



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:07 am GMT

PDB ID : 4Z42  
Title : Crystal structure of urease from Yersinia enterocolitica  
Authors : Studer, G.; Jakob, R.P.; Mahi, M.A.; Wiesand, U.; Schwede, T.; Maier, T.  
Deposited on : 2015-04-01  
Resolution : 3.01 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

<http://wwpdb.org/validation/2016/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) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

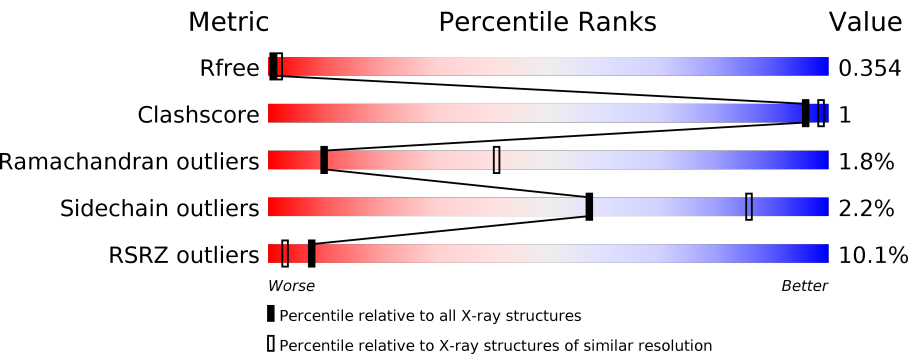
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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))
$R_{free}$	100719	1924 (3.04-3.00)
Clashscore	112137	2279 (3.04-3.00)
Ramachandran outliers	110173	2207 (3.04-3.00)
Sidechain outliers	110143	2210 (3.04-3.00)
RSRZ outliers	101464	1948 (3.04-3.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	100	
1	D	100	
1	G	100	
1	J	100	
2	B	164	
2	E	164	

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Mol	Chain	Length	Quality of chain
2	H	164	<div><div></div><div>34%</div><div></div><div>62%</div><div></div><div>5%</div><div></div><div>30%</div></div>
2	K	164	<div><div></div><div>6%</div><div></div><div>66%</div><div></div><div>• •</div><div></div><div>30%</div></div>
3	C	572	<div><div></div><div>15%</div><div></div><div>95%</div><div></div><div>5%</div></div>
3	F	572	<div><div></div><div>6%</div><div></div><div>94%</div><div></div><div>5%</div></div>
3	I	572	<div><div></div><div>9%</div><div></div><div>95%</div><div></div><div>5%</div></div>
3	L	572	<div><div></div><div>6%</div><div></div><div>94%</div><div></div><div>5%</div></div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 47288 atoms, of which 23471 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 Urease subunit gamma.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	99	Total	C	H	N	O	S	0	0	0
			1555	480	793	128	149	5			
1	D	99	Total	C	H	N	O	S	0	0	0
			1555	480	793	128	149	5			
1	G	99	Total	C	H	N	O	S	0	0	0
			1555	480	793	128	149	5			
1	J	99	Total	C	H	N	O	S	0	0	0
			1555	480	793	128	149	5			

- Molecule 2 is a protein called Urease subunit beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	114	Total	C	H	N	O	S	0	0	0
			1745	560	859	156	169	1			
2	E	114	Total	C	H	N	O	S	0	0	0
			1745	560	859	156	169	1			
2	H	114	Total	C	H	N	O	S	0	0	0
			1744	560	858	156	169	1			
2	K	114	Total	C	H	N	O	S	0	0	0
			1745	560	859	156	169	1			

- Molecule 3 is a protein called Urease subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	571	Total	C	H	N	O	S	0	0	0
			8493	2671	4216	759	822	25			
3	F	571	Total	C	H	N	O	S	0	0	0
			8493	2671	4216	759	822	25			
3	I	571	Total	C	H	N	O	S	0	0	0
			8493	2671	4216	759	822	25			
3	L	571	Total	C	H	N	O	S	0	0	0
			8493	2671	4216	759	822	25			

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	2	Total 2	Ni 2	0	0
4	L	2	Total 2	Ni 2	0	0
4	C	2	Total 2	Ni 2	0	0
4	F	2	Total 2	Ni 2	0	0

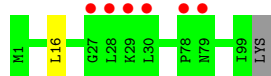
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	8	Total 8	O 8	0	0
5	C	15	Total 15	O 15	0	0
5	D	1	Total 1	O 1	0	0
5	E	8	Total 8	O 8	0	0
5	F	31	Total 31	O 31	0	0
5	I	17	Total 17	O 17	0	0
5	K	4	Total 4	O 4	0	0
5	L	25	Total 25	O 25	0	0

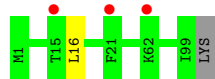
### 3 Residue-property plots [i](#)

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.

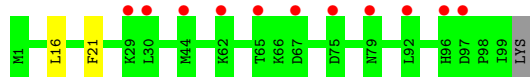
- Molecule 1: Urease subunit gamma



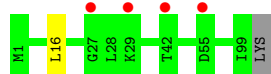
- Molecule 1: Urease subunit gamma



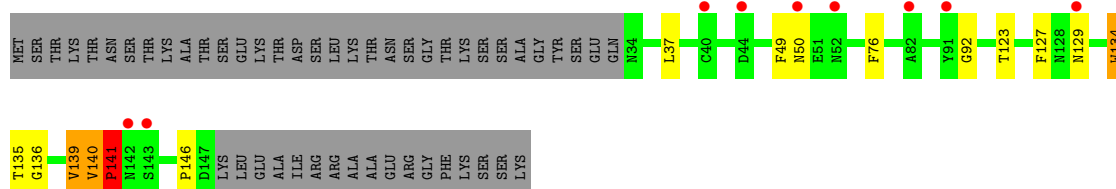
- Molecule 1: Urease subunit gamma



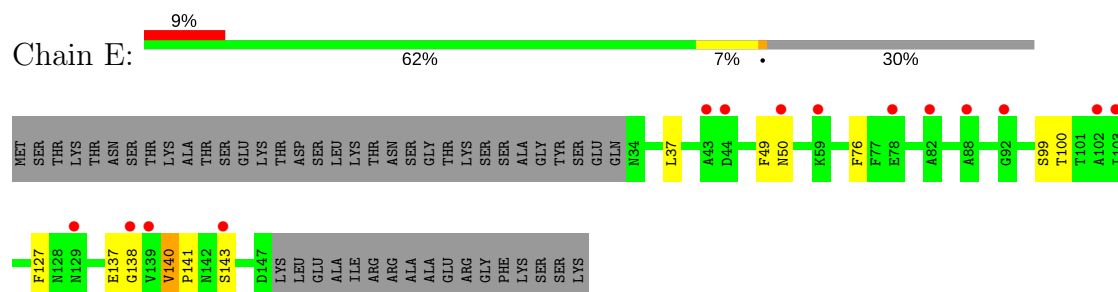
- Molecule 1: Urease subunit gamma



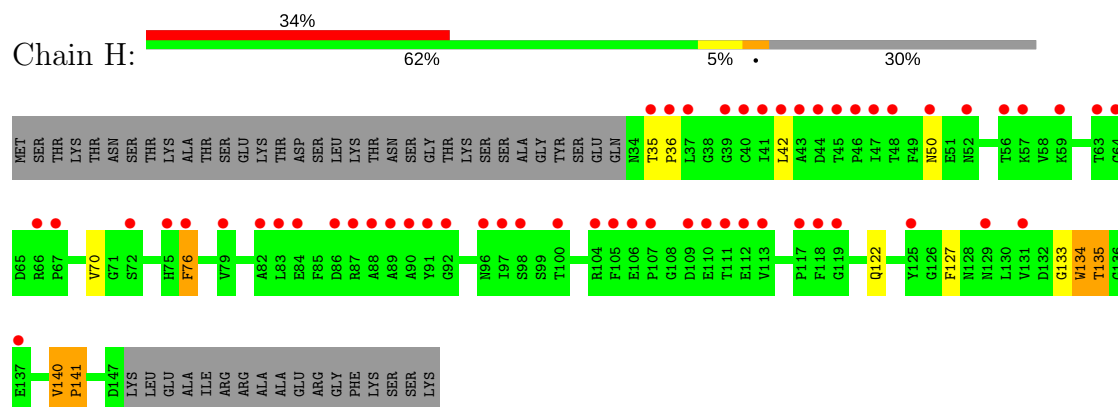
- Molecule 2: Urease subunit beta



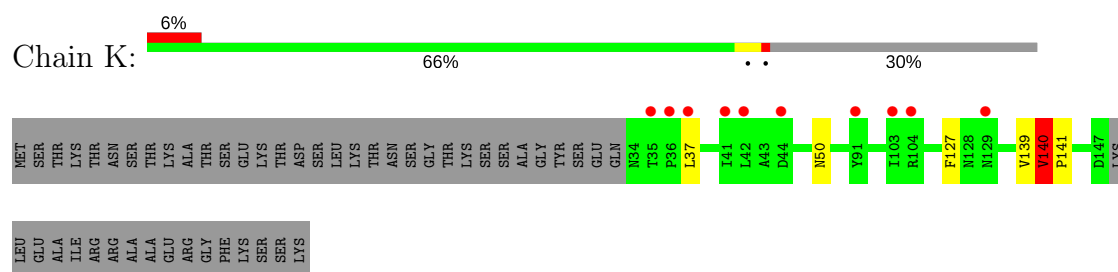
- Molecule 2: Urease subunit beta



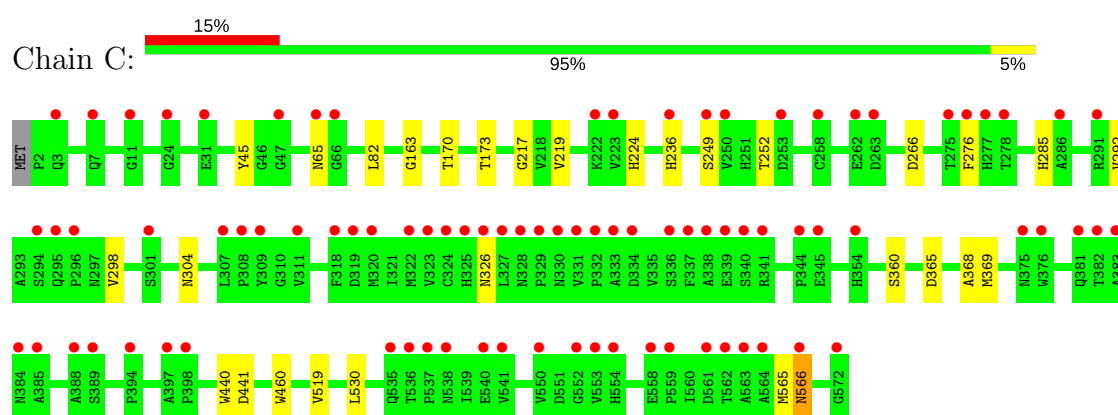
- Molecule 2: Urease subunit beta



- Molecule 2: Urease subunit beta

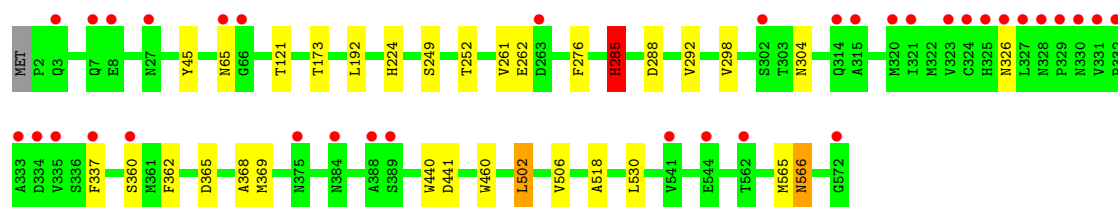


- Molecule 3: Urease subunit alpha

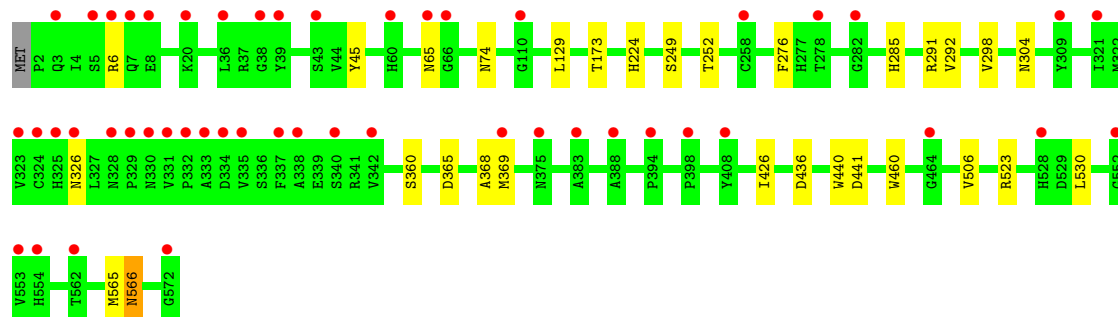
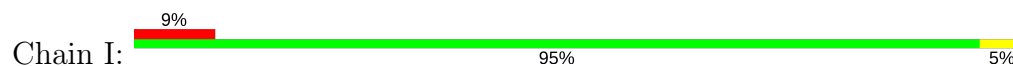


- Molecule 3: Urease subunit alpha

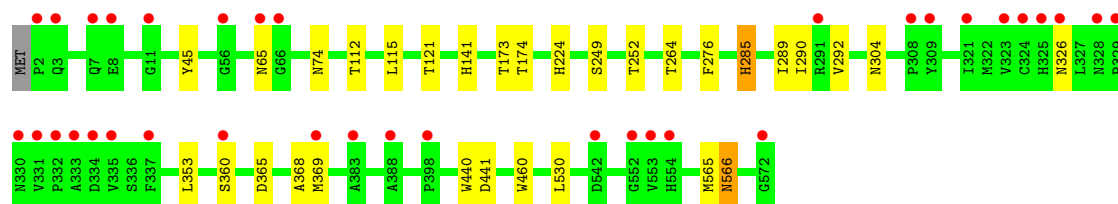




● Molecule 3: Urease subunit alpha



● Molecule 3: Urease subunit alpha





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.20Å 157.20Å 774.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.71 – 3.01 29.71 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.71-3.01) 99.5 (29.71-3.01)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 3.00Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, $R_{free}$	0.277 , 0.298 0.328 , 0.354	Depositor DCC
$R_{free}$ test set	3665 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.0	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 68.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.78	EDS
Total number of atoms	47288	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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

### 5.1 Standard geometry

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

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	0.39	0/770	0.48	0/1040
1	D	0.40	0/770	0.50	0/1040
1	G	0.39	0/770	0.47	0/1040
1	J	0.39	0/770	0.48	0/1040
2	B	0.44	0/908	0.64	1/1235 (0.1%)
2	E	0.43	0/908	0.60	0/1235
2	H	0.42	0/908	0.62	0/1235
2	K	0.41	0/908	0.58	0/1235
3	C	0.37	0/4362	0.56	0/5924
3	F	0.37	0/4362	0.55	0/5924
3	I	0.38	0/4362	0.56	0/5924
3	L	0.38	0/4362	0.56	0/5924
All	All	0.39	0/24160	0.56	1/32796 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	141	PRO	CA-N-CD	-5.05	104.42	111.50

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	762	793	793	0	0
1	D	762	793	793	0	0
1	G	762	793	793	0	0
1	J	762	793	793	0	0
2	B	886	859	859	13	7
2	E	886	859	859	4	0
2	H	886	858	858	9	2
2	K	886	859	859	2	0
3	C	4277	4216	4216	8	2
3	F	4277	4216	4216	10	0
3	I	4277	4216	4216	7	7
3	L	4277	4216	4216	11	0
4	C	2	0	0	0	0
4	F	2	0	0	0	0
4	I	2	0	0	0	0
4	L	2	0	0	0	0
5	B	8	0	0	0	0
5	C	15	0	0	0	0
5	D	1	0	0	0	0
5	E	8	0	0	0	0
5	F	31	0	0	0	0
5	I	17	0	0	0	0
5	K	4	0	0	0	0
5	L	25	0	0	0	0
All	All	23817	23471	23471	62	9

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 1.

All (62) 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:H:122:GLN:HB3	2:H:135:THR:CG2	1.98	0.94
2:H:122:GLN:HB3	2:H:135:THR:HG21	1.61	0.81
2:B:134:TRP:CZ2	2:B:136:GLY:HA2	2.23	0.72
2:B:139:VAL:C	2:B:140:VAL:HG13	2.13	0.68
2:B:92:GLY:HA3	2:B:135:THR:HG21	1.77	0.66
2:B:139:VAL:O	2:B:140:VAL:HG22	1.95	0.66
2:B:92:GLY:CA	2:B:135:THR:HG21	2.26	0.66
2:B:139:VAL:O	2:B:140:VAL:HG13	1.96	0.64
3:F:261:VAL:HG22	3:F:285:HIS:ND1	2.17	0.59
3:F:261:VAL:HG21	3:F:288:ASP:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:THR:HB	2:B:134:TRP:HB2	1.88	0.56
2:B:134:TRP:CZ2	2:B:136:GLY:CA	2.89	0.55
2:E:137:GLU:OE2	2:E:143:SER:O	2.27	0.53
2:B:123:THR:HA	2:B:134:TRP:HA	1.90	0.52
2:B:134:TRP:CE2	2:B:136:GLY:HA2	2.44	0.52
3:C:292:VAL:HG12	3:C:298:VAL:HG21	1.91	0.52
3:L:173:THR:HG22	3:L:224:HIS:CD2	2.45	0.52
3:I:173:THR:HG22	3:I:224:HIS:CD2	2.46	0.51
3:C:173:THR:HG22	3:C:224:HIS:CD2	2.46	0.50
3:F:173:THR:HG22	3:F:224:HIS:CD2	2.47	0.50
3:F:292:VAL:HG12	3:F:298:VAL:HG21	1.94	0.49
2:E:137:GLU:HG3	2:E:138:GLY:N	2.27	0.49
3:L:289:ILE:O	3:L:292:VAL:HG22	2.13	0.48
3:C:219:VAL:CG2	3:C:519:VAL:HG11	2.43	0.48
3:F:502:LEU:HD13	3:F:518:ALA:HB2	1.94	0.48
3:L:360:SER:CB	3:L:530:LEU:HD13	2.44	0.47
3:C:360:SER:CB	3:C:530:LEU:HD13	2.45	0.47
3:F:360:SER:CB	3:F:530:LEU:HD13	2.44	0.47
3:I:360:SER:CB	3:I:530:LEU:HD13	2.44	0.47
3:F:261:VAL:HG22	3:F:285:HIS:CE1	2.48	0.47
2:H:133:GLY:O	2:H:134:TRP:HB3	2.16	0.46
2:H:122:GLN:O	2:H:135:THR:HG23	2.16	0.45
3:L:173:THR:HG22	3:L:224:HIS:CG	2.51	0.45
3:C:173:THR:HG22	3:C:224:HIS:CG	2.52	0.45
2:H:35:THR:HG23	2:H:36:PRO:HD2	1.99	0.45
3:F:262:GLU:CG	2:K:139:VAL:HG21	2.47	0.45
3:I:173:THR:HG22	3:I:224:HIS:CG	2.52	0.44
2:B:134:TRP:O	2:B:134:TRP:CE3	2.70	0.44
3:L:112:THR:CG2	3:L:115:LEU:HD13	2.48	0.44
2:H:133:GLY:O	2:H:134:TRP:CB	2.66	0.44
2:B:139:VAL:C	2:B:141:PRO:HD3	2.38	0.44
3:L:112:THR:HG22	3:L:115:LEU:HD13	2.00	0.44
3:F:249:SER:HB3	3:F:276:PHE:CE2	2.53	0.43
2:B:123:THR:CB	2:B:134:TRP:HB2	2.48	0.43
3:C:249:SER:HB3	3:C:276:PHE:CE2	2.53	0.43
3:I:249:SER:HB3	3:I:276:PHE:CE2	2.53	0.43
3:I:426:ILE:HD13	3:I:436:ASP:HB2	2.01	0.43
2:H:140:VAL:HG22	2:H:141:PRO:HD3	2.00	0.43
3:L:249:SER:HB3	3:L:276:PHE:CE2	2.54	0.43
2:H:42:LEU:HD11	3:I:6:ARG:HB3	2.01	0.43
2:E:140:VAL:HB	2:E:141:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:70:VAL:HG11	2:H:76:PHE:CE1	2.55	0.42
3:C:82:LEU:HD12	3:C:82:LEU:O	2.19	0.42
3:I:292:VAL:HG12	3:I:298:VAL:HG21	2.01	0.42
2:E:99:SER:O	2:E:100:THR:HB	2.20	0.42
3:L:115:LEU:HD12	3:L:115:LEU:N	2.35	0.42
3:F:173:THR:HG22	3:F:224:HIS:CG	2.55	0.41
3:L:141:HIS:CE1	3:L:174:THR:HG23	2.56	0.41
3:L:264:THR:HG21	3:L:285:HIS:CE1	2.56	0.41
3:L:290:ILE:HD11	3:L:353:LEU:CD1	2.51	0.41
3:C:163:GLY:HA3	3:C:170:THR:HG23	2.03	0.40
2:K:140:VAL:HB	2:K:141:PRO:HD3	2.04	0.40

All (9) 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)
2:B:139:VAL:HG12	3:I:291:ARG:NH2[3_545]	0.59	1.01
2:B:139:VAL:HG12	3:I:291:ARG:HH22[3_545]	0.67	0.93
2:B:139:VAL:CG1	3:I:291:ARG:NH2[3_545]	1.31	0.89
2:B:139:VAL:HG12	3:I:291:ARG:HH21[3_545]	0.94	0.66
2:B:139:VAL:CG1	3:I:291:ARG:HH22[3_545]	1.30	0.30
3:C:266:ASP:OD1	2:H:134:TRP:HZ2[3_545]	1.42	0.18
2:B:139:VAL:CG1	3:I:291:ARG:CZ[3_545]	2.10	0.10
3:C:266:ASP:CG	2:H:134:TRP:HZ2[3_545]	1.54	0.06
2:B:139:VAL:HG11	3:I:291:ARG:NH2[3_545]	1.59	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	A	97/100 (97%)	94 (97%)	3 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
1	G	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
1	J	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
2	B	112/164 (68%)	95 (85%)	12 (11%)	5 (4%)	3	16
2	E	112/164 (68%)	96 (86%)	13 (12%)	3 (3%)	6	29
2	H	112/164 (68%)	96 (86%)	11 (10%)	5 (4%)	3	16
2	K	112/164 (68%)	99 (88%)	10 (9%)	3 (3%)	6	29
3	C	569/572 (100%)	512 (90%)	47 (8%)	10 (2%)	10	41
3	F	569/572 (100%)	510 (90%)	50 (9%)	9 (2%)	11	44
3	I	569/572 (100%)	510 (90%)	49 (9%)	10 (2%)	10	41
3	L	569/572 (100%)	511 (90%)	48 (8%)	10 (2%)	10	41
All	All	3112/3344 (93%)	2805 (90%)	252 (8%)	55 (2%)	10	41

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	50	ASN
2	B	140	VAL
2	E	50	ASN
2	E	140	VAL
2	H	140	VAL
3	I	74	ASN
2	K	140	VAL
3	L	285	HIS
2	B	141	PRO
3	C	285	HIS
3	C	365	ASP
3	F	365	ASP
2	H	134	TRP
3	I	285	HIS
3	I	365	ASP
3	C	369	MET
3	F	285	HIS
3	F	369	MET
3	I	369	MET
2	K	50	ASN
3	L	65	ASN
3	L	365	ASP

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Mol	Chain	Res	Type
3	L	369	MET
2	B	127	PHE
3	C	65	ASN
3	C	326	ASN
2	E	127	PHE
3	F	65	ASN
3	F	326	ASN
2	H	127	PHE
3	I	65	ASN
3	I	326	ASN
3	I	566	ASN
2	K	127	PHE
3	L	326	ASN
3	C	565	MET
3	C	566	ASN
3	F	368	ALA
3	F	565	MET
3	F	566	ASN
2	H	50	ASN
3	I	368	ALA
3	I	565	MET
3	L	74	ASN
3	L	368	ALA
3	L	565	MET
3	L	566	ASN
3	C	368	ALA
2	H	141	PRO
2	B	139	VAL
3	C	217	GLY
3	C	304	ASN
3	F	304	ASN
3	I	304	ASN
3	L	304	ASN

### 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	86/87 (99%)	85 (99%)	1 (1%)	75	92
1	D	86/87 (99%)	85 (99%)	1 (1%)	75	92
1	G	86/87 (99%)	84 (98%)	2 (2%)	56	85
1	J	86/87 (99%)	85 (99%)	1 (1%)	75	92
2	B	96/138 (70%)	89 (93%)	7 (7%)	16	48
2	E	96/138 (70%)	93 (97%)	3 (3%)	45	80
2	H	96/138 (70%)	94 (98%)	2 (2%)	59	86
2	K	96/138 (70%)	94 (98%)	2 (2%)	59	86
3	C	457/458 (100%)	450 (98%)	7 (2%)	70	91
3	F	457/458 (100%)	444 (97%)	13 (3%)	49	81
3	I	457/458 (100%)	448 (98%)	9 (2%)	60	87
3	L	457/458 (100%)	450 (98%)	7 (2%)	70	91
All	All	2556/2732 (94%)	2501 (98%)	55 (2%)	57	86

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
2	B	37	LEU
2	B	49	PHE
2	B	76	PHE
2	B	129	ASN
2	B	134	TRP
2	B	141	PRO
2	B	146	PRO
3	C	45	TYR
3	C	236	HIS
3	C	252	THR
3	C	440	TRP
3	C	441	ASP
3	C	460	TRP
3	C	566	ASN
1	D	16	LEU
2	E	37	LEU
2	E	49	PHE
2	E	76	PHE
3	F	45	TYR
3	F	121	THR
3	F	192	LEU

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Mol	Chain	Res	Type
3	F	252	THR
3	F	285	HIS
3	F	337	PHE
3	F	362	PHE
3	F	440	TRP
3	F	441	ASP
3	F	460	TRP
3	F	502	LEU
3	F	506	VAL
3	F	566	ASN
1	G	16	LEU
1	G	21	PHE
2	H	76	PHE
2	H	135	THR
3	I	45	TYR
3	I	129	LEU
3	I	252	THR
3	I	440	TRP
3	I	441	ASP
3	I	460	TRP
3	I	506	VAL
3	I	523	ARG
3	I	566	ASN
1	J	16	LEU
2	K	37	LEU
2	K	140	VAL
3	L	45	TYR
3	L	121	THR
3	L	252	THR
3	L	440	TRP
3	L	441	ASP
3	L	460	TRP
3	L	566	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	L	147	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 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	99/100 (99%)	0.51	6 (6%)	22 8	80, 103, 127, 139	0
1	D	99/100 (99%)	0.55	3 (3%)	51 23	84, 111, 136, 143	0
1	G	99/100 (99%)	0.82	11 (11%)	6 2	90, 116, 137, 144	0
1	J	99/100 (99%)	0.51	4 (4%)	39 16	78, 101, 126, 136	0
2	B	114/164 (69%)	0.73	9 (7%)	13 5	26, 105, 142, 154	0
2	E	114/164 (69%)	0.90	14 (12%)	5 1	65, 105, 146, 161	0
2	H	114/164 (69%)	2.18	56 (49%)	0 0	26, 163, 195, 202	0
2	K	114/164 (69%)	0.71	10 (8%)	11 4	63, 102, 161, 164	0
3	C	571/572 (99%)	0.81	86 (15%)	3 1	28, 99, 202, 232	0
3	F	571/572 (99%)	0.28	35 (6%)	22 8	16, 81, 165, 226	0
3	I	571/572 (99%)	0.53	49 (8%)	11 4	17, 91, 176, 222	0
3	L	571/572 (99%)	0.31	35 (6%)	22 8	15, 82, 169, 202	0
All	All	3136/3344 (93%)	0.59	318 (10%)	8 3	15, 96, 177, 232	0

All (318) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	324	CYS	10.7
3	C	537	PRO	8.5
3	I	326	ASN	8.4
3	C	332	PRO	8.0
3	I	7	GLN	7.8
2	E	44	ASP	7.6
3	L	334	ASP	6.9
3	I	323	VAL	6.7
3	I	325	HIS	6.5
3	L	330	ASN	6.1
3	C	323	VAL	6.1

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Mol	Chain	Res	Type	RSRZ
3	I	552	GLY	5.9
3	L	323	VAL	5.9
3	F	326	ASN	5.9
3	L	324	CYS	5.9
3	F	65	ASN	5.8
3	C	324	CYS	5.8
3	F	325	HIS	5.5
3	I	330	ASN	5.5
3	C	337	PHE	5.4
2	K	44	ASP	5.4
3	C	536	THR	5.3
3	L	552	GLY	5.3
2	H	57	LYS	5.1
2	H	41	ILE	5.1
3	F	330	ASN	5.1
2	H	35	THR	5.0
3	C	558	GLU	5.0
3	L	321	ILE	4.9
2	B	142	ASN	4.8
2	B	129	ASN	4.8
3	C	339	GLU	4.7
3	L	335	VAL	4.7
3	C	538	ASN	4.7
3	L	326	ASN	4.7
2	H	46	PRO	4.7
3	C	562	THR	4.7
2	H	117	PRO	4.6
2	H	44	ASP	4.6
3	F	334	ASP	4.6
3	L	65	ASN	4.6
3	L	66	GLY	4.6
2	H	131	VAL	4.5
2	H	37	LEU	4.5
3	I	332	PRO	4.5
2	H	91	TYR	4.5
3	L	325	HIS	4.5
3	C	344	PRO	4.4
3	F	335	VAL	4.4
3	C	326	ASN	4.4
2	B	52	ASN	4.4
2	H	83	LEU	4.4
3	I	65	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
3	I	334	ASP	4.4
3	C	331	VAL	4.3
3	F	321	ILE	4.3
2	H	42	LEU	4.3
3	C	325	HIS	4.2
3	C	3	GLN	4.2
2	H	52	ASN	4.2
3	L	8	GLU	4.2
3	C	329	PRO	4.2
2	H	89	ALA	4.2
3	C	338	ALA	4.2
3	L	332	PRO	4.1
2	H	86	ASP	4.1
3	I	333	ALA	4.1
3	C	341	ARG	4.1
3	L	3	GLN	4.1
3	L	337	PHE	4.1
3	C	278	THR	4.1
2	B	143	SER	4.1
3	C	540	GLU	4.1
3	F	332	PRO	4.0
2	H	50	ASN	4.0
3	I	331	VAL	4.0
3	C	320	MET	4.0
3	C	383	ALA	4.0
3	C	294	SER	4.0
2	B	40	CYS	3.9
2	H	45	THR	3.9
3	C	394	PRO	3.9
2	E	82	ALA	3.8
3	C	330	ASN	3.8
2	H	109	ASP	3.8
3	I	328	ASN	3.8
2	H	36	PRO	3.7
3	F	331	VAL	3.7
3	F	324	CYS	3.7
2	E	129	ASN	3.7
3	F	388	ALA	3.7
2	E	143	SER	3.7
2	H	96	ASN	3.7
2	H	104	ARG	3.7
3	C	275	THR	3.7

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Mol	Chain	Res	Type	RSRZ
3	I	309	TYR	3.6
3	I	335	VAL	3.6
1	A	27	GLY	3.6
2	K	35	THR	3.6
1	A	30	LEU	3.6
3	C	222	LYS	3.6
3	C	276	PHE	3.6
2	K	41	ILE	3.5
2	H	67	PRO	3.5
3	C	535	GLN	3.5
3	C	333	ALA	3.5
3	I	66	GLY	3.5
2	H	105	PHE	3.5
3	F	360	SER	3.4
3	C	236	HIS	3.4
3	C	328	ASN	3.4
1	D	21	PHE	3.4
3	C	258	CYS	3.4
2	H	63	THR	3.4
2	B	82	ALA	3.4
2	E	139	VAL	3.4
3	C	336	SER	3.4
3	C	553	VAL	3.4
1	G	96	HIS	3.4
3	F	3	GLN	3.4
2	H	43	ALA	3.3
2	H	66	ARG	3.3
3	C	398	PRO	3.3
2	K	103	ILE	3.3
1	A	29	LYS	3.3
2	H	84	GLU	3.3
3	F	302	SER	3.3
1	A	28	LEU	3.3
3	F	8	GLU	3.3
3	C	563	ALA	3.2
2	E	92	GLY	3.2
1	G	67	ASP	3.2
2	H	40	CYS	3.2
3	C	65	ASN	3.2
3	C	564	ALA	3.2
3	F	544	GLU	3.2
1	J	42	THR	3.2

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Mol	Chain	Res	Type	RSRZ
3	I	3	GLN	3.2
3	L	329	PRO	3.1
3	L	333	ALA	3.1
3	L	309	TYR	3.1
3	C	253	ASP	3.1
3	C	566	ASN	3.1
3	L	328	ASN	3.1
3	L	7	GLN	3.1
2	E	88	ALA	3.1
2	K	37	LEU	3.1
3	F	333	ALA	3.1
3	C	375	ASN	3.0
3	C	223	VAL	3.0
3	L	56	GLY	3.0
3	L	11	GLY	3.0
3	I	383	ALA	3.0
3	C	327	LEU	3.0
3	C	11	GLY	3.0
3	I	39	TYR	3.0
3	F	27	ASN	3.0
2	E	138	GLY	2.9
3	L	542	ASP	2.9
3	C	249	SER	2.9
3	C	66	GLY	2.9
3	I	38	GLY	2.9
3	F	263	ASP	2.9
3	I	338	ALA	2.9
3	C	345	GLU	2.9
2	H	106	GLU	2.9
2	K	42	LEU	2.9
3	C	322	MET	2.9
2	H	87	ARG	2.9
3	C	561	ASP	2.8
3	C	550	VAL	2.8
3	C	397	ALA	2.8
2	B	50	ASN	2.8
3	C	262	GLU	2.8
2	H	56	THR	2.8
3	F	7	GLN	2.8
2	E	78	GLU	2.8
1	J	29	LYS	2.8
3	I	572	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	24	GLY	2.8
1	G	75	ASP	2.8
2	H	64	GLY	2.8
3	F	329	PRO	2.8
2	B	91	TYR	2.8
3	F	337	PHE	2.8
3	I	528	HIS	2.8
3	C	385	ALA	2.7
1	G	62	LYS	2.7
2	H	118	PHE	2.7
1	G	79	ASN	2.7
3	I	8	GLU	2.7
3	C	389	SER	2.7
3	I	43	SER	2.7
2	K	91	TYR	2.7
3	I	562	THR	2.7
2	H	47	ILE	2.7
2	H	79	VAL	2.7
3	C	340	SER	2.6
3	C	263	ASP	2.6
3	I	337	PHE	2.6
1	G	92	LEU	2.6
3	I	388	ALA	2.6
3	C	309	TYR	2.6
2	K	36	PRO	2.6
3	I	258	CYS	2.6
3	I	398	PRO	2.6
3	I	282	GLY	2.6
2	K	104	ARG	2.6
2	H	129	ASN	2.6
3	C	334	ASP	2.5
2	H	107	PRO	2.5
2	H	90	ALA	2.5
3	C	7	GLN	2.5
3	C	250	VAL	2.5
3	F	314	GLN	2.5
2	E	59	LYS	2.5
1	D	62	LYS	2.5
3	C	286	ALA	2.5
1	D	15	THR	2.5
3	C	552	GLY	2.5
3	L	2	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
3	I	321	ILE	2.5
2	H	59	LYS	2.5
3	I	394	PRO	2.5
2	H	75	HIS	2.4
2	E	50	ASN	2.4
3	C	296	PRO	2.4
3	C	559	PRO	2.4
3	F	320	MET	2.4
3	C	295	GLN	2.4
3	C	384	ASN	2.4
3	L	388	ALA	2.4
2	H	82	ALA	2.4
2	K	129	ASN	2.4
1	J	55	ASP	2.4
3	I	20	LYS	2.4
3	C	319	ASP	2.4
3	C	308	PRO	2.4
2	H	88	ALA	2.4
2	H	100	THR	2.4
3	I	60	HIS	2.4
2	H	125	TYR	2.3
3	C	376	TRP	2.3
1	G	29	LYS	2.3
3	L	572	GLY	2.3
3	L	554	HIS	2.3
3	C	381	GLN	2.3
2	H	111	THR	2.3
3	I	342	VAL	2.3
2	H	39	GLY	2.3
3	C	318	PHE	2.3
3	L	308	PRO	2.3
3	I	36	LEU	2.3
2	H	92	GLY	2.3
3	I	5	SER	2.3
2	H	112	GLU	2.3
2	H	48	THR	2.3
3	F	323	VAL	2.3
3	L	360	SER	2.3
3	C	382	THR	2.2
2	H	137	GLU	2.2
3	C	301	SER	2.2
3	I	340	SER	2.2

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Mol	Chain	Res	Type	RSRZ
3	L	291	ARG	2.2
3	L	553	VAL	2.2
2	E	43	ALA	2.2
2	H	113	VAL	2.2
3	F	541	VAL	2.2
3	F	384	ASN	2.2
3	F	327	LEU	2.2
3	C	554	HIS	2.2
3	I	554	HIS	2.2
2	E	103	ILE	2.2
2	H	72	SER	2.2
3	I	110	GLY	2.2
1	A	79	ASN	2.2
1	G	65	THR	2.2
3	L	383	ALA	2.2
3	C	277	HIS	2.2
3	I	408	TYR	2.2
3	C	291	ARG	2.2
3	F	572	GLY	2.2
3	L	331	VAL	2.1
3	C	354	HIS	2.1
2	H	110	GLU	2.1
3	C	311	VAL	2.1
2	H	98	SER	2.1
3	C	307	LEU	2.1
3	C	388	ALA	2.1
3	F	562	THR	2.1
3	I	553	VAL	2.1
1	J	27	GLY	2.1
3	F	375	ASN	2.1
3	C	31	GLU	2.1
3	C	541	VAL	2.1
3	F	328	ASN	2.1
3	I	278	THR	2.1
1	A	78	PRO	2.1
3	I	329	PRO	2.1
3	L	398	PRO	2.1
3	I	6	ARG	2.1
3	C	47	GLY	2.1
1	G	44	MET	2.1
3	I	375	ASN	2.1
2	H	97	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	389	SER	2.1
3	F	315	ALA	2.0
2	B	44	ASP	2.0
1	G	30	LEU	2.0
2	H	119	GLY	2.0
1	G	97	ASP	2.0
2	E	102	ALA	2.0
3	F	66	GLY	2.0
3	I	464	GLY	2.0
3	C	572	GLY	2.0
3	I	369	MET	2.0
3	L	369	MET	2.0
2	H	76	PHE	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NI	F	602	1/1	0.77	0.15	-0.76	45,45,45,45	0
4	NI	I	602	1/1	0.98	0.11	-0.94	40,40,40,40	0
4	NI	I	601	1/1	0.96	0.09	-1.22	41,41,41,41	0
4	NI	F	601	1/1	0.91	0.09	-1.27	53,53,53,53	0
4	NI	C	601	1/1	0.93	0.10	-1.39	81,81,81,81	0
4	NI	L	602	1/1	0.83	0.07	-1.41	43,43,43,43	0
4	NI	L	601	1/1	0.95	0.07	-1.46	52,52,52,52	0
4	NI	C	602	1/1	0.90	0.08	-1.47	82,82,82,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.