Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:53 AM GMT

PDB ID	:	3NFI
Title	:	Crystal structure of tandem winged helix domain of RNA polymerase I subunit A49
Authors	:	Geiger, S.R.; Lorenzen, K.; Schreieck, A.; Hanecker, P.; Kostrewa, D.; Heck, A.J.R.; Cramer, P.
Deposited on	:	2010-06-10
Resolution	:	1.90 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:

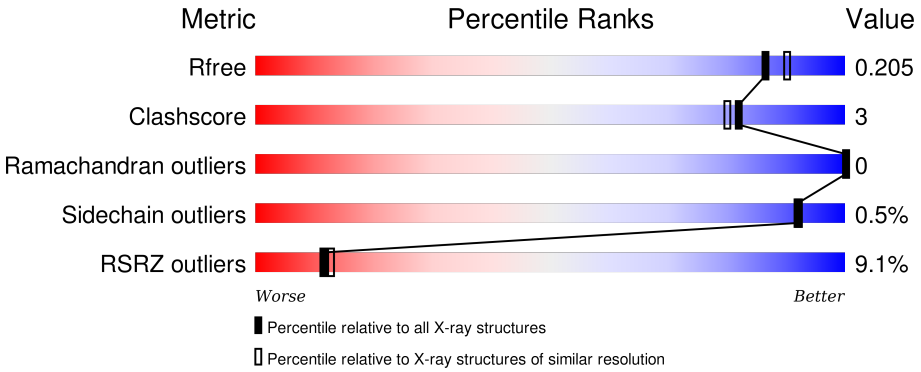
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	237	4%, 84%, 8%, 8%
1	B	237	15%, 89%, 6%, ·
1	C	237	9%, 82%, 8%, 10%
1	D	237	3%, 86%, 7%, 7%
1	E	237	10%, 81%, 8%, 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9695 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 DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	Se	0	9	0
			1798	1167	296	329	1	5			
1	B	227	Total	C	N	O	S	Se	0	5	0
			1838	1189	304	338	1	6			
1	C	214	Total	C	N	O	S	Se	0	9	0
			1750	1139	285	319	1	6			
1	D	220	Total	C	N	O	S	Se	0	6	0
			1790	1161	296	327	1	5			
1	E	212	Total	C	N	O	S	Se	0	7	0
			1721	1120	278	316	1	6			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	167	GLY	-	EXPRESSION TAG	UNP Q01080
A	168	SER	-	EXPRESSION TAG	UNP Q01080
A	169	HIS	-	EXPRESSION TAG	UNP Q01080
A	170	MSE	-	EXPRESSION TAG	UNP Q01080
A	178	MSE	LEU	ENGINEERED MUTATION	UNP Q01080
A	261	MSE	LEU	ENGINEERED MUTATION	UNP Q01080
B	167	GLY	-	EXPRESSION TAG	UNP Q01080
B	168	SER	-	EXPRESSION TAG	UNP Q01080
B	169	HIS	-	EXPRESSION TAG	UNP Q01080
B	170	MSE	-	EXPRESSION TAG	UNP Q01080
B	178	MSE	LEU	ENGINEERED MUTATION	UNP Q01080
B	261	MSE	LEU	ENGINEERED MUTATION	UNP Q01080
C	167	GLY	-	EXPRESSION TAG	UNP Q01080
C	168	SER	-	EXPRESSION TAG	UNP Q01080
C	169	HIS	-	EXPRESSION TAG	UNP Q01080
C	170	MSE	-	EXPRESSION TAG	UNP Q01080
C	178	MSE	LEU	ENGINEERED MUTATION	UNP Q01080
C	261	MSE	LEU	ENGINEERED MUTATION	UNP Q01080
D	167	GLY	-	EXPRESSION TAG	UNP Q01080

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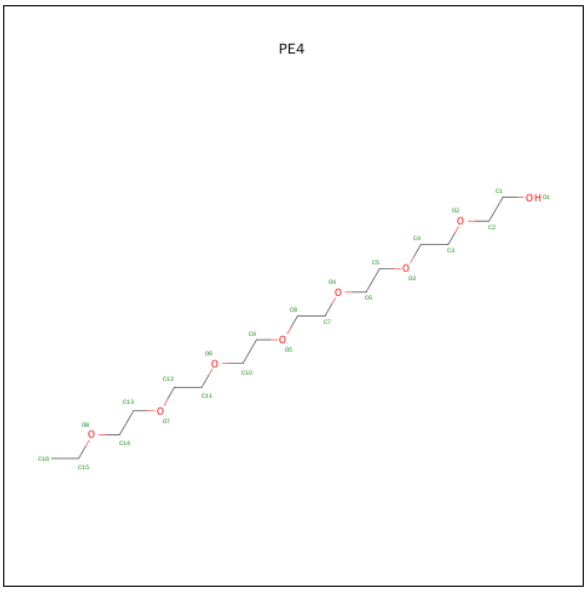
Chain	Residue	Modelled	Actual	Comment	Reference
D	168	SER	-	EXPRESSION TAG	UNP Q01080
D	169	HIS	-	EXPRESSION TAG	UNP Q01080
D	170	MSE	-	EXPRESSION TAG	UNP Q01080
D	178	MSE	LEU	ENGINEERED MUTATION	UNP Q01080
D	261	MSE	LEU	ENGINEERED MUTATION	UNP Q01080
E	167	GLY	-	EXPRESSION TAG	UNP Q01080
E	168	SER	-	EXPRESSION TAG	UNP Q01080
E	169	HIS	-	EXPRESSION TAG	UNP Q01080
E	170	MSE	-	EXPRESSION TAG	UNP Q01080
E	178	MSE	LEU	ENGINEERED MUTATION	UNP Q01080
E	261	MSE	LEU	ENGINEERED MUTATION	UNP Q01080

- Molecule 2 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: $C_{16}H_{34}O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 12 8 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	226	Total O 226 226	0	0
3	B	146	Total O 146 146	0	0

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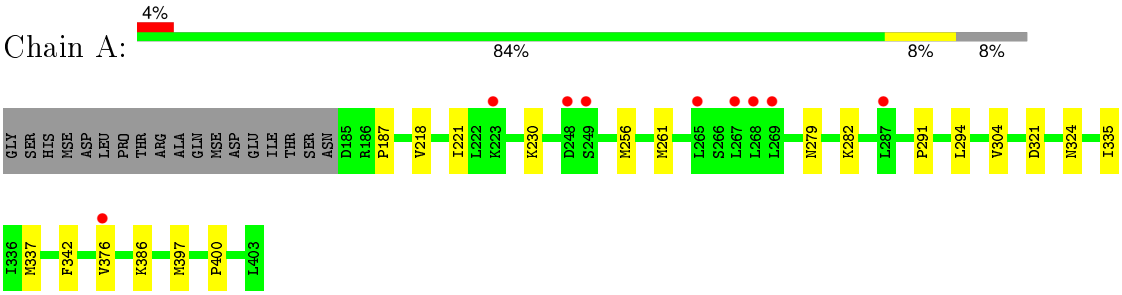
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	116	Total O 116 116	0	0
3	D	156	Total O 156 156	0	0
3	E	142	Total O 142 142	0	0

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.

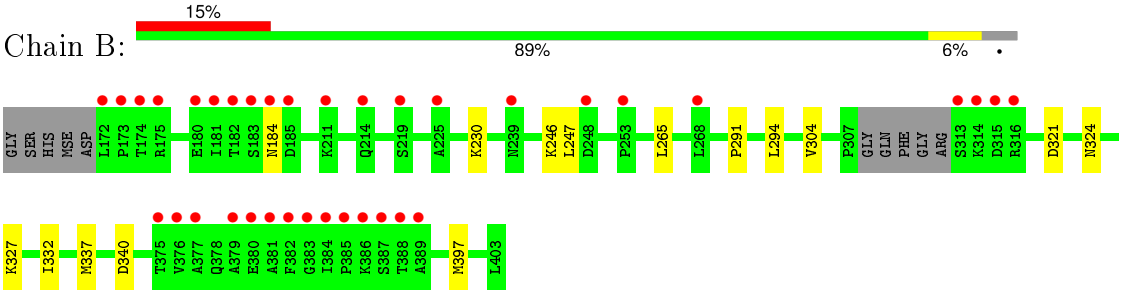
- Molecule 1: DNA-directed RNA polymerase I subunit RPA49

Chain A:



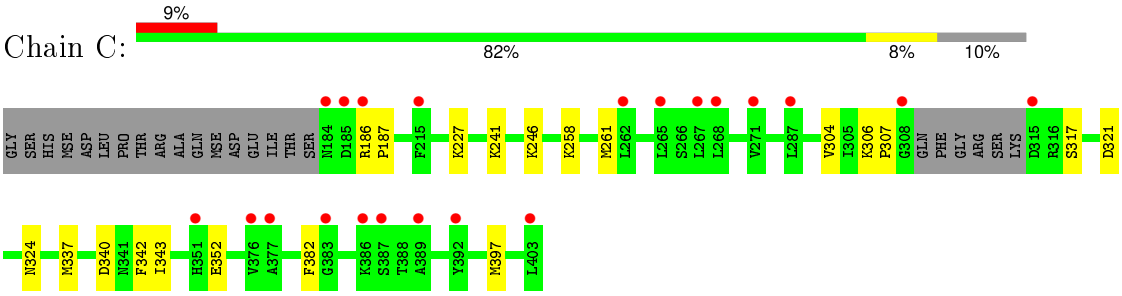
- Molecule 1: DNA-directed RNA polymerase I subunit RPA49

Chain B:



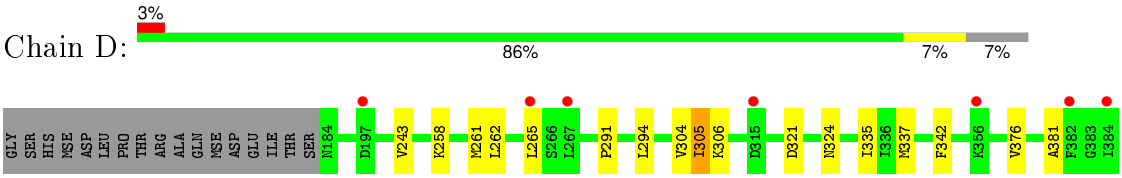
- Molecule 1: DNA-directed RNA polymerase I subunit RPA49

Chain C:



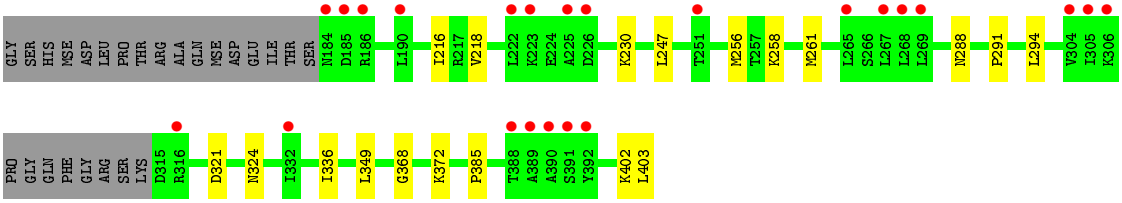
- Molecule 1: DNA-directed RNA polymerase I subunit RPA49

Chain D:



• Molecule 1: DNA-directed RNA polymerase I subunit RPA49

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.11Å 78.10Å 100.67Å 90.00° 113.39° 90.00°	Depositor
Resolution (Å)	27.82 – 1.90 30.87 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (27.82-1.90) 98.3 (30.87-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 1.89Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.189 , 0.224 0.203 , 0.205	Depositor DCC
R_{free} test set	4564 reflections (5.09%)	DCC
Wilson B-factor (Å^2)	29.9	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.2	EDS
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 94401 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9695	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: PE4

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	0/1852	0.61	0/2496
1	B	0.46	0/1878	0.59	0/2531
1	C	0.47	0/1805	0.62	0/2433
1	D	0.51	0/1834	0.62	0/2471
1	E	0.64	1/1768 (0.1%)	0.60	0/2383
All	All	0.52	1/9137 (0.0%)	0.61	0/12314

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	403	LEU	C-OXT	-15.93	0.93	1.23

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	1798	0	1902	15	0
1	B	1838	0	1936	11	0
1	C	1750	0	1861	13	0
1	D	1790	0	1890	9	0
1	E	1721	0	1817	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	12	0	14	1	0
3	A	226	0	0	1	0
3	B	146	0	0	0	0
3	C	116	0	0	0	0
3	D	156	0	0	0	0
3	E	142	0	0	1	0
All	All	9695	0	9420	58	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 3.

All (58) 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:218:VAL:HG23	1:A:256:MSE:SE	2.30	0.80
1:A:337[B]:MSE:SE	1:A:397:MSE:HG3	2.32	0.79
1:C:337[B]:MSE:SE	1:C:397:MSE:SE	3.03	0.77
1:A:187:PRO:HB2	3:A:781:HOH:O	1.85	0.77
1:C:337[B]:MSE:SE	1:C:397:MSE:HG3	2.36	0.76
1:B:184:ASN:HA	1:B:327:LYS:HZ2	1.51	0.75
1:A:337[B]:MSE:SE	1:A:397:MSE:SE	3.05	0.74
1:B:184:ASN:HA	1:B:327:LYS:NZ	2.04	0.72
1:A:304:VAL:HG23	1:A:324:ASN:HD21	1.55	0.70
1:B:304:VAL:HG23	1:B:324:ASN:HD21	1.55	0.70
1:E:218:VAL:HG23	1:E:256[B]:MSE:SE	2.47	0.65
1:B:337[B]:MSE:SE	1:B:397:MSE:SE	3.16	0.63
1:D:304:VAL:HG23	1:D:324:ASN:HD21	1.64	0.62
1:C:304:VAL:HG23	1:C:324:ASN:HD21	1.67	0.60
1:A:337[B]:MSE:SE	1:A:397:MSE:CG	2.99	0.60
1:E:372:LYS:HA	2:E:1:PE4:H121	1.82	0.60
1:E:368:GLY:CA	1:E:402:LYS:HE3	2.32	0.59
1:C:241:LYS:HB2	1:C:352:GLU:OE1	2.03	0.58
1:E:368:GLY:HA2	1:E:402:LYS:HE3	1.84	0.58
1:C:337[B]:MSE:SE	1:C:397:MSE:CG	3.01	0.58
1:A:321:ASP:H	1:A:324:ASN:HD22	1.53	0.55
1:A:218:VAL:CG2	1:A:256:MSE:SE	3.02	0.55
1:D:321:ASP:H	1:D:324:ASN:HD22	1.54	0.54
1:B:321:ASP:H	1:B:324:ASN:HD22	1.55	0.54
1:E:321:ASP:H	1:E:324:ASN:HD22	1.56	0.53
1:A:400:PRO:HB3	1:C:307:PRO:HB2	1.90	0.52
1:A:221:ILE:HG23	1:A:230:LYS:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:MSE:HB3	1:A:335:ILE:HG23	1.94	0.50
1:D:305:ILE:HG12	1:D:306:LYS:N	2.27	0.49
1:B:265[B]:LEU:HD11	1:B:332:ILE:HG23	1.96	0.47
1:C:343:ILE:HG12	1:C:382:PHE:HZ	1.79	0.47
1:D:337:MSE:SE	1:D:342:PHE:HA	2.65	0.47
1:A:337[A]:MSE:SE	1:A:342:PHE:HA	2.65	0.46
1:C:337[A]:MSE:SE	1:C:342:PHE:HA	2.65	0.46
1:D:381:ALA:HA	1:E:385:PRO:HB3	1.98	0.45
1:D:265:LEU:HB2	1:D:335:ILE:HG21	1.98	0.45
1:E:288:ASN:ND2	3:E:503:HOH:O	2.50	0.45
1:D:291:PRO:HD2	1:D:294:LEU:HD12	1.98	0.45
1:B:246:LYS:HE3	1:B:340:ASP:OD1	2.17	0.45
1:E:336:ILE:HD13	1:E:349:LEU:HD11	1.99	0.44
1:D:243:VAL:HA	1:D:262:LEU:HD11	1.99	0.44
1:B:265[B]:LEU:CD1	1:B:332:ILE:HG23	2.47	0.44
1:C:246:LYS:HE3	1:C:340:ASP:OD1	2.18	0.44
1:C:186:ARG:HG3	1:C:187:PRO:HD2	1.99	0.44
1:A:291:PRO:HD2	1:A:294:LEU:HD12	2.00	0.44
1:C:306:LYS:HG3	1:C:317:SER:HB3	1.99	0.43
1:C:258:LYS:HA	1:C:261:MSE:HE3	2.00	0.43
1:E:216:ILE:HG12	1:E:294:LEU:HD11	2.01	0.43
1:E:230:LYS:HB3	1:E:247:LEU:HD21	2.01	0.43
1:B:230:LYS:HB3	1:B:247:LEU:HD21	2.01	0.42
1:C:321:ASP:H	1:C:324:ASN:HD22	1.67	0.42
1:A:337[B]:MSE:CE	1:A:397:MSE:HG3	2.49	0.42
1:D:258:LYS:HA	1:D:261:MSE:HE3	2.02	0.41
1:A:279:ASN:HD21	1:A:282:LYS:HD2	1.85	0.41
1:E:291:PRO:HD2	1:E:294:LEU:HD12	2.02	0.41
1:B:291:PRO:HD2	1:B:294:LEU:HD12	2.02	0.41
1:E:258:LYS:HA	1:E:261:MSE:HE3	2.02	0.40
1:B:337[B]:MSE:SE	1:B:397:MSE:HG3	2.72	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	226/237 (95%)	221 (98%)	5 (2%)	0	100	100
1	B	228/237 (96%)	227 (100%)	1 (0%)	0	100	100
1	C	219/237 (92%)	217 (99%)	2 (1%)	0	100	100
1	D	224/237 (94%)	219 (98%)	5 (2%)	0	100	100
1	E	215/237 (91%)	213 (99%)	2 (1%)	0	100	100
All	All	1112/1185 (94%)	1097 (99%)	15 (1%)	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	207/208 (100%)	205 (99%)	2 (1%)	82	81
1	B	211/208 (101%)	211 (100%)	0	100	100
1	C	203/208 (98%)	202 (100%)	1 (0%)	92	92
1	D	205/208 (99%)	203 (99%)	2 (1%)	82	81
1	E	197/208 (95%)	197 (100%)	0	100	100
All	All	1023/1040 (98%)	1018 (100%)	5 (0%)	92	92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	376	VAL
1	A	386	LYS
1	C	227	LYS
1	D	305	ILE
1	D	376	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	GLN
1	A	278	ASN
1	A	324	ASN
1	B	237	GLN
1	B	324	ASN
1	B	341	ASN
1	C	238	ASN
1	C	252	GLN
1	C	324	ASN
1	D	324	ASN
1	D	341	ASN
1	E	252	GLN
1	E	324	ASN

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

1 ligand is 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	PE4	E	1	-	11,11,23	1.07	0	10,10,22	1.79	3 (30%)

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	PE4	E	1	-	-	0/9/9/21	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	PE4	O5-C8-C7	-2.60	98.48	110.43
2	E	1	PE4	C11-O6-C10	2.50	124.07	113.31
2	E	1	PE4	O7-C12-C11	3.02	123.81	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	PE4	1	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, 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	215/237 (90%)	0.09	9 (4%) 40 44	21, 31, 58, 79	0
1	B	222/237 (93%)	0.72	36 (16%) 3 3	22, 40, 100, 131	0
1	C	210/237 (88%)	0.34	21 (10%) 9 10	24, 40, 70, 100	0
1	D	216/237 (91%)	0.06	8 (3%) 45 49	18, 31, 59, 84	0
1	E	208/237 (87%)	0.31	23 (11%) 7 8	22, 34, 65, 103	0
All	All	1071/1185 (90%)	0.31	97 (9%) 11 13	18, 35, 75, 131	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	174	THR	10.0
1	B	314	LYS	8.4
1	B	313	SER	7.5
1	E	184	ASN	6.5
1	B	315	ASP	6.4
1	B	182	THR	5.6
1	B	386	LYS	5.4
1	E	185	ASP	5.4
1	B	384	ILE	5.2
1	B	253	PRO	5.1
1	B	376	VAL	4.8
1	E	305	ILE	4.8
1	C	389	ALA	4.7
1	C	392	TYR	4.3
1	C	387	SER	4.1
1	B	183	SER	4.1
1	C	308	GLY	4.0
1	B	175	ARG	3.9
1	B	173	PRO	3.9
1	B	316	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	225	ALA	3.6
1	E	316	ARG	3.6
1	D	384	ILE	3.6
1	C	376	VAL	3.5
1	E	388	THR	3.5
1	C	351[A]	HIS	3.4
1	B	219	SER	3.4
1	C	268	LEU	3.4
1	C	185	ASP	3.3
1	B	214	GLN	3.1
1	B	379	ALA	3.1
1	E	222	LEU	3.1
1	B	385	PRO	3.1
1	B	180	GLU	3.0
1	E	269	LEU	3.0
1	E	251	THR	3.0
1	B	381	ALA	2.9
1	A	267	LEU	2.9
1	E	392	TYR	2.9
1	E	389	ALA	2.9
1	B	375	THR	2.9
1	B	380	GLU	2.9
1	A	268	LEU	2.9
1	C	265[A]	LEU	2.8
1	B	181	ILE	2.8
1	E	226	ASP	2.8
1	B	248	ASP	2.7
1	B	172	LEU	2.7
1	B	185	ASP	2.7
1	B	211	LYS	2.7
1	B	184	ASN	2.6
1	B	239	ASN	2.6
1	E	306	LYS	2.6
1	D	197[A]	ASP	2.6
1	C	215	PHE	2.6
1	E	265	LEU	2.6
1	C	184	ASN	2.6
1	C	267	LEU	2.6
1	A	376	VAL	2.6
1	E	304	VAL	2.5
1	B	377	ALA	2.5
1	D	267	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	267	LEU	2.5
1	D	356	LYS	2.5
1	A	265	LEU	2.5
1	C	383	GLY	2.5
1	C	186	ARG	2.5
1	A	287	LEU	2.5
1	B	388	THR	2.4
1	C	386	LYS	2.4
1	A	223	LYS	2.4
1	A	248	ASP	2.3
1	A	269	LEU	2.3
1	C	377	ALA	2.3
1	B	389	ALA	2.3
1	A	249	SER	2.2
1	B	387	SER	2.2
1	C	315	ASP	2.2
1	D	385	PRO	2.2
1	C	262	LEU	2.2
1	C	403	LEU	2.2
1	D	265	LEU	2.2
1	B	382	PHE	2.1
1	D	382	PHE	2.1
1	E	190	LEU	2.1
1	E	268	LEU	2.1
1	E	390	ALA	2.1
1	E	186	ARG	2.1
1	B	225	ALA	2.1
1	B	268	LEU	2.1
1	C	287	LEU	2.1
1	B	383	GLY	2.1
1	D	315	ASP	2.1
1	E	223	LYS	2.0
1	E	391	SER	2.0
1	C	271	VAL	2.0
1	E	332	ILE	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	PE4	E	1	12/24	0.94	0.17	0.49	32,36,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.