Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:43 AM GMT

PDB ID	:	2E50
Title	:	Crystal structure of SET/TAF-1beta/INHAT
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Deposited on	:	2006-12-18
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

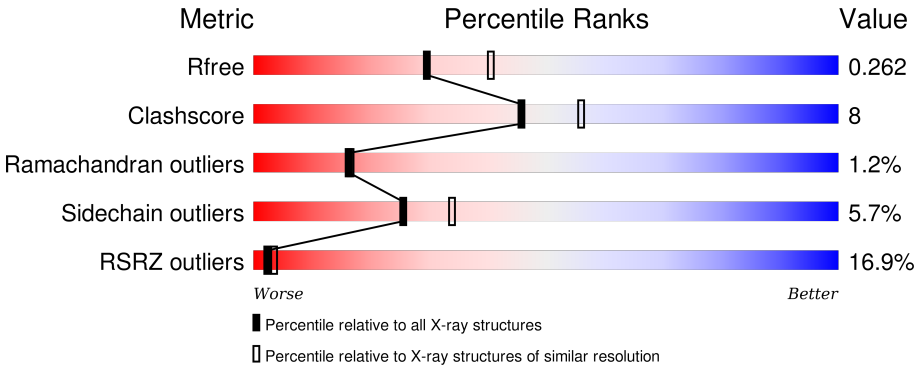
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	225	16% 63% 15% • • 19%
1	B	225	12% 60% 14% • 26%
1	P	225	15% 62% 20% • 17%
1	Q	225	9% 57% 12% • 29%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6064 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.

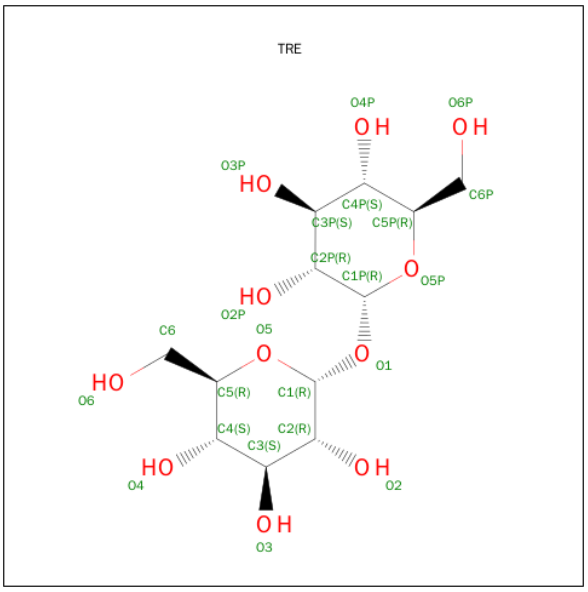
- Molecule 1 is a protein called Protein SET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1526	975	245	303	3			
1	B	167	Total	C	N	O	S	0	0	0
			1409	906	225	276	2			
1	P	186	Total	C	N	O	S	0	0	0
			1550	988	250	309	3			
1	Q	159	Total	C	N	O	S	0	0	0
			1356	875	215	265	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLN	PRO	SEE REMARK 999	UNP Q01105
A	104	MET	LEU	ENGINEERED	UNP Q01105
A	145	MET	LEU	ENGINEERED	UNP Q01105
A	166	MET	LEU	ENGINEERED	UNP Q01105
B	4	GLN	PRO	SEE REMARK 999	UNP Q01105
B	104	MET	LEU	ENGINEERED	UNP Q01105
B	145	MET	LEU	ENGINEERED	UNP Q01105
B	166	MET	LEU	ENGINEERED	UNP Q01105
P	4	GLN	PRO	SEE REMARK 999	UNP Q01105
P	104	MET	LEU	ENGINEERED	UNP Q01105
P	145	MET	LEU	ENGINEERED	UNP Q01105
P	166	MET	LEU	ENGINEERED	UNP Q01105
Q	4	GLN	PRO	SEE REMARK 999	UNP Q01105
Q	104	MET	LEU	ENGINEERED	UNP Q01105
Q	145	MET	LEU	ENGINEERED	UNP Q01105
Q	166	MET	LEU	ENGINEERED	UNP Q01105

- Molecule 2 is TREHALOSE (three-letter code: TRE) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 23 12 11	0	0
2	B	1	Total C O 23 12 11	0	0
2	P	1	Total C O 23 12 11	0	0
2	Q	1	Total C O 23 12 11	0	0

- Molecule 3 is water.

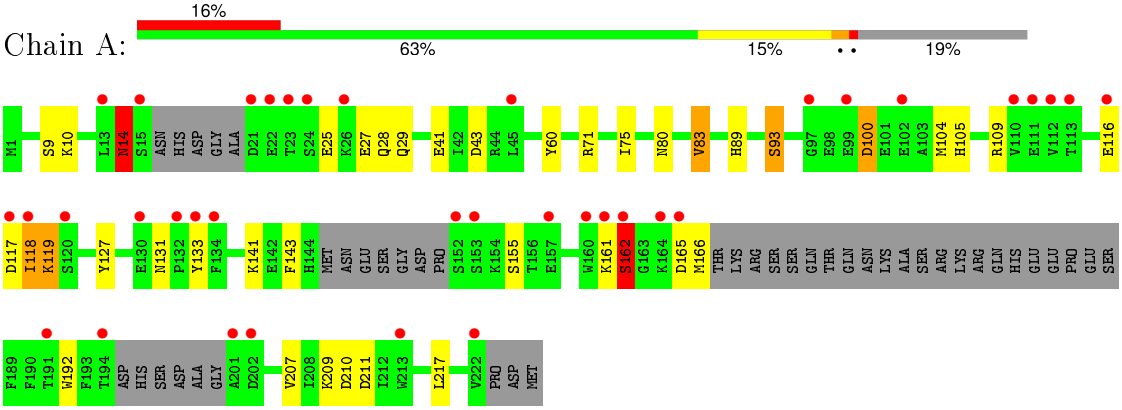
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	35	Total O 35 35	0	0
3	B	31	Total O 31 31	0	0
3	P	37	Total O 37 37	0	0
3	Q	28	Total O 28 28	0	0

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 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.

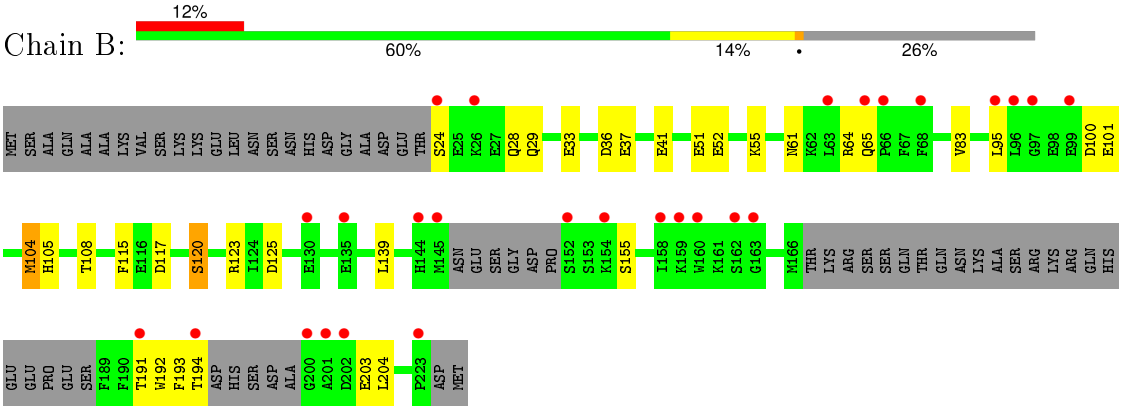
- Molecule 1: Protein SET

Chain A:



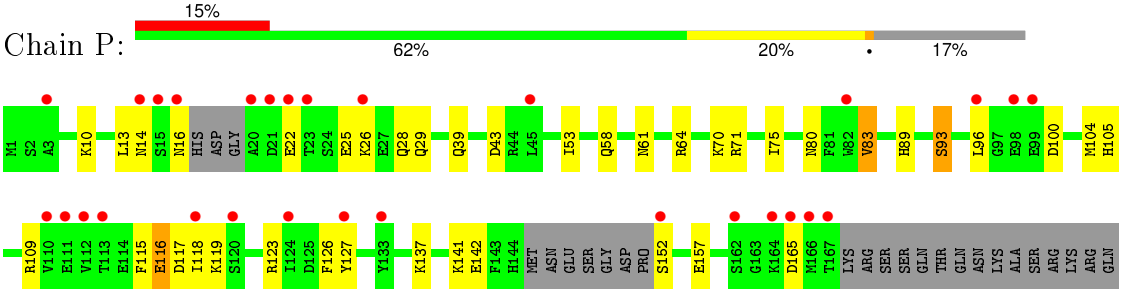
- Molecule 1: Protein SET

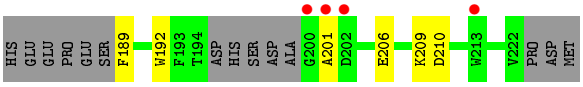
Chain B:



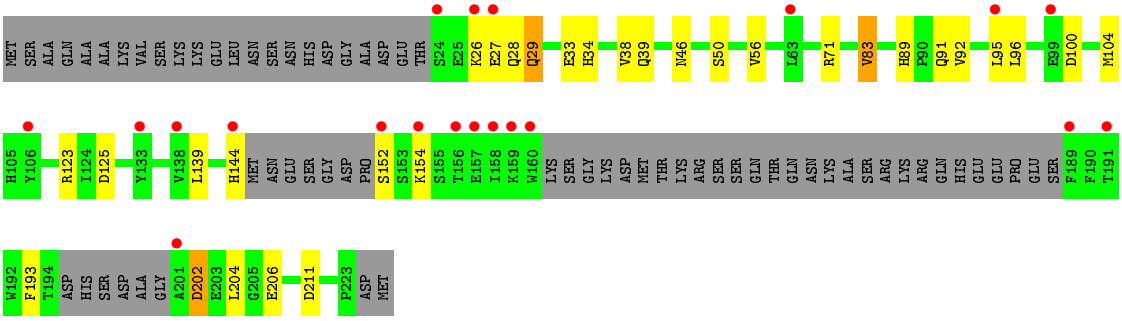
- Molecule 1: Protein SET

Chain P:





- Molecule 1: Protein SET



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.91Å 64.44Å 124.42Å 90.00° 90.85° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 36.25 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-2.30) 96.8 (36.25-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.218 , 0.271 0.210 , 0.262	Depositor DCC
R_{free} test set	2105 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.782	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 70.2	EDS
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	1 of 54742 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6064	wwPDB-VP
Average B, all atoms (Å^2)	47.0	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 41.52 % 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 2.3334e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: TRE

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	0.83	2/1558 (0.1%)	0.75	1/2096 (0.0%)
1	B	0.79	0/1443	0.72	1/1946 (0.1%)
1	P	0.79	2/1582 (0.1%)	0.73	2/2129 (0.1%)
1	Q	0.76	1/1390 (0.1%)	0.68	0/1878
All	All	0.80	5/5973 (0.1%)	0.72	4/8049 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	ASP	CG-OD2	7.11	1.41	1.25
1	A	162	SER	C-O	6.64	1.35	1.23
1	P	165	ASP	CG-OD1	6.57	1.40	1.25
1	Q	38	VAL	CB-CG1	-5.10	1.42	1.52
1	P	165	ASP	CG-OD2	5.06	1.36	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	43	ASP	CB-CG-OD1	6.04	123.74	118.30
1	B	64	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	P	165	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	P	43	ASP	CB-CG-OD1	5.38	123.14	118.30

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	1526	0	1456	24	0
1	B	1409	0	1331	15	0
1	P	1550	0	1477	35	0
1	Q	1356	0	1279	25	0
2	A	23	0	22	0	0
2	B	23	0	22	0	0
2	P	23	0	22	0	0
2	Q	23	0	22	0	0
3	A	35	0	0	0	0
3	B	31	0	0	1	0
3	P	37	0	0	1	0
3	Q	28	0	0	1	0
All	All	6064	0	5631	89	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 8.

All (89) 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:83:VAL:HG13	1:A:104:MET:HB2	1.47	0.95
1:P:39:GLN:HE22	1:Q:71:ARG:HH11	1.16	0.94
1:P:83:VAL:HG13	1:P:104:MET:HB2	1.50	0.93
1:P:83:VAL:HG13	1:P:104:MET:CB	2.06	0.86
1:A:83:VAL:HG13	1:A:104:MET:CB	2.06	0.85
1:Q:89:HIS:HE1	1:Q:211:ASP:OD1	1.63	0.82
1:B:95:LEU:HD13	1:B:204:LEU:HD22	1.68	0.75
1:Q:202:ASP:O	1:Q:206:GLU:HG2	1.87	0.74
1:P:71:ARG:HH11	1:Q:39:GLN:HE22	1.35	0.74
1:P:83:VAL:CG1	1:P:104:MET:HB2	2.20	0.72
1:A:83:VAL:CG1	1:A:104:MET:HB2	2.20	0.71
1:A:25:GLU:OE1	1:A:29:GLN:NE2	2.22	0.71
1:P:89:HIS:O	1:P:93:SER:HB2	1.91	0.71
1:P:39:GLN:NE2	1:Q:71:ARG:HH11	1.86	0.70
1:Q:100:ASP:O	1:Q:104:MET:HG2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:80:ASN:HD21	1:P:105:HIS:HD2	1.41	0.68
1:P:39:GLN:HE22	1:Q:71:ARG:NH1	1.91	0.66
1:P:83:VAL:HG22	3:P:247:HOH:O	1.96	0.65
1:P:64:ARG:HH11	1:Q:46:ASN:HD22	1.43	0.65
1:P:80:ASN:HD21	1:P:105:HIS:CD2	2.15	0.65
1:A:89:HIS:O	1:A:93:SER:HB2	1.97	0.64
1:Q:29:GLN:O	1:Q:33:GLU:HG2	1.97	0.64
1:Q:100:ASP:O	1:Q:104:MET:CG	2.47	0.63
1:A:141:LYS:HE3	1:A:192:TRP:O	2.00	0.62
1:B:192:TRP:CD2	1:B:204:LEU:HD23	2.35	0.60
1:Q:95:LEU:HD12	1:Q:204:LEU:HD13	1.81	0.60
1:A:131:ASN:HD22	1:A:133:TYR:H	1.50	0.60
1:B:115:PHE:HD2	1:B:120:SER:HB3	1.67	0.59
1:Q:33:GLU:HB2	3:Q:241:HOH:O	2.02	0.59
1:A:100:ASP:HA	1:A:166:MET:HE1	1.86	0.58
1:B:123:ARG:NH1	1:B:125:ASP:OD2	2.37	0.58
1:P:83:VAL:HG13	1:P:104:MET:HB3	1.86	0.57
1:B:41:GLU:OE2	3:B:255:HOH:O	2.18	0.56
1:A:100:ASP:O	1:A:104:MET:HG2	2.05	0.56
1:P:10:LYS:HA	1:P:14:ASN:HB2	1.87	0.56
1:P:13:LEU:O	1:P:16:ASN:N	2.39	0.55
1:P:206:GLU:HG3	1:P:210:ASP:OD2	2.06	0.54
1:B:101:GLU:O	1:B:105:HIS:HD2	1.90	0.54
1:A:80:ASN:OD1	1:A:105:HIS:HD2	1.90	0.54
1:A:83:VAL:HG13	1:A:104:MET:HB3	1.90	0.53
1:B:115:PHE:CD2	1:B:120:SER:HB3	2.43	0.53
1:P:70:LYS:HE3	1:Q:34:HIS:CE1	2.43	0.53
1:P:61:ASN:ND2	1:P:64:ARG:HH21	2.06	0.52
1:P:141:LYS:NZ	1:P:201:ALA:HB1	2.24	0.52
1:B:117:ASP:OD1	1:B:120:SER:HB2	2.10	0.51
1:P:123:ARG:HD2	1:P:142:GLU:HG2	1.93	0.51
1:Q:89:HIS:HD2	1:Q:91:GLN:H	1.59	0.51
1:P:61:ASN:HD22	1:P:64:ARG:HH21	1.59	0.51
1:A:14:ASN:N	1:A:14:ASN:OD1	2.44	0.49
1:Q:123:ARG:NH1	1:Q:125:ASP:OD2	2.46	0.49
1:Q:139:LEU:HB3	1:Q:193:PHE:CZ	2.47	0.48
1:Q:144:HIS:HB2	1:Q:152:SER:HB2	1.95	0.48
1:B:139:LEU:HB3	1:B:193:PHE:CZ	2.48	0.48
1:B:33:GLU:O	1:B:37:GLU:HG3	2.14	0.47
1:Q:89:HIS:CE1	1:Q:211:ASP:OD1	2.54	0.47
1:A:207:VAL:O	1:A:211:ASP:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:100:ASP:O	1:P:104:MET:HG2	2.14	0.47
1:B:83:VAL:HG22	1:B:104:MET:O	2.15	0.47
1:A:161:LYS:O	1:A:162:SER:HB2	2.15	0.47
1:Q:83:VAL:HG22	1:Q:104:MET:O	2.15	0.47
1:P:80:ASN:ND2	1:P:105:HIS:HD2	2.09	0.47
1:Q:26:LYS:O	1:Q:29:GLN:HB3	2.16	0.46
1:P:64:ARG:HH11	1:Q:46:ASN:ND2	2.12	0.46
1:A:131:ASN:ND2	1:A:133:TYR:H	2.12	0.45
1:P:53:ILE:HG13	1:Q:56:VAL:HG11	1.98	0.45
1:P:126:PHE:CE1	1:P:192:TRP:HZ3	2.35	0.45
1:P:71:ARG:O	1:P:75:ILE:HG13	2.16	0.44
1:A:71:ARG:O	1:A:75:ILE:HG13	2.17	0.44
1:P:116:GLU:HG3	1:P:119:LYS:HG3	2.00	0.44
1:P:25:GLU:OE1	1:P:29:GLN:NE2	2.47	0.44
1:A:10:LYS:HB2	1:A:10:LYS:HE2	1.87	0.44
1:P:119:LYS:HE3	1:P:119:LYS:HB2	1.72	0.44
1:Q:89:HIS:CD2	1:Q:91:GLN:H	2.35	0.44
1:P:206:GLU:OE1	1:P:209:LYS:NZ	2.49	0.44
1:A:209:LYS:NZ	1:A:210:ASP:OD1	2.51	0.43
1:A:60:TYR:OH	1:B:52:GLU:OE2	2.25	0.43
1:Q:92:VAL:O	1:Q:96:LEU:HD13	2.17	0.43
1:A:109:ARG:HB3	1:A:127:TYR:HB2	2.00	0.43
1:A:143:PHE:HZ	1:A:192:TRP:CZ2	2.37	0.43
1:P:141:LYS:HZ1	1:P:201:ALA:CB	2.32	0.42
1:P:109:ARG:HB3	1:P:127:TYR:HB2	2.01	0.42
1:A:41:GLU:OE2	1:A:41:GLU:HA	2.20	0.42
1:B:51:GLU:O	1:B:55:LYS:HG2	2.20	0.41
1:Q:83:VAL:HG13	1:Q:104:MET:CB	2.50	0.41
1:A:217:LEU:HD21	1:B:36:ASP:HA	2.01	0.41
1:B:61:ASN:O	1:B:65:GLN:HG3	2.20	0.41
1:P:96:LEU:HD23	1:P:189:PHE:HB2	2.01	0.41
1:P:115:PHE:O	1:P:117:ASP:N	2.53	0.41
1:A:207:VAL:O	1:A:211:ASP:CB	2.70	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	172/225 (76%)	162 (94%)	5 (3%)	5 (3%)	6 3
1	B	159/225 (71%)	153 (96%)	6 (4%)	0	100 100
1	P	176/225 (78%)	166 (94%)	7 (4%)	3 (2%)	11 10
1	Q	151/225 (67%)	146 (97%)	5 (3%)	0	100 100
All	All	658/900 (73%)	627 (95%)	23 (4%)	8 (1%)	16 16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	SER
1	P	22	GLU
1	P	116	GLU
1	A	14	ASN
1	A	116	GLU
1	A	119	LYS
1	A	118	ILE
1	P	118	ILE

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	169/206 (82%)	158 (94%)	11 (6%)	21 27
1	B	155/206 (75%)	144 (93%)	11 (7%)	18 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	P	171/206 (83%)	163 (95%)	8 (5%)	32 43
1	Q	150/206 (73%)	143 (95%)	7 (5%)	32 43
All	All	645/824 (78%)	608 (94%)	37 (6%)	25 34

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	14	ASN
1	A	27	GLU
1	A	28	GLN
1	A	83	VAL
1	A	93	SER
1	A	100	ASP
1	A	117	ASP
1	A	118	ILE
1	A	119	LYS
1	A	155	SER
1	B	24	SER
1	B	28	GLN
1	B	29	GLN
1	B	100	ASP
1	B	104	MET
1	B	108	THR
1	B	120	SER
1	B	155	SER
1	B	191	THR
1	B	194	THR
1	B	203	GLU
1	P	26	LYS
1	P	28	GLN
1	P	58	GLN
1	P	83	VAL
1	P	93	SER
1	P	137	LYS
1	P	152	SER
1	P	157	GLU
1	Q	27	GLU
1	Q	28	GLN
1	Q	29	GLN
1	Q	50	SER

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Mol	Chain	Res	Type
1	Q	83	VAL
1	Q	154	LYS
1	Q	202	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	40	ASN
1	A	48	GLN
1	A	61	ASN
1	A	105	HIS
1	A	131	ASN
1	B	34	HIS
1	B	48	GLN
1	B	105	HIS
1	P	28	GLN
1	P	39	GLN
1	P	48	GLN
1	P	61	ASN
1	P	80	ASN
1	P	88	ASN
1	P	105	HIS
1	Q	34	HIS
1	Q	39	GLN
1	Q	46	ASN
1	Q	89	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

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	TRE	A	226	-	24,24,24	0.59	0	35,35,35	1.47	9 (25%)
2	TRE	B	226	-	24,24,24	0.76	0	35,35,35	0.90	2 (5%)
2	TRE	P	226	-	24,24,24	0.68	0	35,35,35	1.13	4 (11%)
2	TRE	Q	226	-	24,24,24	0.53	0	35,35,35	0.95	1 (2%)

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	TRE	A	226	-	-	0/8/48/48	0/2/2/2
2	TRE	B	226	-	-	0/8/48/48	0/2/2/2
2	TRE	P	226	-	-	0/8/48/48	0/2/2/2
2	TRE	Q	226	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	226	TRE	O6P-C6P-C5P	-2.91	101.72	111.33
2	A	226	TRE	O4P-C4P-C5P	-2.62	102.29	109.24
2	A	226	TRE	O1-C1P-O5P	-2.53	104.28	110.68
2	A	226	TRE	C3P-C4P-C5P	-2.53	105.79	110.20
2	P	226	TRE	O6-C6-C5	-2.36	103.53	111.33
2	Q	226	TRE	C3P-C4P-C5P	-2.30	106.19	110.20
2	A	226	TRE	O6-C6-C5	-2.27	103.84	111.33
2	A	226	TRE	O1-C1-O5	-2.04	105.53	110.68
2	P	226	TRE	O2-C2-C3	-2.02	105.78	110.34
2	P	226	TRE	O2-C2-C1	2.05	114.52	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	226	TRE	C1-O5-C5	2.05	117.73	113.75
2	B	226	TRE	O3P-C3P-C4P	2.08	115.01	110.34
2	P	226	TRE	O5-C5-C6	2.14	111.76	106.36
2	B	226	TRE	O5-C5-C6	2.26	112.07	106.36
2	A	226	TRE	O2-C2-C1	2.61	115.74	110.02
2	A	226	TRE	O5-C5-C6	2.68	113.13	106.36

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^{th} 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	182/225 (80%)	0.95	37 (20%)	1 2	26, 47, 64, 86	0
1	B	167/225 (74%)	0.88	27 (16%)	3 4	24, 47, 66, 73	0
1	P	186/225 (82%)	0.95	33 (17%)	2 3	27, 45, 63, 89	0
1	Q	159/225 (70%)	0.72	20 (12%)	5 8	26, 50, 68, 79	0
All	All	694/900 (77%)	0.88	117 (16%)	2 3	24, 47, 66, 89	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	200	GLY	8.4
1	P	20	ALA	7.9
1	A	23	THR	6.9
1	A	162	SER	6.7
1	A	118	ILE	6.3
1	B	201	ALA	6.1
1	P	15	SER	6.0
1	A	152	SER	5.5
1	P	23	THR	5.2
1	P	14	ASN	5.1
1	B	95	LEU	4.9
1	A	22	GLU	4.7
1	P	162	SER	4.7
1	P	167	THR	4.4
1	A	194	THR	4.4
1	B	163	GLY	4.3
1	B	194	THR	4.2
1	P	118	ILE	4.2
1	Q	152	SER	4.2
1	B	96	LEU	4.1
1	B	154	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	Q	160	TRP	4.1
1	P	16	ASN	4.1
1	A	132	PRO	4.0
1	P	201	ALA	3.9
1	Q	201	ALA	3.9
1	Q	24	SER	3.7
1	A	191	THR	3.7
1	B	160	TRP	3.7
1	P	152	SER	3.4
1	B	24	SER	3.4
1	Q	133	TYR	3.3
1	P	22	GLU	3.3
1	A	113	THR	3.3
1	P	120	SER	3.3
1	P	164	LYS	3.2
1	P	98	GLU	3.1
1	Q	157	GLU	3.1
1	Q	106	TYR	3.1
1	A	110	VAL	3.1
1	P	113	THR	3.1
1	A	161	LYS	3.1
1	A	222	VAL	3.1
1	B	162	SER	3.0
1	P	166	MET	3.0
1	B	152	SER	3.0
1	A	15	SER	3.0
1	A	120	SER	3.0
1	A	133	TYR	2.9
1	P	133	TYR	2.9
1	P	21	ASP	2.9
1	B	66	PRO	2.9
1	A	130	GLU	2.9
1	P	45	LEU	2.9
1	Q	144	HIS	2.9
1	Q	158	ILE	2.8
1	A	157	GLU	2.8
1	A	112	VAL	2.8
1	P	110	VAL	2.8
1	B	130	GLU	2.8
1	A	213	TRP	2.8
1	P	112	VAL	2.7
1	B	158	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	P	96	LEU	2.7
1	A	21	ASP	2.7
1	B	63	LEU	2.7
1	Q	154	LYS	2.7
1	P	213	TRP	2.7
1	Q	26	LYS	2.6
1	P	3	ALA	2.6
1	B	65	GLN	2.6
1	A	24	SER	2.5
1	B	26	LYS	2.5
1	P	26	LYS	2.5
1	A	202	ASP	2.5
1	A	99	GLU	2.5
1	B	135	GLU	2.5
1	B	144	HIS	2.5
1	Q	159	LYS	2.5
1	P	127	TYR	2.5
1	Q	63	LEU	2.5
1	Q	156	THR	2.4
1	Q	95	LEU	2.4
1	P	82	TRP	2.4
1	P	165	ASP	2.4
1	A	153	SER	2.4
1	A	45	LEU	2.4
1	B	191	THR	2.4
1	A	201	ALA	2.3
1	Q	27	GLU	2.3
1	A	111	GLU	2.3
1	B	202	ASP	2.3
1	Q	138	VAL	2.3
1	Q	189	PHE	2.3
1	B	159	LYS	2.3
1	A	164	LYS	2.2
1	A	13	LEU	2.2
1	B	223	PRO	2.2
1	P	202	ASP	2.2
1	A	102	GLU	2.2
1	Q	99	GLU	2.2
1	B	68	PHE	2.2
1	A	116	GLU	2.2
1	A	117	ASP	2.2
1	A	165	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	99	GLU	2.1
1	P	111	GLU	2.1
1	A	26	LYS	2.1
1	A	134	PHE	2.1
1	A	160	TRP	2.1
1	P	200	GLY	2.1
1	B	145	MET	2.0
1	P	99	GLU	2.0
1	A	97	GLY	2.0
1	B	97	GLY	2.0
1	P	124	ILE	2.0
1	Q	191	THR	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^{th} 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	TRE	Q	226	23/23	0.91	0.11	-1.06	37,42,45,47	0
2	TRE	P	226	23/23	0.96	0.12	-1.06	22,27,32,34	0
2	TRE	A	226	23/23	0.97	0.11	-1.17	23,25,29,32	0
2	TRE	B	226	23/23	0.95	0.11	-1.32	34,36,37,39	0

6.5 Other polymers (i)

There are no such residues in this entry.