



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:32 AM GMT

PDB ID : 3B87
Title : Complex of T57A Substituted *Drosophila* LUSH protein with Butanol
Authors : Jones, D.N.M; Thode, A.B
Deposited on : 2007-10-31
Resolution : 2.00 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

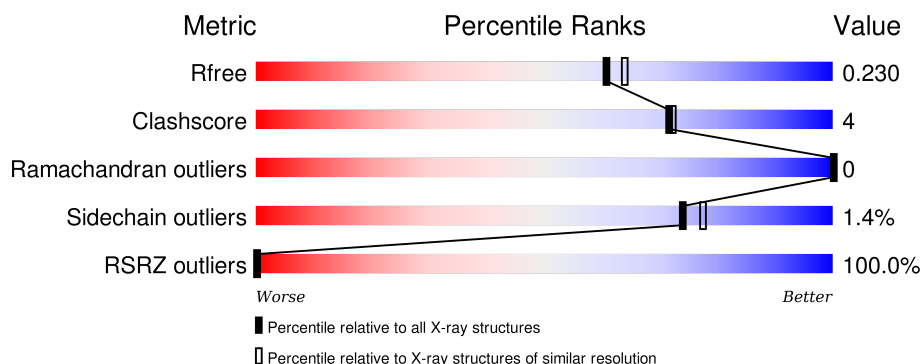
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 $\leq 5\%$. 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	124	<div> <div>100%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>.</div> </div> </div>
1	B	124	<div> <div>100%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	704	-	-	-	X
2	ACT	B	703	-	-	-	X
3	PE8	A	224	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2212 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 General odorant-binding protein lush.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			980	615	167	183	15			
1	B	124	Total	C	N	O	S	0	4	0
			1007	629	172	191	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ALA	THR	ENGINEERED	UNP O02372
B	57	ALA	THR	ENGINEERED	UNP O02372

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



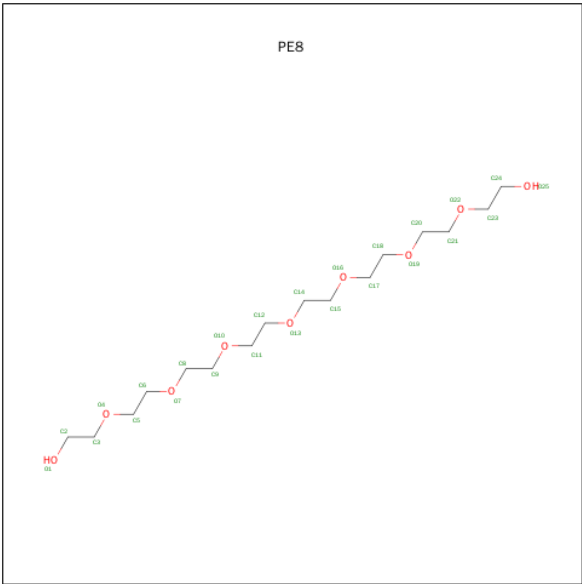
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula: C₁₆H₃₄O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			25	16	9		

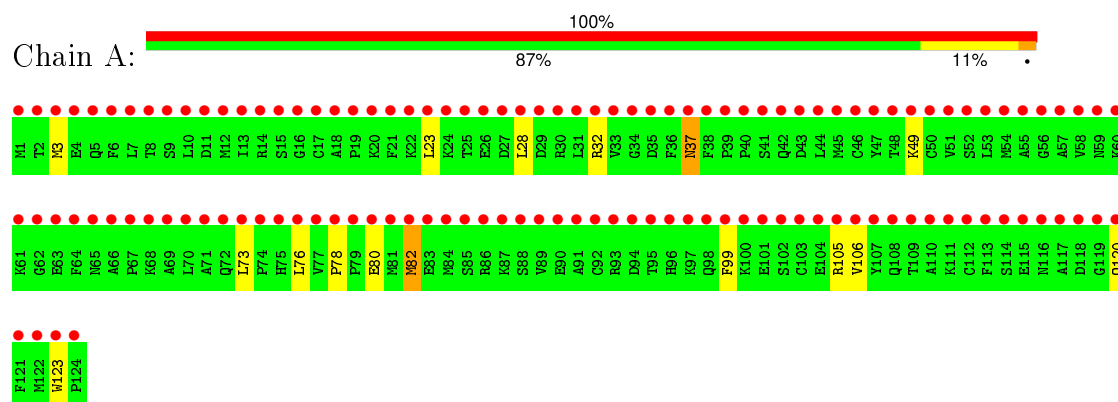
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	98	Total	O	0	0
			98	98		
4	B	90	Total	O	0	0
			90	90		

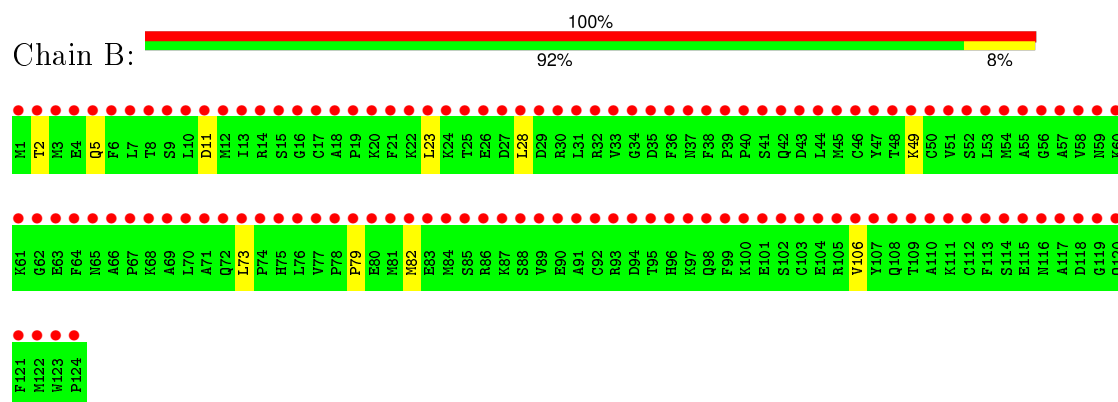
3 Residue-property plots [i](#)

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: General odorant-binding protein lush



- Molecule 1: General odorant-binding protein lush



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	42.66 Å 45.70 Å 114.52 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 45.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.00) 99.9 (45.70-2.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.43 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.187 , 0.229 0.187 , 0.230	Depositor DCC
R_{free} test set	1587 reflections (11.20%)	DCC
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 15811 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2212	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PE8, ACT

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	0.47	0/1001	0.57	0/1343
1	B	0.46	0/1028	0.58	0/1380
All	All	0.47	0/2029	0.57	0/2723

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	980	0	958	13	0
1	B	1007	0	971	5	0
2	A	8	0	6	1	0
2	B	4	0	3	0	0
3	A	25	0	34	1	0
4	A	98	0	0	1	0
4	B	90	0	0	0	0
All	All	2212	0	1972	17	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 4.

All (17) 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:73:LEU:HB3	1:A:82:MET:HE1	1.51	0.90
1:A:76:LEU:HD22	3:A:224:PE8:H182	1.64	0.79
1:A:82:MET:HE3	1:A:82:MET:HA	1.67	0.75
1:A:80:GLU:OE2	2:A:702:ACT:H3	1.91	0.70
1:A:82:MET:HA	1:A:82:MET:CE	2.27	0.65
1:A:23:LEU:HD13	1:A:28:LEU:HD21	1.91	0.53
1:B:2:THR:OG1	1:B:5[A]:GLN:HG3	2.09	0.52
1:B:49:LYS:HA	1:B:106:VAL:HG11	1.92	0.50
1:A:99:PHE:O	1:A:105:ARG:NH1	2.45	0.49
1:B:23:LEU:HD13	1:B:28:LEU:HD21	1.95	0.48
1:A:120:GLN:NE2	1:B:11[B]:ASP:OD2	2.43	0.47
1:A:32:ARG:HA	1:A:123:TRP:O	2.18	0.43
1:A:105:ARG:NH1	4:A:801:HOH:O	2.52	0.43
1:B:79:PRO:HA	1:B:82:MET:HG3	2.01	0.42
1:A:37:ASN:C	1:A:37:ASN:HD22	2.23	0.41
1:A:49:LYS:HA	1:A:106:VAL:HG11	2.03	0.41
1:A:3:MET:SD	1:A:78:PRO:HG2	2.62	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	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	B	126/124 (102%)	126 (100%)	0	0	100	100
All	All	248/248 (100%)	247 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	109/110 (99%)	107 (98%)	2 (2%)	66	69
1	B	112/110 (102%)	111 (99%)	1 (1%)	84	88
All	All	221/220 (100%)	218 (99%)	3 (1%)	74	77

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	82	MET
1	B	73	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	116	ASN
1	B	98	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

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	$\# Z > 2$
3	PE8	A	224	-	24,24,24	0.55	0	23,23,23	0.28	0
2	ACT	A	702	-	1,3,3	0.47	0	0,3,3	0.00	-
2	ACT	A	704	-	1,3,3	1.14	0	0,3,3	0.00	-
2	ACT	B	703	-	1,3,3	1.22	0	0,3,3	0.00	-

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
3	PE8	A	224	-	-	0/22/22/22	0/0/0/0
2	ACT	A	702	-	-	0/0/0/0	0/0/0/0
2	ACT	A	704	-	-	0/0/0/0	0/0/0/0
2	ACT	B	703	-	-	0/0/0/0	0/0/0/0

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
3	A	224	PE8	1	0
2	A	702	ACT	1	0

5.7 Other polymers

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	124/124 (100%)	22.11	124 (100%) 0 0	11, 19, 28, 35	0
1	B	124/124 (100%)	23.38	124 (100%) 0 0	11, 18, 31, 38	0
All	All	248/248 (100%)	22.75	248 (100%) 0 0	11, 19, 30, 38	0

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	TRP	81.1
1	B	6	PHE	75.0
1	A	77	VAL	71.5
1	B	70	LEU	68.1
1	B	2	THR	64.0
1	B	123	TRP	62.5
1	B	23	LEU	61.9
1	A	70	LEU	59.9
1	A	67	PRO	59.6
1	B	78	PRO	59.1
1	B	43	ASP	58.9
1	A	66	ALA	58.9
1	A	107	TYR	57.9
1	A	64	PHE	57.3
1	A	31	LEU	57.0
1	B	99	PHE	57.0
1	B	38	PHE	57.0
1	B	77	VAL	56.2
1	B	73	LEU	54.4
1	B	109	THR	54.3
1	A	19	PRO	54.2
1	A	27	ASP	53.1
1	B	107	TYR	53.1
1	A	69	ALA	52.5

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Mol	Chain	Res	Type	RSRZ
1	B	3	MET	52.2
1	A	73	LEU	52.0
1	A	118	ASP	52.0
1	B	96	HIS	51.1
1	A	16	GLY	49.3
1	A	17	CYS	48.2
1	A	29	ASP	47.5
1	A	106	VAL	46.5
1	B	97	LYS	45.2
1	B	74	PRO	45.0
1	B	66	ALA	44.6
1	A	6	PHE	44.1
1	A	26	GLU	43.5
1	B	104	GLU	43.5
1	B	118	ASP	43.5
1	B	7	LEU	43.1
1	B	64	PHE	43.1
1	A	102	SER	42.8
1	B	35	ASP	42.3
1	A	20	LYS	42.1
1	B	42	GLN	41.1
1	B	110	ALA	40.1
1	A	28	LEU	39.4
1	B	33	VAL	38.7
1	B	119	GLY	38.5
1	B	22	LYS	38.3
1	A	15	SER	38.2
1	A	74	PRO	37.1
1	B	106	VAL	36.5
1	A	5	GLN	36.4
1	B	47	TYR	35.7
1	A	8	THR	35.6
1	B	1	MET	35.2
1	B	30	ARG	33.8
1	A	109	THR	33.6
1	A	98	GLN	33.1
1	B	60	LYS	33.1
1	B	54	MET	33.0
1	B	4	GLU	32.1
1	A	32	ARG	32.1
1	A	116	ASN	32.1
1	B	95	THR	31.7

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Mol	Chain	Res	Type	RSRZ
1	A	44	LEU	31.6
1	A	103	CYS	31.6
1	B	53	LEU	31.2
1	B	67	PRO	31.2
1	B	108	GLN	31.0
1	B	69	ALA	30.9
1	A	122	MET	30.5
1	B	10	LEU	30.1
1	A	62	GLY	29.6
1	B	93	ARG	28.8
1	B	11[A]	ASP	28.8
1	B	39	PRO	28.4
1	A	119	GLY	27.8
1	B	117	ALA	27.8
1	B	124	PRO	27.5
1	B	36	PHE	27.3
1	A	117	ALA	27.0
1	A	21	PHE	26.9
1	B	122	MET	26.7
1	A	78	PRO	26.5
1	A	18	ALA	26.1
1	B	37[A]	ASN	25.7
1	A	63	GLU	25.3
1	B	94	ASP	24.9
1	A	65	ASN	24.5
1	B	46	CYS	24.5
1	A	110	ALA	24.4
1	B	45	MET	24.1
1	B	71	ALA	23.5
1	A	42	GLN	23.4
1	A	10	LEU	23.4
1	B	18	ALA	23.2
1	B	48	THR	23.0
1	B	17	CYS	23.0
1	A	25	THR	22.9
1	B	50	CYS	22.8
1	B	14	ARG	22.7
1	A	101	GLU	22.4
1	A	124	PRO	22.2
1	A	45	MET	21.5
1	A	79	PRO	21.2
1	A	71	ALA	21.2

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Mol	Chain	Res	Type	RSRZ
1	B	12	MET	21.1
1	A	1	MET	20.6
1	B	31	LEU	20.6
1	A	40	PRO	19.9
1	B	44	LEU	19.7
1	A	39	PRO	19.7
1	B	21	PHE	19.3
1	A	80	GLU	19.2
1	A	95	THR	19.2
1	A	48	THR	19.0
1	B	76	LEU	18.9
1	A	61	LYS	18.7
1	A	41	SER	18.3
1	B	79	PRO	18.0
1	A	108	GLN	17.8
1	B	98	GLN	17.7
1	A	7	LEU	17.5
1	B	116	ASN	17.5
1	B	8	THR	17.0
1	B	105	ARG	17.0
1	A	115	GLU	16.7
1	A	94	ASP	16.3
1	A	50	CYS	16.3
1	A	82	MET	16.2
1	B	113	PHE	15.7
1	A	12	MET	15.5
1	A	46	CYS	15.4
1	B	34	GLY	15.3
1	B	15[A]	SER	15.2
1	A	99	PHE	15.1
1	A	89	VAL	14.8
1	A	59	ASN	14.6
1	A	96	HIS	14.5
1	A	2	THR	14.4
1	A	54	MET	14.4
1	B	89	VAL	14.3
1	A	24	LYS	14.0
1	A	9	SER	13.7
1	A	113	PHE	13.6
1	B	41	SER	13.6
1	B	103	CYS	13.4
1	A	53	LEU	13.3

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Mol	Chain	Res	Type	RSRZ
1	A	38	PHE	13.3
1	A	76	LEU	13.0
1	A	81	MET	12.9
1	A	60	LYS	12.7
1	B	32	ARG	12.5
1	B	16	GLY	12.2
1	B	13	ILE	12.2
1	A	105	ARG	12.1
1	B	115	GLU	11.4
1	B	28	LEU	11.4
1	A	43	ASP	11.1
1	B	61	LYS	11.0
1	B	87	LYS	10.8
1	B	82	MET	10.4
1	B	59	ASN	10.1
1	A	30	ARG	10.0
1	A	3	MET	10.0
1	B	9	SER	9.9
1	A	36	PHE	9.8
1	B	121	PHE	9.6
1	B	51	VAL	9.4
1	A	4	GLU	9.4
1	A	87	LYS	9.3
1	B	92	CYS	9.2
1	A	93	ARG	9.0
1	B	5[A]	GLN	9.0
1	A	91	ALA	8.9
1	A	83	GLU	8.9
1	A	92	CYS	8.9
1	B	40	PRO	8.8
1	A	97	LYS	8.3
1	A	85	SER	8.2
1	A	58	VAL	8.2
1	A	68	LYS	8.1
1	A	112	CYS	7.9
1	A	11	ASP	7.7
1	A	13	ILE	7.7
1	A	33	VAL	7.7
1	A	22	LYS	7.2
1	A	104	GLU	7.2
1	A	52	SER	7.1
1	B	55	ALA	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	25	THR	6.7
1	B	100	LYS	6.7
1	B	112	CYS	6.6
1	B	120	GLN	6.6
1	B	52	SER	6.5
1	B	114	SER	6.5
1	A	47	TYR	6.5
1	A	14	ARG	6.5
1	A	121	PHE	6.3
1	B	111	LYS	6.2
1	B	65	ASN	6.1
1	B	85	SER	6.0
1	A	57	ALA	5.9
1	B	24	LYS	5.9
1	B	58	VAL	5.8
1	B	29	ASP	5.8
1	A	72	GLN	5.8
1	A	120	GLN	5.7
1	A	75	HIS	5.7
1	A	37	ASN	5.6
1	B	68	LYS	5.6
1	B	62	GLY	5.4
1	A	88	SER	5.4
1	B	20	LYS	5.4
1	A	114	SER	5.4
1	B	72	GLN	5.3
1	A	23	LEU	5.3
1	B	81	MET	5.2
1	B	19	PRO	5.1
1	A	51	VAL	5.0
1	B	49	LYS	5.0
1	A	49	LYS	4.9
1	B	56	GLY	4.9
1	A	84	MET	4.8
1	A	55	ALA	4.8
1	A	111	LYS	4.8
1	B	101	GLU	4.8
1	B	102	SER	4.7
1	B	75	HIS	4.7
1	A	34	GLY	4.5
1	B	88	SER	4.5
1	B	57	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	86	ARG	4.2
1	B	84	MET	4.1
1	B	91	ALA	3.8
1	A	100	LYS	3.6
1	A	90	GLU	3.5
1	B	83	GLU	3.4
1	A	86	ARG	3.3
1	B	63	GLU	3.3
1	B	80	GLU	3.2
1	A	35	ASP	3.2
1	B	27	ASP	3.1
1	A	56	GLY	2.9
1	B	90	GLU	2.8
1	B	26	GLU	2.7

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, 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	ACT	A	704	4/4	-0.35	2.47	0.78	26,27,27,28	0
3	PE8	A	224	25/25	0.02	1.50	0.18	32,37,45,46	0
2	ACT	B	703	4/4	-0.06	0.63	-0.83	58,58,58,58	0
2	ACT	A	702	4/4	-0.33	0.36	-1.17	23,23,24,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.