



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:03 PM GMT

PDB ID : 4E4M
Title : JAK2 kinase (JH1 domain) in complex with compound 30
Authors : Eigenbrot, C.
Deposited on : 2012-03-13
Resolution : 2.25 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

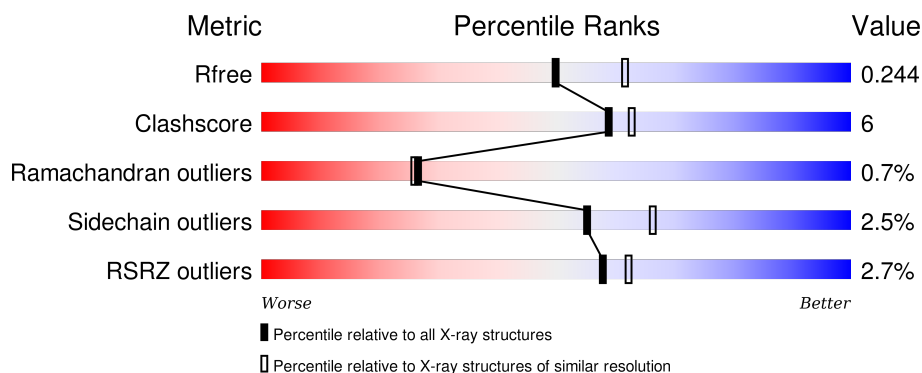
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	302	<div> <div>2%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	B	302	<div> <div>3%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	D	302	<div> <div>3%</div> <div>87%</div> <div>11%</div> <div>..</div> </div>
1	E	302	<div> <div>3%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10417 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.

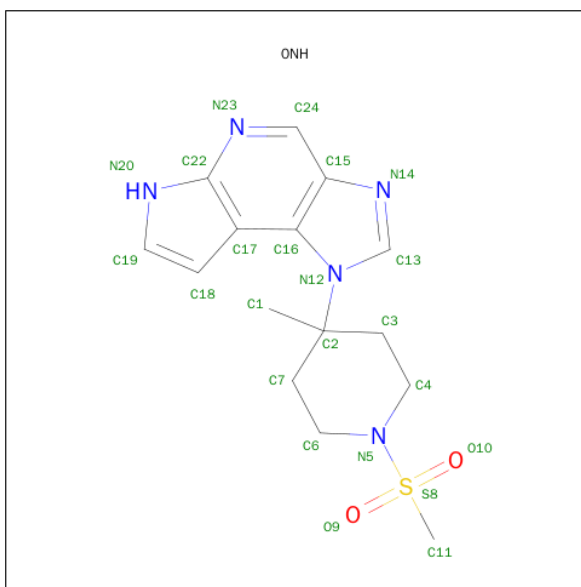
- Molecule 1 is a protein called Tyrosine-protein kinase JAK2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	P	S	0	0	0
			2469	1563	429	461	2	14			
1	B	298	Total	C	N	O	P	S	0	0	0
			2469	1563	429	461	2	14			
1	D	298	Total	C	N	O	P	S	0	0	0
			2469	1563	429	461	2	14			
1	E	298	Total	C	N	O	P	S	0	0	0
			2469	1563	429	461	2	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	831	GLY	-	EXPRESSION TAG	UNP O60674
A	832	SER	-	EXPRESSION TAG	UNP O60674
B	831	GLY	-	EXPRESSION TAG	UNP O60674
B	832	SER	-	EXPRESSION TAG	UNP O60674
D	831	GLY	-	EXPRESSION TAG	UNP O60674
D	832	SER	-	EXPRESSION TAG	UNP O60674
E	831	GLY	-	EXPRESSION TAG	UNP O60674
E	832	SER	-	EXPRESSION TAG	UNP O60674

- Molecule 2 is 1-[4-METHYL-1-(METHYLSULFONYL)PIPERIDIN-4-YL]-1,6-DIHYDROIMIDAZO[4,5-D]PYRROLO[2,3-B]PYRIDINE (three-letter code: 0NH) (formula: C₁₅H₁₉N₅O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			23	15	5	2	1		
2	B	1	Total	C	N	O	S	0	0
			23	15	5	2	1		
2	D	1	Total	C	N	O	S	0	0
			23	15	5	2	1		
2	E	1	Total	C	N	O	S	0	0
			23	15	5	2	1		

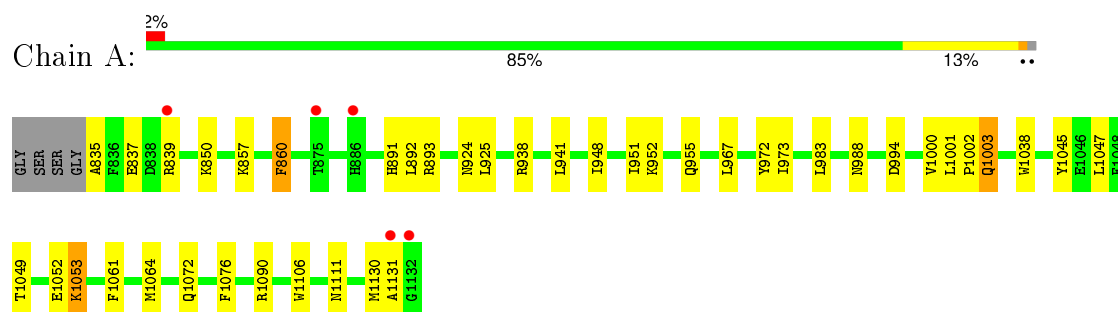
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	114	Total	O	0	0
			114	114		
3	B	115	Total	O	0	0
			115	115		
3	D	115	Total	O	0	0
			115	115		
3	E	105	Total	O	0	0
			105	105		

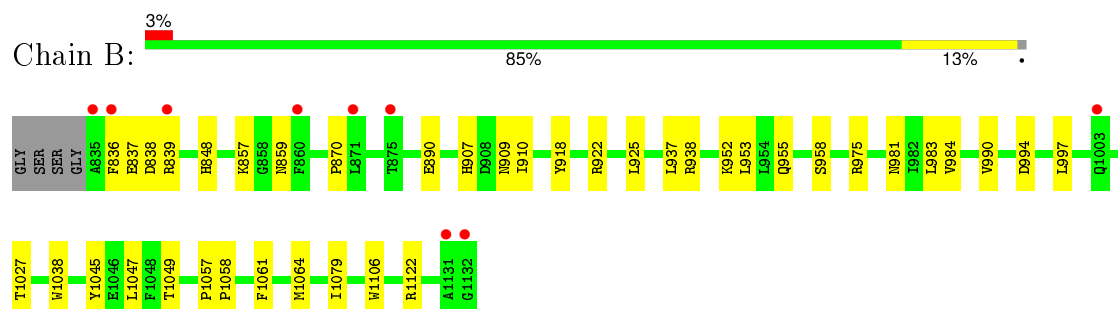
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

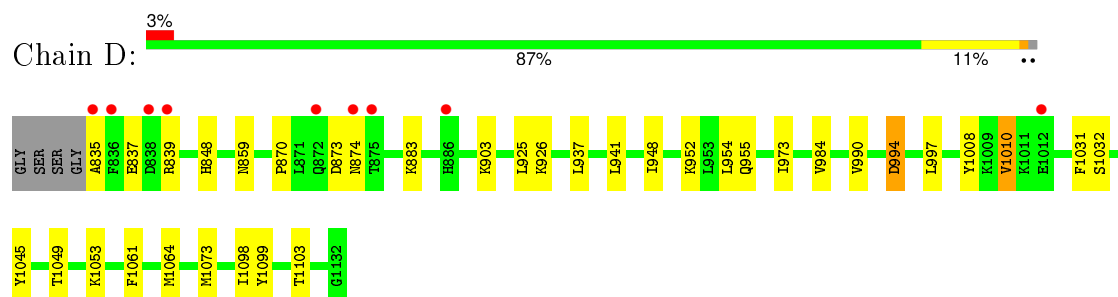
• Molecule 1: Tyrosine-protein kinase JAK2



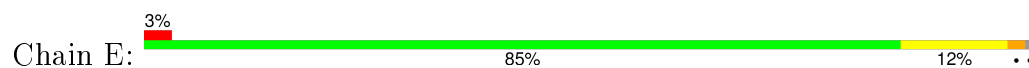
• Molecule 1: Tyrosine-protein kinase JAK2

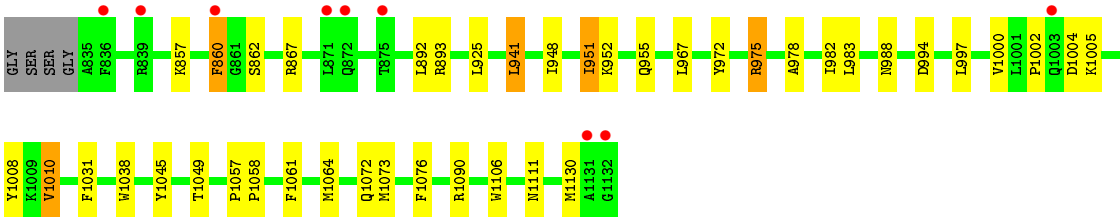


• Molecule 1: Tyrosine-protein kinase JAK2



• Molecule 1: Tyrosine-protein kinase JAK2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.37Å 76.31Å 87.28Å 75.27° 66.62° 62.96°	Depositor
Resolution (Å)	50.00 – 2.25 34.68 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-2.25) 93.1 (34.68-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.250 0.198 , 0.244	Depositor DCC
R_{free} test set	691 reflections (1.05%)	DCC
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 23.4	EDS
Estimated twinning fraction	0.457 for h,h-k,h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 66342 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10417	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 74.40 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.5387e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 0NH, PTR

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	0.50	0/2488	0.64	0/3347
1	B	0.50	0/2488	0.63	0/3347
1	D	0.49	0/2488	0.65	0/3347
1	E	0.51	0/2488	0.64	1/3347 (0.0%)
All	All	0.50	0/9952	0.64	1/13388 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	975	ARG	NE-CZ-NH1	6.08	123.34	120.30

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	2469	0	2433	37	0
1	B	2469	0	2433	27	0
1	D	2469	0	2433	19	0
1	E	2469	0	2433	40	0
2	A	23	0	19	4	0
2	B	23	0	19	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	23	0	19	1	0
2	E	23	0	19	3	0
3	A	114	0	0	2	0
3	B	115	0	0	3	0
3	D	115	0	0	4	0
3	E	105	0	0	3	0
All	All	10417	0	9808	115	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 6.

All (115) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:GLU:OE1	1:A:839:ARG:HD2	1.66	0.94
1:A:941:LEU:HD23	1:A:948:ILE:HD13	1.59	0.85
1:A:837:GLU:OE1	1:A:839:ARG:CD	2.31	0.78
1:B:1061:PHE:HA	1:B:1064:MET:HE3	1.68	0.76
1:A:835:ALA:HB2	1:E:1002:PRO:HG2	1.70	0.74
1:A:951:ILE:HD11	1:A:1130:MET:HE2	1.70	0.73
1:D:1061:PHE:HA	1:D:1064:MET:HE3	1.71	0.72
1:A:892:LEU:HD21	1:E:1076:PHE:HE2	1.56	0.69
1:E:983:LEU:HD11	2:E:1201:ONH:H7	1.73	0.69
1:E:941:LEU:HD12	1:E:948:ILE:HD13	1.76	0.67
1:B:907:HIS:HB3	1:B:910:ILE:HD12	1.77	0.66
1:E:952:LYS:NZ	1:E:955:GLN:HE22	1.93	0.66
1:A:835:ALA:CB	1:E:1002:PRO:HG2	2.26	0.66
1:E:1061:PHE:HA	1:E:1064:MET:HE3	1.78	0.65
1:A:835:ALA:HB2	1:E:1002:PRO:CD	2.27	0.64
1:A:952:LYS:NZ	1:A:988:ASN:OD1	2.31	0.63
1:B:952:LYS:NZ	1:B:955:GLN:HE22	1.98	0.62
1:B:983:LEU:HD11	2:B:1201:ONH:H7	1.80	0.62
1:B:983:LEU:HD11	2:B:1201:ONH:C7	2.30	0.61
1:A:835:ALA:HB2	1:E:1002:PRO:CG	2.30	0.61
1:A:892:LEU:HD21	1:E:1076:PHE:CE2	2.36	0.60
1:B:859:ASN:ND2	1:B:994:ASP:OD2	2.35	0.59
1:A:835:ALA:HB2	1:E:1002:PRO:HD2	1.84	0.59
1:B:836:PHE:CE2	1:B:838:ASP:HB2	2.38	0.58
1:B:984:VAL:HG22	1:B:990:VAL:HG12	1.85	0.58
1:D:984:VAL:HG22	1:D:990:VAL:HG12	1.87	0.56
1:D:903:LYS:HE2	3:D:1399:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1027:THR:HG22	1:B:1079:ILE:HD13	1.88	0.55
1:A:941:LEU:HD11	1:A:1047:LEU:HD23	1.89	0.54
1:B:836:PHE:CZ	1:B:838:ASP:HB2	2.42	0.54
1:A:938:ARG:HD2	3:A:1392:HOH:O	2.07	0.54
1:A:972:TYR:CD2	1:A:1000:VAL:HG22	2.43	0.53
1:B:937:LEU:HD21	1:B:1047:LEU:HD21	1.90	0.53
1:D:1099:TYR:O	1:D:1103:THR:HG23	2.08	0.52
1:E:952:LYS:HZ2	1:E:955:GLN:HE22	1.56	0.52
1:B:994:ASP:CG	3:B:1333:HOH:O	2.48	0.52
1:E:952:LYS:HZ2	1:E:955:GLN:NE2	2.08	0.51
1:A:1111:ASN:HB2	3:A:1389:HOH:O	2.08	0.51
1:D:848:HIS:CG	1:D:870:PRO:HA	2.45	0.51
1:E:972:TYR:CD2	1:E:1000:VAL:HG22	2.45	0.51
1:B:1057:PRO:HB2	1:B:1058:PRO:HD3	1.93	0.51
1:E:972:TYR:CE2	1:E:1000:VAL:HG22	2.46	0.51
1:E:951:ILE:CD1	1:E:1130:MET:HE2	2.41	0.51
1:A:973:ILE:HD11	1:A:1001:LEU:HD21	1.93	0.50
1:A:835:ALA:CB	1:E:1002:PRO:CG	2.90	0.50
1:D:952:LYS:NZ	1:D:955:GLN:HE22	2.09	0.50
1:B:952:LYS:HD3	1:B:955:GLN:HE21	1.76	0.50
1:D:994:ASP:HB3	3:D:1389:HOH:O	2.11	0.50
1:A:837:GLU:OE2	1:E:1008:PTR:OH	2.30	0.49
1:B:837:GLU:CD	1:B:839:ARG:HD2	2.33	0.49
1:A:952:LYS:NZ	1:A:955:GLN:HE22	2.11	0.49
1:A:835:ALA:CB	1:E:1002:PRO:CD	2.90	0.49
1:A:1072:GLN:HG3	1:A:1076:PHE:CE1	2.48	0.48
1:A:835:ALA:HB3	1:E:1008:PTR:HA	1.95	0.48
1:A:951:ILE:CD1	1:A:1130:MET:HE2	2.41	0.48
1:B:848:HIS:CG	1:B:870:PRO:HA	2.47	0.48
1:A:972:TYR:CE2	1:A:1000:VAL:HG22	2.49	0.48
1:A:1038:TRP:CE3	1:A:1106:TRP:HA	2.49	0.48
1:A:952:LYS:HZ3	1:A:955:GLN:HE22	1.62	0.48
1:E:1038:TRP:CE3	1:E:1106:TRP:HA	2.49	0.47
1:E:1111:ASN:HB2	3:E:1352:HOH:O	2.14	0.47
1:A:835:ALA:N	1:E:1005:LYS:HG2	2.28	0.47
1:E:951:ILE:HD11	3:E:1324:HOH:O	2.15	0.46
1:D:883:LYS:HB3	1:D:926:LYS:HD3	1.98	0.46
1:D:941:LEU:HD12	1:D:948:ILE:HD13	1.98	0.46
1:E:1045:TYR:O	1:E:1049:THR:HG23	2.15	0.46
1:A:1045:TYR:O	1:A:1049:THR:HG23	2.15	0.46
1:B:918:TYR:HB3	1:B:922:ARG:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:952:LYS:HZ3	1:B:955:GLN:HE22	1.64	0.45
2:A:1201:0NH:C18	2:A:1201:0NH:H3A	2.46	0.45
1:A:892:LEU:HD23	1:E:1073:MET:HG2	1.98	0.45
2:B:1201:0NH:H11	2:B:1201:0NH:H6A	1.76	0.45
1:D:835:ALA:N	3:D:1396:HOH:O	2.51	0.44
1:A:857:LYS:HA	1:A:857:LYS:HD3	1.85	0.44
1:E:1010:VAL:HG13	1:E:1031:PHE:CE1	2.53	0.44
1:D:1073:MET:HG3	3:D:1384:HOH:O	2.16	0.44
1:E:951:ILE:HD12	1:E:1130:MET:CE	2.48	0.44
1:D:837:GLU:OE1	1:D:839:ARG:HD2	2.17	0.44
1:D:954:LEU:HD21	1:D:1098:ILE:HD12	1.99	0.44
1:B:907:HIS:HE1	1:B:909:ASN:HD22	1.65	0.44
1:B:983:LEU:HD11	2:B:1201:0NH:H7A	1.98	0.43
1:B:981:ASN:HA	2:B:1201:0NH:H11A	2.00	0.43
1:E:1045:TYR:CE2	1:E:1049:THR:HG21	2.52	0.43
1:E:1057:PRO:HB2	1:E:1058:PRO:HD3	2.00	0.43
2:A:1201:0NH:H18	2:A:1201:0NH:H3A	1.99	0.43
1:A:1002:PRO:O	1:A:1003:GLN:CB	2.67	0.43
2:A:1201:0NH:H7	2:A:1201:0NH:C18	2.49	0.43
1:A:1052:GLU:O	1:A:1053:LYS:HB3	2.18	0.43
1:E:952:LYS:NZ	1:E:988:ASN:OD1	2.43	0.43
1:E:1072:GLN:HG3	1:E:1076:PHE:CE1	2.54	0.42
1:A:983:LEU:HD11	2:A:1201:0NH:H7	2.01	0.42
1:D:1045:TYR:O	1:D:1049:THR:HG23	2.20	0.42
1:D:873:ASP:O	1:D:874:ASN:CB	2.67	0.42
1:E:978:ALA:O	1:E:982:ILE:HG12	2.19	0.42
1:B:1038:TRP:CE3	1:B:1106:TRP:HA	2.54	0.42
1:A:837:GLU:OE2	1:E:1008:PTR:P	2.78	0.41
1:B:1122:ARG:HD2	3:B:1347:HOH:O	2.20	0.41
1:E:951:ILE:HD11	1:E:1130:MET:HE2	2.03	0.41
1:A:1061:PHE:CD2	1:A:1064:MET:HE3	2.56	0.41
1:B:890:GLU:HG3	3:B:1412:HOH:O	2.19	0.41
2:E:1201:0NH:H3A	2:E:1201:0NH:C18	2.50	0.41
1:B:975:ARG:HD3	1:B:997:LEU:O	2.20	0.41
1:E:1004:ASP:N	1:E:1004:ASP:OD1	2.52	0.41
1:D:1010:VAL:HG13	1:D:1031:PHE:CE1	2.56	0.41
1:A:1045:TYR:CE2	1:A:1049:THR:HG21	2.56	0.41
1:D:859:ASN:ND2	1:D:997:LEU:HG	2.35	0.41
1:E:857:LYS:HD2	3:E:1397:HOH:O	2.21	0.41
2:D:1201:0NH:C18	2:D:1201:0NH:H7	2.51	0.41
1:D:973:ILE:HD12	1:D:1032:SER:C	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:975:ARG:HD3	1:E:997:LEU:O	2.21	0.40
1:E:983:LEU:HD11	2:E:1201:ONH:C7	2.48	0.40
1:B:953:LEU:HD22	1:B:1047:LEU:HB3	2.03	0.40
1:E:951:ILE:HD12	1:E:1130:MET:HE2	2.02	0.40
1:D:1008:PTR:HE2	1:D:1010:VAL:HB	2.04	0.40
1:B:1045:TYR:O	1:B:1049:THR:HG23	2.21	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	294/302 (97%)	283 (96%)	6 (2%)	5 (2%)	11	6
1	B	294/302 (97%)	286 (97%)	8 (3%)	0	100	100
1	D	294/302 (97%)	288 (98%)	5 (2%)	1 (0%)	46	52
1	E	294/302 (97%)	287 (98%)	5 (2%)	2 (1%)	26	26
All	All	1176/1208 (97%)	1144 (97%)	24 (2%)	8 (1%)	26	26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	860	PHE
1	A	994	ASP
1	A	1131	ALA
1	D	994	ASP
1	E	994	ASP
1	A	1003	GLN
1	E	860	PHE
1	A	1053	LYS

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	269/271 (99%)	261 (97%)	8 (3%)	48	59
1	B	269/271 (99%)	265 (98%)	4 (2%)	72	82
1	D	269/271 (99%)	265 (98%)	4 (2%)	72	82
1	E	269/271 (99%)	258 (96%)	11 (4%)	37	44
All	All	1076/1084 (99%)	1049 (98%)	27 (2%)	55	66

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	850	LYS
1	A	860	PHE
1	A	891	HIS
1	A	893	ARG
1	A	924	ASN
1	A	925	LEU
1	A	967	LEU
1	A	1090	ARG
1	B	857	LYS
1	B	925	LEU
1	B	938	ARG
1	B	958	SER
1	D	925	LEU
1	D	937	LEU
1	D	1010	VAL
1	D	1053	LYS
1	E	860	PHE
1	E	862	SER
1	E	867	ARG
1	E	892	LEU
1	E	893	ARG
1	E	925	LEU
1	E	941	LEU
1	E	951	ILE

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Mol	Chain	Res	Type
1	E	967	LEU
1	E	1010	VAL
1	E	1090	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	909	ASN
1	A	924	ASN
1	A	955	GLN
1	B	872	GLN
1	B	909	ASN
1	B	924	ASN
1	B	955	GLN
1	D	909	ASN
1	D	955	GLN
1	E	848	HIS
1	E	854	GLN
1	E	872	GLN
1	E	891	HIS
1	E	950	HIS
1	E	955	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues 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
1	PTR	A	1007	1	14,16,17	1.88	1 (7%)	18,22,24	0.64	0
1	PTR	A	1008	1	14,16,17	1.87	1 (7%)	18,22,24	1.10	2 (11%)
1	PTR	B	1007	1	14,16,17	1.90	1 (7%)	18,22,24	0.86	1 (5%)
1	PTR	B	1008	1	14,16,17	1.85	1 (7%)	18,22,24	0.77	0
1	PTR	D	1007	1	14,16,17	1.87	1 (7%)	18,22,24	0.73	0
1	PTR	D	1008	1	14,16,17	1.88	1 (7%)	18,22,24	0.72	0
1	PTR	E	1007	1	14,16,17	1.87	1 (7%)	18,22,24	0.65	0
1	PTR	E	1008	1	14,16,17	1.83	1 (7%)	18,22,24	0.90	0

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
1	PTR	A	1007	1	-	0/9/11/13	0/1/1/1
1	PTR	A	1008	1	-	0/9/11/13	0/1/1/1
1	PTR	B	1007	1	-	0/9/11/13	0/1/1/1
1	PTR	B	1008	1	-	0/9/11/13	0/1/1/1
1	PTR	D	1007	1	-	0/9/11/13	0/1/1/1
1	PTR	D	1008	1	-	0/9/11/13	0/1/1/1
1	PTR	E	1007	1	-	0/9/11/13	0/1/1/1
1	PTR	E	1008	1	-	0/9/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1007	PTR	OH-CZ	-6.85	1.24	1.40
1	B	1008	PTR	OH-CZ	-6.76	1.24	1.40
1	A	1008	PTR	OH-CZ	-6.75	1.24	1.40
1	B	1007	PTR	OH-CZ	-6.75	1.24	1.40
1	D	1008	PTR	OH-CZ	-6.65	1.24	1.40
1	E	1007	PTR	OH-CZ	-6.61	1.24	1.40
1	A	1007	PTR	OH-CZ	-6.61	1.24	1.40
1	E	1008	PTR	OH-CZ	-6.50	1.25	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1007	PTR	O-C-CA	-2.34	119.38	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1008	PTR	P-OH-CZ	2.41	130.70	123.76
1	A	1008	PTR	OH-CZ-CE1	2.48	126.86	119.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	1008	PTR	1	0
1	E	1008	PTR	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
2	0NH	A	1201	-	20,26,26	3.75	9 (45%)	21,41,41	2.92	11 (52%)
2	0NH	B	1201	-	20,26,26	3.57	9 (45%)	21,41,41	2.90	12 (57%)
2	0NH	D	1201	-	20,26,26	3.58	9 (45%)	21,41,41	3.02	12 (57%)
2	0NH	E	1201	-	20,26,26	3.66	9 (45%)	21,41,41	2.93	12 (57%)

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
2	0NH	A	1201	-	-	0/10/24/24	0/4/4/4
2	0NH	B	1201	-	-	0/10/24/24	0/4/4/4
2	0NH	D	1201	-	-	0/10/24/24	0/4/4/4
2	0NH	E	1201	-	-	0/10/24/24	0/4/4/4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1201	0NH	C24-N23	-9.68	1.31	1.47
2	A	1201	0NH	C24-N23	-9.38	1.31	1.47
2	D	1201	0NH	C24-N23	-9.33	1.31	1.47
2	A	1201	0NH	C17-C16	-9.20	1.41	1.54
2	B	1201	0NH	C24-N23	-9.04	1.32	1.47
2	E	1201	0NH	C17-C16	-8.47	1.42	1.54
2	B	1201	0NH	C17-C16	-8.25	1.42	1.54
2	D	1201	0NH	C17-C16	-8.09	1.42	1.54
2	A	1201	0NH	C16-N12	-6.09	1.38	1.48
2	E	1201	0NH	C16-N12	-5.82	1.39	1.48
2	B	1201	0NH	C16-N12	-5.65	1.39	1.48
2	D	1201	0NH	C16-N12	-5.60	1.39	1.48
2	A	1201	0NH	C15-N14	-4.73	1.36	1.48
2	B	1201	0NH	C15-N14	-4.67	1.36	1.48
2	E	1201	0NH	C15-N14	-4.60	1.36	1.48
2	D	1201	0NH	C15-N14	-4.58	1.36	1.48
2	E	1201	0NH	C19-N20	-3.47	1.36	1.48
2	A	1201	0NH	C19-N20	-3.40	1.36	1.48
2	B	1201	0NH	C13-N12	-3.36	1.37	1.46
2	A	1201	0NH	C13-N12	-3.31	1.37	1.46
2	E	1201	0NH	C13-N12	-3.22	1.37	1.46
2	D	1201	0NH	C13-N12	-3.21	1.37	1.46
2	B	1201	0NH	C19-N20	-3.21	1.37	1.48
2	D	1201	0NH	C19-N20	-3.16	1.37	1.48
2	A	1201	0NH	C18-C17	-2.63	1.46	1.54
2	E	1201	0NH	C18-C17	-2.62	1.46	1.54
2	B	1201	0NH	C18-C17	-2.54	1.46	1.54
2	D	1201	0NH	C18-C17	-2.34	1.47	1.54
2	B	1201	0NH	S8-N5	2.05	1.66	1.63
2	E	1201	0NH	S8-N5	2.21	1.66	1.63
2	D	1201	0NH	S8-N5	2.54	1.66	1.63
2	A	1201	0NH	C11-S8	2.57	1.80	1.75
2	E	1201	0NH	C11-S8	2.81	1.80	1.75
2	A	1201	0NH	S8-N5	2.81	1.67	1.63
2	B	1201	0NH	C11-S8	3.35	1.81	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1201	0NH	C11-S8	3.43	1.82	1.75

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	0NH	O10-S8-N5	-5.35	101.62	106.99
2	E	1201	0NH	O10-S8-N5	-4.85	102.13	106.99
2	D	1201	0NH	O9-S8-N5	-4.74	102.23	106.99
2	B	1201	0NH	O10-S8-N5	-3.53	103.45	106.99
2	B	1201	0NH	C11-S8-N5	-2.43	105.10	107.35
2	E	1201	0NH	O9-S8-N5	-2.27	104.71	106.99
2	D	1201	0NH	O10-S8-N5	-2.16	104.82	106.99
2	A	1201	0NH	O9-S8-N5	-2.07	104.91	106.99
2	A	1201	0NH	O9-S8-C11	2.02	111.50	108.70
2	A	1201	0NH	C13-N12-C16	2.13	107.07	104.75
2	B	1201	0NH	C13-N12-C16	2.15	107.09	104.75
2	E	1201	0NH	C13-N12-C16	2.36	107.32	104.75
2	D	1201	0NH	C6-N5-S8	2.37	118.46	115.99
2	D	1201	0NH	O10-S8-C11	2.50	112.15	108.70
2	E	1201	0NH	C7-C2-C3	2.51	111.91	108.23
2	B	1201	0NH	C7-C2-C3	2.65	112.11	108.23
2	D	1201	0NH	C13-N12-C16	2.78	107.77	104.75
2	E	1201	0NH	C19-C18-C17	2.82	107.34	104.02
2	B	1201	0NH	C19-C18-C17	2.89	107.42	104.02
2	A	1201	0NH	C19-C18-C17	2.90	107.43	104.02
2	D	1201	0NH	C7-C2-C3	2.92	112.51	108.23
2	E	1201	0NH	O9-S8-C11	2.99	112.83	108.70
2	B	1201	0NH	O10-S8-C11	3.00	112.85	108.70
2	E	1201	0NH	C24-C15-N14	3.05	133.21	117.69
2	D	1201	0NH	C24-C15-N14	3.06	133.28	117.69
2	B	1201	0NH	C24-C15-N14	3.08	133.38	117.69
2	B	1201	0NH	C6-N5-S8	3.11	119.24	115.99
2	D	1201	0NH	C19-C18-C17	3.13	107.70	104.02
2	A	1201	0NH	C24-C15-N14	3.20	133.98	117.69
2	E	1201	0NH	C4-N5-S8	3.46	119.60	115.99
2	A	1201	0NH	C6-N5-S8	3.54	119.69	115.99
2	E	1201	0NH	C19-N20-C22	3.55	109.44	105.40
2	E	1201	0NH	C6-N5-S8	3.91	120.08	115.99
2	D	1201	0NH	C19-N20-C22	4.00	109.96	105.40
2	B	1201	0NH	C19-N20-C22	4.03	110.00	105.40
2	A	1201	0NH	C19-N20-C22	4.11	110.08	105.40
2	E	1201	0NH	C24-C15-C16	4.23	118.72	111.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	0NH	C24-C15-C16	4.26	118.79	111.15
2	B	1201	0NH	C4-N5-S8	4.47	120.66	115.99
2	D	1201	0NH	C24-C15-C16	4.49	119.20	111.15
2	A	1201	0NH	C4-N5-S8	4.56	120.75	115.99
2	B	1201	0NH	C24-C15-C16	4.63	119.44	111.15
2	D	1201	0NH	C4-N5-S8	5.57	121.81	115.99
2	A	1201	0NH	C6-N5-C4	6.02	119.51	112.20
2	D	1201	0NH	C6-N5-C4	6.17	119.69	112.20
2	B	1201	0NH	C6-N5-C4	6.50	120.10	112.20
2	E	1201	0NH	C6-N5-C4	6.59	120.21	112.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	0NH	4	0
2	B	1201	0NH	5	0
2	D	1201	0NH	1	0
2	E	1201	0NH	3	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	296/302 (98%)	-0.40	5 (1%) 73 77	10, 22, 60, 89	0
1	B	296/302 (98%)	-0.32	9 (3%) 54 58	10, 24, 65, 94	0
1	D	296/302 (98%)	-0.31	9 (3%) 54 58	10, 23, 68, 94	0
1	E	296/302 (98%)	-0.30	9 (3%) 54 58	10, 23, 61, 95	0
All	All	1184/1208 (98%)	-0.33	32 (2%) 58 62	10, 23, 65, 95	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1132	GLY	16.8
1	D	835	ALA	10.2
1	E	1131	ALA	8.5
1	A	1131	ALA	6.0
1	A	839	ARG	4.0
1	B	835	ALA	3.5
1	D	836	PHE	3.5
1	E	839	ARG	3.4
1	B	860	PHE	3.1
1	D	872	GLN	3.0
1	D	874	ASN	3.0
1	D	838	ASP	2.9
1	E	860	PHE	2.7
1	D	839	ARG	2.6
1	D	875	THR	2.5
1	A	1132	GLY	2.5
1	B	1131	ALA	2.3
1	D	886	HIS	2.3
1	B	1003	GLN	2.3
1	E	1003	GLN	2.3
1	B	871	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	871	LEU	2.2
1	E	872	GLN	2.2
1	B	1132	GLY	2.2
1	A	875	THR	2.1
1	B	836	PHE	2.1
1	E	836	PHE	2.1
1	D	1012	GLU	2.1
1	B	839	ARG	2.1
1	A	886	HIS	2.1
1	B	875	THR	2.0
1	E	875	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	LLDF	B-factors(Å ²)	Q<0.9
1	PTR	B	1007	16/17	0.92	0.14	-	30,47,64,64	0
1	PTR	A	1007	16/17	0.92	0.13	-	17,40,60,61	0
1	PTR	D	1007	16/17	0.92	0.14	-	29,48,63,64	0
1	PTR	A	1008	16/17	0.91	0.16	-	17,43,75,75	0
1	PTR	B	1008	16/17	0.89	0.17	-	20,46,70,71	0
1	PTR	E	1008	16/17	0.89	0.15	-	24,37,59,59	0
1	PTR	D	1008	16/17	0.89	0.15	-	19,45,70,72	0
1	PTR	E	1007	16/17	0.93	0.12	-	18,43,65,66	0

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	0NH	A	1201	23/23	0.97	0.11	0.20	17,27,36,42	0
2	0NH	E	1201	23/23	0.97	0.11	0.16	16,24,34,38	0
2	0NH	B	1201	23/23	0.97	0.11	-0.17	18,24,41,53	0
2	0NH	D	1201	23/23	0.97	0.09	-0.89	20,25,42,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.