	I	204	LEU	2.1
1	M	205	GLY	2.1
2	D	170	LEU	2.1
1	I	201	SER	2.1
1	I	67	TYR	2.1
1	O	208	THR	2.1
2	L	166	VAL	2.1
2	P	76	PHE	2.0
2	P	29	VAL	2.0
1	E	114	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	CL	J	301	1/1	0.83	0.09	89,89,89,89	0
3	CL	G	301	1/1	0.86	0.08	76,76,76,76	0
3	CL	K	301	1/1	0.86	0.21	82,82,82,82	0
3	CL	C	301	1/1	0.95	0.16	67,67,67,67	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.