



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:47 pm BST

PDB ID : 4LEP
Title : Structural insights into substrate recognition in proton dependent oligopeptide transporters
Authors : Guettou, F.; Quistgaard, E.M.; Tresaugues, L.; Moberg, P.; Jegerschold, C.; Zhu, L.; Jong, A.J.; Nordlund, P.; Low, C.
Deposited on : 2013-06-26
Resolution : 3.20 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

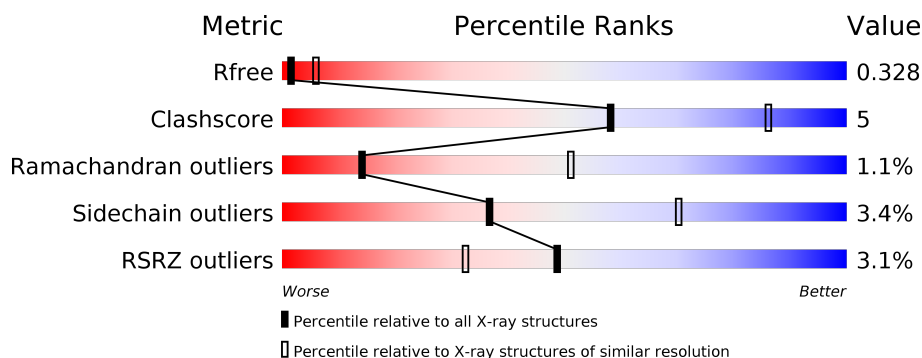
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 respectively. 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	523	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>13%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	523	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>13%</div> <div>•</div> <div>14%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6858 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.

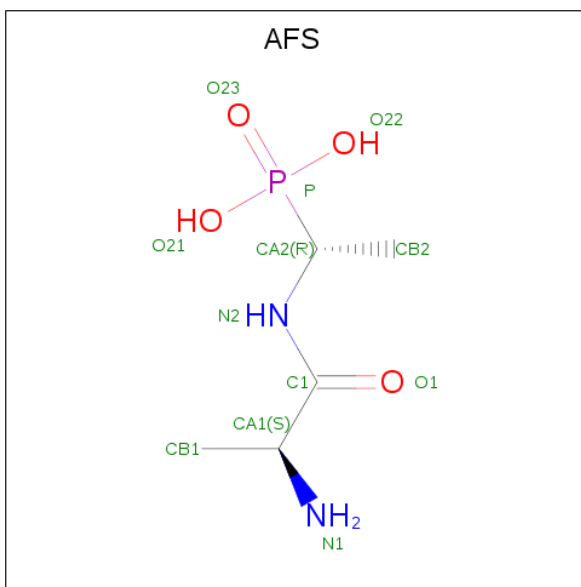
- Molecule 1 is a protein called Proton:oligopeptide symporter POT family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3434	2280	552	582	20			
1	B	452	Total	C	N	O	S	0	0	0
			3399	2255	543	581	20			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	517	ALA	-	EXPRESSION TAG	UNP Q8EHE6
A	518	GLU	-	EXPRESSION TAG	UNP Q8EHE6
A	519	ASN	-	EXPRESSION TAG	UNP Q8EHE6
A	520	LEU	-	EXPRESSION TAG	UNP Q8EHE6
A	521	TYR	-	EXPRESSION TAG	UNP Q8EHE6
A	522	PHE	-	EXPRESSION TAG	UNP Q8EHE6
A	523	GLN	-	EXPRESSION TAG	UNP Q8EHE6
B	517	ALA	-	EXPRESSION TAG	UNP Q8EHE6
B	518	GLU	-	EXPRESSION TAG	UNP Q8EHE6
B	519	ASN	-	EXPRESSION TAG	UNP Q8EHE6
B	520	LEU	-	EXPRESSION TAG	UNP Q8EHE6
B	521	TYR	-	EXPRESSION TAG	UNP Q8EHE6
B	522	PHE	-	EXPRESSION TAG	UNP Q8EHE6
B	523	GLN	-	EXPRESSION TAG	UNP Q8EHE6

- Molecule 2 is N-[(1R)-1-phosphonoethyl]-L-alaninamide (three-letter code: AFS) (formula: C₅H₁₃N₂O₄P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			12	5	2	4	1		
2	B	1	Total	C	N	O	P	0	0
			12	5	2	4	1		

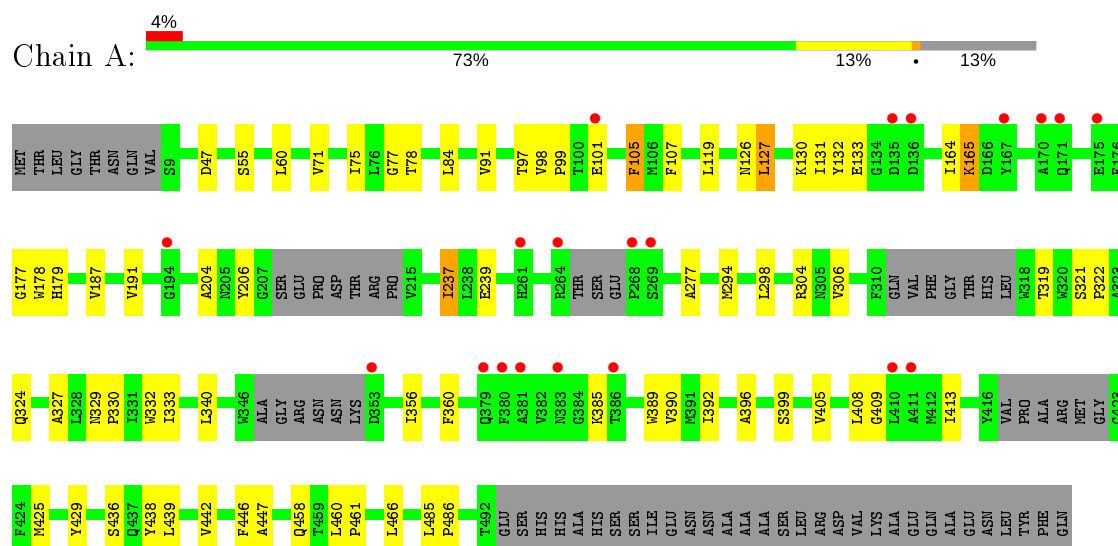
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

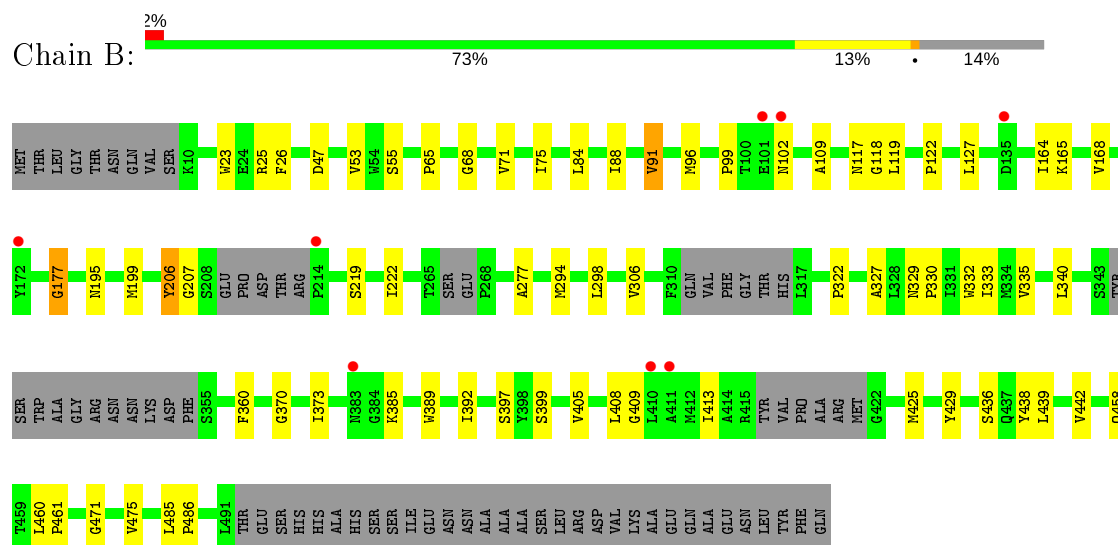
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Proton:oligopeptide symporter POT family



- Molecule 1: Proton:oligopeptide symporter POT family



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.24Å 107.73Å 205.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 3.20 29.86 – 3.10	Depositor EDS
% Data completeness (in resolution range)	77.6 (29.86-3.20) 71.5 (29.86-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.11Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.275 , 0.325 0.277 , 0.328	Depositor DCC
R_{free} test set	1258 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	81.4	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6858	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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, 0.333 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: ZN, AFS

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	0.56	0/3517	0.61	0/4787
1	B	0.58	0/3480	0.63	0/4738
All	All	0.57	0/6997	0.62	0/9525

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	3434	0	3450	35	0
1	B	3399	0	3420	31	0
2	A	12	0	11	0	0
2	B	12	0	11	0	0
3	A	1	0	0	0	0
All	All	6858	0	6892	66	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 (66) 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:101:GLU:OE1	1:A:105:PHE:CE2	1.86	1.28
1:A:101:GLU:OE1	1:A:105:PHE:CD2	2.28	0.85
1:A:389:TRP:HA	1:A:392:ILE:HD12	1.76	0.67
1:B:294:MET:HA	1:B:298:LEU:HB3	1.78	0.65
1:B:389:TRP:HA	1:B:392:ILE:HD12	1.77	0.65
1:B:55:SER:HB3	1:B:438:TYR:HA	1.79	0.65
1:B:425:MET:O	1:B:429:TYR:HB3	1.97	0.64
1:A:294:MET:HA	1:A:298:LEU:HB3	1.81	0.62
1:B:436:SER:HA	1:B:439:LEU:HD12	1.82	0.62
1:B:306:VAL:HG22	1:B:322:PRO:HG3	1.85	0.59
1:B:277:ALA:HB1	1:B:413:ILE:HD12	1.87	0.57
1:A:306:VAL:HG22	1:A:322:PRO:HG3	1.86	0.56
1:A:78:THR:HB	1:A:204:ALA:HB1	1.86	0.56
1:A:436:SER:HA	1:A:439:LEU:HD12	1.89	0.55
1:A:71:VAL:HA	1:A:75:ILE:HD12	1.89	0.55
1:A:55:SER:HB3	1:A:438:TYR:HA	1.91	0.53
1:A:77:GLY:HA2	1:A:206:TYR:HB2	1.92	0.52
1:B:385:LYS:HG3	1:B:460:LEU:HD13	1.91	0.52
1:A:329:ASN:HB3	1:A:330:PRO:HD3	1.92	0.51
1:A:132:TYR:N	1:A:133:GLU:HA	2.26	0.50
1:A:385:LYS:HG3	1:A:460:LEU:HD13	1.93	0.50
1:A:333:ILE:HG13	1:A:399:SER:HB2	1.93	0.50
1:A:439:LEU:O	1:A:442:VAL:HG22	2.12	0.50
1:B:329:ASN:HB3	1:B:330:PRO:HD3	1.94	0.50
1:B:84:LEU:HD23	1:B:119:LEU:HD13	1.95	0.49
1:B:458:GLN:O	1:B:461:PRO:HD2	2.12	0.49
1:B:327:ALA:O	1:B:330:PRO:HD2	2.14	0.48
1:A:126:ASN:O	1:A:130:LYS:HG2	2.12	0.48
1:A:60:LEU:HD11	1:A:237:ILE:HD11	1.96	0.48
1:B:370:GLY:HA2	1:B:373:ILE:HD12	1.96	0.48
1:A:84:LEU:HD23	1:A:119:LEU:HD13	1.96	0.48
1:B:333:ILE:HG13	1:B:399:SER:HB2	1.96	0.47
1:A:107:PHE:CE2	1:A:239:GLU:HG2	2.48	0.47
1:B:306:VAL:HG13	1:B:322:PRO:HD3	1.96	0.47
1:B:195:ASN:O	1:B:199:MET:HG2	2.14	0.47
1:B:460:LEU:HB3	1:B:461:PRO:HD3	1.98	0.46
1:A:277:ALA:HB1	1:A:413:ILE:HD12	1.95	0.46
1:B:68:GLY:HA3	1:B:118:GLY:O	2.14	0.46
1:A:165:LYS:HD2	1:A:178:TRP:CZ3	2.50	0.46
1:A:327:ALA:O	1:A:330:PRO:HD2	2.16	0.46
1:B:485:LEU:N	1:B:486:PRO:HD2	2.31	0.46
1:A:127:LEU:O	1:A:131:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:THR:HA	1:A:179:HIS:HB3	1.98	0.45
1:A:458:GLN:O	1:A:461:PRO:HD2	2.17	0.45
1:B:168:VAL:HG12	1:B:177:GLY:H	1.81	0.45
1:B:206:TYR:HB3	1:B:207:GLY:H	1.62	0.45
1:B:219:SER:HA	1:B:222:ILE:HG22	1.99	0.45
1:A:425:MET:O	1:A:429:TYR:HB3	2.17	0.44
1:A:304:ARG:O	1:A:385:LYS:NZ	2.42	0.44
1:B:439:LEU:O	1:B:442:VAL:HG22	2.17	0.44
1:B:65:PRO:HB3	1:B:122:PRO:HD3	1.99	0.44
1:B:471:GLY:O	1:B:475:VAL:HG23	2.18	0.44
1:A:332:TRP:CE2	1:A:396:ALA:HB2	2.52	0.43
1:A:446:PHE:HB2	1:A:466:LEU:HD13	2.02	0.42
1:A:101:GLU:OE1	1:A:105:PHE:HE2	1.78	0.42
1:A:98:VAL:HG11	1:A:105:PHE:CE1	2.54	0.42
1:B:23:TRP:O	1:B:26:PHE:HB3	2.20	0.42
1:B:88:ILE:O	1:B:91:VAL:HG12	2.20	0.42
1:A:187:VAL:O	1:A:191:VAL:HG23	2.21	0.41
1:B:96:MET:HG2	1:B:109:ALA:HB1	2.03	0.41
1:A:485:LEU:N	1:A:486:PRO:HD2	2.36	0.41
1:B:71:VAL:HA	1:B:75:ILE:HD12	2.02	0.41
1:B:25:ARG:HH22	1:B:117:ASN:ND2	2.18	0.41
1:A:321:SER:HB3	1:A:324:GLN:HG3	2.03	0.41
1:A:447:ALA:HB2	1:A:466:LEU:HD22	2.03	0.40
1:B:332:TRP:HA	1:B:335:VAL:HG12	2.02	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	443/523 (85%)	412 (93%)	25 (6%)	6 (1%)	11 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	440/523 (84%)	406 (92%)	30 (7%)	4 (1%)	17	56
All	All	883/1046 (84%)	818 (93%)	55 (6%)	10 (1%)	14	51

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	PRO
1	B	99	PRO
1	B	177	GLY
1	A	177	GLY
1	A	409	GLY
1	B	409	GLY
1	A	319	THR
1	A	356	ILE
1	A	405	VAL
1	B	405	VAL

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	342/417 (82%)	331 (97%)	11 (3%)	39	71
1	B	340/417 (82%)	328 (96%)	12 (4%)	36	69
All	All	682/834 (82%)	659 (97%)	23 (3%)	37	70

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ASP
1	A	91	VAL
1	A	105	PHE
1	A	127	LEU
1	A	164	ILE
1	A	165	LYS

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Mol	Chain	Res	Type
1	A	237	ILE
1	A	340	LEU
1	A	360	PHE
1	A	390	VAL
1	A	408	LEU
1	B	47	ASP
1	B	53	VAL
1	B	91	VAL
1	B	102	ASN
1	B	127	LEU
1	B	164	ILE
1	B	165	LYS
1	B	206	TYR
1	B	340	LEU
1	B	360	PHE
1	B	397	SER
1	B	408	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	AFS	A	601	-	9,11,11	2.58	3 (33%)	9,16,16	0.98	1 (11%)
2	AFS	B	601	-	9,11,11	3.49	5 (55%)	9,16,16	1.11	1 (11%)

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	AFS	A	601	-	-	0/14/14/14	-
2	AFS	B	601	-	-	2/14/14/14	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	AFS	P-O23	6.93	1.61	1.49
2	A	601	AFS	P-O21	5.10	1.62	1.54
2	B	601	AFS	P-CA2	-4.92	1.79	1.84
2	A	601	AFS	P-O22	4.89	1.62	1.54
2	B	601	AFS	P-O22	4.59	1.62	1.54
2	B	601	AFS	P-O21	-3.37	1.49	1.54
2	A	601	AFS	P-CA2	2.89	1.87	1.84
2	B	601	AFS	CB2-CA2	2.04	1.56	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	AFS	O22-P-O23	-2.60	106.91	113.45
2	A	601	AFS	O21-P-O23	-2.48	107.21	113.45

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	AFS	P-CA2-N2-C1
2	B	601	AFS	CB2-CA2-N2-C1

There are no ring outliers.

No monomer is involved in short contacts.

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	455/523 (86%)	-0.23	20 (4%) 34 21	55, 98, 161, 186	0
1	B	452/523 (86%)	-0.28	8 (1%) 68 55	54, 98, 161, 186	0
All	All	907/1046 (86%)	-0.25	28 (3%) 49 32	54, 98, 161, 186	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	ASP	8.5
1	B	383	ASN	7.1
1	B	102	ASN	5.4
1	B	410	LEU	5.3
1	A	171	GLN	4.3
1	A	383	ASN	4.3
1	A	353	ASP	4.2
1	B	411	ALA	3.9
1	B	135	ASP	3.7
1	A	268	PRO	3.5
1	B	214	PRO	3.5
1	A	101	GLU	3.1
1	A	380	PHE	3.1
1	A	194	GLY	3.0
1	A	411	ALA	3.0
1	A	264	ARG	2.9
1	A	386	THR	2.8
1	A	269	SER	2.8
1	B	172	TYR	2.7
1	A	170	ALA	2.6
1	A	136	ASP	2.6
1	A	379	GLN	2.5
1	B	101	GLU	2.5
1	A	167	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	381	ALA	2.4
1	A	175	GLU	2.2
1	A	410	LEU	2.1
1	A	261	HIS	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. 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	B-factors(\AA^2)	Q<0.9
2	AFS	B	601	12/12	0.93	0.20	53,99,191,192	0
2	AFS	A	601	12/12	0.94	0.23	69,113,137,178	0
3	ZN	A	602	1/1	0.97	0.11	121,121,121,121	0

6.5 Other polymers [i](#)

There are no such residues in this entry.