W O R L D W I D E
wwPDB
P R O T E I N D A T A B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:56 pm GMT

PDB ID	:	4E4L
Title	:	JAK1 kinase (JH1 domain) in complex with compound 30
Authors	:	Eigenbrot, C.
Deposited on	:	2012-03-13
Resolution	:	2.00 Å(reported)

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

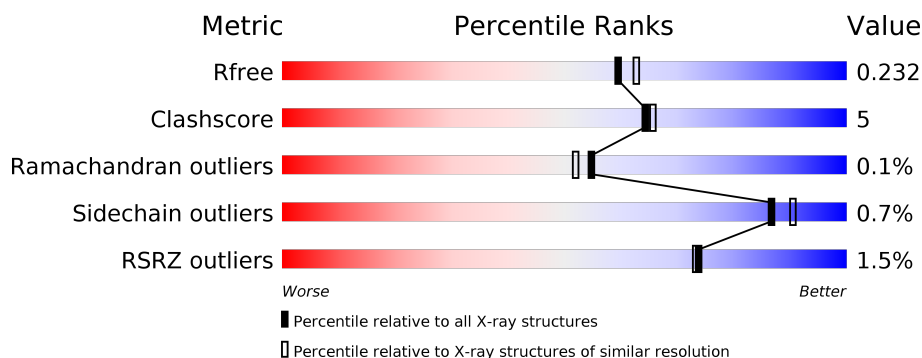|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	Percentile Ranks	Value
Rfree		0.232
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		0.7%
RSRZ outliers		1.5%

Worse ◄ ► Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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 >=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 <=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	% 84% 8% 8%
1	B	302	2% 84% 8% 7%
1	D	302	2% 82% 12% 6%
1	E	302	% 83% 10% 7%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 9949 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 JAK1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	P	S	0	3	0
			2301	1466	393	425	2	15			
1	B	281	Total	C	N	O	P	S	0	5	0
			2337	1488	399	433	2	15			
1	E	282	Total	C	N	O	P	S	0	4	0
			2333	1484	399	433	2	15			
1	D	283	Total	C	N	O	P	S	0	4	0
			2334	1483	400	434	2	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	853	GLY	-	EXPRESSION TAG	UNP P23458
B	853	GLY	-	EXPRESSION TAG	UNP P23458
E	853	GLY	-	EXPRESSION TAG	UNP P23458
D	853	GLY	-	EXPRESSION TAG	UNP P23458

- Molecule 2 is 1-[4-METHYL-1-(METHYLSULFONYL)PIPERIDIN-4-YL]-1,6-DIHY DROIMIDAZO[4,5-D]PYRROLO[2,3-B]PYRIDINE (three-letter code: 0NH) (formula: $C_{15}H_{19}N_5O_2S$).
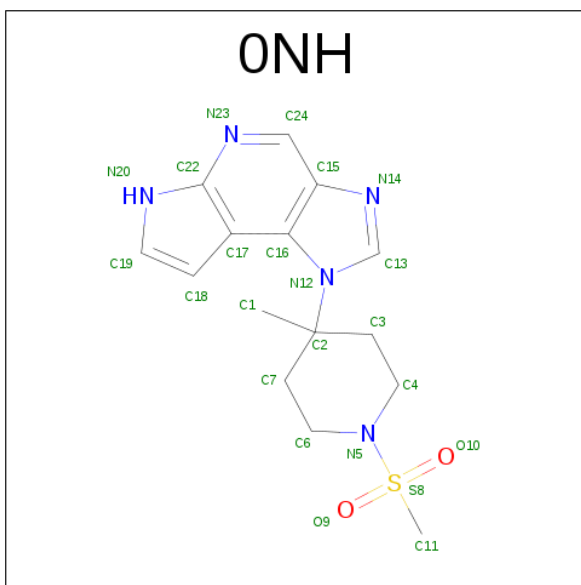
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			23	15	5	2	1		
2	A	1	Total	C	N	O	S	0	0
			23	15	5	2	1		
2	B	1	Total	C	N	O	S	0	0
			23	15	5	2	1		
2	D	1	Total	C	N	O	S	0	0
			23	15	5	2	1		

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	143	Total	O	0	0
			143	143		
3	B	140	Total	O	0	0
			140	140		
3	E	132	Total	O	0	0
			132	132		
3	D	137	Total	O	0	0
			137	137		

3 Residue-property plots ⓘ

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: Tyrosine-protein kinase JAK1
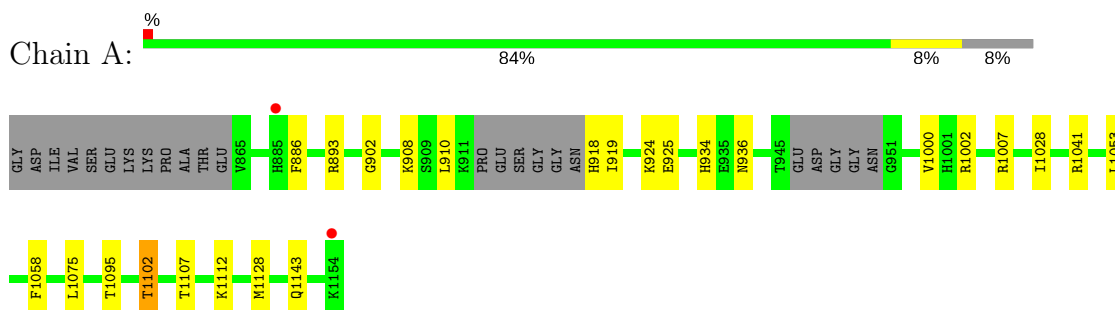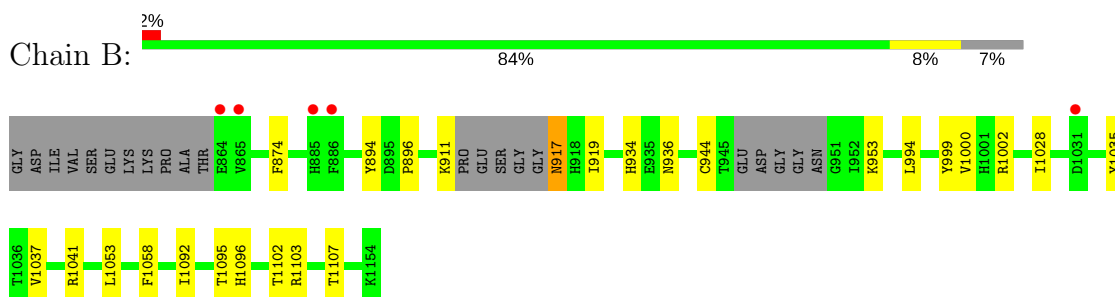
• Molecule 1: Tyrosine-protein kinase JAK1

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• Molecule 1: Tyrosine-protein kinase JAK1

L1053 S1056 K1057 F1058 W1065 L1075 L1089 K1090 P1094 T1102 T1107 K1112 P1118 M1128 W1132 S1137 N1144 K1154

4 Data and refinement statistics (i)

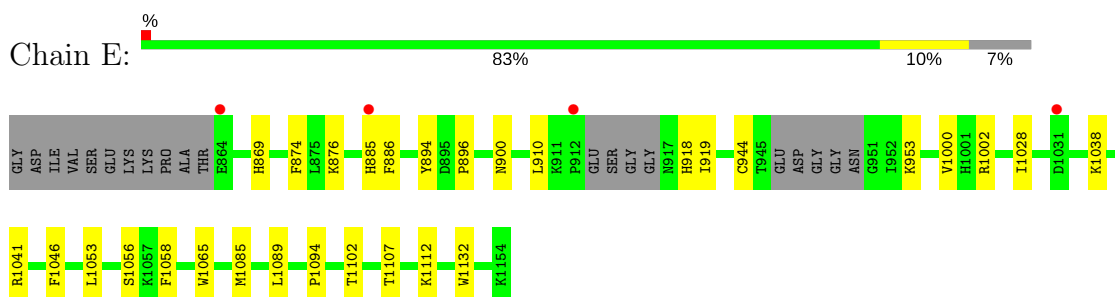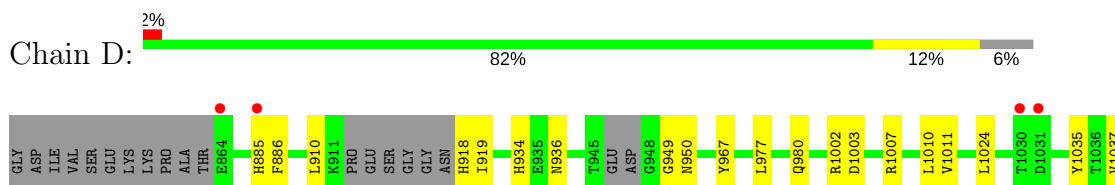| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.84Å 171.76Å 87.82Å 90.00° 92.15° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 47.95 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.5 (50.00-2.00) 94.6 (47.95-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.190 , 0.228 0.194 , 0.232	Depositor DCC
R_{free} test set	3725 reflections (4.85%)	DCC
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.5	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.107 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9949	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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 53.86 % 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 3.9670e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: 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	0.51	0/2315	0.62	0/3112
1	B	0.50	0/2352	0.60	0/3162
1	D	0.49	0/2348	0.61	0/3156
1	E	0.49	0/2348	0.61	0/3158
All	All	0.50	0/9363	0.61	0/12588

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2301	0	2301	17	0
1	B	2337	0	2326	22	0
1	D	2334	0	2324	28	0
1	E	2333	0	2325	29	0
2	A	46	0	38	1	0
2	B	23	0	19	1	0
2	D	23	0	19	1	0
3	A	143	0	0	1	0
3	B	140	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	137	0	0	5	0
3	E	132	0	0	6	0
All	All	9949	0	9352	90	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 5.

All (90) 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:E:900:ASN:HB2	3:E:1432:HOH:O	1.66	0.94
1:A:1053:LEU:O	1:B:1102:THR:HG21	1.75	0.87
1:B:1000:VAL:HB	1:B:1058[B]:PHE:CE2	2.19	0.78
1:B:1000:VAL:HB	1:B:1058[B]:PHE:CD2	2.20	0.77
1:E:885:HIS:HD2	1:E:886:PHE:CZ	2.07	0.72
1:E:910:LEU:CD1	1:E:919:ILE:HD13	2.20	0.71
1:D:1144[B]:ASN:ND2	3:D:1419:HOH:O	2.25	0.69
1:E:885:HIS:CD2	1:E:886:PHE:CZ	2.81	0.69
1:A:1000:VAL:HG13	1:A:1028:ILE:HD11	1.75	0.68
1:E:910:LEU:HD12	1:E:919:ILE:HD13	1.76	0.68
1:A:1002:ARG:HA	1:A:1058:PHE:CZ	2.28	0.67
1:E:1000:VAL:HG13	1:E:1028:ILE:HD11	1.77	0.66
1:D:1035:PTR:HE1	1:D:1037:VAL:HG12	1.77	0.65
1:E:1053:LEU:O	1:D:1102:THR:HG21	1.97	0.64
1:D:1107:THR:HG23	1:D:1112:LYS:HD2	1.82	0.60
1:B:1035:PTR:HE1	1:B:1037:VAL:HG22	1.82	0.60
1:E:1107:THR:HG22	1:E:1112:LYS:HB2	1.83	0.58
1:D:1107:THR:HG22	1:D:1112:LYS:HB2	1.86	0.58
1:A:924:LYS:NZ	3:A:1434:HOH:O	2.36	0.58
1:D:1002:ARG:NH2	1:D:1037:VAL:HG11	2.18	0.57
1:E:1002:ARG:HA	1:E:1058:PHE:CZ	2.40	0.56
1:B:1000:VAL:HG13	1:B:1028:ILE:HD11	1.87	0.55
1:D:910:LEU:HD11	1:D:919:ILE:HA	1.89	0.54
1:D:1002:ARG:HA	1:D:1058:PHE:CZ	2.44	0.53
1:D:1075:LEU:HD12	1:D:1128:MET:CE	2.38	0.53
1:E:1107:THR:HG23	1:E:1112:LYS:HD2	1.90	0.53
1:D:886:PHE:CD2	1:D:918:HIS:NE2	2.78	0.51
1:A:1041:ARG:HG3	1:B:1095:THR:O	2.11	0.51
1:A:910:LEU:HD11	1:A:919:ILE:HA	1.92	0.50
1:B:934:HIS:HE1	1:B:936:ASN:HD22	1.59	0.50
1:D:934:HIS:HE1	1:D:936:ASN:HD22	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1102:THR:HG21	1:D:1053:LEU:O	2.12	0.50
1:D:1107:THR:HG23	1:D:1112:LYS:CD	2.42	0.50
1:A:1095:THR:O	1:B:1041:ARG:HG3	2.11	0.49
1:D:1003:ASP:HB2	1:D:1024:LEU:HD12	1.93	0.49
1:B:1002:ARG:HA	1:B:1058[B]:PHE:CZ	2.48	0.49
1:D:1007:ARG:NE	3:D:1343:HOH:O	2.44	0.49
1:E:885:HIS:CD2	1:E:886:PHE:CE1	3.01	0.49
1:E:885:HIS:HD2	1:E:886:PHE:CE2	2.31	0.48
1:B:1000:VAL:CG1	1:B:1028:ILE:HD11	2.44	0.48
1:B:874:PHE:CD1	1:B:896:PRO:HA	2.50	0.47
1:A:934:HIS:HE1	1:A:936:ASN:HD22	1.61	0.47
1:D:1037:VAL:HG23	1:D:1056:SER:HB3	1.95	0.47
1:A:1143:GLN:HE22	1:E:900:ASN:HD21	1.63	0.47
1:A:1107:THR:HG22	1:A:1112:LYS:HB2	1.96	0.47
1:A:886:PHE:CD2	1:A:918:HIS:NE2	2.82	0.47
1:E:1038:LYS:HG3	3:E:1400:HOH:O	2.14	0.46
1:B:1096:HIS:CD2	1:B:1103:ARG:HD2	2.50	0.46
1:B:994:LEU:HG	1:B:999:TYR:HB2	1.98	0.46
1:E:1089:LEU:HD22	1:E:1094:PRO:HA	1.97	0.46
1:D:886:PHE:CE2	1:D:918:HIS:NE2	2.82	0.46
1:A:1075:LEU:HD12	1:A:1128:MET:CE	2.46	0.46
1:E:869:HIS:HB3	3:E:1424:HOH:O	2.14	0.46
1:E:876:LYS:HD2	3:E:1375:HOH:O	2.16	0.45
2:A:1201:0NH:H7A	2:A:1201:0NH:H18	1.99	0.45
1:B:911:LYS:C	3:B:1383:HOH:O	2.54	0.45
1:B:944:CYS:HB3	1:B:953:LYS:HB2	1.98	0.45
1:E:1000:VAL:CG1	1:E:1028:ILE:HD11	2.45	0.45
1:E:910:LEU:HD22	1:E:918:HIS:HB2	1.99	0.44
1:E:944:CYS:HB3	1:E:953:LYS:HB2	1.99	0.44
1:B:1000:VAL:CB	1:B:1058[B]:PHE:CD2	2.98	0.44
1:E:874:PHE:CG	1:E:896:PRO:HA	2.53	0.44
1:A:893:ARG:NH1	1:A:902:GLY:O	2.51	0.43
1:A:908:LYS:NZ	1:A:925:GLU:OE2	2.37	0.43
1:B:874:PHE:HB2	1:B:894:TYR:CE1	2.53	0.43
1:E:874:PHE:CD1	1:E:896:PRO:HA	2.53	0.43
1:D:1089:LEU:HD22	1:D:1094:PRO:HA	2.00	0.42
1:A:1143:GLN:NE2	1:E:900:ASN:HD21	2.18	0.42
1:D:977:LEU:HA	1:D:980:GLN:OE1	2.19	0.42
1:D:1010:LEU:HD21	2:D:1201:0NH:C16	2.49	0.42
1:A:1000:VAL:CG1	1:A:1028:ILE:HD11	2.48	0.42
1:B:1000:VAL:HB	1:B:1058[B]:PHE:HE2	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:886:PHE:CD2	1:D:918:HIS:CD2	3.08	0.41
1:E:876:LYS:CD	3:E:1375:HOH:O	2.68	0.41
1:B:1092:ILE:HG22	1:B:1107:THR:OG1	2.19	0.41
1:D:919:ILE:HD13	3:D:1415:HOH:O	2.20	0.41
1:E:1046:PHE:CE2	1:E:1085:MET:HG3	2.55	0.41
1:A:1102:THR:HG21	1:B:1053:LEU:O	2.19	0.41
1:E:1065:TRP:CE3	1:E:1132:TRP:HA	2.55	0.41
1:D:1065:TRP:CE3	1:D:1132:TRP:HA	2.56	0.41
2:B:1201:0NH:H18	2:B:1201:0NH:H1	2.03	0.41
1:D:1090:LYS:HD2	3:D:1379:HOH:O	2.21	0.41
1:D:1002:ARG:HH21	1:D:1037:VAL:HG11	1.85	0.41
1:D:1118:PRO:HG2	3:D:1414:HOH:O	2.21	0.41
1:B:917:ASN:HD21	1:B:919:ILE:HB	1.85	0.40
1:D:1075:LEU:HD12	1:D:1128:MET:HE1	2.03	0.40
1:D:967:TYR:CG	1:D:1011:VAL:HG21	2.56	0.40
1:B:1037:VAL:HG23	1:B:1058[A]:PHE:CD1	2.56	0.40
1:E:1041:ARG:CZ	3:E:1394:HOH:O	2.69	0.40
1:E:874:PHE:HB2	1:E:894:TYR:CE1	2.57	0.40

There are no symmetry-related clashes.

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	274/302 (91%)	271 (99%)	3 (1%)	0	100	100
1	B	278/302 (92%)	276 (99%)	2 (1%)	0	100	100
1	D	279/302 (92%)	275 (99%)	3 (1%)	1 (0%)	38	33
1	E	278/302 (92%)	274 (99%)	4 (1%)	0	100	100
All	All	1109/1208 (92%)	1096 (99%)	12 (1%)	1 (0%)	55	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	949	GLY

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	253/267 (95%)	251 (99%)	2 (1%)	85	88
1	B	257/267 (96%)	256 (100%)	1 (0%)	93	95
1	D	256/267 (96%)	253 (99%)	3 (1%)	75	80
1	E	257/267 (96%)	256 (100%)	1 (0%)	93	95
All	All	1023/1068 (96%)	1016 (99%)	7 (1%)	87	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1007	ARG
1	A	1102	THR
1	B	917	ASN
1	E	1056	SER
1	D	885	HIS
1	D	950	ASN
1	D	1137	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	936	ASN
1	A	1143	GLN
1	B	885	HIS
1	B	936	ASN
1	E	885	HIS
1	E	900	ASN
1	E	936	ASN
1	D	936	ASN

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	1034	1	15,16,17	0.63	0	19,22,24	0.92	0
1	PTR	A	1035	1	15,16,17	0.69	0	19,22,24	0.80	0
1	PTR	B	1034	1	15,16,17	0.67	0	19,22,24	0.82	0
1	PTR	B	1035	1	15,16,17	0.75	0	19,22,24	0.92	0
1	PTR	D	1034	1	15,16,17	0.61	0	19,22,24	0.81	0
1	PTR	D	1035	1	15,16,17	0.63	0	19,22,24	0.77	0
1	PTR	E	1034	1	15,16,17	0.67	0	19,22,24	0.86	0
1	PTR	E	1035	1	15,16,17	0.69	0	19,22,24	0.89	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	1034	1	-	0/9/11/13	0/1/1/1
1	PTR	A	1035	1	-	0/9/11/13	0/1/1/1
1	PTR	B	1034	1	-	0/9/11/13	0/1/1/1
1	PTR	B	1035	1	-	0/9/11/13	0/1/1/1
1	PTR	D	1034	1	-	0/9/11/13	0/1/1/1
1	PTR	D	1035	1	-	0/9/11/13	0/1/1/1
1	PTR	E	1034	1	-	0/9/11/13	0/1/1/1
1	PTR	E	1035	1	-	0/9/11/13	0/1/1/1

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1035	PTR	1	0
1	D	1035	PTR	1	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	-	22,26,26	4.79	12 (54%)	23,41,41	3.08	12 (52%)
2	0NH	A	1202	-	22,26,26	4.78	12 (54%)	23,41,41	3.01	12 (52%)
2	0NH	B	1201	-	22,26,26	4.73	12 (54%)	23,41,41	3.12	12 (52%)
2	0NH	D	1201	-	22,26,26	4.59	14 (63%)	23,41,41	4.18	18 (78%)

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	A	1202	-	-	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

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	0NH	C18-C19	-12.28	1.33	1.53
2	B	1201	0NH	C18-C19	-11.54	1.34	1.53
2	A	1202	0NH	C18-C19	-11.38	1.34	1.53
2	D	1201	0NH	C18-C19	-10.85	1.35	1.53
2	A	1202	0NH	C24-N23	-10.16	1.32	1.47
2	D	1201	0NH	C24-N23	-9.81	1.32	1.47
2	B	1201	0NH	C24-N23	-9.74	1.32	1.47
2	A	1201	0NH	C17-C16	-9.40	1.41	1.54
2	A	1202	0NH	C22-N23	-9.18	1.33	1.45
2	B	1201	0NH	C17-C16	-9.15	1.41	1.54
2	A	1201	0NH	C24-N23	-9.11	1.33	1.47
2	B	1201	0NH	C22-N23	-8.56	1.34	1.45
2	A	1202	0NH	C17-C16	-8.48	1.42	1.54
2	A	1201	0NH	C22-N23	-8.27	1.34	1.45
2	D	1201	0NH	C17-C16	-7.67	1.43	1.54
2	D	1201	0NH	C22-N23	-7.56	1.35	1.45
2	A	1202	0NH	C16-N12	-6.36	1.38	1.48
2	A	1201	0NH	C16-N12	-6.26	1.38	1.48
2	B	1201	0NH	C16-N12	-6.00	1.39	1.48
2	A	1202	0NH	C15-N14	-5.16	1.36	1.48
2	D	1201	0NH	C15-N14	-5.15	1.36	1.48
2	A	1201	0NH	C15-N14	-5.07	1.36	1.48
2	B	1201	0NH	C15-N14	-4.64	1.37	1.48
2	D	1201	0NH	C16-N12	-4.10	1.41	1.48
2	D	1201	0NH	C3-C2	-3.80	1.50	1.53
2	D	1201	0NH	C7-C2	-3.72	1.50	1.53
2	D	1201	0NH	C19-N20	-3.27	1.37	1.49
2	A	1202	0NH	C19-N20	-3.26	1.37	1.49
2	A	1201	0NH	C19-N20	-3.26	1.37	1.49
2	B	1201	0NH	C19-N20	-3.05	1.38	1.49
2	A	1202	0NH	C13-N12	-2.81	1.38	1.46
2	B	1201	0NH	C13-N12	-2.75	1.38	1.46
2	A	1201	0NH	C13-N12	-2.74	1.38	1.46
2	D	1201	0NH	C13-N12	-2.61	1.38	1.46
2	A	1202	0NH	C18-C17	-2.48	1.47	1.54
2	A	1201	0NH	C18-C17	-2.22	1.48	1.54
2	A	1201	0NH	C7-C2	-2.16	1.52	1.53
2	D	1201	0NH	C18-C17	-2.11	1.48	1.54
2	B	1201	0NH	C18-C17	-2.11	1.48	1.54
2	B	1201	0NH	S8-N5	2.01	1.66	1.63
2	B	1201	0NH	C1-C2	2.07	1.56	1.53
2	A	1202	0NH	S8-N5	2.09	1.66	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1202	0NH	C3-C2	2.33	1.55	1.53
2	A	1202	0NH	C11-S8	2.40	1.81	1.75
2	D	1201	0NH	C11-S8	2.42	1.81	1.75
2	B	1201	0NH	C3-C2	2.72	1.55	1.53
2	A	1201	0NH	C11-S8	2.79	1.82	1.75
2	D	1201	0NH	C4-N5	2.89	1.51	1.47
2	A	1201	0NH	C1-C2	2.95	1.57	1.53
2	D	1201	0NH	S8-N5	3.69	1.68	1.63

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1201	0NH	C7-C2-N12	-5.99	94.11	110.72
2	D	1201	0NH	C3-C2-N12	-4.65	97.85	110.72
2	D	1201	0NH	C11-S8-N5	-4.35	103.54	107.48
2	B	1201	0NH	C11-S8-N5	-3.93	103.91	107.48
2	A	1202	0NH	C11-S8-N5	-3.77	104.06	107.48
2	A	1201	0NH	C11-S8-N5	-3.11	104.66	107.48
2	D	1201	0NH	O9-S8-N5	-2.46	104.77	107.02
2	D	1201	0NH	C6-N5-S8	2.02	117.96	115.96
2	A	1202	0NH	C13-N12-C16	2.03	107.01	104.53
2	A	1201	0NH	C4-N5-S8	2.06	118.00	115.96
2	B	1201	0NH	C13-N12-C16	2.06	107.04	104.53
2	A	1201	0NH	C7-C2-C3	2.06	111.32	108.36
2	D	1201	0NH	O10-S8-O9	2.08	121.68	118.61
2	B	1201	0NH	O10-S8-O9	2.14	121.76	118.61
2	A	1201	0NH	C19-C18-C17	2.27	106.44	104.01
2	B	1201	0NH	C3-C4-N5	2.35	112.44	109.27
2	A	1202	0NH	O9-S8-N5	2.39	109.21	107.02
2	A	1201	0NH	C13-N12-C16	2.48	107.55	104.53
2	A	1202	0NH	C7-C6-N5	2.53	112.68	109.27
2	A	1202	0NH	C4-N5-S8	2.54	118.48	115.96
2	B	1201	0NH	C6-N5-S8	2.59	118.52	115.96
2	D	1201	0NH	C3-C4-N5	2.62	112.80	109.27
2	B	1201	0NH	C4-N5-S8	2.87	118.80	115.96
2	D	1201	0NH	C19-C18-C17	2.95	107.16	104.01
2	D	1201	0NH	O9-S8-C11	3.08	112.86	108.59
2	D	1201	0NH	C7-C2-C3	3.32	113.12	108.36
2	A	1201	0NH	C6-N5-S8	3.34	119.26	115.96
2	A	1201	0NH	C7-C6-N5	3.38	113.83	109.27
2	D	1201	0NH	C4-N5-S8	3.51	119.43	115.96
2	A	1201	0NH	C3-C4-N5	3.51	114.01	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1202	0NH	C17-C22-N23	3.56	120.21	111.22
2	B	1201	0NH	C19-C18-C17	3.58	107.83	104.01
2	B	1201	0NH	C17-C22-N23	3.79	120.80	111.22
2	B	1201	0NH	C22-C17-C16	3.91	118.42	111.53
2	D	1201	0NH	C17-C22-N23	3.98	121.26	111.22
2	A	1202	0NH	C22-C17-C16	4.07	118.71	111.53
2	A	1202	0NH	C19-N20-C22	4.09	109.98	105.27
2	B	1201	0NH	C7-C6-N5	4.13	114.86	109.27
2	A	1201	0NH	C17-C22-N23	4.15	121.70	111.22
2	A	1201	0NH	C22-C17-C16	4.19	118.92	111.53
2	A	1202	0NH	C19-C18-C17	4.25	108.55	104.01
2	A	1202	0NH	C6-N5-S8	4.40	120.32	115.96
2	D	1201	0NH	C7-C6-N5	4.53	115.39	109.27
2	D	1201	0NH	C19-N20-C22	4.53	110.50	105.27
2	A	1202	0NH	C3-C4-N5	4.84	115.81	109.27
2	D	1201	0NH	C22-C17-C16	4.94	120.23	111.53
2	A	1201	0NH	C19-N20-C22	4.99	111.02	105.27
2	B	1201	0NH	C19-N20-C22	5.22	111.29	105.27
2	D	1201	0NH	C1-C2-C7	5.35	120.12	110.51
2	A	1202	0NH	C6-N5-C4	7.62	120.76	112.11
2	D	1201	0NH	C1-C2-C3	7.79	124.50	110.51
2	A	1201	0NH	C6-N5-C4	9.06	122.39	112.11
2	B	1201	0NH	C6-N5-C4	9.11	122.45	112.11
2	D	1201	0NH	C6-N5-C4	9.20	122.56	112.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	0NH	1	0
2	B	1201	0NH	1	0
2	D	1201	0NH	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	277/302 (91%)	-0.26	2 (0%)	87	87	12, 28, 49, 71	6 (2%)
1	B	279/302 (92%)	-0.32	5 (1%)	69	68	12, 27, 51, 76	9 (3%)
1	D	281/302 (93%)	-0.19	6 (2%)	64	63	14, 31, 56, 78	9 (3%)
1	E	280/302 (92%)	-0.22	4 (1%)	75	75	12, 30, 54, 79	8 (2%)
All	All	1117/1208 (92%)	-0.25	17 (1%)	74	73	12, 29, 53, 79	32 (2%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	885	HIS	4.0
1	E	1031	ASP	3.7
1	D	885	HIS	3.2
1	E	885	HIS	3.1
1	D	1154	LYS	3.1
1	D	864	GLU	3.0
1	E	912	PRO	2.9
1	D	1031	ASP	2.9
1	E	864	GLU	2.8
1	A	885	HIS	2.7
1	D	1030	THR	2.7
1	B	864	GLU	2.5
1	B	886	PHE	2.3
1	B	865	VAL	2.2
1	D	1058	PHE	2.2
1	B	1031	ASP	2.1
1	A	1154	LYS	2.1

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	D	1035	16/17	0.92	0.11	-	34,40,51,53	0
1	PTR	D	1034	16/17	0.92	0.12	-	35,54,71,75	0
1	PTR	A	1034	16/17	0.93	0.10	-	31,43,61,61	0
1	PTR	B	1034	16/17	0.89	0.12	-	30,43,58,60	0
1	PTR	A	1035	16/17	0.94	0.10	-	25,32,42,45	0
1	PTR	E	1034	16/17	0.91	0.14	-	38,51,67,72	0
1	PTR	E	1035	16/17	0.90	0.11	-	34,38,49,54	0
1	PTR	B	1035	16/17	0.95	0.09	-	28,35,44,44	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(Å^2)	Q<0.9
2	0NH	A	1201	23/23	0.98	0.10	-0.44	7,12,17,18	0
2	0NH	D	1201	23/23	0.98	0.09	-0.48	7,15,19,23	0
2	0NH	A	1202	23/23	0.98	0.09	-0.51	8,12,16,18	0
2	0NH	B	1201	23/23	0.98	0.08	-0.64	10,15,19,24	0

6.5 Other polymers (i)

There are no such residues in this entry.